

# L'origine des comètes riches en N2: nouvelles contraintes fournis par la comète C/2016 R2 (PanSTARRS)

Sarah Anderson

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### THÈSE DE DOCTORAT DE L'ÉTABLISSEMENT UNIVERSITÉ BOURGOGNE FRANCHE-COMTÉ PRÉPARÉE À L'UNIVERSITÉ DE FRANCHE-COMTÉ

École doctorale n° 553 Carnot-Pasteur

Doctorat d'Astrophysique

Par Mme. Sarah E. Anderson

### The Origin of N2 -rich comets: new constraints from comet C/2016 R2 (PanSTARRS)

 $\label{eq:lorigine} \begin{array}{l} \mbox{L'origine des comètes riches en $N_2$} : \\ \mbox{Nouvelles contraintes fournis par la comète $C/2016 R2$ (PanSTARRS)} \end{array}$ 

Thèse présentée et soutenue à l'Observatoire de Besançon, le 25 Octobre 2022

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Titre : L'origine des comètes riches en N<sub>2</sub> : nouvelles contraintes fournis par la comète C/2016 R2 (PanSTARRS). Mots clés : comète, C/2016 R2 (PanSTARRS), spectroscopie, mécanique céleste, disques protoplanétaires

de la formation du Système Solaire, s'étant agglomérées à (pour 1 ua). Il s'agit de la première mesure directe de tels partir de différents grains de glace et particules de pous- paramètres. On déduit que le taux de production d'azote sière restants du processus de formation planétaire et ayant moléculaire résultant est  $Q(N_2) \sim 1 \times 10^{28}$  molécules.s<sup>-1</sup>, subi peu d'altérations depuis. À mesure que les comètes le plus élevé de toutes les comètes connues. Avec un taux s'approchent du Soleil, la sublimation de leurs glaces crée de production de Q(CO)  $\sim 1.1 \times 10^{29}$  molécules.s<sup>-1</sup>, an un grand nuage gazeux qui, avec l'interaction avec le ray- trouve alors un  $Q(N_2)/Q(CO) \sim 0.09$ , ce qui est cohérent onnement solaire, conduit à diverses émissions spectro- avec le rapport  $N_2^{++}/CO^{+}$  déduit des intensités observées scopiques. Cela nous permet d'étudier la composition des raies d'émission  $N_2^+$  et CO<sup>+</sup>. glaces cométaires et de déterminer les conditions physicochimiques de leur formation, fournissant ainsi un aperçu supplémentaire de la nature du Système Solaire primitif retracer avec certitude la trajectoire des comètes riches au moment et à l'endroit où ces comètes se sont formées. en N2<sup>+</sup> en raison de leurs interactions avec les planètes Les observations de la comète C/2016 R2 (PanSTARRS) ont révélé des bandes d'émission exceptionnellement brillantes de N<sub>2</sub><sup>+</sup>, les plus fortes jamais observées dans un spectre de comète, ainsi qu'un fort appauvrissement en H2O.

tion de N<sub>2</sub> à partir des raies d'émission N<sub>2</sub><sup>+</sup> en utilisant le S'agissant de la zone de formation susceptible de produire modèle de Haser et un nouveau modèle de fluorescence des comètes de même composition que C/2016 R2, ce pro- $N_2^+$  que nous avons créé pour une utilisation sur les futures cessus pourrait expliquer l'absence de comètes similaires comètes. J'ai calculé des longueurs d'échelle effectives de la observées dans le Système Solaire. molécule-mère (N<sub>2</sub>) et de son produit d'ionisation (N<sub>2</sub><sup>+</sup>) de

Les comètes sont parmi les reliques les plus inchangés  $l_m = 2,8 \times 10^6$  km et  $l_f = 3,8 \times 10^6$  km respectivement

J'ai étudié l'origine dynamique de C/2016 R2, constatant que les modèles dynamiques sont incapables de géantes. À l'aide d'une simulation numérique de la formation du Système Solaire, j'ai suivi les cometesimaux dans le scénario Jumping Neptune et j'ai découvert que la majorité des objets formés entre 8 et 12 ua étaient éjectés au Lors de cette thèse, j'ai quantifié le taux de produc- début de la chronologie de la formation du système solaire.

#### Title: The Origin of N2-rich comets: new constraints from comet C/2016 R2 (PanSTARRS) Keywords: Comet, C/2016 R2 (PanSTARRS), Spectroscopy, Celestial Mechanics, Protoplanetary Disks

mation of the Solar System, having agglomerated from dif- the first direct measurement of such parameters. Using a ferent icy grains and dust particles leftover from the plane- revised fluorescence efficiency for N2<sup>+</sup>, the resulting productary formation process and undergone little alteration since. tion rate of molecular nitrogen is inferred to be  $Q(N_2) \sim 1$ As comets approach the Sun, the sublimation of their ices  $\times 10^{28}$  molecules.s<sup>-1</sup>, the highest for any known comet. creates a large gaseous coma, which, along with the inter- Based on a CO production rate of  $Q(CO) \sim 1.1 \times 10^{29}$ action with solar radiation, leads to various spectroscopic molecules. $s^{-1}$ , we find  $Q(N_2)/Q(CO) \sim 0.09$ , which is conemissions. This allows us to investigate the composition of sistent with the  $N_2^+/CO^+$  ratio derived from the observed cometary ices and determine the physico-chemical condi- intensities of  $N_2^+$  and  $CO^+$ emission lines. tions of their formation, thus providing further insight to the nature of the early Solar System at the time and place these comets formed. Observations of comet C/2016 R2 (PanSTARRS) have revealed exceptionally bright emission bands of N<sub>2</sub><sup>+</sup>, the strongest ever observed in a comet spectrum. Alternatively, it appears to be remarkably depleted in H<sub>2</sub>O.

rived effective parent  $(N_2)$  and daughter  $(N_2^+)$  scalelengths similar comets observed in the Solar System. of  $l_p = 2.8 \times 10^6$  km and  $l_d = 3.8 \times 10^6$  km respec-

Comets are among the most pristine relics of the for- tively (for 1 au, when using a scaling with  $r_h^2$ ). This is

I explored the dynamical origin of C/2016 R2, finding that dynamic models are unable to trace back the trajectory of any N2<sup>+</sup> rich comet with certainty due to their interactions with the giant planets. Using a numerical simulation of early Solar System formation, I instead tracked the dynamical evolution of the objects in the Jumping Neptune scenario and found that objects formed between 8-12 au In this thesis, I quantified the N<sub>2</sub> production rate from were predominantly ejected early in the formation time- $N_2^+$  emission lines using the Haser model and a new  $N_2^+$  flu-line. As this is the formation zone likely to produce comets orescence model we created for use on future comets. I de- of this composition, this process could explain the lack of



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### List of Publications

### **Publications in refereed journals**

- S. E. Anderson, P. Rousselot, B. Noyelles, C. Opitom, E. Jehin, D. Hutsemékers, and J. Manfroid. Accepted for Publication. *N*<sub>2</sub> *Production Rate in Comet C/2016 R2 (Pan-STARRS)*. Monthly Notices of the Royal Astronomical Society.
- P. Rousselot, S. E. Anderson, A. Alijah, B. Noyelles, C. Opitom, E. Jehin, D. Hutsemékers, and J. Manfroid. (2022). N<sub>2</sub><sup>+</sup> fluorescence spectrum of comet C/2016 R2 (PanSTARRS). Astronomy and Astrophysics.
- P. Rousselot, A. Kryszczyńska, P. Bartczak, I. Kulyk, K. Kamiński, G. Dudziński, **S. E. Anderson**, B. Noyelles, A. Guilbert-Lepoutre, (2021). *New constraints on the physical properties and dynamical history of Centaur 174P/Echeclus*. Monthly Notices of the Royal Astronomical Society.
- S. E. Anderson, O. Mousis, and T. Ronnet, (2021). *Formation conditions of Titan and Enceladus' building blocks in Saturn's circumplanetary disk*. The Planetary Science Journal.

### Papers in preparation

- **S. E. Anderson**, P. Rousselot, and B.Noyelles. In preparation. *Cracking a comet cold case; a reanalysis of comet C/1908 R1 (Morehouse) with modern methods*. Astronomy and Astrophysics.
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### **Conference Abstracts**

- S. E. Anderson, P. Rousselot, B. Noyelles, C. Opitom, E. Jehin, D. Hutsemékers, and J. Manfroid, (2022). *The N<sub>2</sub> Production Rate in C/2016 R2 (PanSTARRS)*. EPSC Abstracts Vol. 16, EPSC2022-538, 2022, Europlanet Science Congress 2022
- S. E. Anderson, J.-M. Petit, B. Noyelles, O. Mousis, and P. Rousselot, (2022). *Volatile-rich comets ejected early in Solar System formation*. EPSC Abstracts Vol. 16, EPSC2022-521, 2022, Europlanet Science Congress 2022

- S. E. Anderson, J.-M. Petit, B. Noyelles, O. Mousis, and P. Rousselot, (2022). *Peculiar comets ejected early in Solar System formation*. EGU General Assembly 2022, Vienna, Austria, 23–27 May 2022, EGU22-7975, 2022.
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To continue along the line of unnecessary analogies, they say writing a thesis is like running a marathon, but I feel as if I've been in a different kind of race, driving a derby car against Formula 1: I'm not going very fast and I'm not going to win, but I'll burn some rubber along the way and hopefully leave my mark. I'm forever grateful to my pit crew for keeping me stocked on fresh tires.

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### Résumé Français

#### Introduction

Les comètes sont parmi les corps les plus remarquables du Système Solaire, étant restés relativement inchangés depuis leur formation il y a plus de 4 milliards d'années. Les noyaux cométaires conservent un aperçu de la composition du disque protoplanétaire (PPD) grâce à leurs rapports d'abondance isotopique, puisque leur composition reflète les conditions physico-chimiques du disque au moment et à l'endroit de leur formation dans la nébuleuse protosolaire (PSN). Comprendre où chaque comète s'est formée révèle des détails quant à l'évolution du Système Solaire. À mesure que les comètes s'approchent du Soleil, la sublimation de leurs glaces crée une grande chevelure, appelée 'coma,' composée de gaz et de poussières qui, avec l'interaction avec le rayonnement solaire, conduit à diverses émissions spectroscopiques. Cela nous permet d'étudier la composition des glaces cométaires et de déterminer les conditions physico-chimiques de leur formation. Des décennies de télédétection des comètes ont révélé que ces objets sont riches en glace d'eau, avec une composition typique de monoxyde de carbone de  $CO/H_2O = 4\%$ , et appauvris en N<sub>2</sub>, malgré l'abondance de ce dernier dans les atmosphères et les surfaces des corps extérieurs du Système Solaire tels que Triton ou Pluton.

#### La composition unique de la comète C/2016 R2 (PanSTARRS)

La comète de longue période C/2016 R2 (PanSTARRS) a démontré une morphologie de coma atypique avant son passage près du périhélie (~ 2.6 ua) en décembre 2017, émettant fortement dans les longueurs d'onde optiques bleues en raison de l'émission d'ions dominant dans le coma. Les observations radio ont révélé que le spectre était dominé par des bandes de CO<sup>+</sup> et qu'elle était remarquablement appauvrie en eau, avec un rapport H<sub>2</sub>O/CO de seulement ~ 0, 32%. De plus, il avait une abondance particulière de N<sub>2</sub><sup>+</sup>, qui n'avait jamais été vu en telle abondance dans les comètes auparavant. Il s'est également avéré qu'il était à la fois faible en CN et peu poussiéreux.

Le déficit apparent de N<sub>2</sub> dans les comètes a longtemps été un sujet de grand débat. Très peu d'observations au sol ont permis la détection du N<sub>2</sub><sup>+</sup> dans les spectres cométaires. Non seulement les raies spectrales de cet ion ont été observées dans C/2016 R2, mais elles sont aussi les plus brillantes jamais vues dans un spectre cométaire. La quantité de N<sub>2</sub> présente est donc d'une importance significative. En mesurant l'intensité de bande du N<sub>2</sub><sup>+</sup> observée dans le spectre de C/2016 R2 (en supposant que la fluorescence de résonance solaire est la seule source d'excitation)

les flux d'émission observés ont été utilisés pour calculer les rapports ioniques de  $N_2^+/CO^+$  dans le coma entre  $0.06\pm0.01$  et  $0.08\pm0.01$ . C'est bien plus que la meilleure mesure de la comète 67P, avec un rapport  $N_2/CO$  de  $\sim 2,87 \times 10^{-2}$ , bien que ces mesures aient été obtenues beaucoup plus près du noyau.

Cette composition ouvre de nombreuses pistes de questionnement quant à notre compréhension de la formation des comètes. Cette composition riche en CO et pauvre en eau, ainsi qu'aucun des composés neutres habituels observés dans la plupart des spectres cométaires, fait de C/2016 R2 un spécimen unique et intrigant. Comprendre l'histoire dynamique de cette comète est donc d'une importance essentielle pour comprendre la chronologie de la formation des planétésimaux dans notre Système Solaire.

#### Conclusions

Lors de cette thèse, nous avons créé un nouveau modèle de fluorescence pour  $N_2^+$  dans les spectres cométaires. Il est évident que  $N_2$  et  $N_2^+$  mettent beaucoup de temps à atteindre l'équilibre, car nous avons une forte variation entre la production au noyau et le bord de la fente spectroscopique. En utilisant les nouveaux facteurs de fluorescence, j'ai ensuite réestimé les rapports N<sub>2</sub>/CO des comètes riches en  $N_2$ . Mon estimation des nouvelles longueurs d'échelle des espèces mère ( $N_2$ ) et fille (N<sub>2</sub><sup>+</sup>) donne  $l_p = 2,8 \times 10^6$  km et  $l_d = 3,8 \times 10^6$  km respectivement (pour 1 ua, lors d'une mise à l'échelle avec  $r_h^2$ ). Cela fournit un taux de production N<sub>2</sub> de  $Q(N_2) \sim 10^{28}$  molecules.s<sup>-1</sup>, exceptionnellement élevé, compatible avec les valeurs estimées par d'autres équipes à partir du ratio  $N_2^+/CO^+$ . Comparé à un taux de production de CO de  $Q(CO) \sim 1.1 \times 10^{29}$  molecules.s<sup>-1</sup>, je trouve un rapport N<sub>2</sub>/CO de 0,09, ce qui correspond aux rapports d'intensité observés. C'est le plus élevé de ces rapports observés pour une comète jusqu'à présent avec une spectroscopie à haute résolution. Il existe également une forte variabilité au cours des trois nuits d'observation, probablement due à la répartition non uniforme des zones actives riches en  $N_2$  à la surface du noyau.

J'ai étudié si les comètes de notre étude avaient une histoire dynamique partagée qui pourrait indiquer une région de formation particulière, ou à tout le moins, un point d'origine partagé qui pourrait aider à identifier leur zone de formation d'origine. Les résultats sont malheureusement peu concluants. Il semble n'y avoir aucune corrélation entre les comètes de notre étude, sauf qu'elles ont des orbites très excentriques. Il est clair que chaque interaction successive avec les planètes géantes efface la memoire dynamique de la dernière. Nous avons également cherché à savoir si le passage de ces comètes dans le Système Solaire interne pouvait être retracé au passage d'une seule étoile. Nous n'avons pas trouvé d'événement partagé qui aurait pu provoquer leur afflux. Nous avons constaté que la probabilité d'une collision récente était si faible qu'elle serait insignifiante.

Une hypothèse vraisemblable serait que ces objets sont originaires du nuage d'Oort, capturés alors qu'ils visitaient le Système Solaire interne, bien que nous ne puissions pas déterminer précisément où dans le nuage d'Oort ils ont été stockés pendant la majeure partie de ces quatre derniers de millards d'années. Il ne semble pas y avoir de lien entre le rapport  $N_2/CO$  et l'histoire dynamique de la comète ni le nombre moyen d'orbites dans le Système Solaire interne : il ne semble pas y avoir de ligne de base  $N_2/CO$  à partir duquel ces comètes se seraient érodées à chaque passage successif près du soleil. Comme les flocons de neige, ils sont tout simplement uniques.

En utilisant un modèle déjà établi de la formation de la ceinture d'Edgeworth-Kuiper, ainsi que des estimations des zones de formation possibles de C/2016 R2 si elle s'était formée dans des pics d'abondance liés aux lignes de glace dans le disque, j'ai étudié le sort des objets formés dans ces régions. Ces objets sont presque entièrement éjectés du Système Solaire dans des délais astronomiquement courts. Si ces objets se sont effectivement formés dans une région de formation étroite de notre propre Système Solaire, ils auraient été éjectés, ce qui pourrait expliquer pourquoi nous ne voyons pas ces comètes aujourd'hui.

#### **Ouverture**

Il y a peut-être plus à apprendre des comètes que nous n'observons pas plutôt que de celles que nous observons. Avant la découverte de C/2016 R2 (PanSTARRS), un tel appauvrissement de  $H_2O$  dans les comètes était impensable. Après tout, c'est le composant le plus important des glaces cométaires et dans la définition même des comètes. Cela nous oblige à examiner la possibilité de l'existence d'autres types de comètes, comme C/2016 R2, que nous n'avons pas (encore) observées, des comètes aux compositions exotiques telles que l'enrichissement en gaz nobles ou autres glaces volatiles, dues à des formations dans des petits réservoirs autour de leurs lignes de glace avec des pics d'abondance. Comprendre pourquoi ces comètes n'ont pas été observées sera essentiel pour révéler la structure de notre Système Solaire primitif et imposer des contraintes à son évolution dynamique.

### Introduction

### **Motivation**

Comets are some of the most pristine bodies in the Solar System, having remained relatively unchanged since their formation 4.6 billion years ago. Cometary nuclei preserve insight into the composition of the early protoplanetary disk (PPD) through their isotopic abundance ratios. As their composition reflects the physico-chemical conditions of the disk at the location of their formation in the protosolar nebula (PSN), understanding where each comet was formed reveals details as to the evolution of the Solar System. As comets approach the Sun, the sublimation of their ices creates a large gaseous coma, which, along with the interaction with solar radiation, leads to various spectroscopic emissions. Decades of remote-sensing of comets have revealed these objects to be water-ice rich, with a typical carbon monoxide composition of CO/H<sub>2</sub>O = 4%, and depleted in N<sub>2</sub>, despite the abundance of the latter in the atmospheres and surfaces of the outer Solar System bodies such as Triton or Pluto.

Long period comet C/2016 R2 (PanSTARRS) displayed atypical coma morphology in optical images since its passage near perihelion (~ 3.0 au) in December 2017, emitting strongly in blue optical wavelengths due to ion emission dominating in the coma. Radio observations revealed that the spectrum dominated by bands of CO<sup>+</sup> and remarkably depleted in water, with a H<sub>2</sub>O/CO ratio of only ~ 0.32%. Further, it had a peculiar abundance of N<sub>2</sub><sup>+</sup>: by measuring the band intensity of the observed N<sub>2</sub><sup>+</sup> in C/2016 R2's spectrum, assuming that solar resonance fluorescence is the only excitation source, the observed emission fluxes have been used to calculate ionic ratios of N<sub>2</sub><sup>+</sup>/CO<sup>+</sup> in the coma between  $0.06 \pm 0.01$  and  $0.08 \pm 0.01$ . This is larger than the best measurement in comet 67P, with a N<sub>2</sub>/CO ratio of ~  $2.87 \times 10^{-2}$ , though these measurements were obtained much closer to the nucleus. It was also found to be both CN-weak and dust-poor.

The apparent N<sub>2</sub> deficiency in comets has long been a matter of great debate. Despite Pluto and Triton — which also formed in the outer Solar System — both exhibiting a N<sub>2</sub>-rich surface, very few ground-based facilities have ever observed N<sub>2</sub><sup>+</sup> in cometary spectra. The detection of N<sub>2</sub> in comets using spectroscopic methods has been challenging: as a diatomic, symmetrical molecule, N<sub>2</sub> has no permanent dipole moment, which results in the absence of pure rotational transitions. It emits no radiation at millimeter-wavelengths, making the molecule invisible to observations in that range. The electronic transitions are visible in the UV through instruments placed outside of our atmosphere. The presence of N<sub>2</sub> in comet 67P/ Churyumov-Gerasimenko was not detected through any transition but using the ROSINA mass spectrometer in-situ measurements. However, its daughter-species  $N_2^+$  is detectable in the optical range through the bands of the first negative group  $(B^2\Sigma_u^+ - X^2\Sigma_g^+)$  with the (0,0) bandhead located at 3914 Å. Not only have this ion's spectral lines been observed in C/2016 R2, they are also the brightest ever seen in a cometary spectrum. The quantity of  $N_2$  present is thus of significant importance.

This composition opens many avenues of questioning as to our understanding of comet formation, as it was understood that CO ice was unlikely to be freezing out without abundant water ice, which has a higher binding energy than CO. Most volatile species would also be expected to deplete with each subsequent passage of this comet within the inner Solar System. This CO-rich and water-poor composition, along with none of the usual neutrals seen in most cometary spectra, makes C/2016 R2 a unique and intriguing specimen. Understanding the dynamical history of this comet is thus of essential importance to understanding the timeline of planetesimal formation in our Solar System.

### **Objectives of this Work**

Comet C/2016 R2 (PanSTARRS) is, so far, the only known  $N_2$ - and CO-rich,  $H_2O$ -poor comet ever observed. Since comets are some of the most pristine bodies in the Solar System, understanding where each comet was formed reveals details as to the evolution of the Solar System. An exact composition of this comet is essential to determine the likelihood of each formation scenario, adding additional insight into the composition of the early Solar System, helping us to further understand the structure of the PSN and explain the  $N_2$  depletion in comets.

My goal is to create a fluorescence model of  $N_2^+$  in comets and test it against the observed  $N_2^+$  in C/2016 R2 in order to see if this model can be used on future  $N_2$ -rich comets we may observe. Once this model is complete, I will determine the quantity of  $N_2$  produced by this comet and use it as a new baseline for  $N_2$ -rich comets. This makes up the spectroscopy aspect of my research.

I would then like to use tie this composition to a specific formation reservoir. I will evaluate different numerical integrators in order to find if such a reservoir of N<sub>2</sub>-rich comets can be found. Tying the composition to a specific formation zone in the PPD will allow us to impose new constraints on Solar System formation models. This makes up the dynamical aspect of my research.

With both a spectroscopic view of C/2016 R2, and a dynamical history, I compare it to other  $N_2$ -rich comets or  $H_2O$ -poor comets to see if any conclusions can be drawn for this population of rare, exotic comets. The benefit of this two-pronged approach is a wide perspective and the possibility of tying together two seemingly unrelated fields of cometary research.

### **Organization of the Dissertation**

In Part I, I first present the context in which this work is conceived. A brief review of the history of comet science is told so as to show much is yet to be understood about these objects. This is further exemplified in our presentation of the physical characteristics of comets. This sets the stage for our investigation of C/2016 R2-like comets. I will synthesize what is known about N<sub>2</sub>-rich and H<sub>2</sub>O-poor comets, presenting the comets in our study and investigating the first obvious links with comet C/2016 R2.

In Part II, we create a new fluorescence model of  $N_2^+$  in comets in order to better understand the  $N_2$  composition in future  $N_2$ -rich comets. I begin by presenting the model and the methods used to create it. I then apply it to comet C/2016 R2 and estimate the new scale lengths of  $N_2$  and  $N_2^+$ . I evaluate the production rate of comet C/2016 R2 and re-estimate the  $N_2$ /CO ratios of  $N_2$ -rich comets using new fluorescence factors derived from our fluorescence model.

Then, in Part III, we run a dynamical evolution model on the comets in our sample in an attempt to identify a potential shared origin point, which could lead to a reservoir of  $N_2$ -rich comets. We then examine alternative formation models and hypotheses for the peculiar nature of comet R2. One suggestion in particular, that comet C/2016 R2 is a natural by-product of our own Solar System's formation process, lead us to adapt a dynamical model of early planet migration so as to investigate the evolution of planetesimals formed in this system.

Finally, in Part IV, we conclude as to what we heave learned about R2-like comets, and what they can teach us about the formation of the Solar System.

### PART I

### CONTEXT

*II* The man will come one day who will explain in what regions the comets move, why they diverge so much from the other stars, what is their size and their nature.

Many discoveries are reserved for the ages still to be when our memory shall have perished. The world is a poor affair if it does not contain matter for investigation for the whole world in every age... Nature does not reveal her secrets at once. We imagine we are initiated in her mysteries. We are, as of yet, hanging around her outer courts.

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Seneca, On Comets

## 1 A Brief History of Comets

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COMETS ARE SOME OF the first celestial objects to have captured mankind's attention, and yet remain some of the least well understood. Here, we follow the birth of astronomy as a science through the lens of cometary observation so as to better understand the questions we still have today.

### 1.1 Early Comet Observational History

Mankind's interest in comets is as old as astronomy itself. At a time when skies were clear enough for the Milky Way to be seen as spilled milk amongst the heavens, the slightest variation would stand out to any observer. And comets were in no way a *slight* variation: larger than a star, but smaller than the Sun and moon; fuzzy, with a tail, not like the pinpricks that make up the stars; remaining in the skies for weeks, if not months, unlike fleeting shooting stars; but ever changing, slowly, enough to make it difficult to determine if it belonged to the clouds rather than the stars. In most early belief systems, the sky was seen as immutable, eternal, the realm of the gods: Any change within reflected a disruption to the harmony of the celestial plane. Some believed change was a message from the gods, usually omens of doom: deaths of kings or noble men, or coming catastrophes. Whether they were superstitious or not, the presence of a comet was significant enough to warrant being recorded: observations have been recorded as early as the first millennia BCE, in every continent and across multiple civilizations.

Ancient Chinese astronomers first inscribed their observations on ox shoulderblades and the flat under-part of turtle shells, a record we now call the *Oracle Bones*, dated as far back as  $\sim$ 1400-1200 BCE. Under the theory of *Wu Xing* (five elements),

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**Figure 1.1** – Detail of descriptions and illustrations of seven comets from and astrology manuscript unearthed from Mawangdui tomb. 29 comets in total were detailed in this manuscript *Ink on silk, 2nd century BC, Han dynasty. China Arts, Volume 1st, Wen Wu Publishing, Beijing, China,* 1979-10.



**Figure 1.2** – Possible representation of Comet 1P/Halley during its return in 1066 (Bottom). Petroglyphs at Chaco Canyon, Penasco Blanco, New Mexico. The star-like image represents the supernova of 1054 which produced the Crab Nebula. *Michael Lloyd of Wild Light Imaging Studio.* 

comets were thought to signify an imbalance of yin and yang (Needham et al., 1974). The first dated observations of comets originate from 613 BC, though there is one potential record from 2316 BCE (Ho Peng Yoke & Ho Ping-Yü, 1962). There is even a possible sighting of Halley's Comet dated 1059 BCE. The Mawangdui Silk Texts, an almanac transcribed on silk in the IV<sup>th</sup> century BC, is the first known illustrated catalog of comets (Fig.1.1): This book documents a variety of them in great detail, commenting on the appearance, path, and their peculiar properties such as the number of tails, along with the details of the catastrophe or disaster thought to be associated with each one. These texts only recorded the time, position, and brightness of each comet's passing, but additionally contained meteorological and astronomical data, including the earliest records of a solar eclipse (Zhen-Tao et al., 1995). They are accurate often to within half a degree of right ascension, and consistent over three millennia, to the point where they have retroactively been used to find periodicity of modern comets today. These astronomers were also the first to observe that comet tails point away from the Sun, many centuries before the phenomenon was understood in the West. The detailed observations were important to the astrologers of the time, and Chinese emperors employed observers specifically to watch for them as they might indicate important orders from the heavens: Emperor Ruizong of Tang abdicated after a comet appearance in 712 CE.

In the Americas, a pair of disks with long tails located on the wall of a cave produced by the Ventureño tribelet of the Chumash at Burro Flats have been interpreted as portraits of a comet "seen over an interval of a few days or weeks" (Hudson & Underhay, 1978). A depiction of a comet is carved in Penasco Blanco Train, in Chaco Canyon, New Mexico, USA, thought to be Halley's Comet (Fig.1.2). In Mexico, they were described as "smoking stars," usually signaling the death of a ruler. Curiously, this interpretation is shared by most —if not all —ancient civilizations with recorded comet observations. As later said by Shakespeare, "When beggars die there are no comets seen; The heavens themselves blaze forth the death of princes." Julius Caesar (II, 30-31), 1599.

Throughout history, different names were given to describe the apparition of a comet: The word *comet* derives from the Greek χομήτης, *kometes*, meaning "the hairy one" or "wearing long hair" due to its wispy tail in the night sky. Similarly, early Chinese records call comets *beixing* as in "bushy star" or "sparkling star" and distinguish the *huixing*, "broom star," that is comets without and with a tail respectively. The Ojibwa of the upper Great Lakes region passed down through oral history the observations of a *Genondahwayanung*, which meant "Long Tailed Heavenly Climbing Star," though it's observation cannot be dated. The Norse believed comets were flakes of the giant Ymir's skull falling from the sky and then disintegrating.



**Figure 1.3** – Roman silver coin with a depiction of the head of emperor Augustus. The comet of 44 BC is shown on the reverse. *Trustees of the British Museum*.



**Figure 1.4** – Portion of the Bayeux tapestry, Section 32, depicting the passage of Halley's comet in 1066. The text translates to 'These men wonder at the star'.

The first dated records of comets in Europe come from the IV<sup>th</sup> century BCE. In the Greek Era, the nature of the comets was intensely debated: were they astronomical, or meteorological? Did it belong to the "Cosmos," the perfectly ordered heavens, or to "Chaos," and the realm of man? Aristotle (384-322 BCE) was the first to attempt a consistent, structured cosmological theory of comets, firmly of the opinion that comets were meteorological in nature, due to the fact that comets could appear outside of the Zodiac and vary in brightness over the course of a few days. He described comets as a phenomenon of the upper atmosphere, where hot, dry "windy exhalations" from the Earth that reached out into our atmosphere, gathered, and occasionally burst into flame. Aristotle held this mechanism responsible for not only comets, but also meteors, the aurora borealis, and even the Milky Way, as all celestial objects were perfect and changeless, thus anything that changed must exist below the moon. Meanwhile, Seneca the Younger (4 BCE-65 CE), in his Natural Questions, observed that comets moved regularly through the sky and were undisturbed by the wind, behavior more typical of celestial than atmospheric phenomena, seeing no reason that a planet-like object couldn't move through any part of the sky. However, the Aristotelean view on comets was upheld during the following millennium.

Despite this step towards a scientific understanding of the nature of comets, these phenomena were still widely seen as omens from above. *Great Comets*, so called because of their exceptional brightness, were frequently associated with recent events, interpreted by those who had the most to gain. The appearance of a Great Comet<sup>1</sup> in the sky soon after Caesar's death in 44 BCE was taken by many Romans as evidence his soul was accepted among the immortal gods, which was then used as propaganda (Fig. 1.3) by his great nephew Augustus (63 BCE -14 CE)

<sup>&</sup>lt;sup>1</sup>Official designation: C/-43 K1, known colloquially as Caesar's Comet.

in order to cement his reign. In the epic poem *the Aeneid* Virgil describes how "a star appeared in the daytime, and Augustus persuaded people to believe it was Caesar". It did help to be related to a god when trying to rule the Roman Empire.

This fear of the unknown only intensified in the middle ages, when scientific study in Europe was at a standstill. While scientists in the middle east (such as Persia) and Asian countries (such as China and India) made great strides in astronomy, Europe suffered through the dark ages, and further descended into astrology, as the fear of this "heavy hand of God" reached its pinnacle. Halley's comet (1P/Halley) played a prominent role in history because of its large nucleus and therefore great brightness and longevity, making it the only periodic comet that can regularly be seen from earth by the naked eye. Its passage in 1066 was one of the greatest ever recorded, with four unique Chinese accounts of the observation, as well as Japanese, Korean, Italian, and English records which give us a clear idea of its position and appearance. The latter was recorded in the Bayeux Tapestry (Fig. 1.4) which chronicles the Battle of Hastings, for whom both William the Conqueror (1028-1087) and King Harold II of England (1022-1066) were convinced the comet was a sign of their victory. Only William was correct.

The first doubts to the Aristotelean view were expressed by Thomas Aquinas (1225–1274) and by Roger Bacon (1214-1294) in his *Opus Tertium* from 1267<sup>2</sup>. It was only when Paolo Toscanelli (1397–1482) observed P/Halley in 1456<sup>3</sup> and several other comets between 1433 and 1472 with improved accuracy that they were deemed astronomical, inaugurating the renaissance of European observational astronomy.

# 1.2 The Copernican Revolution and the Cometary Renaissance

The first major advancement in understanding the nature of comets came from the observations of the Great Comet of 1577 (C/1577 V1) by Tycho Brahe (1546–1601) at Uraniborg observatory, who demonstrated that comets must exist outside the Earth's atmosphere by measuring that its parallax was smaller than 15', corresponding to a distance of  $\sim 230$  Earth radii, placing it farther away than the Moon (Fig. 1.6) (Christianson, 1979). He also calculated that the tail must be millions of kilometers long, and realized (a Petrus Apianus (1495-1552) had first suggested) it was always

<sup>&</sup>lt;sup>2</sup>Though, like their predecessors, they firmly believed comets to be evil omens despite their more scientific approach.

<sup>&</sup>lt;sup>3</sup>It was in this year 1456 that Halley's comet was supposedly excommunicated as an agent of the devil by Pope Calixtus III (1378–1458) (Wallace, 1908). This is potentially an urban myth, supported by the fact that Halley's comet has continued to return.



**Figure 1.5** – The great comet of 1527 as depicted in "Ausburg Book of Miracles". Many pages were devoted to comets, each bearing a physical description, and the catastrophe they were believed to have caused. Here, it reads: "In the year 1527, on the eleventh of October, at four o'clock in the morning, this comet was seen in Westrich for five quarters of an hour and then it disappeared again. It was extremely long and yellowish-red, like a diluted blood in colour. At the front the head was like a bent arm, as if it had a sword in its hand and was poised to start striking with it. And at the point of the sword there were three big stars and from the stars there issued a cloud-coloured stream, which was longer than the comet's tail, just as it is painted here." Details like these can hint at comet composition even hundreds of years since their singular passage.



**Figure 1.6** – Left: Diagram of the Great Comet of 1577's orbit by Tycho Brahe. Right: Image of the Great Comet of 1577 as it appeared in the sky, by Jiri Dashitzki.

pointing away from the Sun<sup>4</sup>. This was made possible by a new international cooperation and communication between astronomers across Europe, giving Brahe access to observational data from by geographically separated observers. This was a major step in creating the analytic system of scientific research and the international astronomical community as a whole.

Nicolaus Copernicus (1473–1543) was the first to propose that comets have a heliocentric orbit. When the next great comet made its appearance in 1610, Italian astronomer Galileo Galilei (1564-1642), who had revolutionized astronomy by creating his telescope only a year before, supported this theory through his improved observations<sup>5</sup>. Johannes Kepler (1571–1630), who had worked with Brahe as his assistant before his death, built upon the precision of this research when building the laws of planetary motion, though he believed comets to be interstellar objects moving along straight lines, so the dynamics did not fit with his model. This linear model was challenged by the work of Johann Hevelius (1611-1687), who presented his *Cometographia* in which he studied the trajectories of the comets between 1652 and 1680 and determined that they must originate in the outer regions of our Solar System and travel in a parabolic trajectory. Based on the work of Kepler and Galileo, Sir Isaac Newton (1642–1726) determined that comets are attracted by the gravitation of the Sun, demonstrating that they could have elliptical, parabolic, or hyperbolic orbits (Newton, 1687). He proved his theory by calculating the orbit of comet C/1680 V1 (Kirch), determining that it had a parabolic orbit around the Sun, which was then confirmed by observation.

Edmond Halley<sup>6</sup> (1656-1742) was the first to suggest that comets may be moving along very elongated ellipses rather than parabolic paths<sup>7</sup>. He found that the great comet of 1682 appeared to be periodic, estimating a period of about 76 years, and predicting its return between 1758 and 1759 (Halley, 1706). Unfortunately, he did not live to see the event, though the passage of 'his' comet as predicted proved not only that his hypothesis was correct, but that Newton's laws of gravitation were indeed valid far beyond the observable planets. The perihelion passage itself was calculated Nicole-Reine Lepaute (1723-1788), a clockmaker, along with her colleagues Alexis Clairaut (1713-1765) and Joseph Lalande (1732-1807) who presented their result in

<sup>&</sup>lt;sup>4</sup>Despite this, the second half of his manuscript about the comet dealt with the astrological and apocalyptic aspects of the comet, making his own predictions of dire political events in the near future.

<sup>&</sup>lt;sup>5</sup>Very much a simplification of the events. An entire chapter could be devoted to Galileo's thoughts on comets, as, despite his observations, he still defended the Aristotlean view. This may have had less to do with personal belief and more with the oppressive doctrine of the church.

<sup>&</sup>lt;sup>6</sup>Alternatively Edmond or Edmund, Halley, Hailey, or Hawley.

<sup>&</sup>lt;sup>7</sup>Though it has been suggested that this knowledge was known long before and lost though the rise and decline of civilizations. There is a reference in the Talmud to "one star that rises once in seventy years and misleads sailors at sea." (Brodetsky, 1911)

front of the *Académie des Sciences* after six months of arduous calculations, manually accounting for the gravitational pull of each of the planets. While their prediction was for 13 April 1759, the comet arrived on 13 March; only one month off (Lynn, 1911). This was the birth of the field of comet dynamics.

Over the next 200 years, as the precision of their instruments improved, astronomers were able to better constrain the periods of the comets. There seemed to be two distinct groups: those with a period under 200 years, which they called short-period comets (SPCs), and those with periods longer, or long-period comets (LPCs). The science done on comets at the time consisted of predicting their orbits and describing their morphology: their true nature was still a mystery.

## 1.3 Spectroscopy and the Pioneering Age

The next great leap in cometary research came with the advent of spectroscopy. Until then, the composition of comets was completely unknown. While Newton's *Opticks* (1704) demonstrated how white light could be split up into component colors using a prism, and that these components could be recombined to generate white light, and Robert Hooke (1635–1703) and Christiaan Huygens (1629–1695) demonstrated how spectra was representative of the chemical constituents producing the light, it would take over a hundred years for optical instruments to deliver high enough resolution to see into the composition of astronomical bodies.

The first spectrometer was built by William Hyde Wollaston (1766-1828) in 1802. Using a a lens to focus the Sun's spectrum on a screen, he discovered dark bands obscuring the continuum of color, which Joseph von Fraunhofer (1787-1826) later revealed using diffraction grating in 1815 to belong to specific wavelengths. To this day, these are referred to as Fraunhofer lines. Léon Foucault (1819-1868) then experimentally demonstrated that absorption and emission lines appearing at the same wavelength are both due to the same material in 1849, almost at the same times as Anders Jonas Ångström (1814-1874) who, in 1853 postulated that an incandescent gas emits rays of the same wavelength as those it can absorb.

The systematic attribution of spectra to chemical elements began in the 1860s with the work of German physicists Robert Bunsen (1811-1899) and Gustav Kirchhoff (1824–1871), who found that Fraunhofer lines correspond to emission spectral lines observed in laboratory light sources. This laid way for spectrochemical analysis in laboratory and astrophysical science. Bunsen and Kirchhoff applied the optical techniques of Fraunhofer and established the linkage between chemical elements and their unique spectral patterns. In the process, they established the technique of analytical spectroscopy. In 1860, they published their findings on the spectra of eight

elements and identified these elements' presence in several natural compounds. They demonstrated that spectroscopy could be used for trace chemical analysis and several of the chemical elements they discovered were previously unknown. Kirchhoff and Bunsen also definitively established the link between absorption and emission lines, including attributing solar absorption lines to particular elements based on their corresponding spectra.

The first reported use of spectroscopy on a comet was from August 5th, 1864, when Italian astronomer Giovanni Battista Donati (1826–1873) turned his telescope on Tempel's Comet of 1864 (Modern designation C/1864 N1, alternatively 1864 II or 1864 a). Donati had built a small visual spectroscope and adapted it to his refractor in order to examine the spectra of stars and nebulae. In Tempel's comet, he observed three bright rays, assimilating them to those produced by metals (Donati, 1864): in truth, those were the Swan bands of carbon. This set off decades of visual observations of cometary spectra (Swings, 1965).

Sir William Huggins (1824-1910), a notable spectroscopist, turned his attention from nebulae (from which he had already identified the 'nebular lines') to Tempel's Comet of 1866 (Modern designation 55P/Tempel–Tuttle, alternatively 1866 I or 1865 f), the first of what would be six comets he would observe from 1865 to 1871, publishing their spectra. He would place a spark in gas and hold it in his eyepiece beside the comet's so as to align them perfectly. Using this method he correctly identified the D-doublet of sodium. He remarked on the difference between the spectra of nebulae and those of comets, and even realized how the spectrum could be different when observing separate sections of a single comet. It was here that the continuous spectrum was found.

Cometary spectroscopy's first golden age came in the early 1880's, when a boon of four incredibly bright comets —some considered Great Comets —made their appearance at the same time as photographic plates became more widely available: C/1881 K1, C/1881 N1, C/1882 F1 (Huggins, 1882), and C/1882 R1 (Christie, 1882). C/1882 R1 was calculated to have been only 0.0032 au from the solar surface and reached an estimated magnitude of -17, and lead to the discovery of the Kreutz Sungrazers. The four comets lead to 80 different papers published in this time period, a most of which using photographic plates to capture their spectra. Huggins identified CN bands in C/1881 K1, along with OH,  $C_3$ , and was able to separate the P and R branches of CN. He found similar results in the other comets of this period. This helped establish a baseline for the composition of comet heads. They were now known to be made of up CN,  $C_2$ ,  $C_3$ , CH, while the tails remained a mystery, as they were too weak to develop on spectroscopic plates.

Finding cyanogen in a comet might have been exciting for scientists, but terrifying for the public. Camille Flammarion (1842-1925) shared the presence of this



**Figure 1.7** – Spectrum drawn by Huggins in 1868 (bottom) where Donati's bands can be found. The spectrum of the comet is compared with spectra of carbonaceous products traversed by sparks. Here, the bands are due to the  $C_2$ . It was quite fortunate that Huggins was examining the bands of  $C_2$ , as these are similar both in the comet and in the laboratory. Had he chosen another molecule (such as the CN (0,0) band) he may not have had such impressive results.

compound in comet Halley, along with the fact that, should a sufficient quantity of hydrogen in the comet's tail be combined with our atmospheric oxygen, all animal life could suffocate in just a few moments. And here, in 1910 the tail lay stretched in the path of the Earth, mankind helpless to change its course. "We can admit that we ignore what fate has in store for next May. [...] The human race would perish in a paroxysm of universal joy, delirium and madness, probably very enchanted with its fate," he said, expressing his small doubt at the diffusive nature of the tail. The press ran with this, causing a panic: The night of 18-19 May 1910, when the Earth traveled through the tail of the comet, people feared they would be poisoned. Flammarion denied the rumor, citing how the press quoted him out of context and sensationalized his claims, but the apocalyptic news was already out. Charlatans seized the opportunity to sell anti-comet pills, umbrellas, gas-masks, and even an anti-Halley's comet elixir to hapless citizens who believed it was their only change of survival (see examples Fig. 1.8). The tail did prove to be extremely diffuse, and there was no effect when the planet passed through it<sup>8</sup>. It would seem the fear associated with comets would not be diminished with scientific understanding, only be seen through a different lens. That, and that fake news will always tail astronomers.

*"The literature of comets' tails may be likened to the literature of the Free Trade and Tariff Reform in the world of Politics: it is superabundant and more than superabundant."* 

<sup>&</sup>lt;sup>8</sup>Ironically, after-the-fact calculations determined that the Earth did not pass through the comet's tail in 1910. We missed it by at least 400,000 km due to errors in the comet's predicted orbit and the curve of the tail. While we missed the tail, perhaps we did not miss the point.



**Figure 1.8** – Examples of the apocalyptic headlines and solutions surrounding the 1910 return of Halley's comet.

(Chambers, 1909). This quote from a comet reference book at the turn of the century offers a snapshot the field of comet research at the time. But while entire books were dedicated to comet tail morphology, almost nothing was known about their composition. That was until the invention of objective prisms in the early 1900's. Count Aymar de la Baume Pluvinel (1860–1938) adapted the technology to comets, and began using them for hour-long exposures of comets starting with C/1907 L2 (Daniel), in which he found massive amounts of CO<sup>+</sup> in the tail, followed by the spectacular C/1908 R1 (Morehouse). This comet displayed a brilliant tail which rapidly shifted in morphology. This allowed for a shocking discovery: CN and  $C_2$  were resigned to the head, while the tail proved to be rich in CO<sup>+</sup> and N<sub>2</sub><sup>+</sup>.

It was becoming clear that cometary activity was linked to the solar activity. With increasingly powerful instruments, astronomers observed how the radial velocity of a comet affected its rotational profiles; how heliocentric distance  $r_h$  affects the rotational temperatures; how the solar wind affects the behavior of the ion tail. International teams began to be put in place in the 1940s-1950s in order to systematically survey every comet's spectra. The McDonald observatory in Texas, the Dominion Astrophysical Observatory in Canada, and the Observatoire de Haute Provence in France were some of the most notable in the early-mid XX<sup>th</sup> century, using split spectrograms to investigate the UV region. They discovered that the rotational bands of OH and NH corresponded to a low temperature. Comet C/1947

S1 (Bester) provided the first real look into comet tails using modern spectroscopy:  $CO^+$  bands were once again identified, and  $N_2^+$ , "as expected" (Swings, 1965), and it was the first time  $CO_2^+$  emission was identified in the optical spectrum of a comet. Astronomy textbooks at the time described comet tails to be both  $CO^+$  and  $N_2^+$  rich, "as is well known" and these were "the two characteristic molecules of the comet-tail spectra" (Swings & Page, 1950). Since the method of obtaining cometary spectra using objective prisms was used until the 1940's, the only spectra of tails obtained before 1940 were of C/1908 R1 (Morehouse), and C/1911 O1 (Brooks), which also had a  $CO^+$  tail, comet tails were thought to have this ionic composition until the mid XX<sup>th</sup> century. It was only when applying these spectroscopy techniques to comets using their modern technology that they discovered this was an outlier, not the rule: these ionic tails were incredibly bright, thus enabling spectroscopic measurements to be taken, creating an observational bias<sup>9</sup>.

One of the greatest mysteries still waiting to be uncovered was that of the perturbations in Uranus and Neptune's orbit. After French astronomer Urbain Le Verrier (1811–1877) discovered Neptune in 1846 on the basis of disturbances observed in the trajectory of Uranus (the first discovery of a celestial object made through mathematical calculation) it was understood there had to be another perturbing element in the distant Solar System in order to explain the discordance in the math. Percival Lowell presented the hypothesis of a planet X to explain these anomalies, building an observatory in 1894 in Arizona to look for it, but died in 1916 before finding it. By using the 'blink method', Clyde Tombaugh (1906–1997) discovered Pluto at the Lowell observatory in 1930, but it was quickly shown to not have the mass required for these perturbations. Frederick C. Leonard (1896-1960) speculated that it was "not likely that in Pluto there has come to light the first of a series of ultra-Neptunian bodies, the remaining members of which still await discovery but which are destined eventually to be detected" (Leonard, 1930).

## 1.4 The Modern Era of Cometary Science

The year 1950 was a turning point in cometary science, as it marked the emergence of the modern collective view of comets. Fred Lawrence Whipple (1906–2004) wrote a series of influential papers entitled *A Comet Model* in which he put forward the "dirty snowball" hypothesis of comets, postulating that comets were icy conglomerates

<sup>&</sup>lt;sup>9</sup>Personal speculation. Comet tails were thought to be rich in  $N_2^+$  until the 1980's; then, it seems the  $N_2$  depletion became more apparent. However, I could not find any transitional articles, though Lutz et al. (1993) say that  $N_2^+$  is 'rarely reported' in cometary plasma. This leads me to believe in the observational bias of bright  $N_2^+$ - rich tails being easier to study with spectroscopy before the use of high spectral and geometrical resolution. I discus this in section 3.3



**Figure 1.9** – The 1992 discovery of Kuiper Belt Object 1992 QB<sub>1</sub> (15760 Albion) by Jewitt and Luu. From Jewitt (1992), modified to fit this page.

(Whipple, 1950, 1951, 1955). At the same time, in 1951, Ludwig Biermann (1907-1986) hypothesized that the motions of features in the tails of comets were caused by their interactions with a flow of charged particles emanating from the Sun: the solar wind (Biermann, 1951).

The installation of coudée spectrograms in large observatories ~1957 allowed for more precise analysis further from the comet head, revealing gas emissions could extend >200,000 km from the nucleus and tails could be ~10<sup>7</sup> km long. The increased resolution improved the precision of measured wavelengths and intensities: the rotational structure became more clear, there was better separation between the bands, and it was easier to subtract the solar continuum, revealing bands that were previously so weak as to be hidden. It was around this time that the field of cometary physics experienced a true 'revival' (Arpigny, 1964; Swings, 1965).

Also in 1951, Gerard Kuiper (1905–1973) famously put forward the idea of a disc having formed at the beginning of the evolution of the Solar System in the region beyond Neptune. The material in the solar nebula was too far apart to condense into planets, so it instead formed a disk of small bodies that would no longer exist. However, Kenneth Edgeworth had already posited that the area between 35 and 50 au would be a reservoir of short period comets (Edgeworth, 1943), still present today. Whipple and Al Cameron both independently conjectured that this 'comet ring' was still present and would account for the number of comets observed (Cameron, 1962; Whipple, 1964). Julio Fernandez used numerical simulations to demonstrate that the Kuiper belt would indeed exist and correctly predicted its shape, crediting Kuiper for the original hypothesis (Fernandez, 1980) which lead Duncan et al. (1988) to coin the name Kuiper belt<sup>10</sup>. David Jewitt and Jane Luu conducted research trying to find this disk with a blinking comparator, like Clyde Tombaugh. After five years of searching, Jewitt and Luu announced in 1992 the discovery of candidate Kuiper Belt Object 1992 QB<sub>1</sub> (Fig 1.9) (Jewitt & Luu, 1993), now called 15760 Albion, first trans-Neptunian object other than Pluto, shortly hailed as the tenth planet by the press. Six months later, they discovered a second object, 1993 FW. The Edgworth-Kuiper Belt was confirmed, finally placing Pluto in its proper perspective.

If this was the source of short period comets, then where did long period comets come from? In 1932, Ernst Öpik (1893–1985) postulated that long-period comets originated in an orbiting cloud at the outermost edge of the Solar System; Jan Oort (1900–1992) independently revived the idea in 1950, reasoning that a comet could not have formed while in its current orbit while keeping their volatile composition (Oort, 1950). However, comets at this distance would be too small, cold, and faint to be observed with modern telescopes.

Starting in the 1980s with the so-called Halley Armada 1.5, a handful of missions were launched to investigate comets. At this stage, optical spectroscopy had become quantitative photoelectric spectrophotometry and had been extended to the radio and ultraviolet (A'Hearn, 1982) and the inventory of materials contained within comets grew slowly and steadily. Then, in 1983, the IRAS spacecraft detected excess infrared radiation from young A-type main-sequence star  $\beta$  Pictoris which was soon determined to be a debris disk, seen edge-on. Strange, hour-long variations in the calcium H and K lines in this spectrum was revealed to be the result of passing comets, or exo-comets, also called Falling Evaporating Body (FEB), the first observed outside of our own Solar System (Ferlet et al., 1987; Beust et al., 1990; Vidal-Madjar et al., 1994). To date, there are over 30 known systems to present exo-comets.

These are not to be confused with Interstellar comets, which originate from outside of our Solar System, but are observed during their passage through our own. 1I/'Oumuamua, discovered in 2017, was the first certified object of this type, traveling with an eccentricity e of 1.2 (the highest ever observed at the time) and at a velocity exceeding the escape velocity of our Solar System. Eccentricities > 1 represent hyperbolic orbits, and objects on these trajectories are unbound from the Solar System. This discovery was followed shortly by that of 2I/Borisov in 2019, with an astounding eccentricity of e = 3.4, making it clearly a visitor from another system. With two interstellar objects discovered at only a two year interval, we must

<sup>&</sup>lt;sup>10</sup>An example of inconsistent literature review, which has lead to the over-crediting of Kuiper despite having never spoken about this ring still being present. Duncan, Quinn, and Tremaine regret having coined the name and would have preferred the Fernandez belt. In fact, we could (and perhaps should) add the names Cameron, Whipple, and Leonard to give credit where credit is due, though creating an amalgam of these names would not be an easy feat. *International Comet Quarterly* propose the LEdgeKWhip belt(s). It just might be catchy enough to work.

ask ourselves how many others may have come and gone without our knowledge of their alien nature.

We are aided in our search for comets by new full-sky surveys, starting with NASA's initiation of the Near-Earth Object (NEO) Observations program in 1998. Some of these programs include Catalina Sky Survey (CSS) and Spacewatch near Tucson Arizona, the Lincoln Near-Earth Asteroid Research (LINEAR) project near Socorro New Mexico, the Panoramic Survey Telescope and Rapid Response System (Pan-STARRS1 and 2) on Haleakala, Maui, Hawaii, Lowell Observatory Near-Earth-Object Search (LONEOS) near Flagstaff Arizona and the Near-Earth Asteroid Tracking (NEAT) project run by NASA/JPL. The number of long-period comets discovered with these surveys is shown in Fig. 1.10. While the goal of these large telescope arrays is to sweep the sky every night in order to search for the motion of small bodies, with the intent to give prior warning in case of a collision, an added benefit is the discovery of comets. As a result, the quantity of known comets has skyrocketed in the 21<sup>st</sup> century, while also providing us with longer windows to observe and understand them better. As of writing this thesis, 4415 comets are







**Figure 1.11** – Comet Halley's nucleus as imaged by the *Giotto* spacecraft, at only ~ 2000 km. *Halley Multicolor Camera Team, Giotto Project, ESA* 

known and cataloged by the *IAU Minor Planet Center*, and more are discovered every day.

## 1.5 Comets in the Space Age: Spacecraft Encounters

Comets are particular difficult to visit with probes, particularly long-period comets, whose arrival in the inner Solar System is unpredictable. As the process of planning a mission is long and arduous, only short-period comets can currently be candidates for probes —though this is about to change —and even then, constraints abound.

Launched in 1978, the International Cometary Explorer (ICE), originally known as ISEE-3 (International Sun-Earth Explorer), completed its original intended mission of studying the interaction between the Earth's magnetic field and the solar wind along with its sister probes ISEE and ISEE-2. Afterwards, it was placed in a halo orbit at the L1 Earth-Sun Lagrange point in order to be reactivated, renamed, and diverted to pass through Comet 21P/Giacobini–Zinner's tail on September 11<sup>th</sup> 1985, within about 7,800 km of the nucleus.

The 1986 return of comet 1P/Halley offered a once-in-a-lifetime opportunity to rendez-vous with a comet as its nearest approach to Earth occurred at a distance of 0.42 au. Not only was Halley's orbit well known, but it had already gained the public's attention. As a result, eight different probes were sent to rendez-vous, sometimes called the "Halley Armada". The NASA Pioneer Venus Orbiter, already in orbit of Venus, was positioned perfectly to take measurements of the comet during

its perihelion February 9<sup>th</sup>, 1986. Its UV-spectrometer observed the water loss when Halley's Comet was difficult to observe from the Earth. Russian spacecrafts Vega-1 and Vega-2, launched to drop probes on Venus in 1984, continued on their journey to investigate and photograph Comet Halley. Vega-1 made its closest approach to the comet on March 6<sup>th</sup> 1986 at a distance of 8890 km and Vega-2 flew in closer to the comet nucleus at a distance of 8030 km on March 9<sup>th</sup>. These were followed by twin spacecraft Sakigake and Suisei, Japan's first deep-space missions. Suisei approached to within  $1.5 \times 10^5$  km of Comet Halley on March 8<sup>th</sup> specifically to observe the interactions of the coma with the solar wind, followed by Sakigake which approached to within  $7 \times 10^6$  km of the comet on March 11<sup>th</sup>. Next, ESA's *Giotto* spacecraft, the first European deep space mission, flew past the nucleus of Comet Halley at a distance of only 600 km on March 13<sup>th</sup>, revealing a dark, potato-shaped object with jets of gas and dust blasting into space (Fig. 1.11). The sight of this nucleus was monumental, as it proved the accepted hypothesis of the nature of a comet's active core. NASA's Pioneer 7 -launched in 1966 by NASA -was also redirected from its study of the solar magnetic field and flew within  $12.3 \times 10^6$  of Halley's Comet and monitored the interaction between the cometary hydrogen tail and the solar wind; NASA's Pioneer 12 was also redirected for this purpose. Finally, ICE passed through the tail within  $30 \times 10^6$  km from the nucleus. Overall, this collection of missions offered the first true insight into the nature of a comet's nucleus, ushering in a new era of cometary science.

It was also the mission of the Space Shuttle Challenger STS-51-L crew to observe the comet from space for six days, carrying the "Shuttle Pointed Autonomous Research Tool for Astronomy" (SPARTAN-203), Halley's Comet Experiment, and Comet Halley Active Monitoring Program (CHAMP). The shuttle failed to reach orbit, resulting in the total loss of crew and vehicle. This launch failure led to the cancellation of multiple scheduled missions, including ASTRO-1 observatory, which was intended to make astronomical observations of Halley's Comet.

The NASA Galileo mission was able to image Shoemaker-Levy 9 —D/1993 F2 (Shoemaker-Levy) or SL9 —then on its way to a rendezvous with Jupiter scheduled for 1995. This comet was orbiting the gas giant when it was discovered by Carolyn and Eugene M. Shoemaker and David Levy in 1993, but calculations showed that its unusual fragmented form was due to a previous closer approach to Jupiter in July 1992 when it passed within Jupiter's Roche limit and was ripped apart by Jupiter's tidal forces. It was predicted with an extremely high probability that SL9 would collide with Jupiter in July 1994, and several space observatories oriented to observe, including the Hubble Space Telescope (See Fig. 1.12), the ROSAT X-ray-observing satellite, and the W. M. Keck Observatory. The first impact occurred at July 16<sup>th</sup>, 1994, creating a massive fireball visible with Earth-based telescopes. 21 distinct



**Figure 1.12** – The individual nuclei of Comet Shoemaker-Levy 9, as imaged by the Hubble Space Telescope on May 17, 1994. *NASA*.

impacts were observed over the next 6 days, allowing for chemical studies of the atmosphere of Jupiter.

The next missions allowed us to explore a variety of comets. Deep Space 1, the first spacecraft in NASA's New Millennium program, approached within 26 km of Asteroid 9969 Braille on July 19th 1999 and encountered comet 19P/Borrelly on September 22<sup>nd</sup> 2001, returning images and other science data from  $\sim 2200$  km from the nucleus. The NASA Stardust mission launched 7 February 1999, flew through the coma of Wild 2 (81P/Wild, pronounced 'vilt two') -a long period comet which became a short period comet in 1974 when a close-encounter with Jupiter changed its orbit —offering a rare opportunity to observe a once-long-period comet. The spacecraft came to within 240 km of the nucleus on January 2<sup>nd</sup> 2004, where it trapped particle samples from the comet's coma in ultra low density aerogel, which it returned to Earth in 2006 along with interstellar material it collected during the journey, later revealed to contain seven particles of interstellar dust (Westphal et al., 2014) and the amino acid glycine (Elsila et al., 2009). In an extended mission phase known as Stardust-NExT (New Exploration of Tempel 1), the spacecraft visited Comet Tempel 1 in 2011, in order to evaluate the results of the 2005 Deep Impact mission (See Fig. 1.13).

A few missions were not so successful. Contact was lost with CONTOUR (Comet Nucleus Tour), a NASA mission to improve our understanding of comet nuclei launched in July 2002, when it began maneuvers to move onto a heliocentric, comet-chasing orbit, and was considered lost. Other times, spacecraft had unexpected encounters with a comet, such as the *Ulysses* spacecraft which made an unexpected pass through the ion tail of C/1996 B2 Hyakutake on May 1<sup>st</sup> 1996. Later, in 1999 a coronal mass ejection carried the cometary material of C/1999



**Figure 1.13** – Images taken by NASA's *Deep Impact* after dropping the impactor. The impact was so bright and dusty it made visualizing the crater difficult. Image from A'Hearn et al. (2005).

T1 (McNaught–Hartley) to the spacecraft, before it reached the tail of C/2006 P1 (McNaught) on February 3<sup>rd</sup> 2007.

All missions up to this point had been flyby missions. Comet comas were beginning to be well understood, but the nucleus was still a mystery below the surface. In order to investigate comet interiors, NASA's *Deep Impact*<sup>11</sup> missions was launched in 2005 to study the interior composition of the comet Tempel 1 (9P/Tempel) by releasing an impactor into the comet. On July 4<sup>th</sup> 2005, the first impactor was crashed into the nucleus, while the flyby module took photographs, though the dust cloud produced was so thick and bright that the size of the impact created a crater was not known until 2007, when rendez-vous-ed by the Stardust-NExT mission, which helped determine it to be 150 m in diameter. The comet was also more dusty and less icy than had been expected, suggesting they may be less 'dirty snowballs' as Whipple (1950) suggested and more 'icy dirtballs,' though composition varies from comet to comet. It presented a very fluffy structure made up of a fine dust held together by gravity, weaker than a bank of powder snow.

*Deep Impact* was then renamed EPOXI (Extrasolar Planet Observation and Deep Impact Extended Investigation) before it embarked on an extended mission designated to visit other comets. After a failed encounter with Comet 85D/Boethin, it was redirected once again, this time to Hartley 2 (103P/Hartley). EPOXI came within 700 km of the nucleus, returning detailed photographs of the "peanut" shaped

<sup>&</sup>lt;sup>11</sup>No relation to the film, however the mission took place seven years after the movie, and NASA is known to take inspiration from pop culture, though is usually more subtle about it.



**Figure 1.14** – Left: 67P/Churyumov–Gerasimenko seen by the Rosetta orbiter. Right: Surface of 67P/Churyumov–Gerasimenko seen by the Philae lander, with depth cues. *ESA* / *Rosetta* / *Philae* / *CIVA* / *Mattias Malmer*.

cometary nucleus and several bright jets, along with spectroscopic data of the coma. It then observed Comet Garradd (C/2009 P1) from February to April 2012 through a variety of filters while it was 1.87–1.30 au away, revealing that the outgassing from the comet varies with a period of 10.4 hours, which helped determine the rotation period of the nucleus. A CO/H<sub>2</sub>O of ~10% was also found. It was also able to complete some observations of comet ISON (C/2012 S1). Unfortunately, communication with this spacecraft was lost in 2013.

The most monumental comet mission of this generation is the ESA Rosetta-Philae mission, with the intention to place a lander on comet 67P/Churyumov–Gerasimenko. They were named for the Rosetta Stone and the Philae obelisk, which were used to decrypt ancient languages: in that same way, it was hoped that these spacecraft would help decrypt the Solar System. Launched in 2004, it took the spacecraft ten years to reach the comet, arriving in 2014. It dove into the coma and returned photos of 67P's peanut-like bilobal nature (shown in Fig. 1.14) before becoming the first spacecraft to orbit a comet. On November 12<sup>th</sup>, its lander module Philae performed the first successful landing on a comet, conducting the first soft landing on a comet nucleus. Due to the low escape velocity of only around 1 m/s, two harpoons were meant to fire into the comet on contact with the surface to prevent the lander from bouncing off: however, the surface at the initial touchdown site was relatively soft, covered with a 0.25m layer of granular material<sup>12</sup>, and the harpoons failed. The

<sup>&</sup>lt;sup>12</sup>An amusing analogy of comets is that they resemble 'deep fried ice cream', with only a very thinly 'fried' layer and a soft icy center.

lander rebounded, bouncing twice on the comet's surface, before it finally settled —in the shadow of a cliff. The solar panels were not able to function as the lander sits on its side wedged into a dark crevice as observed by the Rosetta orbiter. The lander was still able to return astounding pictures of the surface, giving us the first look of a comet's surface. The comet became too distant from the sun in 2016, preventing the orbiter from obtaining enough sunlight. On September 29<sup>th</sup> 2016, it was de-orbited and crashed into the surface, its closest photo ~20 m from the surface.

This mission provided the community with a plethora of data still being analyzed today. In many ways, it opened up a whole new era of comet research, separating the pre- and post-Rosetta eras. The Rosetta orbiter featured 12 instruments, and the Philae lander contained nine additional instruments. There was evidence of nonvolatile organic compounds everywhere on the surface with little to no water ice visible.

Sadly, no new comet spacecraft have been launched since 2005. But all that is about to change with the adoption of the Comet Interceptor mission, and on an impressive scale. Until now, the only comets which were good candidates for a probe were periodic comets, as spacecraft missions are time-consuming and costly, limiting the window of opportunity for investigation. It is simpler to prepare a mission for an already known comet with a set return date. The downside of this is that our spacecraft would only be able to visit comets that have already been altered by their multiple passages within the inner Solar System. This ESA-JAXA mission is slated for launch in 2029 and would allow us to place a spacecraft at the L2 Lagrange point, where it would wait in standby for a dynamically new comet to be discovered. Then, we would effectively skip the process of waiting for assembly and have the probe ready to go investigate right away. This would also allow us to visit interstellar objects were they to pass through our Solar System on a suitable trajectory.

\* \* \*

Despite being some of the oldest known celestial objects, comets are still some of the least well understood. While the general public is at least aware of the existence of comets, and will occasionally look up in awe at the beauty of a beautiful comet in the sky, the nature of these objects is not a primary focus of science education. This leads to a lack of public interest which in turn leads to a lack of funding for cometary science. Worse, due to the persistence of folklore and astrology, comets are still blamed for modern day disasters, just as they were centuries ago. A heartbreaking example of this would the Heaven's Gate cult, who believed comet C/1995 C1 Hale-Bopp was hiding a UFO, and committed mass suicide in March 1997 in an

#### 🛲 San Francisco Chronicle





**Figure 1.15** – Headline from the San Francisco Chronicle after the mass suicide of the Heaven's Gate cult members. To this day, their website still flashes with "Red Alert: HALE-BOPP Brings Closure to Heaven's Gate."

**Figure 1.16** – Twitter graphic from the 2016 Brexit leave vote. The UK is represented as a comet.

attempt to join the spaceship (Fig 1.15). This event was less then 30 years ago, and a heartbreaking example of rampant science distortion. I hesitate to call it misinformation, as their understanding of the comet may have been scientifically sound, only symbolically motivated. Fig. 1.16 was one of many memes made after the Brexit vote of 2016, when the UK vote to leave the EU<sup>13</sup>. Here, the UK is represented as a comet. Even if this image was probably made in good fun, it displays the lingering willful association of comets with the supernatural and the astrological.

It is easy to understand how comets can still captivate us: galaxies can not be seen by the naked eye, and shooting stars require a fair bit of luck to be observed, but comets? They remain as beautiful and otherworldly in the sky as they appeared to our ancestors before us. So why then are they not common knowledge? Hopefully, a mission like Comet Interceptor will be able to ignite more interest in the general public and encourage new generations of scientists to explore this fascinating field, which still has many mysteries waiting to be explored.

<sup>&</sup>lt;sup>13</sup>Ironically, C/2016 R2 was discovered in 2016 — Coincidence?

# 2 General Overview

#### Contents

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## 2.1 Classification of Comets

Comets formed in the early Protosolar Nebula (PSN) by agglomeration of dust grains and condensation of gas. These comets (or cometesimals) were the building blocks of the cores of the giant planets. It is generally accepted that they delivered water and organics to the terrestrial planets. As they are thought to have formed from the materials available to them in the PSN at the location of their birth, they preserve the composition of the disk at that precise area and moment in time: a core sample of the PSN. Tracing back comets we see today to their formation area allows us to better understand the formation of the Solar System and establish constraints on the formation of the planets.

Their formation area is estimated to range from the area of the giant planets —beyond the water iceline, the radius where the disk temperature is equal to the sublimation/condensation temperature of water-ice —to the outer part of the PSN, approximately 5-50 au. Beyond that point, there would not be enough material to build comets, while inwards of the iceline, cometary ices would not survive. No comets would have formed in the Öpik–Oort Cloud (OC) as there was no material that far from the Sun: instead, this reservoir was filled during the period of dynamic instability when a large part of the planetesimals formed in the region of the giant planets were sent outwards on highly elliptical orbits (Tsiganis et al., 2005). Those which remained make up the Edgeworth-Kuiper Belt (EKB). These are the two distant reservoirs in which comets are stored, and each new comet brings a new piece of the puzzle to our understanding of their shape and structure.

#### 2.1.1 Dynamical Origin of Comets

Historically, the most widely used classification divides comets in two main families: Short-period comets (SPCs) are those with P < 200 years (P/ comets) while longperiod comets (LPCs)have P> 200 years (C/ comets). The use of 200 years is arbitrary, but roughly corresponds to the time since systematic observations with instruments could be made, and it effectively divides which comets came from the Edgeworth-Kuiper Belt (SPCs) and those from the Opik–Oort Cloud (LPCs) (see Fig. 2.1), as these comets appear to originate from a spherical reservoir extending to  $\sim 2 \times 10^5$  au (Fouchard et al., 2006). However, this division is misleading, as some so-called "long-period" comets are not periodic at all, and can have highly elliptical or nearly-hyperbolic orbits taking them on a single pass through the inner Solar System. There are also comets with the P/ designation such as 153P/Ikeya-Zhang with a period > 200 years. In order to more accurately divide these comets into a binary, we classify them into dynamical families based on specific orbital elements (Levison, 1996). Due to their small scale compared to the giant planets, it is important to distinguish the likelihood of comets to interact with these, as it will determine their orbit. For this, we have the Tisserand parameter:

$$T_P = \frac{a_P}{a} + 2\cos(i)\sqrt{\frac{a}{a_P}(1-e^2)}$$
(2.1)

where *a* is the semi-major axis of the interplanetary body's orbit, *e* its eccentricity, *i* its inclination with respect to the ecliptic plane, and  $a_P$  the semi-major axis of the perturbing body's orbit. This parameter defines the interaction between the interplanetary body and a larger perturbing body: in comet dynamics, this perturbing body is Jupiter, as it is the most massive planet in the Solar System and exerts the greatest dynamical influence on the comets and asteroids. The lower the Tisserand parameter, the less an object is influenced by the perturbing body. This allows us to re-classify these "long-period" comets as Nearly-Isotropic Comets (NICs) with a  $T_J < 2$ , less likely to interact with Jupiter, and "short-period" comets as Ecliptic comets (ECs) with  $T_J > 2$ , more likely to interact with Jupiter.

Within this binary, we further classify comets by groups of orbital elements, or 'families.' These families are shown in 2.2. Comets having a  $2 < T_J < 3$  are considered Jupiter Family comets (JFCs) and their dynamics are controlled by the giant planet; these tend to have perihelia interior to Jupiter (q < 5.2 au) and aphelia well separated from Saturn (Q < 7 au). Within NICs, we have both New ( $a > 10^4$ 



**Figure 2.1** – The Edgeworth-Kuiper Belt and the Öpik–Oort Cloud shown to scale with the orbit of the planets. The orbit of the trans-Neptunian object 90377 Sedna is shown to better exemplify the scope of the Öpik–Oort Cloud. *NASA / JPL-Caltech*.



Figure 2.2 – The Levison (1996) classification of comets.

au) and Returning ( $a < 10^4$  au) comets, the latter split into those with semi-major axes a > 40 au, or External comets, and Halley-type comets (HTCs) with semi-major axes a < 40 au, that is a period typically between 20 and 200 years. Many will have an eccentricity such that they only make one pass through the Solar System. These comets are further divided into near-Parabolic ( $e \simeq 1$ ), which do not have a high enough velocity to escape the Solar System, and Hyperbolic (e > 1) comets, which are not likely to ever return. Once a comet is beyond 250 au from the sun, it is outside of the influence of the inner Solar System, in the sense that its orbital elements will remain unaltered until its next passage, assuming there is one. At this stage we can use 1/a as a proxy for orbital energy (Oort, 1950; Thomas, 2020). If it is positive, the comet is unbound from the Solar System.

Asteroids are distinguished from comets by usually having a  $T_J > 3$ , though some comets also fit this criterion, specifically Encke type comets (with  $a < a_J$ ) and Chiron Type comets (CTSs) with  $a > a_J$ . These are sometimes referred to as Main Belt Comets (MBCs). Comets can transition between these families (Duncan et al., 2004), though in doing so can occasionally undergo tidal-disruption and breakup if they pass through the Roche limit of Jupiter, as was the case with Comet Levi-Shoemaker 9 (see Sec. 1.5), and other ancient comets as evidenced by crater patterns on some of Jupiter's moons.

A unique family are the centaurs, a transient population of icy bodies that dynamically link the outer Solar System's trans-Neptunian objects (TNO) population with the JFCs (Jewitt, 2009). They are named after the mythological centaurs that were a chimera of horse and human as they typically exhibit the characteristics of both asteroids and comets. Centaurs have perihelion distance q and semi-major axis a between the semi-major axis of Jupiter and Neptune( $a_J < q$  and  $a < a_N$ ). Frequent gravitational perturbations from the giant planets drive their dynamical evolution.

We now know that the reservoir of trans-Neptunian objects has a complex structure, separated between the EKB and the Scattered Disk. The EKB is a relatively thick torus and sits between ~30-50 au, composed of trans-Neptunian objects which do not cross the orbit of Neptune. These objects are dynamically stable over long time scales (Levison et al., 2008). It can be divided between objects in 2:3 and 1:2 resonances with Neptune and those in between. The Classical Belt (42-48 au) is comprised of those in between these two resonances, and objects within rarely have their orbits altered. The first TNO found, (15760) 1992  $QB_1$  is one of these objects: as a result, objects in this category are sometimes called 'Cubewanos.' This population can be subdivided even further into the 'dynamically cold' with  $i < 4^{\circ}$  and e < 0.1, and the 'dynamically hot' which are much more inclined, with 4 < i < 30. The Classical Belt is banded by the mean motion resonances with Neptune, with the 2:3 resonance at 39.4 au, containing Pluto, giving this population the name 'plutinos', and the 1:2 resonance at 47.7 au, amusingly called 'twotinos'. Meanwhile, the Scattered Disk contains objects on more eccentric orbits, with a > 50 au and q > 30, making them easily influenced by Neptune. Sedna is an example of this population, with a = 506 au and q = 76.2 au (Morbidelli & Brown, 2004).

Less is known about the Öpik–Oort Cloud as its distance and low albedo of its objects make it impossible to observe direction. Based on their random distribution in inclinations, this so-called cloud is believed to be an isotropic reservoir of icy objects ranging from approximately 10,000 to 50,000 au and may contain as many as 10<sup>11</sup> comets (Dones et al., 2015). There appeared to be a spike in population between 27 and 36 kau (Dones et al., 2004). These are loosely bound gravitationally to our Sun, easily perturbed by the Galactic Mass Distribution (galactic tides) and stellar encounters, which can place them on trajectories which bring them into the inner Solar System (Fouchard et al., 2011). Occasionally, a very close passage of a star can trigger a comet shower, which would re-shuffle the placement of OC members and send many OC comets into the inner Solar System. Comets entering the inner Solar System for the first time since their placement in the Opik–Oort Cloud are called dynamically new comets and are the most pristine remnants of the PSN, likely unaltered (save for by the interstellar medium) since their formation and placement in the OC. Depending on their passage near Jupiter, these can be captured by a new comet families; be kicked out of the Solar System; or return to the OC unaltered. The latter are not likely to return to the inner Solar System. OC comets with gently perturbed orbits may have a low perehelion distance for quite a few orbits before

a similar passage with a giant planet increases this distance and returns them to the OC. This shuffling of objects makes identifying the original formation zones of these comets from the early inner Solar System difficult.

#### 2.1.2 Comet Nomenclature

Prior to the early XX<sup>th</sup> century, comet discoveries infrequent enough that no true standard of nomenclature was needed or established. In most cases no first observer could be identified, so it would be called "comet of X year." In the case of particularly bright comets, the name "great comet of X year" could be attributed. While these might later earn a more official designation, the colloquial term was clear to both the professional and amateur astronomer. The first come to bear the name of a scientist was Halley's comet, after it returned as predicted in 1759. This was then followed by Encke and Biaela as they calculated the trajectories of the comets that now bear their name. The first comet to be named after its discoverer was Comet Faye, discovered by Hervé Faye in 1843: This tradition slowly caught on, leading to comets such as Tempel's comet or Daniel's comet<sup>1</sup>. Dual discoverers were also able to hyphen their names, giving us Comet Swift-Tuttle<sup>2</sup>. However, this became confusing if an astronomer was particularly good at spotting comets, thus requiring the need to differentiate the comets by their moment of discovery. For most of the 20<sup>th</sup> century, comets were given an additional designation consisting of the year of their discovery, followed by a lowercase letter indicating its order of discovery in that year. This dating system soon transitioned into a more complicated process: once the comet's orbit had been established, it was given a designation comprised of the year of its perihelion, followed by a Roman numeral indicating its order of perihelion passage in that year. Comet 1969i (Bennett) became Comet 1970 II, since it was the second comet to pass perihelion in 1970.

Since the process of waiting for comets to pass perihelion could be time consuming and confusing, a new nomenclature needed to be established. The International Astronomical Union approved a new naming system in 1994 which is currently in use today:

<sup>&</sup>lt;sup>1</sup>Some interesting outliers would be Caesar's comet of 44 BCE, as mentioned in sec. 1.1, which was not discovered by Caesar, but forever linked in the minds of the roman populace after having marked his death.

<sup>&</sup>lt;sup>2</sup>In our modern day designations, hyphens remain for dual discoverers, but are removed when a single discoverer has an already hyphened name to avoid confusion. i.e. The comet discovered by Stephen Singer-Brewster becomes 105P/Singer Brewster, while Comet Swift–Tuttle remains 109P/Swift–Tuttle. This is also why, despite having been discovered by Pan-STARRS, comets discovered by this System are named PanSTARRS, sans-hyphen.



The first letter in a comet's name, the prefix, identifies the nature of the comet:

- P/ indicates a multiple-apparition or periodic comet. This would be a comet with a a short-period comet (SPCs) (<200 yrs) if they were recovered via prediction (or re-discovered accidentally) after having not been seen for some years. It is preceded by the chronological or historical order in which it was confirmed as returning to perihelion two or more times: the first would be Halley's Comet<sup>3</sup>, with the designation 1P/ Halley. As of May 2022, 443 periodic comets are officially referenced by the Minor Planet Center.
- **C**/ indicates a single apparition or non-periodic comet. These are usually longperiod comets (LPCs), or comets for which a period cannot be determined. Most comets are in this category.
- X/ indicates a comet for which no orbit could be reasonably established. In general, this is used for historic comets, though rarely seen as their colloquial designations suffice.
- D/ indicates a periodic comet that has disappeared. Comets can break up due to their fragile composition or collide with another body at any time. They can also be 'lost' to calculation errors. A recent example is Comet Shoemaker–Levy 9 (D/1993 F2), which broke apart in July 1992 and collided with Jupiter in July 1994. At the time of writing this, there are currently eight comets with this designation. In unique cases, a lost comet can be found and its classification changes: take for instance D/1783 W1 (Pigott), which was found and now bears the designation 226P/Pigott-LINEAR-Kowalski.
- A/ indicates an object first identified as a comet, but later recognized as a minor planet. An unused option for many years, this classification was first applied in 2017 for 'Oumuamua (A/2017 U1) and subsequently to all asteroids on comet-like orbits.
- I/ is the newest designation and indicates an interstellar object. 'Oumuamua (1I/2017 U1) is the first object of this kind, and its discovery in 2017 lead to the new addition to table. As of writing, the only other object with this classification is Comet 2I/2019 Q4 Borisov.

<sup>&</sup>lt;sup>3</sup>The *International Comet Quarterly* specifies though the name "Halley" is pronounced with a short "a", so that it rhymes with the English word "alley", not like the long "a" in "Haley" of "Bill Haley and the Comets" fame.

In order to differentiate between the plethora of comets discovered each year, the second element in a comet's name is the year in which it is found, preceded by the half-month in which it was discovered (represented by a letter, so the first two weeks of January would be A, the second two weeks would be B, and so on and so forth). Finally, it is given a number to designate in which order in this two week period it was found. A negative year represents comets observed BCE. Thus, a comet with the designation C/1995 O1 (Hale-Bopp) would be a long period or (non-periodic) comet, the first one discovered in the second half of July 1995 by astronomers Alan Hale and Thomas Bopp.

Here, I will frequently refer to comets by their C/xxxx yy designation rather than their full name.



**Figure 2.3** – Structure of a comet (not to scale). In simple terms, a comet can be split into three parts: the nucleus, the coma, and the tail(s).

## 2.2 Comet Structure and Composition

In essence, a comet can be split into three features: the nucleus, the coma, and the tail(s), shown in Fig. 2.3. The nucleus is the true comet, present both at small and large heliocentric distances; the coma and tail are by-products of the nucleus's passage near the sun.

#### 2.2.1 The Nucleus

The nucleus is the solid structure of the comet, composed of dust and ice. These ices are generally 80% of H<sub>2</sub>O, 10- to 20% of CO<sub>2</sub> and CO, along with complex organic molecules in minor quantities (See Fig. 2.5). The nucleus is usually only a few kilometers large, and on general <10 km in diameter, though some extremely rare 'megacomets' with radii in excess of 50 km do exist, such as C/1995 O1 Hale-Bopp with a diameter of 30-80 km (Weaver et al., 1997; Fernández, 2003) and the recently discovered C/2014 UN271 (Bernardinelli-Bernstein) with a diameter of over 120 km (Hui et al., 2022). Despite improved instrument sensitivity, very few nuclei with diameters < 100 m have been observed. In the outer Solar System, nuclei remain inert and are extremely difficult to detect from Earth due to their small size and low reflectivity of ~4%, among the least reflective objects found in the Solar System (Sagdeev et al., 1986). By comparison, asphalt reflects ~7%. As the cometary ice



**Figure 2.4** – Collage of all cometary nuclei imaged by spacecraft and planetary radars, to scale. *Daniel Macháček and The Planetary Society. Individual credits for source images are directly in the collage.* 



**Figure 2.5** – Range of abundances of molecules detected via spectroscopy in comets, relative to water. The number of comets used to establish this range is indicated at right. Figure from Bockelée-Morvan & Biver (2017).

sublimates, solar heating drives off lighter volatile compounds, leaving behind heavier dark organic compounds which then unevenly coat the comet's surface, creating regions which are more active than others. This low reflectivity causes them to absorb the heat that further drives their outgassing processes. Active zones are also believed to be the origin of jets, some of which can be seen in the image of 1P/Halley's nucleus, in the center of Fig.2.4.

Due to their low reflectivity and small size, cometary nuclei are nearly impossible to resolve at high heliocentric distances beyond the thermal influence of the sun. As they approach the sun, heat causes them to sublimate, forming the coma. The comet is suddenly brilliantly visible, as the dust scatters sunlight directly while the gases glow from ionization. However, the nucleus remains hidden in this coma, and we are only able to gain size estimates from radio observations if the contrast between nucleus and coma is high. The true shape of a nucleus can only be seen clearly during a flyby event, when a spacecraft plunges into the coma for a better view. These missions were described in Sec. 1.5, and the observed nuclei are shown to scale in Fig.2.4. Due to their low mass, cometary nuclei are not spherical, and instead tend to be elongated<sup>4</sup>, and in some cases bilobal, such as 67P/Churyumov-Gerasimenko: this was most likely due to a slow and gentle collision in the early Solar System, which fused two comets into one. Known comets have been estimated to have an average density of 0.6 g/cm<sup>3</sup>, with masses in the range  $10^{10} - 10^{15}$  kg (Britt et al., 2006). This low density would seem to favor the fluffy aggregate (Donn et al., 1985) and rubble pile (Weissman, 1986) models, that is to say that the nucleus is made up of loosely gravitationally bound ice and dust particles with large cavities between the various blocs (see Fig. 2.6). This would help explain their fragile nature, as they are prone to fracturing and outbursts. A benefit of the Philae lander's 'bounce' on 67P was that the density of two sites could be investigated instead of just one: the first with a 30-cm fluffy sediment layer made of conglomerates of particles of dust and ice, and the second with a tough crust, revealing the diversity of surfaces even on such a small area.

#### 2.2.2 The Coma

The coma or 'head' of the comet is a bright, roundish, nebulous shape in the night sky and can be seen as a temporary atmosphere of  $10^5 - 10^6$ km in diameter. On some occasions —i.e. 17P/Holmes and Great Comet of 1811 —the coma is near or larger than the size of the Sun ( $1 \times 10^6$ ,  $1.6 \times 10^6$  km, and  $1.3 \times 10^6$  km, respectively). However, the hydrogen envelope that surrounds it can be much larger, and its actual size much more difficult to estimate, as well as its shape as it greatly depends on

<sup>&</sup>lt;sup>4</sup>Sometimes referred to as'potato shaped' or 'peanut shaped'.



**Figure 2.6** – Possible comet nucleus formation scenarios. From A'Hearn (2011). (a) Whipple (1950)'s original dirty snowball model. (b) Donn & Hughes (1986)'s fractal aggregate model. (c) Weissman (1986)'s primordial rubble pile model. (d) The icy glue model of Gombosi & Houpis (1986). (e) Belton et al. (2007)'s TALPS model.



**Figure 2.7** – The Rosetta cometary zoo: a humorous approach to displaying the variety of species detected around by ROSINA onboard Rosetta in the gas around Comet 67P/C-G. *K. Altwegg and the ROSINA team, ESA.* 

solar radiation. The coma is constituted of sublimated gas that made up the nucleus and the dust that was liberated in this reaction, with H<sub>2</sub>O generally making up to 90% of the sublimated iced that outflow from the nucleus when the comet is < 2.5au. At larger heliocentric distances, the coma is dominated by CO and CO<sub>2</sub> (Press, 2000). Occasionally a comet may experience a huge and sudden outburst during which the size of the coma greatly increases for a period of time.

Molecules released directly from the nucleus are referred to as parent species, the daughter-species being by-products of parent-species chemistry in the coma. As a result, the composition of the coma varies over nucleocentric distance, with more densely-packed molecules nearer the surface, emitting mainly through fluorescence processes, and more diffuse concentrations further from the nucleus, where interactions with the solar radiation strip electrons lead to photodissociation, and interactions with the solar wind to photoionization of these molecules into daughter-species. At 1 au, the coma can be divided into four zones (Lutz et al., 1993): Within the first few  $10^3$ km of the surface, neutral molecules dominate and there is no interaction with the solar wind. This region of pure plasma is cometary ion-dominated and extends then to  $10^5$  km, before reaching the 'cometopause', where the plasma interaction becomes dominated by solar wind, leading to a tangle of magnetic lines at this transition (Gringauz et al., 1986). It's within the inner region  $< 10^5$  km that the gas is dense enough for ion-molecule chemistry to occur (Huebner & Giguere, 1980). This cometary ionosphere is then bounded in the solar-facing direction by the bow-shock at  $\sim 10^6$  km, where the solar wind passes through this hydrogen-ion -dominated coma, separating it from pure solar wind.

Coma are also compost of generally chondritic dust dislodged by the sublimation of cometary ices. These are mainly refractory materials such as silicates (pyroxene, olivine), organics, and carbon, ranging 0.1-1  $\mu$ m in size (Mukai et al., 1987). These particles fill what is called the 'dust shell' before the difference in velocity between these and the lighter molecules in the coma effectively blow them away. The gas and dust released from these comets diffuse into the Solar System, feeding the Zodiacal cloud, a collection of interplanetary dust which slowly disperses along the ecliptic plane.

The variety of these species found in the coma has lead some to humorously refer to a "cometary zoo" (see Fig. 2.7).

#### 2.2.3 The Tail(s)

The 'comet's tail' is a misnomer: comets possess multiple tails, containing different sized particles. The motion of ions is influenced by their interaction with the solar wind (electric interaction between charged particles) and oriented in slightly



**Figure 2.8** – A comparison of the average comet tail length with the sun-planet distances. Comet C/1996 B2 Hyakutake was the longest tail ever recorded at a whopping 3.8 au, when the *Ulysses* spacecraft unexpectedly crossed the tail on May 1<sup>st</sup> 1996.

different directions due to their interaction with the solar radiation and wind. The ion tail, or type I tail, is made up of gas ionized by interaction with the solar wind, and always points in the anti-sunward direction rather than an orbital trajectory. As a result, this tail will be in front of the comet as its trajectory leaves it away from the Sun. This tail is usually  $\sim 10^6$ km, sometimes exceeding 1 au, with the longest ever recorded at 3.8 au (see Fig. 2.8). Its color depends on its ion composition, and the morphology can vary over time more or less quickly due to magnetic field of the solar wind, and the ion tail can even be entirely stripped during tail disconnection events. If the comet crosses the orbit of Mars  $\sim 1.5$  au, the solar wind becomes strong enough to blow the gas and dust away from the coma, enlarging the tail.

Type II tails are composed of dust ejected from the surface of a comet by the gas jets. The velocity differences between the comet this dust tends to produce a curved tail along the comet's path. Because the ratio between radiation pressure and gravitational force is inversely proportional to the radius of the grains, smaller grains are more affected by radiation pressure, leading to a 'fountain effect,' particle size distribution in the dust tail compared to the regions near the nuclesu. Heavier particles which are less influenced by the radiation pressure of the solar photons are left behind in the comet's wake. The Earth occasionally passes through these ancient comet tails, causing beautiful meteor showers as these larger particles interact with our atmosphere. On occasions such as when Earth passes through a comet's orbital plane, the antitail, pointing in the opposite direction to the ion and dust tails, may be seen.

# 3 N<sub>2</sub> in Comets

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SINCE COMETS ARE THOUGHT to have agglomerated from planetesimals within reach of one another, they should represent the composition of the disk at the location in which they were formed. Finding these specific formation areas would effectively be reconstructing the puzzle that represents a snapshot of the Protoplanetary Disk (PPD) at the moment of their formation. This snapshot will reveal the composition of the PPD and sources of those components which would answer how the Solar System came to be in the configuration we have now.

# 3.1 The N<sub>2</sub> Deficiency in Comets

By examining the composition of comets as they pass through the inner Solar System, we have the unique opportunity to look back in time at this early PPD. The present-day Sun should be representative of the PSN, and thus is used as a point of comparison. While most elements in comets seem on par with this expectation,
nitrogen is apparently low and thus particularly puzzling: the ratio of carbon-tonitrogen within comets should be similar to that of the Sun, but comets appear to be nitrogen-deficient by comparison. For example, the elemental N/O abundance measured in the dust of Comet 1P/Halley is depleted by a factor of 3 with respect to the solar abundance (N/O)<sub> $\odot$ </sub> = 0.13 (Jessberger & Kissel, 1991). The depletion is even stronger when combining measurements of various N-bearing molecules: Wyckoff et al. (1991) estimated that there is a deficiency in the ice component of Comet Halley by a factor of 75 with respect to (N/O)<sub> $\odot$ </sub> and an overall (dust+ice) elemental nitrogen deficiency of 6. From the detection of a few new N-bearing volatile species, Bockelée-Morvan et al. (2000) inferred an N/O elemental depletion of 15 relative to the solar ratio in the gas phase of Comet C/1995 O1 (Hale–Bopp). Since N<sub>2</sub> is the least reactive of all N-bearing species, and believed to be the main carrier of nitrogen in the PSN, the low abundance of elementary nitrogen must be due to a depletion of N<sub>2</sub> (Feldman et al., 2004). The protosolar nebula value for N<sub>2</sub>/CO is estimated at 0.145 ± 0.048 (Lodders et al., 2009).

The N<sub>2</sub> depletion in comets has long been a matter of great debate. Despite both Pluto and Triton, which also formed in the outer Solar System, exhibiting N<sub>2</sub>-rich surfaces (Cruikshank et al., 1993; Owen et al., 1993; Quirico et al., 1999; Merlin et al., 2018), very few ground-based facilities have ever observed  $N_2^+$  in cometary spectra<sup>1</sup>. Owen & Bar-Nun (1995) studied the deposition of gases into amorphous water ice in the laboratory and determined that ices incorporated into comets at around 50K would have  $N_2/CO \approx 0.06$  if  $N_2/CO$  is  $\approx 1$  in the solar nebula. For comparison, Cochran et al. (2000) found an upper limit for  $N_2/CO$  as only  $3 \times 10^{-4}$  for comet deVico and  $6 \times 10^{-5}$  for comet Hale-Bopp, which is at least  $100 \times$  lower than expected. It is unknown whether this depletion occurs before or after the formation of comets: phenomena that could deplete the N<sub>2</sub> post-formation are yet unknown, and it is unclear how cometary icy grains depleted in N<sub>2</sub> could originate from a presolar cloud in which N<sub>2</sub> is currently estimated to be more abundant than NH<sub>3</sub>, which is currently valid for most chemical models of the interstellar medium. Charnley & Rodgers (2002) showed that it is possible that much of the available nitrogen in the presolar cloud was in atomic nitrogen, with a significant contribution in ammonia ice, and little in N<sub>2</sub>. Irvine et al. (2000) found evidence that at least part of the genuine interstellar material was reprocessed in the solar nebula prior to the formation of pre-cometary grains. But these hypotheses are not enough to explain where the  $N_2$  could have gone.

One possibility is that these volatiles were trapped in water ice in the form of clathrate hydrates during the nebular phase of planet formation (Iro et al., 2003). Based on the  $H_2O/H_2$  ratio, which sets the amount of water ice which could trap

<sup>&</sup>lt;sup>1</sup>Save those early comet spectra, as discussed in section 1.3

the gaseous volatiles, they determined water ice decreases the relative abundances of  $N_2$  with respect to  $H_2O$  since there is no more  $N_2$  in the gas phase left to trap. CO was also preferentially incorporated in clathrates compared to N<sub>2</sub>. This opens up the possibility of there being two types of comets: typical comets, with a low  $N_2/CO$  ratio, formed in the region of the PSN where the  $H_2O/H_2$  ratio was less than 2.8  $(O/H)_{\odot}$ , the value of the ratio for maximum trapped N<sub>2</sub>, and a second type, formed around 5 au, which would exhibit PSN  $N_2/CO$  ratios, assuming that they have the same composition as the planetesimals that enriched the envelope of Jupiter in heavy elements, since the C/N/S/Ar/Kr/Xe/S ratios observed in Jupiter are approximately solar. The oversolar abundance of water required to interpret the composition of Jupiter formed at 5 au may imply a subsolar abundance in other regions of the nebula. They also determined that the CO abundance measured in comets is related to the abundance of ice available in the nebula, at the heliocentric distance where cometesimals were produced. This hypothesis is consistent if the nebula's temperature never cooled down below ~45 K in their formation region, which impedes the formation of  $N_2$ -bearing ice. However, this mechanism is not consistent with the fact that Pluto and Triton possess thick nitrogen ice covers while they are both expected to have been formed in the same region of the primitive nebula as ecliptic comets (Lellouch et al., 2011). At the very least, it is evident that the distribution of water ice varied substantially with radius throughout the nebula.

A decade later, Mousis et al. (2012) argued that the  $N_2$  deficiency might be a consequence of poor trapping efficiency of  $N_2$  and postaccretion internal heating generated by the decay of radiogenic nuclides. They found that molecular nitrogen is a poor clathrate former when considering a plausible gas-phase composition of the primordial nebula, and its trapping into cometesimals requires a low disk temperature ( $\sim 20$  K) in order to allow the formation of its pure condensate.

The question is puzzling: where did all this N<sub>2</sub> go?

# 3.2 The Peculiar Composition of Comet C/2016 R2

#### 3.2.1 Chronology of Observations

When comet C/2016 R2 (PanSTARRS), henceforth C/2016 R2, was first discovered using the Pan-STARRS telescopes in Haleakalā, Hawaii on September 7 2016 (Weryk & Wainscoat, 2016), its unique properties were not immediately apparent. It was evidently a long period comet, with period of 18,709 years and a semi-major axis of 704 au<sup>2</sup>. It was not a dynamically new comet, as it was estimated to have undergone

<sup>&</sup>lt;sup>2</sup>First estimated as an orbital period of 21,600 years with a semi-major axis of  $\sim$ 1500 au.



**Figure 3.1** – Comet C/2016 R2 (PanSTARRS) taken by the SPECULOOS observatory on 18 January 2018. *ESO/SPECULOOS Team/E. Jehin*.

a few journeys through the inner Solar System. However, it proved to be unusual insofar as it has an extremely eccentric orbit, with an eccentricity of 0.996. The orbital elements of this comet are displayed in Table 3.1. It was already outgassing at r=6.3 au: since water is dominant in comets and usually does not sublimate efficiently until it is under r~2-3 au. This would indicate we were not observing water-ice sublimation, but instead a more hypervolatile species (Ootsubo et al., 2012; Reach et al., 2013; Bauer et al., 2015; Wierzchos & Womack, 2017; Womack et al., 2017).

It was only in autumn 2017 that its unusual composition came to light —quite literally —as it approached perihelion. As R2 approached the Sun at >3 au, it revealed a bright and vibrant coma, which was a distinct shade of blue, garnering it the unofficial name of 'The Blue Comet.' In contrast, usual comets show a dust tail and a white or yellowish color coma, produced by the dust scattering of solar radiation. Its tail also presented multiple rapidly changing structures. To make this composition even more fascinating, Wierzchos & Womack (2017) made a stunning new detection: or, rather, a lack of detection. They calculated a 3-sigma upper limit of  $Q(\text{HCN}) < 3.6 \times 10^{25}$  molecules.s<sup>-1</sup>at r = 2.9 au and  $\Delta$  = 2.1 au. They estimated a Q(CO)/Q(HCN) > 1300, which was unheard of in comets. For comparison, this comet produced almost half of the CO that comet C/1995 O1 (Hale-Bopp) did at the same heliocentric distance (Wierzchos & Womack, 2017), and prompted a flurry of observations.

Cochran & McKay (2018) conducted optical imaging and spectroscopic observations of R2 at The University of Texas McDonald Observatory in November and

**Table 3.1** – Orbital elements of comet C/2016 R2 (PanSTARRS) as given by the JPL small body browser, at Epoch 2458267.5 (2018-May-29.0) Barycentric Dynamical Time (TDB). Perihelion was on 9.6 May 2018 UT at 2.60 au.

Element	Value	Uncertainty (1-sigma)	Units
е	0.9963073873895085	$1.9501 \times 10^{-6}$	
а	704.7487057333195	.37245	au
q	2.602363958018401	$1.1386 \times 10^{-6}$	au
i	58.22406306808122	$8.7863 \times 10^{-6}$	deg
node	80.56902872443624	$6.748 \times 10^{-6}$	deg
peri	33.19189859773018	$2.0025 \times 10^{-5}$	deg
M	0.001022899290845507	$8.1319 \times 10^{-7}$	deg
tp	2458248.083084792859	$9.1186 \times 10^{-5}$	TDB
-	2018-May-09.58308479		
period	6833604.771387515	5417.3	d
1	18709.39020229299	14.832	У
n	$5.268083420734685 \times 10^{-5}$	$4.1762 \times 10^{-8}$	deg/d
Q	1406.895047508621	.74353	au

Reference: JPL 43 (heliocentric IAU76/J2000 ecliptic). Solution Date 2021-Jul-01 22:12:39.

**Table 3.2** – Composition of comet C/2016 R2 as determined by different observations. Many of these observations were conducted at the same time (between December 2017 and February 2018), but published months apart. Here I have tried to place them in order of heliocentric distance r as R2 approached perihelion.

Reference	r	$\Delta$	Q(CO)	$Q(N_2)$	N <sub>2</sub> /CO
	(au)	(au)	$(mols.sec^{-1})$	$(mols.sec^{-1})$	
Cochran & McKay (2018)	3.1	2.1	-	-	$0.06\pm0.01$
Wierzchos & Womack (2017)	2.9	2.1	$4.7 \times 10^{28}$	-	-
Wierzchos & Womack (2018)	2.9	2.1	$4.6 \times 10^{28}$	$2.8 \times 10^{27}$	-
Biver et al. (2018)	2.8	2.2	$1.1 \times 10^{29}$	-	$0.08\pm0.01$
McKay et al. (2019)	2.8	2.4	$9.5 \times 10^{28}$	$4.8 \times 10^{27}$	$0.05\pm0.01$
Opitom et al. (2019)	2.8	2.4	-	-	$0.06\pm0.01$

December 2017 with the 0.8 m and 2.7 m telescopes, respectively. They found R2's tail revealed little dust or other emission lines, including a lack of  $C_2$  Swan bands, if any at this heliocentric distance, which are not seen here. Comet tails are rarely this well resolved at such a high heliocentric distance, and even stranger, this tail presented stronger as more developed in the CN filter than in the  $C_2$  filter.

The unique shade suggested it was an ion tail. As such a well-resolved ion tail would be uncommon at such a large heliocentric distance, Cochran & McKay (2018) used the Tull 2DCoude spectrograph (Tull et al., 1995) on the Harlan J. Smith 2.7 m telescope of McDonald Observatory on 2017 December 8–10 UT in order to confirm their hypothesis of ionic emission contaminating their narrowband imaging. It was immediately apparent that the spectrum was peculiar when compared to comets seen before. The CN band at 3880 Å was missing, despite usually being one of the strongest emission features observed in optical spectra of comets. The other usual neutrals seen in most cometary spectra,  $C_2$ ,  $C_3$ , CH, or NH<sub>2</sub> were also absent.

Instead, R2's spectrum was dominated by the bands of CO<sup>+</sup>, which was rarely seen in comets. The strongest observed could be attributed to CO<sup>+</sup> (4, 0), (3, 0), (2, 0), (1, 0), (4, 2), (3, 2), (2, 1), and (1, 1) A<sup>2</sup> $\Pi$ —X<sup>2</sup> $\Sigma$  bands. Perhaps the most surprising feature was the source of the stunning blue hue: the blue degrading band can be attributed to the B<sup>2</sup> $\Sigma$ –X<sup>2</sup> $\Sigma$  (0, 0) band of N<sub>2</sub><sup>+</sup> with a bandhead at 3914 Å. It is rare that such strong CO<sup>+</sup> and N<sub>2</sub><sup>+</sup> are ever observed together in the spectrum of a comet.

After further observations in December 2017 and January 2018, Wierzchos & Womack (2018) refined their measurement of the HCN production rate, finding  $Q(\text{HCN}) = 8 \times 10^{24}$  molecules.s<sup>-1</sup>, or a quarter of what they published in their 2017 telegraph. This raises the Q(CO)/Q(HCN) to >5000, much higher than any comet ever previously measured (Fig. 3.2). No search for OH or H<sub>2</sub>O emission was successful: no water-ice sublimation was detected. Comets typically present a CO/H<sub>2</sub>O ratio of ~8% (Dello Russo et al., 2016), but since H<sub>2</sub>O eludes detection in R2, the CO/H<sub>2</sub>O ratio could be much, much higher. However, these observations were made while R2 was at  $r \sim 2.9$  au, so perhaps the water-ice was not sublimating efficiently. Meanwhile, they found a  $Q(N_2) \sim 2.8 \times 10^{27}$  molecules.sec<sup>-1</sup>based on the N<sub>2</sub>/CO column density ratio calculated by Cochran & McKay (2018).

A team of astronomers observed R2 on January 23-24, 2018 with the 30-m telescope of the *Institut de radioastronomie millimetrique* (IRAM), and in January to March 2018 with the Nançay radio telescope (Biver et al., 2018). They found a N<sub>2</sub><sup>+</sup>/CO<sup>+</sup> column density ratio of 0.08, in line with Cochran & McKay (2018) and a CO production rate twice as large as Wierzchos & Womack (2018), with CO production in the order of ~  $10^{29}$ . molecules.sec<sup>-1</sup>. They also confirmed the very low dust production based on the Af $\rho$  which is lower than values measured in comets of similar gaseous activity at ~3 au from the Sun by more than a factor of 15. They agreed with the depletion of  $H_2O$ ,  $CH_3$  OH,  $H_2CO$ , HCN and  $H_2S$  relative to CO (by more than one order of magnitude) compared with other comets observed at a similar heliocentric distance.

The last set of observations was made by Opitom et al. (2019) in February 2018 with the Ultra-Violet Echelle Spectrograph (UVES) mounted on the ESO 8.2m UT2 telescope of the VLT. By using the TRAPPIST-North (TN) and TRAPPIST-South (TS) telescopes, they also observed  $CO^+$ ,  $C_2$ , and CN through narrowband filters. The coma was ever-changing through the  $CO^+$  filter, with structures moving night after night, enhanced in the anti-sunward direction: further evidence of the tail's ionic nature. Meanwhile, the CN coma wasn't diffuse and symmetrical as usually observed in comets: instead, it presented similar morphology to the  $CO^+$  image, indicating that the CN filter is contaminated by the  $N_2^+$  ion. They were able to derive an upper limit of about 0.4 for the  $H_2O^+/CO^+$  ratio. This was the last set of published observations, and the spectra that we will use in this study.

### 3.2.2 N<sub>2</sub><sup>+</sup> and subsequently N<sub>2</sub> in C/2016 R2

The detection of N<sub>2</sub> in comets using spectroscopic methods has been challenging: as a diatomic, symmetrical molecule,  $N_2$  has no permanent dipole moment, which results in the absence of pure rotational transitions. It emits no radiation at millimeter-wavelengths, making the molecule invisible to observations in that range. These transitions are visible in the UV through instruments placed outside of our atmosphere. The presence of N<sub>2</sub> was confirmed in comet 67P/Churyumov-Gerasimenko from Rosetta in-situ surface measurements (Rubin et al., 2015) using the ROSINA spectroscope. With ground-based telescopes, any indication as to the presence of N<sub>2</sub> comes from the observation of one of its by-products, a daughtermolecule or daughter-ion that could be visible under certain conditions. In the case of C/2016 R2 we observed strong emission of  $N_2^+$  in the coma, an ion that can only have been produced by the photoionization of  $N_2$  by the solar UV photos.  $N_2^+$  is detectable in the optical range thanks to the bands of the first negative group ( $B^2\Sigma_u^+$ ) -  $X^2\Sigma_a^+$ ) with the (0,0) bandhead at 3914 Å. However, to make matters even more complicated,  $N_2^+$  is excited by the Earth's atmosphere, especially near dusk and dawn. These telluric lines can appear in cometary spectra. The lines observed in the spectra of R2 were precisely at the correct wavelength for the cometary Doppler shift which was convincing evidence that they were truly cometary in nature.

Methods of estimating these quantities were established for multiple species over the past decades of comet spectra observation. However, as  $N_2$  was previously unidentified — or in such small quantities as to be seen as little to no importance — no fluorescence model of  $N_2^+$  had yet been made. In order to estimate the quantity

of N<sub>2</sub> until now, we have relied on abundance ratios with other, already quantified, components.

In the case of C/2016 R2, an estimate of the quantity of  $N_2$  was made through the abundance ratio with CO (Cochran & McKay, 2018). Since the column density of a species is given as:

$$N = \frac{I_{v'v"}}{g_{v'v"}}$$

where N is the column density,  $I_{v'v"}$  the integrated band intensity, and  $g_{v'v"}$  the excitation factor. We can determine the ratio of column density for these two species to be:

$$\frac{\mathbf{N}_2^+}{\mathbf{CO}^+} = \frac{g_{CO^+}}{g_{N_2^+}} \frac{I_{N_2^+}}{I_{CO^+}}.$$
(3.1)

This gives us our first estimate of the quantity of  $N_2^+$  present in the coma of C/2016 R2. By measuring the band intensity of the observed  $N_2^+$  in R2's spectra, assuming that solar resonance fluorescence is the only excitation source, the observed emission fluxes have been used to calculate ionic ratios of  $N_2^+/CO^+$  in the coma. This would be the same ratio for  $N_2/CO$  since  $N_2$  and CO should be released in the same proportion as they exist in the ices because their photoionization rates are similar(Bar-Nun et al., 1988; Huebner et al., 1992). CO could be produced by the dissociation of CO<sub>2</sub>: in that case, we would expect to see  $CO_2^+$  in our spectra, but none was detected. CO and  $N_2$  should then be ionized in proportion to the amount of neutrals and  $N_2/CO = N_2^+/CO^+$  in the coma. Thus, Cochran & McKay (2018) derived that  $N_2/CO = 0.15$ , later corrected to  $N_2/CO = 0.06$  (Erratum Cochran & McKay (2018)).

While the ratio of species seen in the gas phase is not necessarily representative of the ratio of the ices in the nucleus, neither CO nor N<sub>2</sub> are terribly reactive with other species. Chemical reactions probably would not alter this ratio much, and the ratio is not expected to change with heliocentric distance. Owen & Bar-Nun (1995) determined that ices incorporated into comets at around 50K would have N<sub>2</sub>/CO $\approx$ 0.06 if N<sub>2</sub>/CO is  $\approx$ 1 in the solar nebula: this is the exact measurement of N<sub>2</sub>/CO found by Cochran & McKay (2018), and one of the the highest such ratio reported for a comet, while being the cleanest detection of N<sub>2</sub><sup>+</sup> ever made as it is both digital and at high spectral resolution.



**Figure 3.2** – The range of CO/HCN ratios among Solar System comets. The unusually high concentration detected in Comet C/2016 R2 (PanSTARRS) is shown on the far left; that of 2I/Borisov, the first interstellar comet, is shown in orange. Figure from Cordiner et al. (2020) with the values of C/2016 R2 from McKay et al. (2019) (CO/HCN=26,400).

#### 3.2.3 C/2016 R2's water depletion

With an H<sub>2</sub>O/CO upper limit of <0.1 (Biver et al., 2018) or <0.4 (Opitom et al., 2019), this comet is incredibly depleted in water, thousands of times more so than usual comets. This is at least 5 times higher than in any other comet observed inside the water ice line at ~2.5 au (Lisse et al., 2022). Typical comets have a CO/H<sub>2</sub>O ratio of between about 0.2% to 23% relative to water, with a typical value around 4% (Bockelée-Morvan & Biver, 2017). McKay et al. (2019) constrained  $Q(H_2O)$  in C/2016 R2 to less than ~  $10^{27}$  molecules.s<sup>-1</sup> with a most likely value of  $(3.1 \pm 0.2) \times 10^{26}$  molecules.s<sup>-1</sup>, resulting in an CO/H<sub>2</sub>O ratio of (3.08 ± 0.35) ×10<sup>4</sup> %. For such an active comet, with such a high production rate of CO, H<sub>2</sub>O is always detected (Lisse et al., 2021). When H<sub>2</sub>O cannot be detected, HCN is frequently used as a proxy, since it can be seen in infrared wavelengths, yet it too was barely identified in C/2016 R2 (Fig. 3.2).

The depletion of  $H_2O$  is highly peculiar, as it is usually the fundamental composition of a comet, making up ~80% of a comet's ice. While some ice-less comets have been found, such as C/2014 S3 (PANSTARRS)<sup>3</sup>, this was most likely formed in the

<sup>&</sup>lt;sup>3</sup>As this comet had no tail, it became the first of a new category of tail-less comets, dubbed Manx objects.



**Figure 3.3** – Composition of comet C/2016 R2 (right) compared to that of an ordinary comet (left) as derived using mixing ratios from Dello Russo et al. (2016) and Ootsubo et al. (2012). Figure by McKay et al. (2019). This CO- and N<sub>2</sub>-rich, H<sub>2</sub>O-poor composition makes it truly one of a kind.

inner Solar System and ejected at a very early stage, making it more akin to asteroids (Meech et al., 2016). As of today, C/2016 R2 is the only confirmed water-poor comet that has been identified.

\* \* \*

C/2016 R2 is one of the most unique comet specimens ever observed. It stands out as being, CO-rich; N<sub>2</sub>-rich; and H<sub>2</sub>O-depleted. A comparison between the composition of C/2016 R2 and usual comets is shown in Fig. 3.3.

While other outliers with high CO have been observed, and a handful with N<sub>2</sub>, none are this depleted in water. The combination of these three attributes makes C/2016 R2 one of a kind and implies that C/2016 R2 formed very cold, and was maintained at temperatures  $\leq 20$  K for the duration of its lifetime (Cordiner et al., 2022). With a multitude of cometary spectra, C/2016 R2 is our first glimpse into this rare comet type, and the information it tells us about the far reaches of the Oort Cloud will bring us invaluable insight into our Solar System's formation.

# 3.3 Observed N<sub>2</sub>-rich Comets

Three comets supposed to have an N<sub>2</sub>-rich composition were observed pre-High-Resolution spectrographs: C/1908 R1 (Morehouse) (de La Baume Pluvinel & Baldet, 1911), C/1947 S1 (Bester) (Swings & Page, 1950), and C/1961 R1 (Humason) (Greenstein, 1962). While their observation was done through the use of photographic plates, thus the color was not visible to the naked eye, the intensity of their spectra convinced astronomers that they were blue-ish in nature. Glancy (1909) mentions that while comet Daniel 1907 (another vibrant comet at the time) was visually brighter, comet Morehouse photographed more readily, due to stronger emissions in the blue and violet 'photographic regions.' However, none had been observed with modern astronomical facilities.

Others presenting a high N<sub>2</sub>/CO ratio would be C/2002 VQ94 (LINEAR) —a comet active at >8 au —with N<sub>2</sub>/CO = 0.06 (Korsun et al., 2014). This is twice as much as the next candidate, comet C/2001 Q4 (NEAT), for which Feldman (2015) placed a  $3\sigma$  upper limit on N<sub>2</sub>/CO of 0.027 using FUSE observations. While Ivanova et al. (2016) measured N<sub>2</sub><sup>+</sup>/CO<sup>+</sup> as 0.013 for comet 29P/Schwassmann-Wachmann 1 at 5.25 au, the N<sub>2</sub><sup>+</sup> feature is not well defined in these low-resolution spectra. Rubin et al. (2015) measured a N<sub>2</sub>/CO ratio of (5.70±0.66) ×10<sup>-3</sup> at the comet using the ROSINA Mass Spectrometer from the ROSETTA probe: however, this ratio was measured at a heliocentric distance beyond far perihelion, and Rubin et al. (2020) later derived a N<sub>2</sub>/CO ratio of ~2.87 ×10<sup>-2</sup>. This was from a direct in-situ read at the comet's surface. These values are shown in Table 3.4 to offer a point of comparison. It would appear comet C/2016 R2 and comet C/2002 VQ94 (LINEAR) present identical N<sub>2</sub>/CO ratios, and are representative of Owen & Bar-Nun (1995)'s prediction. This would seem to suggest they would have had a colder formation temperature, possibly >50K.

Cochran et al. (2000) also list other N<sub>2</sub>-rich comets and estimated their N<sub>2</sub>/CO ratios based on their photographic plates: C/1940 R2 Cunningham, C/1956 R1 Arend-Roland, C/1957 P1 Mrkos, C/1969 T1 Tago-Sato-Kosaka, C/1969 Y1 Bennett, C/1973 E1 Kohoutek, C/1975 V1-A West, and C/1986 P1 Wilson. Their N<sub>2</sub>/CO ratios were calculated in conjunction with their personal communication with Claude Arpigny and their N<sub>2</sub><sup>+</sup>/CO<sup>+</sup> ratios were adapted to use the CO<sup>+</sup>(2,0) bands. Unfortunately, these were a late edition to our sample, and thus will not be explores as thoroughly as the previously cited comets.



**Figure 3.4** – Images of comet C/1908 R1 Morehouse between 30/09/1908 and 29/11/1908 in chronological order. The outburst of October 15<sup>th</sup> can be seen starting on the second row. From the Lick, Juvisy, and Heidelberg, and Greenwich observatories.

#### 3.3.1 Comet C/1908 R1 (Morehouse)

Comet C/1908 R1 Morehouse (1908c in literature of the time) was a bright, nonperiodic comet first observed on September 1, 1908 by Daniel Walter Morehouse<sup>4</sup>. The tail had become visible beyond 2 au, which was a first at this time. Once discovered, it was photographed by the global astronomical community, providing us with a photo record of its life history as it traveled pole to pole over the course of three months. An attempt to order the photographs from books at the time into chronological order is shown in Fig. 3.4.

It was spectacular in that its tail presented unexpected and rapid variations. On October 1<sup>st</sup>, the comet lost its tail entirely, while the nucleus remained unchanged, potentially caused by a reversal of the ion tail's magnetic field; The next day, it regrew not one, but 3 tails, all faint and changing slowly; Then, on October 15<sup>th</sup>, within the 12 hours that separated two observations, the comet split in two, each mass with its own separate tail, flimsily connected. A month later on November 16<sup>th</sup> comet Morehouse once again underwent a shocking transformation: firstly, the tail made an abrupt right turn "as if it has encountered a resisting medium" before the coma became massive, sending pulsations down the tail. The tail broke into waves with a "conspicuous" dark streak extending down its side (Chambers, 1909). This odd behavior continued along its months of visual observation, recorded by both professional and amateur astronomers of the time. Comet Morehouse repeatedly lost its tail and formed new ones; at times, the tail seemed to split into up to six or eight separate tails, depending on the source. Many tail features that had never been seen before made comet Morehouse a spectacular sight: waves, twisted funnels like cyclones. It cycled through active and inactive phases (Christie, 1908).

The ion tail highlighted the effects of the solar wind, which was not yet understood: astronomers, who were just beginning to understand the link between solar activity and comet activity, hypothesized the existence of a "Light Pressure" capable of interacting with the plasma tail (Chambers, 1909). By ripping the ions in the tail, the solar photons produced shockwaves which created the variety of tail morphologies which captivated the world.

It should come as no surprise then that this comet's composition was as spectacular as its tail:

In place of the familiar hydrogen gas was found the poisonous cyanogen element. Other ingredients not recognized seem to be present. Altogether it gave astronomers a wealth of data which it will require years to digest and interpret properly. (Chambers, 1909)

<sup>&</sup>lt;sup>4</sup>It was also observed by the French astronomy M. Borrelly in Marseille on September 3<sup>rd</sup>, and in French journals of the time it is sometimes referred to as Comet Morehouse-Borrelly.

The "other ingredients not recognized" proved to be CO<sup>+</sup>. Using negatives obtained with objective-prisms, de La Baume Pluvinel & Baldet (1911) were able to photograph this comet on October 18<sup>th</sup> 1908 and obtain a clear spectrum. When these negatives were taken, CO<sup>+</sup> had not yet been modeled in the lab: it was only after, based on the research of Fowler (1909), that it could be identified. In addition, no continuous spectrum was visible, and the images were located in the blue, violet, and ultra-violet: comet Morehouse was "consequently blue" and even to the naked eye had a "blueish sheen" (Guillaume, 1908). The spectrum extended to a considerable height, and the various images of the tail could be separated as far as 34' from the nucleus, approximately  $8.5 \times 10^8$  km (Motherwell, 1909).

In order to estimate the  $N_2/CO$  ratio, we take defined intensities from the literature:

	Deslandes et al. (1909)	Campbell & Albrecht (1909)	Swings & Page (1950)
$I(N_2^+)(0,0)$	7	2	7
I(CO <sup>+</sup> )(2,0)	10+9	10+8	10
$N_2^{+}/CO^{+}$	0.02	0.005	0.04

**Table 3.3** – Measured intensities and resulting  $N_2^+/CO^+$  ratio from the literature.

with the intensities in arbitrary units. Swings & Page (1950) recalculated the intensities in 1950 when estimating the values of comet C/1947 S1 (Bester). The first two intensities of the CO<sup>+</sup>(2,0) are too high, as the transition at 4273 Å is contaminated by the N<sub>2</sub><sup>+</sup> (0,1) group. This is corrected for Swings & Page (1950). We continue with the same coefficients as Opitom et al. (2019) ( $g_{CO^+} = 3.55 \times 10^{-3}$  and  $g_{N_2^+} = 7 \times 10^{-2}$  photons.ion<sup>-1</sup>.s<sup>-1</sup>) and eq. 3.1 and find that N<sub>2</sub><sup>+</sup>/CO<sup>+</sup> is between 0.01 and 0.04.

The results point to a higher than usual  $N_2/CO$  ratio. The value estimated with the intensities given by Swings & Page (1950) are more reasonable as they remove the  $N_2^+$  contamination and are more aware of the complications regarding spectroscopy of the era. These values were later re-estimated by Cochran et al. (2000), who estimate a  $N_2^+/CO^+$  ratio of 0.06. This is the same ratio as in C/2016 R2.



**Figure 3.5** – C/1947 S1 (Bester), date not given. *Hieronim Hurnik, Kometa Halleya, Państwowe Wydawnictwo Naukowe, Warszawa* 



**Figure 3.6** – Comet C/1961 R1 (Humason) as seen on September 5, 1962, Palomar Observatory. *C.E. Kearnes and K. Rudnicki with 48inch Schmidt at Palomar Observatory, California.* 

#### 3.3.2 Comet C/1947 S1 (Bester)

Comet C/1947 S1 (Bester) (Fig. 3.5), also known as Comet 1947 k or 1948 I, was a late addition to this sample, as it is rarely mentioned in papers, despite the early success of spectroscopic study of its tail (See Sec. 1.3). It was discovered on 25 September 1947 by Michiel J. Bester, and it emitted strongly in the UV range. It made its closest approach to the Earth on 5 April 1948 (0.740 au), about 1.5 months after its perihelion passage at 0.748 au from the sun (van Biesbroeck, 1961). It seemed to escape the comet from the Solar System on a hyperbolic orbit (Królikowska, 2014).

Based on tables 11 and 12 of Swings & Page (1950), we see a  $I(N_2^+(0,0))$  of 4 and  $I(CO^+(2,0))$  of 5+4 in the spectrum of the tail. This gives us a value of  $N_2/CO$  of about 0.02.

### 3.3.3 Comet C/1961 R1 (Humason)

Similar to C/2016 R2, Comet C/1961 R1 (Humason) (Fig. 3.6), also known as 1962 VIII and 1961e, presented a bright and defined coma already at a large heliocentric distance ( $r \sim 2.6$  au). It was shown to exhibit exceptionally intense activity with rapid variation of its brightness. With a magnitude of  $m_0 = 3.5$ , the radius of its nucleus was estimated between 30 and 41 km, making it a massive comet (Öpik, 1964, 1963). It had an unusually disrupted or "turbulent" appearance (Brandt & Chapman, 2004). At one point, between two observations in July 1962, the tail broke off the nucleus (van Biesbroeck, 1962). It also presented a strong CO<sup>+</sup> and  $N_2^+$  emission with a 'tremendously active' tail (Swings, 1965), and weak emission in the continuum. CO<sup>+</sup>, CN, and C<sub>3</sub> were present but weaker than expected, with only a 'trace' of CH<sup>+</sup>. Usually CO<sup>+</sup> is observed only in the tail, but here, it was detected

even in the coma (Warner & Harding, 1963).  $N_2^+$  was found to be strong while  $CO_2^+$  was weak (Greenstein, 1962).

We were first able to make a crude estimate of the N<sub>2</sub>/CO ratio of comet Humason thanks to Table 1 of Greenstein (1962). This table presents the wavelengths and their respective intensities observed at the Palomar Observatory. Two spectra were made, one on August 1<sup>st</sup> (N1695), and the second on August 2<sup>nd</sup> (N1702), both while the comet was at r = 2.6 au and  $\Delta = 1.7$  au. This was the first time that CO<sup>+</sup> had been seen in a comet's tail with such a high resolution.

We once again selected the bands used by Opitom et al. (2019) to calculate this ratio for C/2016 R2, the  $N_2^+(0,0)$  band with the head at 3914Å (here, identified at 3912Å) and the CO<sup>+</sup>(2,0) band at 4252 and 4273, we have:

 $- I(N_2^+)(0,0) = 4$ 

 $- I(CO^{+})(2,0) = 10 + 10 = 20$ 

with the intensity in arbitrary units. We continue with the same coefficients as Opitom et al. (2019) and eq. 3.1 and find the  $N_2^+/CO^+$  ratio is in the order of:

$$\frac{N_2^+}{CO^+} = \frac{3.55 \times 10^{-3}}{7 \times 10^{-2}} \times \frac{4}{20} = 0.01$$

or 6 times lower than C/2016 R2, however still much higher than the norm. Even if we were to try to separate the relative intensities contributing to the intensity of the 4273 line, knowing that  $N_2^+$  is also a contributor,  $I(CO^+)(2,0) \simeq 14$ , and the  $N_2^+/CO^+$  ratio would become 0.014.

Arpigny (1964) calculated the molecular abundances present in the tail at  $10^4$  km and found N(CO<sup>+</sup>) in the order of  $10^{13}$  cm<sup>-2</sup> and N(N<sub>2</sub><sup>+</sup>) in the order of  $10^{11}$  cm<sup>-2</sup>, giving us a N<sub>2</sub><sup>+</sup>/CO<sup>+</sup>  $\simeq 0.01$ , in the same order as what we estimated based on the observations of Greenstein (1962). He estimates his uncertainties on the molecular abundances N(N<sub>2</sub><sup>+</sup>) in the order of  $\pm 2 \times 10^{11}$  cm<sup>-2</sup>, which would give us an uncertainty on the N<sub>2</sub><sup>+</sup>/CO<sup>+</sup> ratio of  $\pm 0.01$ . These values were also re-estimated by Cochran et al. (2000).

#### 3.3.4 Comet C/1987 P1 (Bradfield)

Otherwise known as Comet Bradfield 1987s (Fig. 3.7), this comet was discovered on the evening of August 11, 1987 by William A. Bradfield in Australia, and soon became bright enough to be seen with the naked eye. Two events of plasma tail separation occurred on October 19-20<sup>th</sup> 1987 (Cimati, 1989), and December 20, 1987 (Cremonese & Fulle, 1988).



**Figure 3.7** – Comet C/1987 P1 (Bradfield) on Nov 21 1987. *Edwin Faughn* 



**Figure 3.8** – Comet C/2001 Q4 (NEAT), April 18, Alcohuaz, Chile. *Loke Kun Tan (Star-ryScapes)* 

Spectra of Comet C/1987 P1 were obtained with the Ohio State University Image Dissector Scanner (IDS) on the Perkins 1.8 m telescope at Lowell observatory, when the comet was at  $r_h = 0.9$  and  $\Delta = 0.9$  au. Both CO<sup>+</sup> and N<sub>2</sub><sup>+</sup> were identified in the tail, along with CH<sup>+</sup> and H<sub>2</sub>O<sup>+</sup> (Lutz et al., 1993). It had an impressive temporal variability, with the CO<sup>+</sup>, N<sub>2</sub><sup>+</sup>, and H<sub>2</sub>O<sup>+</sup> increasing by more than 50% from 1987 November 24-25 but then dropping by half again until December 9<sup>th</sup>.

An average abundance ratio of  $N_2^+/CO^+$  was calculated as  $0.02 \pm 0.01$  in the tail at  $6 \times 10^4$  km from the nucleus (Lutz et al., 1993). This was the first time a *g* factor could be established for  $N_2^+$  in comets, and  $g = 7 \times 10^{-2}$  photons.ion<sup>-1</sup>.s<sup>-1</sup>at 1 au has been used ever since. Unlike C/2016 R2, it would appear to not have stronger CN bands at 3883 Å. It did not appear to be depleted in water-ice, as the lowest measured CO<sup>+</sup>/H<sub>2</sub>O<sup>+</sup> ratio was ~ 0.2 ± 0.1, assuming the CO<sup>+</sup> parent was CO and not CO<sub>2</sub>.

### 3.3.5 Comet C/2001 Q4 (NEAT)

Comet C/2001 Q4 (NEAT) (Fig 3.8) was discovered on August 24, 2001 by the Near-Earth Asteroid Tracking program (NEAT). Cometary activity was first detected at the end of August 2003 when the comet was 8.8 au from the Sun (Korsun et al., 2014). It was bright and observable with the naked eye in the southern hemisphere,

only 0.32 au from Earth in May 2004. Much like C/2016 R2, it was seen to have a low CN production rate,  $< 1.4 \times 10^{25}$  mol.s<sup>-1</sup>(Tozzi et al., 2003).

Cochran et al. (2000) and Cochran & Cochran (2002) could not find any N<sub>2</sub><sup>+</sup>, and placed an upper limit of N<sub>2</sub><sup>+</sup>/CO<sup>+</sup>  $\leq 5 \times 10^4$ . By using the N<sub>2</sub> (0,0) band of the Carroll-Yoshino ( $c'_4 \Sigma_u^+ - X^1 \Sigma_g^+$ ) system at 958 Å, Feldman (2015) find an N<sub>2</sub><sup>+</sup>/CO<sup>+</sup> ratio of 0.027, with an optically-thin fluorescence efficiency of  $g = 5.1 \times 10^{-8}$  photons.s<sup>-1</sup>.molecule<sup>-1</sup>at 1 au.

N.B.: Using the methods I will later describe in section 5, I do not manage to find any  $N_2^+$  in the spectrum available to us with the  $B^2\Sigma - X^2\Sigma$  (0, 0) band of  $N_2^+$  with a bandhead at 3914 Å.

#### 3.3.6 Comet C/2002 VQ94 (LINEAR)

C/2002 VQ94 (LINEAR) was first discovered by the LINEAR team in November 2002, when the comet was at a distance of  $r_h = 10.02$  au (Tichy et al., 2002), may be one of the largest comets ever observed, with a nucleus estimated to be ~100 km in diameter. Cometary activity was first detected at the end of August 2003 when the comet was at  $r_h = 8.36$  au, displaying CO<sup>+</sup> and N<sub>2</sub><sup>+</sup>, with an estimated N<sub>2</sub><sup>+</sup>/CO<sup>+</sup> of 0.06 (Korsun et al., 2014). This was the first time these ionic emissions had been observed in such great quantities, and at such a large heliocentric distance.

Unfortunately, the comet's orbit did not bring it into the inner Solar System, with its perihelion at 6.8 au. Thus, no study on the emission of water-ice can be done. As it left the Solar System, the spectra obtained in 2009 showed no emission lines above continuum at a distance of 9.86 au from the Sun.

#### 3.3.7 Comet 29P/Schwassmann-Wachmann 1

Comet 29P/Schwassmann-Wachmann 1 (hereafter 29P) was discovered in 1927 by the German astronomers A. Schwassmann and A. Wachmann while it was outbursting. Unlike the other comets in this list, 29P has a short-period, belonging to the Jupiter family of comets. It has a period of only 14.6 years, and an eccentricity of only 0.04; nothing like the nearly-parabolic comets on this list. This quasi-circular orbit lies between Jupiter and Saturn, and it was the first observed small body with an orbit entirely beyond Jupiter. Its perihelion is at 5.7 au, meaning its volatiles continue to sublimate rapidly: it has had a persistent coma since its discovery. This can be seen in Fig. 3.9. It has an incredibly large nucleus of 60 km (Schambeau et al., 2015), and frequently undergoes massive outbursts may be caused by seasonal cryovolcanic activity (Miles, 2016).



**Figure 3.9** – Comet 29P/Schwassmann-Wachmann 1 (left) from Spitzer (infrared image in false colours) and its quasi-circular orbit just beyond Jupiter (right) from the SBD.



**Figure 3.10** – Eccentricity as a function of perihelion for all known comets (Elements retrieved from the SBD) with the comets of our sample in red.

The spectra revealed the presence of  $CO^+$  and  $N_2^+$  emissions in the cometary coma while it was at a distance of 5.25 au from the Sun, with an estimated  $N_2^+/CO^+$  ratio of 0.013 within the projected slit.

#### 3.3.8 Shared traits of N<sub>2</sub>-rich comets

Table 3.2 presents a comparison of all known volatile-rich comets. A comparison of their orbital elements is shown in Fig. 3.10. All values of the orbital elements are retrieved from the JPL Small Body Database (SBD) Lookup tool.

To expand our sample, included are CO-rich/H<sub>2</sub>O-poor comets such as C/2009 P1 Garrard and 2I/Borisov for which  $N_2^+$  was not observed, but as they are some of

Comet	P (Yrs)	q (au)	e	inc(deg°)	D (km)	H <sub>2</sub> O/CO	N <sub>2</sub> /CO
C/1908 R1	-	0.945	1.0009	140.17	-	-	≥0.06 <sup>a</sup>
C/1940 R2	-	0.368	1.0005	49.89	-	-	$\geq 0.04^{a}$
C/1947 S1	-	0.748	1.0003	140.56	37*	-	$0.05-0.09^{a}$
C/1956 R1	-	0.316	1.0002	119.94	-	-	>0.09 <sup>a</sup>
C/1957 R1	12415	0.355	0.9992	93.96	24*	-	0.02 <sup>a</sup>
C/1961 R1	2944	2.133	0.9896	153.28	30-41	$5^{\mathrm{b}}$	0.02-0.03 <sup>a</sup>
C/1969 T1	512287	0.472	0.9999	75.82	-	-	≤0.03ª
C/1969 Y1	1747	0.538	0.9962	90.04	-	-	0.03 <sup>a</sup>
C/1973 E1	-	0.142	1.000	14.30	-	-	$0.07^{a}$
C/1986 P1	-	1.199	1.0003	147.12	33*	-	$0.07^{a}$
C/1987 P1	2122	0.869	1.000	34.09	-	-	$0.02\pm0.07^{c}$
C/2001 Q4	-	0.962	1.0007	99.64	-	13.88 <sup>d</sup>	0.03 <sup>d</sup>
C/2002 VQ94	2863	6.797	0.9663	70.52	$96 \pm 4^{\text{e}}$	-	0.06 <sup>e</sup>
C/2016 R2	18709	2.602	0.9963	58.22	38	$< 0.1^{f}$	$0.06\pm0.01^{\rm g}$
1P	76	0.586	0.9671	162	11	-	0.005 <sup>h</sup>
29P	14.6	5.734	0.0440	9.37	$60.4^{i}$	0.22 <sup>j</sup>	0.01 <sup>k</sup>
67P	6.43	1.2432	0.6497	3.87	4	32.25	$0.03^{1}$
11	-	0.256	1.2011	122.74	$0.2\times0.04\times0.04^m$	-	-
2I	-	2.007	3.3562	44.05	$<1^n$	1.73	-
C/2009 P1	-	1.551	1.0009	106.18	115*	0.6-1.6°	-
C/2014 UN271	$4.47 \times 10^{6}$	10.95	0.9994	95.460	$119\pm15^{\rm p}$	-	-

**Table 3.4** – Orbital elements along with  $H_2O/CO$ ,  $N_2/CO$  abundance ratios of comets with peculiar  $N_2$ - rich and/or  $H_2O$ -poor compositions.

<sup>a</sup> Values from Table III of Cochran et al. (2000) based on their personal communication with C. Arpigny and photographic plates, save for C/1973 E1 (Fourier Transform spectrometer) and C/1986 P1 (CCD). <sup>b</sup> Estimated from Greenstein (1962) & Arpigny (1964).

<sup>c</sup> Lutz et al. (1993).

<sup>d</sup> Feldman (2015) from the N<sub>2</sub>(0,0) band of the  $(c_4' \Sigma_u^+ - X^1 \Sigma_g^+)$  system at 958Å.

<sup>e</sup> Korsun et al. (2014)

<sup>f</sup> Biver et al. (2018). McKay et al. (2019) estimate a  $H_2O/CO$  of 0.0032.

<sup>g</sup> Opitom et al. (2019).

 $^{\rm h}$  Wyckoff et al. (1991): CO/N $_2 \sim 200.$ 

<sup>i</sup> Schambeau et al. (2015).

- <sup>j</sup> Ootsubo et al. (2012).
- <sup>k</sup> Ivanova et al. (2016).

<sup>1</sup> Rubin et al. (2020),  $CO/H_2O = 0.031$ .

<sup>m</sup> Jewitt et al. (2017).

<sup>n</sup> Jewitt et al. (2020).

° Feaga et al. (2014): CO/H<sub>2</sub>O of 63% that of water; Bodewits et al. (2020) CO/H<sub>2</sub>O = 173%.

<sup>p</sup> Hui et al. (2022).

the rare comets that are depleted in water. The former has a CO/H<sub>2</sub>O abundance ratio of 63%, the highest ever observed for any comet inside the water snow line before the discovery of C/2016 R2, and displayed variation in relative abundance of different species with heliocentric distance (Feaga et al., 2014). 2I/Borisov contains significantly more CO than H<sub>2</sub>O gas, with a CO/H<sub>2</sub>O ratio of at between 35% and 173% (Cordiner et al., 2020; Bodewits et al., 2020), more than three times higher than previously measured for any comet in the inner (<2.5 au) Solar System. Comet C/2016 R2 is the extreme, with no water detected. Since the CO iceline is near the N<sub>2</sub> iceline, it's worth investigating these comets and this theory, as it may be expanded to other "exotic" species. Although these comets represent a very small fraction of the comets for which CO/H<sub>2</sub>O has been measured, they are more difficult to explain.

Comet C/2014 UN271 Bernadelli-Bernstein has also been added, despite no estimations of its composition having been done as yet, due to the fact that is it already outgassing at > 20 au, and must therefor have a hypervolatile-rich composition.

Based on the nucleus magnitude provided by the ephemeris and a realistic geometric albedo of about 0.04, we can estimate effective radii ( $R_n$ ) of our sample comets from their absolute nuclear magnitude using the standard methodology devised by Russell (1916) and reformulated by Lamy et al. (2004):

$$R_n = \frac{1.496 \times 10^{11}}{\sqrt{p}} 10^{0.2(m_{\odot} - H)}$$
(3.2)

where  $R_n$  is the comet's nucleus in meters, p is the geometric albedo,  $m_{\odot}$  the apparent magnitude of the Sun, and H the absolute magnitude of the comet's nucleus, i.e., the magnitude at  $r_h = \Delta = 1$  au,  $\alpha = 0^{\circ}$ ), where *alpha* represents the phase angle (angle made between the Earth-Comet-Sun). We take -26.93 for the r'-band magnitude of the Sun (Colina et al., 1996), and 11.2 for the absolute magnitude of comet nucleus from the SBD. Comet sizes I have estimated based on the nucleus absolute magnitude are marked with a \*.

Overall, there is no immediate link between these comets. The non-periodic comets are quasi parabolic, with high eccentricities nearing or superior to 1, but their inclinations vary from  $34^{\circ}$  to  $150^{\circ}$ . They appear to have larger than common nucleus size, with C/2016 R2 and C/1961 R1 the smallest of the set, at only ~35 km. Visual observations also seem to indicate that these comets are active at higher heliocentric distances and have rapidly changing tail morphology. If this were the entirety of our sample size, then we could say these are large, long-period comets originating from the distant Oort cloud. Seeing their volatile-rich composition, they should be dynamically new, and perhaps represent some of the oldest comets available to us, offering us a pristine look at the early Solar System.

However, the in-situ detection of  $N_2$  in comet 67P by Rubin et al. (2020), along with elevated  $N_2/CO$  ratios in comets 1P and 29P, make us wonder how the periodic comets fit into this puzzle. It is possible  $N_2$  could be found in many other comets if we were to directly measure at their surfaces. More in-situ probes are required. 1P is a Halley-type comet, while 29P and 67P are part of the Jupiter family of comets. Short period comets move backwards and forwards from the Jupiter family to the Halley (intermediate-period) family on average about 12 times during their dynamical lifetime (Levison & Duncan, 1994), meaning these two families are intrinsically linked. We will investigate their dynamical history and nature in chapter 6.

If we refer back to Table 3.4, there seems to be a cluster of N<sub>2</sub>-rich comets with high-eccentricities and a perihelion between 0.7 and 1 au, with 1P just outside this cluster. A plot of these diameters along with the known diameters of other comets is shown Fig. 3.11. in The only N<sub>2</sub>-rich comets we have observed with a perihelion > 3 au are extremely large comets: comet 29P with a confirmed 60.4 km diameter (Schambeau et al., 2015); comet C/2002 VQ94 with an anticipated 96 km diameter (Korsun et al., 2014), and comet C/2014 UN271 with a calculated diameter of 119 km (Jewitt et al., 2017). At first glance, this would seem natural: despite outgassing at large heliocentric distances, we would miss small comets with large q due to the limitations of our observational technology. Large cometary nuclei are brighter than small cometary nuclei and are thus easier to detect, and since the amount of gas and dust emitted by a comet varies as a function of the heliocentric distance, its perihelion distance plays a key role in its discoverability. However, many of these small q comets are seen on approach at much larger heliocentric distances than the qof these large comets; we should also be observing many more massive volatile-rich comets with small q, especially if they are such powerful outgassers. In short: why are the mega-comets not approaching any closer<sup>5</sup>? Is it possible that comets of this size would not survive such a close approach to the Sun, due to their potential fragile nature?

In a study of 105 short-period comets (here, P<20 yr) with known nuclei radii, Hughes (2003) found that a value of  $q \simeq 2.7$  au divides the comets into an outer Solar System group which are hardly affected by decay, and an inner Solar System group which are decaying quickly. This distance separates comets which have negligible water sublimation from comets that are decaying speedily. This is interesting, as the cluster of N<sub>2</sub>-rich comets has a q < 2.7 au.



**Figure 3.11** – Estimated diameters of all comets in our study (red) compared to all known comet nucleus diameters as a function of perihelion distance. Our comets are larger than typical. 67P is within the average range of nucleus diameters, but the  $N_2$  was measured in-situ.

#### 3.3.9 Observational Bias

There exists a possibility that our Solar System is rife with volatile-rich comets, but we are simply not observing them. However, since these comets are more productive at higher heliocentric distances, they should, in fact, be easier to detect, unless there is a process that would prevent  $N_2$  outgassing from being observed: as with the in-situ measurements of  $N_2$  on 67P's surface, there is perhaps much more  $N_2$  in comets than than our spectroscopes can observe.

A possible observational bias —or a strange coincidence —arises from the fact that of these comets (before this sample was complimented by the Cochran et al. (2000) list) were detected between the same six-week period of August 1<sup>st</sup> and September 25<sup>th</sup>, hence their P,Q,R,S designations. In the case of older comets (pre-Sky Surveys) perhaps this could be linked to ideal observational conditions, at least in the northern hemisphere, which would better permit the discovery of such comets: as we saw with the first spectroscopic observations of comet tails creating the false assumption that N<sub>2</sub><sup>+</sup> was one of the main components, which persisted over 50 years. However, even with the advent of NEAR, LINEAR, and Pan-STARRS, these comets were still found within the same six-weeks of each other. Once the list from Cochran et al. (2000) was added, these comets were complimented by more

<sup>&</sup>lt;sup>5</sup>I am not complaining, this is probably a good thing for Earth.

seasons, yet they were still predominantly discovered in this small window. At the very least, this is strange: I cannot speculate further.

All three H<sub>2</sub>O-poor comets have only been discovered in the past decade: One, an interstellar visitor (2I/Borisov); one, enriched in N<sub>2</sub> (C/2016 R2), and one presenting as a usual comet in every other way (C/2009 P1). There may be some selection bias that causes CO-poor comets to be observed more frequently. This could be a result of our modern observational technology: while our spectrometers have higher resolution, they usually require a smaller slit. The first comet tails were observed with photo plates with a long slit and medium resolution; since the implementation of CCDs ~ 1990, we have much higher resolution spectroscopy, but the caveat is that spectra have a short slit centered on the nucleus, in the order of arcseconds rather than arcminutes. With UVES short slit, one never sees CO<sup>+</sup> or N<sub>2</sub><sup>+</sup> while still seeing H<sub>2</sub>O<sup>+</sup>, OH<sup>+</sup> and CH<sup>+</sup>. No CO<sup>+</sup> is seen in the centered spectrum of DE Vico (Cochran et al., 2000), but it is weakly present in the offset spectrum. However, using long-slit spectroscopy raises the possibility of contamination by atmospheric N<sub>2</sub><sup>+</sup> lines and strong CN lines. This compromise may have cost us multiple N<sub>2</sub><sup>+</sup>-rich comets.

#### PART II

# NEW FLUORESCENCE MODEL OF N<sub>2</sub> AND APPLICATION TO COMET C/2016 R2 PANSTARRS

// — I am like a slip of comet, Scarce worth discovery, in some corner seen Bridging the slender difference of two stars, *Come out of space, or suddenly engender'd By heady elements, for no man knows:* But when she sights the sun she grows and sizes And spins her skirts out, while her central star Shakes its cocooning mists; and so she comes To fields of light; millions of travelling rays Pierce her; she hangs upon the flame-cased sun, And sucks the light as full as Gideon's fleece: But then her tether calls her; she falls off, And as she dwindles shreds her smock of gold *Amidst the sistering planets, till she comes To single Saturn, last and solitary;* And then goes out into the cavernous dark. So I go out: my little sweet is done: *I have drawn heat from this contagious sun:* To not ungentle death now forth I run.

11

Gerard Manley Hopkins, After observing Temple's Comet in 1864.

# 4 Towards a Fluorescence model of N<sub>2</sub><sup>+</sup>

#### Contents

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4.4	New 1	Fluorescence Efficiencies

UNDERSTANDING THE PRESENCE (OR LACK OF)  $N_2$  in comets allows us to investigate key features in the timeline of planetesimal formation. An object such as C/2016 R2 provides us with a unique opportunity to improve our  $N_2$  identification process in cometary spectra. In order to improve upon this measurement in C/2016 R2 and calculate its production rate of  $N_2$ , we must first improve upon the measurement itself of the quantity of  $N_2^+$ . Our first step in identifying which spectral lines belong to  $N_2^+$  must then be the creation of a  $N_2^+$  fluorescence model, as none has yet been made for comets as of today.

This chapter is published as Rousselot et al. (2022).

# 4.1 Spectroscopy Notions

Spectroscopy is the study of the matter as it interacts with electromagnetic radiation, which allows us to understand the composition, quantity, motion, pressure, and temperature of distant astronomical objects. The absorption of a photon results in the excitation of molecules, which can in turn dissipate their energy by decomposition, reaction, or re-emission, as they relax from the excited state (higher energy) to the ground state (lower energy). In most cases the emitted light has a longer wavelength than the absorbed radiation. The photon energy *E* of each transition corresponds to a difference in energy levels and is proportional to its frequency  $\nu$  following  $E = h\nu = E_1 - E_2$ , where *h* is Planck's constant. The position of these discrete

energy levels  $E_1$  and  $E_2$  is determined by the structure of each molecule. Following  $\lambda = c/\nu$ , the photon is emitted at a unique wavelength which allows us to determine which transition was at its source, and from there, identify which species are present. Through the observation of a collection of wavelengths emitted (or re-emitted) from a celestial object, we obtain the spectrum of of its light, and are able to determine its composition through spectroscopy. As each species has its own unique structure, only certain transitions are allowed between energy levels: rotational, vibrational, and electronic transitions, or a combination thereof, each emitting — or absorbing, if the transition is from a lower to a higher energy level — a photon with a unique frequency. Rotational levels exist within the vibrational levels, which exist within the electronic levels. An example of this structure is shown in Fig. 4.1. What we observe depends on the type of transition:



**Figure 4.1** – Potential energy curve representing the potential energy of interaction between the two nucleii as a function of atom-atom distance inside a molecule. This gives the structure of electronic, vibrational, and rotational levels. The arrow indicates a transition between the v' = 1 vibrational level from one excited state to the v'' = 0 ground state of a molecule.



**Figure 4.2** – A diatomic molecule. This rigid rotor model has two masses attached to each other with a fixed distance between the two masses. It can rotate around the center of mass.

- An electronic transition defines a system;
- A vibrational transition defines a **band**;
- A rotational transition defines a line.

The energy of each level is determined by:

$$E_{\text{int}} = E_{\text{elec}} + E_{\text{vib}}(v) + E_{\text{rot}}(J)$$

where E is the energy of each level. We must determine the energy functions of molecules based on their structure and geometry so as to find the positions of these discrete energy levels.

In a molecule, the electrons orbit around the nuclei of their atoms. Here, as we are dealing solely with N<sub>2</sub> and N<sub>2</sub><sup>+</sup>, we are considering the case of a linear diatomic molecule, meaning it has a cylindrical symmetry. Each electron has an angular momentum  $\vec{l}$  projected as  $\vec{\lambda}$  on the internuclear axis. This value can be positive or negative for a linear molecule and be degenerate, meaning multiple different configurations of electrons in their molecular orbitals giving the same result. The sum of these projections gives us  $\vec{\Lambda}$ , the projection of the electronic orbital angular momentum along the internuclear axis. We take its modulus:

$$|\overrightarrow{\Lambda}| = \Lambda \frac{h}{2\pi}$$

where *h* is Planck's constant, and  $\Lambda$  will be an integer. Spectroscopic notation uses Greek letters to identify the state of a molecule by this quantum number  $\Lambda = 0, 1, 2, 3, ...$  represented by the letters  $\Sigma, \Pi, \Delta, \Phi, ...$  respectively.

The spins of electrons will couple together to give  $\vec{S}$  corresponding to an integer *S* through the relation:

$$\left|\overrightarrow{S}\right| = S^* \frac{h}{2\pi}$$

where  $S^* = \sqrt{S(S+1)}$ . By projecting  $\vec{S}$  onto the internuclear axis we obtain  $\vec{\Sigma}$  and its corresponding  $\Sigma$  from  $|\vec{\Sigma}| = \Sigma \frac{h}{2\pi}$ .  $\Sigma$  can only take on 2S + 1 values, such as -S, -S + 1...S. The total angular momentum is thus represented by  $\vec{\Omega} = \vec{\Sigma} + \vec{\Lambda}$ . The molecular term symbol is then defined as:

$$^{2S+1}\Lambda_{\Omega,(q,u)}$$

where  $\Lambda$  is represented by its greek letter counterpart, i.e.  $\Pi$  if  $\Lambda = 1$ . In the case of homonuclear molecules (all atoms are the same) we use *g* and *u* to identify if the wavefunction changes the state of the molecule around its center of symmetry (*u* or not (*g*). homonuclear molecules can only transition from *g* to *u* states or from *u* to *g* states.

Spin-orbit coupling occurs when the *z*-component of spin interacts with the *z*-component of the orbital angular momentum. This gives us twice the number of degenerate states. When  $\Lambda = 0$ , we have no spin-orbit coupling. All  $\Lambda = 0$  states are either symmetric under any plane containing the internuclear axis, or antisymmetric. These two situations are labeled as  $\Sigma^+$  or  $\Sigma^-$ . The number of degenerate states, or 'multiplicity,' is given as:

- $(2S+1) \times 2$  for  $\Lambda \neq 0$
- (2S+1) for  $\Lambda = 0$

A same molecule can have many different electronic states with the same multiplicity (the same  $\Sigma$ ). To identify them, we use X for the ground state and A,B,C, and so on for excited states of the same multiplicity (having the same spin quantum *S* number) in ascending order of energy. If *S* is not the same, the level is indicated with a,b,c, etc.

Let us first identify the positions of the rotational levels. In the gas phase, a molecule may rotate freely around a set of mutually orthogonal axes of fixed orientation centered on the center of mass of the molecule. We first simplify our linear molecule as a 'rigid rotor' configuration: it can be seen as two masses attached to each other where the internuclear separation  $r_e$  (atom-atom distance) is constant. We start with the Hamiltonian solution to a rigid rotor problem in which H = T + Vwhere T is the kinetic energy and V is potential energy. Since we are in the gas



**Figure 4.3** – Energy level diagram showing the N<sub>2</sub><sup>+</sup> first negative group  $B^2\Sigma_u^+ \rightarrow X^2\Sigma_g^+$ and the different types of lines allowed by the selection rules. The number in brackets corresponds to the N'' value (N value in the  $X^2\Sigma_g^+$  state).

phase, there is no resistance to the rotation and V = 0. H = T where T is the kinetic energy. This energy can be expressed as:

$$E = \frac{1}{2}I\omega_x^2 + \frac{1}{2}I_y\omega_y^2 + \frac{1}{2}I_z\omega_z^2$$
(4.1)

where  $\omega_i$  is the angular frequency for the rotation around each axis ( $\omega_i = \nu_{rot}/c$ ), called the harmonic wavenumber. In the case of a rigid rotor, the molecule can rotate around its three axes, but its moment of inertia remains constant. This inertia can be expressed as:

$$I = \mu r_e^2$$

where  $\mu$  the reduced mass of the system, or  $\mu = \frac{m_1m_2}{m_1+m_2}$ . We can simplify this using the modulus of the angular momentum  $|\vec{L}| = I\omega_e$  so that:

$$E = \frac{1}{2} \frac{|\vec{L}|^2}{I}$$
(4.2)

We use the rotational quantum number J which defines the magnitude of the rotational angular momentum, where  $\vec{J} = \vec{L} + \vec{\Omega}$ , and  $|\vec{J}| = \sqrt{J(J+1)}(h/2\pi)$ . J = L + S is the total angular momentum. Now eq.4.2 becomes:

$$E = \frac{1}{2}I\omega_{\rm rot}^2 = \frac{J(J+1)h}{8\pi^2 I}$$
(4.3)

Since  $E = hc/\lambda = hc\overline{\nu}$ , where  $\overline{\nu}$  is the wavenumber in cm<sup>-1</sup>. The convention is to give the rotational energy as  $F(J)/\text{cm}^{-1}$ , we must convert  $E_{\text{rot}}$  into the proper units.

$$F(J) = \frac{E_{\text{rot}}}{hc} = \frac{1}{hc} \frac{J(J+1)h}{8\pi^2 I} = BJ(J+1)$$
(4.4)

where *B* the rotational constant  $B = \frac{h}{8\pi^2 I_c}$ . For pure rotational transitions, selection rules require that transitions fulfill  $\Delta J = \pm 1$ , so the difference between these levels will always be 2*B*.

When  $\overrightarrow{\Omega} = \overrightarrow{\Sigma} + \overrightarrow{\Lambda}$  exists, we say we are in Hund's coupling case a. F(J) = BJ(J+1) becomes  $F(J) = B[J(J+1) - \overrightarrow{\Omega}]^2$ , and J can take on values of  $J = \Omega, \Omega + 1, \Omega + 2, ...$ 

In the case where the molecule is spinning,  $\vec{S}$  is no longer coupled with  $\vec{\Lambda}$  and  $\vec{\Omega}$  does not exist. We are in Hund's coupling case b. We need to consider  $\vec{N}$  where  $\vec{N} = \vec{\Lambda} + \vec{L}$ . *N* is quantified by  $|\vec{N}| = \sqrt{N(N+1)}(h/2\pi)$ , and can take the values  $N = \Lambda, \Lambda + 1, \dots$  We find  $\vec{J}$  by  $\vec{J} = \vec{S} + \vec{N}$ . *J* now takes on values of  $J = |N - S|, N - (S + 1), \dots, N + S$  and we have spin a multiplicity for these levels

of 2S + 1. All  $\Lambda = 0$  states ( $\Sigma$  states) are in this case, and transitions between them require a  $\Delta N = \pm 1$ . The difference between *J* and *N* levels is illustrated by Fig. 4.3.

In the case where S = 1/2, we have two new values of F: for J = N + 1/2:

$$F_1(N) = B[N(N+1) - \Lambda^2] + \frac{1}{2}\gamma N$$
(4.5)

where  $\gamma$  is a correcting term,  $\gamma \ll B$ . For J = N - 1/2:

$$F_2(N) = B[N(N+1) - \Lambda^2] + \frac{1}{2}\gamma(N+1)$$
(4.6)

However, bonds do not act like a rod with a fixed distance, but like a spring. This means that the angular velocity of the molecule increases as the distance between the atoms increases, and we are in the case of a non-rigid rotor. We use the centrifugal distribution constant D, a small correction, where  $D = \frac{4B^3}{\omega_e^2} \ll B$  so that:

$$F_v(J) = B_v J(J+1) - D_v J^2 (J+1)^2$$
(4.7)

This is where we must account for vibrational transitions, represented by the vibrational quantum number v = 0, 1, 2, ... Transitions between these levels are caused by the vibration or 'stretch' of molecules in this structure. These emit in the infrared. The collection of lines produced by a vibrational transition is called a band. It is spectroscopic convention for a transition to label the upper state quantum number by a single prime and the lower state quantum number by a double prime. Each band is designated by two integers, v' the starting vibrational level, and v''the arriving level, so that the transition that creates them is called the (v', v'') band. A single molecule can be responsible for multiple band systems. Transitions from one vibrational level to another are accompanied by a change in rotational levels (ro-vibrational transitions). For pure rotational transitions, selection rules impose that  $\Delta J = \pm 1$ : rotational transitions may be P branches ( $\Delta J = -1$ , transitions from a higher J" to a lower J' (poorer)) or R branches ( $\Delta J = +1$ , transitions from a lower J" to a higher J' (richer)). For ro-vibrational spectroscopy, vibrational transitions are accompanied by rotational transitions, both P and R branches, as well as the vibrational-only Q branches, transitions from a J'' level to a J' level of the same value. These transitions are shown in Fig. 4.3.

We simplify the problem as a Simple Harmonic Oscillator (SHO). Here the vibrational energy *G* is G = U/hc where *U* is the potential energy. Following the potential energy equation for an SHO, we have:

$$U = \frac{1}{2}k(r - r_e)^2$$
(4.8)

where k is the force constant of the bond and  $r_e$  the equilibrium distance. The vibrational energy G is then:

$$G(v) = \omega_e(v + \frac{1}{2}) \tag{4.9}$$

In the case where the molecule is not a harmonic oscillator, we must account for a different potential, such as:

$$U = f(r - r_e)^2 - g(r - r_e)^3$$
(4.10)

where *f* and *g* are two constants, and  $f \gg g$ . This gives us a final value of the energy of a ro-vibrational level:

$$G(v) = \omega_e(v + \frac{1}{2}) + \omega_e x_e(v + \frac{1}{2})^2 + \omega_e y_e(v + \frac{1}{2})^3$$
(4.11)

where  $\omega_e$ ,  $\omega_e x_e$  and  $\omega_e y_e$  are three vibrational constants, in cm<sup>-1</sup>(the first harmonic, the second to, ahormonic constants). The selection rules for pure vibrational transitions requires  $\Delta v = \pm 1$ .

The final type of transition is that between two electronic states, or rotational-vibrational-electronic transitions. These are the most powerful, and are emitted in the Visible-UV wavelength range. A photon is absorbed and excites an electron to higher energy molecular orbitals, giving rise to an excited state, i.e. the  ${}^{2S+1}\Lambda_{\Omega,(g,u)}$  states.

The spectrum observed in a cometary coma is made up of two elements:

- A continuum made up of sunlight scattered by dust grains, which reddens the light.
- Emission lines due to the fluorescence mechanism of the species present in the coma.

Finding which lines belong to which process, and which species contribute to which line, is the greatest challenge for spectroscopists. Since the chemical makeup of these objects is varied, many of these bands can overlap, making distinguishing the species complicated. The spectrum is also Doppler shifted due to the relative motion of the comet when viewed from Earth. The field of spectroscopy continues to evolve as our instruments improve and our understanding of the behaviors of these species increases.

#### 4.2 Observational data

The spectra used for this study were obtained over a five night run at the ESO 8.2 m UT2 telescope by Opitom et al. (2019) using the Ultraviolet-Visual Echelle Spectrograph (UVES) for its scope of the full optical range. The dichroic #1 (390+580) setting covered the range 326 to 454 nm in the blue and 476 to 684 nm in the red, for three dates, February 11, 13, and 14, for a total of five exposures. The dichroic #2(437+860) setting covered the range 373 to 499 nm in the blue and 660 to 1060 nm in the red for February 15 and 16. The dates and observing circumstances of the 5 spectra are summarized in Table 4.1. All observations were with 0.44"-wide slit, providing a resolving power  $R \sim 80\ 000$ . The smallest slit length of 8" sampled about 14500 km at the distance of the comet ( $\Delta$  = 2.5 au).

The data reduction was made using the ESO UVES pipeline<sup>1</sup>, combined with custom routines to perform the extraction, cosmic rays removal, and correct for the Doppler shift due to the relative velocity of the comet with respect to the Earth. The final comet spectrum contains the gas component only. More details regarding data reduction can be found in Manfroid et al. (2009) and Opitom et al. (2019). The TRAPPIST 60-cm telescopes were used in addition to the UVES spectra (Jehin et al., 2011) to monitor the general activity of the comet. More details about the TRAPPIST data reduction procedure can be found in Opitom et al. (2015).

For each day of observation, we have a 2D spectra: a spectrum is taken every pixel along the slit, 0.25" apart, giving us 30 spectra per observation date, centered on the nucleus. At this distance, each 0.25'' corresponds to 435km, so the slit extends over  $1.4 \times 10^4$  km centered on the nucleus. The 1D spectra used are a line by line extraction of the 2D spectra, so the units are the same, with flux in erg.s<sup>-1</sup>.cm<sup>-2</sup>.Å<sup>-1</sup>. Before we use them for our model, we subtract the solar continuum.

<sup>&</sup>lt;sup>1</sup>More details can be found at ftp://ftp.eso.org/pub/dfs/pipelines/uves/ uves-pipeline-manual-22.17.pdf

<b>Fable 4.1</b> – Observing circumstances of	/2016 R2 with VLT	/UVES by O	pitom et al.	(2019)
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Date	$r_h(au)$	$\dot{r}_h$ (km.s <sup>-1</sup> )	$\Delta(AU)$	$\dot{\Delta}$ (km.s <sup>-1</sup> )	Exptime(s)	UVES Setup	UVES slit
2018-02-11T00:27:07.326	2.76	-6.09	2.40	19.7	4800	DIC1-390+580	0.44"×8" - 0.44"×12"
2018-02-13T00:46:23.196	2.76	-5.97	2.43	19.9	4800	DIC1-390+580	0.44"×8" - 0.44"×12"
2018-02-14T00:47:40.759	2.75	-5.91	2.44	20.1	4800	DIC1-390+580	0.44"×8" - 0.44"×12"
2018-02-15T00:23:16.493	2.75	-5.85	2.45	20.1	3000	DIC1-390+580	0.44"×10" - 0.44"×12"
2018-02-16T00:16:08.672	2.75	-5.97	2.46	20.2	3000	DIC1-390+580	0.44"×10" - 0.44"×12"

### 4.3 The Fluorescence of N<sub>2</sub><sup>+</sup>

Fluorescence is the emission of a photon by a substance that has absorbed a photon (or other electromagnetic radiation), rather than emission via radiation solely through its own heat source (incandescence). The resonance fluorescence process occurs when a molecule de-excites by directly emitting a photon at the same wavelength as the one that was absorbed, thus returning to the ground state in a single step. It is this process which allows the species present in a comet's coma to absorb solar radiation and re-emit the light that we then observe as the band spectra of various molecules and interpret with our instruments.

In the case of N<sub>2</sub>, we have two identical N atoms in a linear arrangement, or a centrosymmetric diatomic homeonucleic molecule. It is non-polar, and we have no permanent electric dipole moment, or 'push and pull' within the molecule, the pure rotational and vibrational transitions are forbidden. As a result, it only emits in UV, which is difficult to see with our ground based instruments. However, the electronic transitions of the N<sub>2</sub><sup>+</sup> ion are in the blue-optical part of the spectrum, instead of UV spectrum. The transition visible in comets is the first negative group,  $B^2\Sigma_u^+ - X^2\Sigma_g^+$  with the (0,0) bandhead at 3914 Å, which emits in the visible wavelengths.

#### 4.3.1 Calculating the Energy Levels

The most common method used to compute a fluorescence spectrum in such cases consists of solving a set of equations describing an equilibrium between the radicals leaving a state *i* to the ones reaching the same state, as described in Zucconi & Festou (1985). In order to create our model of the N<sub>2</sub><sup>+</sup> spectrum, we must first build the matrix containing the transition probabilities of all electronic levels the photons of this ion can occupy. We start by examining only the X<sup>2</sup> $\Sigma_g^+$  and B<sup>2</sup> $\Sigma_u^+$  levels and will later take into account the A levels.

Because these are  $\Sigma$  states, they follow Hund's coupling case b: we have  $J = N \pm 1/2$ . The selection rules for these types of transitions imply that  $\Delta N = \pm 1$ . Because of the existence of two different J values for each value of N ( $F_1$  and  $F_2$  levels) it is possible to have  $\Delta N = \Delta J$  (main lines labeled  $P_1$ ,  $P_2$ ,  $R_1$  and  $R_2$ ) or  $\Delta N \neq \Delta J$  (satellite lines  ${}^PQ_{12}$  and  ${}^RQ_{21}$ ). Fig. 4.3 presents the energy levels diagram with the different types of lines involved in this group.

For  ${}^{14}N_2^+$  the energy levels can be determined from Dick et al. (1978), who cataloged the energies of P and R transitions for multiple combinations of v' and v''. These have not yet been digitized. I manually input the line energies for each (v', v'') transition: (0,0), (0,1), (0,2), (1,1), (1,2), (1,3), (2,3), (2,4), (3,5), (4,6) and (5,7) for both P and R branches. Q branches are also possible but the line energies are not

available to us in the literature. From these line energies, we are able to calculate the energy levels for both the (X) and (B) electronic states by use of the different wavenumbers. We use parameters published by Zhang et al. (2015) for the  $X^2\Sigma_g^+$ state and Gottscho et al. (1979) for the  $B^2\Sigma_u^+$  state. Our harmonic wavenumbers are  $\omega_e = 2207.19$ ,  $\omega_e x_e = 16.136$  and  $\omega_e y_e = -0.04$  (Wood & Dieke, 1938). The rotational constants  $B_v$  and the centrifugal distortion constant  $D_v$  values are given in Table 72 (p 248) of Lofthus & Krupenie (1977). For  ${}^{15}N_2^{14}N_2^+$ , we use the wavelengths of Wood & Dieke (1938) and the parameters appearing in the same paper so as to compute the first  $X^2\Sigma_q^+$  level E(N):

$$E(N) = G_v + B_v N(N+1) - D_v N^2 (N+1)^2$$
(4.12)

where  $G_v$ , the vibrational term (eq. 4.11), is  $G_v = \omega_e(v + 0.5) - \omega_e x_e(v + 0.5)^2 + \omega_e y_e(v + 0.5)^3$ .

For v = 0, we use  $B_0 = 192229$  and  $D_0 = 5.92 \times 10^{-6}$  (Lofthus & Krupenie, 1977). Equation 4.12 now becomes:

$$E(N) = \omega_e(0.5) - \omega_e x_e(0.5)^2 + \omega_e y_e(0.5)^3 + B_0 N(N+1) - D_0 N^2 (N+1)^2$$
(4.13)

From this first level, using the line energies from Dick et al. (1978), we can determine the next energy level of the (X) electronic state:

$$E_X(N) = E_X(N-2) + \Delta R(N-2) - \Delta P(N)$$
(4.14)

And we can similarly determine the energy levels of the (B) electronic state:

$$E_B(N) = E_B(N+1) + \Delta P(N)$$
 (4.15)

Using equations 4.14 and 4.15, we calculate the X and B energy levels  $E_X$  and  $E_B$  for v = 0, 1, 2 and for  $N = 0 \rightarrow 40$  for a total of 186 levels. These energy levels are shown in the appendix, in tables 8.4, 8.5, 8.6.

#### 4.3.2 Estimating Transition Probabilities

The intensity of an observed line is related to the probability that the molecule or atom will undergo the transition when illuminated by light at the proper frequency. This probability is proportional to the population of the initial state involved in the transition. Now that we have the energy levels, we need to estimate the probabilities
**Table 4.2** – Hönl-London factors for a  ${}^{2}\Sigma - {}^{2}\Sigma$  transition. *N* corresponds to *N*" (rotational quantum number of the lower state). This factor indicates the relative intensity of R-, P- and Q-branches for a transition. Values from Mulliken (1931).

Line	$P_1$	$P_2$	$R_1$	$R_2$	${}^{P}Q_{12}$	${}^{R}Q_{21}$
HL factor	$\left  \begin{array}{c} \frac{2N(N+1)}{2N+1} \end{array} \right $	$\tfrac{2N(N-1)}{2N-1}$	$\frac{2(N+1)(N+2)}{2N+3}$	$\frac{2N(N+1)}{2N+1}$	$\frac{2N}{(2N-1)(2N+1)}$	$\frac{2(N+1)}{(2N+1)(2N+3)}$

of each possible transition between them in order to determine the associated line intensity. For this, we need the Einstein coefficients: these provide the relationship between spontaneous emission by atoms or molecules that are in quantum states above the ground state,  $A_{v'v''}$  for the spontaneous desxcitation emission (without the presence of inducing radiation) and  $B_{v'v''}$  for the induced (application of electromagnetic radiation of frequency  $\nu$ ) absorption and emission. They are expressed in  $s^{-1}$ .

The spontaneous transition probability for a given line is given by the Einstein coefficients  $A_{v'J' \rightarrow v''J''}$  such that:

$$A_{v'J' \to v''J''} = \frac{\nu^3}{\nu^{*3}} \times \frac{S_{J'J''}}{g_i} \times A_{v' \to v''}$$
(4.16)

where  $\nu$  the transition frequency in cm<sup>-1</sup>,  $\nu^*$  the transition frequency of the band (in this case N'=0  $\rightarrow$  N"= 0 in cm<sup>-1</sup> and  $A_{v'J' \rightarrow v''J''}$ ) the Einstein coefficient of spontaneous emission in s<sup>-1</sup>, and  $S_{J'J''}$  is the Hönl-London factor, given for the general doublet transition in a diatomic molecule. The statistical weight  $g_i$  of the upper level is the product between the statistical weight related to the nuclear spin  $g_{ns}$  and (2J + 1) such that  $g_i = g_{ns}(2J + 1)$ . It can be computed by considering the nuclear spin, and depends on the considered isotopolog and N value. For <sup>14</sup>N<sub>2</sub><sup>+</sup> we have  $g_{ns} = 6$  for even N values and  $g_{ns} = 3$  for odd N values for the  $X^2\Sigma_g^+$  levels. For  $B^2\Sigma^+$  it is the opposite ( $g_{ns} = 3$  for even N values and  $g_{ns} = 6$  for odd N values).

The Einstein coefficients for  $N_2^+$  first needed to be revisited with modern mathematical methods in order to provide the precision we need for our fluorescence modeling. We collaborated with Ferchichi et al. (2022) who recomputed the potential energy curves and transition dipole moment function at a very high level of ab initio theory, which is to say calculate the many electron function which is the solution of the non-relativistic electronic Schrödinger equation. We use their new  $\tilde{A}$ , a and bcoefficients to create our model.

With the standard normalization for the Hönl-London factors (shown in Table 4.2):

$$\sum_{J''} S_{J'J''} = (2 - \delta_{0,\Delta' + \Delta''})(2S' + 1)(2J' + 1)$$
(4.17)

The final calculation of the Einstein  $A_{v'J' \rightarrow v''J''}$  coefficients can then be written: For even N' values:

$$A_{v'J' \to v''J''} = \frac{\nu^3}{\nu^{*3}} \times \frac{S_{J'J''}}{3(2J'+1)} \times A_{v' \to v''}$$
(4.18)

For odd N' values:

$$A_{v'J' \to v''J''} = \frac{\nu^3}{\nu^{*3}} \times \frac{S_{J'J''}}{6(2J'+1)} \times A_{v' \to v''}$$
(4.19)

For a  $\Sigma \rightarrow \Sigma$  transition, this equation can be written:

$$A_{v'J' \to v''J''} = F \frac{S_{J'J''}}{2J'+1}$$
(4.20)

with *F* being defined by  $F = \tilde{A}(1 + aN + bN^2)$ .

The Einstein absorption coefficients  $B_{v''J'' \rightarrow v'J'}$  can be computed with:

$$B_{v''J'' \to v'J'} = \frac{(2J'+1)}{(2J''+1)} \frac{1}{8\pi h\sigma^3} \times A_{v'J' \to v''J''}$$
(4.21)

where  $h = 6.67 \times 10^{-27}$  erg. $s^{-1}$  is Planck's constant and  $\sigma$  the transition frequency (in cm<sup>-1</sup>). The absorption probability is then given by  $B_x \rho_\nu$ , where  $\rho_\nu$  is the solar radiation computed for the wavelength shifted by the Doppler effect.

It is worth mentioning that this formula does not change with different statistical weight for even and odd N values, because transitions with  $\Delta N = 0$  are forbidden for N<sub>2</sub><sup>+</sup>. Consequently the statistical weight due to the different nuclear spins is always the same for the lower and upper level.

While we could possibly ignore the contribution of the Meinel bands, i.e. the  $A^2\Pi_u - X^2\Sigma_g^+$  transitions, it is worth computing them as well since they allow us to get a more complete view of the spectrum. The AII levels add a level of complexity because they are split between the  ${}^2\Pi_{1/2}$  and  ${}^2\Pi_{3/2}$  sub bands. These transitions are shown in Fig. 4.4. If the lambda-doubling (interaction between the electronic and rotational motions when  $\Lambda \neq 0$ ) is neglected it is possible to write:

For state  ${}^{2}\Pi_{1/2}$ :

$$F_2(J) = T + A/2 + BJ(J+1) - 3B/4$$
(4.22)



**Figure 4.4** – Energy level diagram showing the  $N_2^+ A^2 \Pi_u - X^2 \Sigma_g^+$  group and the different types of lines allowed by the selection rules. The number in brackets corresponds to the J'' value (J value in the  $X^2 \Sigma_g^+$  state).

For state  ${}^{2}\Pi_{3/2}$ :

$$F_2(J) = T - A/2 + BJ(J+1) - 3B/4$$
(4.23)

where T, A, and B are constants. They are taken for the different vibrational levels from Table II of Zhang et al. (2015).

#### 4.3.3 Probability Matrix Method

The classic method to solve the population problem is to compute the matrix that contains the transition probabilities for a given heliocentric distance  $r_h$  and velocity v. This matrix gives the probabilities of transitioning from one state to another in a single time unit. Pure vibrational transitional probabilities are forbidden (very low probability), as well as pure rotational transition probabilities, so they can be neglected. From this matrix we will compute the relative populations for the ground electronic state. To do this we split the original matrix into smaller matrices using the method given by Zucconi & Festou (1985) in order to optimize calculation time for the inversion, as these matrices can be quite large and computationally heavy. The final spectrum, including emission lines and spectrum convolved by the right Gaussian instrument response function, is then calculated from the relative populations we compute.

To fill the probability matrix, we calculate every possible transition from level i (of energy  $E_i$ ) to level j (of energy  $E_j$ ):

$$p_{ij} = A_{ij} \frac{\sum^3}{\sum^3_0 \frac{2J' + 1}{2J' + 1}}$$
(4.24)

where  $\Sigma$  is the wavenumber in cm<sup>-1</sup>and  $\sigma_0$  is the wavenumber of the first line in cm<sup>-1</sup>, and  $p_{ij}$  the probability that a transition from level *i* to level *j* occurs.  $p_{ij}$  can represent ether spontaneous emission (i.e.  $A_{ij}$ ) or the absorption mechanism (i.e.  $B_{ij}\rho_{\nu ij}$ ).

Once this probability matrix is filled, we can determine the population of each level. We first calculate the temporal evolution of the population n of a sublevel i of the molecule using the following equation, which expresses the balance between emissions and absorptions of that level:

$$n_i = -n_i \sum_{j=1}^{N} p_{ij} + \sum_{j=1}^{N} n_j p_{ji} \quad i = 1, N$$
(4.25)

Solving equation 4.25 is complicated due to the large number of transitions involved. Using the procedure outlined by Zucconi & Festou (1985), let:

$$T_{ij} = p_{ji} - \delta_{ij} \sum_{k=1}^{N} p_{ik} \quad i, j = 1, N$$
(4.26)

with  $\delta_{ij}$  the Kronecker symbol. Equation 4.25 then becomes:

$$\dot{n_i} = T_{ij} n_j \tag{4.27}$$

or in matrix form:  $\dot{n}_i = Tn$  where *n* represents the column vector of the energy levels and *T* is a  $N \times N$  matrix.

The levels are split into two categories: The electronic ground state sublevels  $n_X$  (for which the lifetime is in the order of a second), and the excited electronic states of the molecule  $n_E$ , (for which the lifetime is expressed in nanoseconds, and where rovibrational and pure rotational transitions can be neglected.) These two populations are split into separate matrices  $n_X = (n_1, ..., n_{N_X})$  and  $n_E = (n_{X+1}, ..., n_N)$ . This allows us to treat these populations separately and radically reduce computation time. Now we can rewrite equation 4.27:

$$\begin{pmatrix} n_{X} \\ n_{E} \end{pmatrix} = \begin{pmatrix} T_{XX} & T_{XE} \\ T_{EX} & T_{EE} \end{pmatrix} \cdot \begin{pmatrix} n_{X} \\ n_{E} \end{pmatrix}$$
(4.28)

where  $T_{EE}$  is diagonal, since non-electronic transitions are negligible in excited electronic states. From here, we get the relationship  $\dot{n_E} = T_{EX}n_X + T_{EE}n_E$ .

We then assume the population of ground state sublevels is constant over small time intervals. Thus, we can say that  $n_X$  is constant over these time intervals since the non-excited states have a longer lifetime than the interval itself. Since the lifetime of the excited states is much shorter than these intervals, we assume  $n_E$  will have reached equilibrium. As a result, we can consider  $n_E$  as negligible before  $n_X$ , and the total population of the ground levels would be equal to 1. We obtain:

$$\dot{n_E} = -T_{EE}^{-1} T_{EX} n_X$$
 (4.29)

which, combined with eq. 4.27 becomes:

$$\dot{n_X} = (T_{XX} - T_{XE}T_{EE}^{-1}T_{EX})n_X$$
 (4.30)

Using this formulation, the number of equations we need to solve is reduced to the number of ground state sublevels. This can now be easily done through computation.

We now need to compute the relative population of the upper states and the ground states. We can do this by stating:

$$\sum_{j=1}^{N_x} B_{ji} \rho_{\nu} = \sum_{j=1}^{N_x} A_{ij} x_i$$
(4.31)

with  $N_X$  being the number of considered levels in the ground electronic state  $X^2\Sigma_g^+$ , and *i* and *j* corresponding to the *i*<sup>th</sup> and *j*<sup>th</sup> levels. From this equation it is possible to compute the relative populations  $x_i$  of the levels belonging to the upper electronic state:

$$x_{i} = \sum_{j=1}^{N_{X}} B_{ji} \rho_{\nu} \sum_{j=1}^{N_{X}} A_{ij}$$
(4.32)

The last step is to compute the final spectrum. We obtain the wavelengths by calculating  $\Delta E = h\nu$  and adjusting for the comet's motion with respect to the earth:

$$\lambda = \frac{1 \times 10^8}{E_i - E_j} \frac{1}{n_\lambda} \frac{1 + \Delta}{c}$$
(4.33)

The luminosity per molecule of a given emission line, also called fluorescence efficiency or 'g factor' is given by:

$$I = x_i A_{ij} \tag{4.34}$$

with  $x_i$  being the relative population of the upper level *i* and  $A_{ij}$  the Einstein coefficient corresponding to the transition from the level *i* to the level *j*.

This provides a 'stem' model in which each line is reduced to a wavelength and its intensity. We now convolve this spectrum by the instrument response, in this case a Gaussian, with a FWHM of 0.06Å. This constitutes our model of the  $N_2^+$  spectrum, as shown in Fig 4.5. While visually it seems like a good fit, this was due to liberal scaling and a naïve and hopeful author. In reality, while the wavelengths are accurate, the intensities are not. We proceeded to add in the effect of the A levels, to no avail. These added an imperceptible variation to the final spectrum. This method does not produce an accurate modeling of the  $N_2^+$  spectrum we observe.

The issue lies with the fact that we have modeled the N<sub>2</sub><sup>+</sup> fluorescence equilibrium spectrum: However, this model functions *only* for a species at equilibrium. N<sub>2</sub><sup>+</sup> having no permanent dipole moment the pure rotational transitions are forbidden, or have a very low probability through quadrupolar transitions (not taken into account in our model), thus excited ions cannot deexcite and need longer absorptionemission cycles between the  $X^2\Sigma_g^+$  and  $B^2\Sigma_u^+$  states to reach their equilibrium. Such cycles imply a time in the order of  $10^4$ s. For the N<sub>2</sub><sup>+</sup> ions inside the coma at the he-



**Figure 4.5** – Final convolved  $N_2^+$  model. While we have access to the full spectrum all the way up to  $4.7 \times 10^6$ Å, Here, we show only the portion of the spectrum obtained from C/2016 R2. We do not have access to the  $N_2^+$  (0,1) band as it is beyond the scope of this observation, with the bandhead at 4729 Å. The intensities of the bands are manually scaled to better see the fit as they do not accurately represent observation.

liocentric distances of C/2016 R2 (>2.7 au) this requires a few thousand kilometers. The spectrum obtained on the nucleus being significantly different to the one obtained at the end of the slit (See Fig. 4.6) it is evident that fluorescence equilibrium is not reached in our spectra. Unlike most of the diatomic radicals present in cometary coma (such as OH or CN), we need to take into account the evolution of relative population with time in order to compute the  $N_2^+$  fluorescence spectrum. While the locations of the wavelengths are correct, the intensity is not realistic. In order to create a proper model, we must employ a different method.

#### 4.3.4 Monte-Carlo Method

We use the method described by Rousselot et al. (1994, 2000). It is a probability simulation starting from an initial large relative population (~  $10^5$  molecules), described, for example, by a Boltzmann distribution at a temperature representative of the kinetic coma temperature. We then follow the behavior of a given molecule (or ion in our case) step by step as it absorbs and emits photons between its different energy levels. The exact time of absorption and emission is computed via repeated random sampling using the traditional Monte Carlo method.



**Figure 4.6** – Comparison in red of the observed average spectrum of C/2016 R2 extracted on the nucleus (corresponding to about 250 km on either side of the nucleus) and in blue at the extremity of the slit (cometocentric distance ~6000 km). The R branch of the (0, 0) band starts at 3909.7 Å and is degraded to the blue side (i.e., lines appear at shorter wavelengths for increasing values of quantum number N), and the P branch starts at 3910.9 Åand returns at the bandhead at 3914.3 Å to shorter wavelengths. The two spectra are different.

The initial population distribution is in the v = 0 vibrational level of the ground electronic state and follows a Boltzmann distribution such that:

$$x_i = \frac{g_i}{Q} e^{-\frac{E_i}{kT}},\tag{4.35}$$

with *T* the Boltzmann temperature,  $E_i$  the energy value for the level *i*,  $g_i$  the statistical weight of the considered level. *Q* is the partition function, or the statistical properties of the system in thermodynamic equilibrium, given by:

$$Q = \sum_{i} g_i e^{-\frac{E_i}{kT}}.$$
(4.36)

with the statistical weight  $g_i$  is given in Section 4.3.

We use a Boltzmann temperature close to the kinetic temperature of the gas in the inner coma of 80 K. This parameter has little influence on the final result: The range  $\sim 30$  to  $\sim 200$  K provides similar results for times in the order of a few thousands of seconds.

Our Monte-Carlo modeling starts with a Boltzmann distribution for the lower states  $(X^2\Sigma_g^+)$  and provides the relative populations of the levels belonging to this state. That is to say, at a time t = 0:

1. All the molecules are distributed so that each i level has an  $x_i$  population following eq. 4.35; Each level has a given number of possible transitions following the selection rules. These transitions have a probability regulated by



**Figure 4.7** – Comparison of the observed spectra of C/2016 R2 obtained at the ends of the slit (nucleocentric distance ~ 6000 km, averaged at 4 different positions at both extremities of the slit) with our model. The upper and lower parts correspond to two different wavelengths intervals. Some CN emission lines, not reproduced by the model, appear in the region around 3880 Å. The observational data is shown in blue while the model appears in red. Wavelengths are given by the vertical bars appearing above the spectra. The R branch is degraded to the blue while the P branch is first degraded to the red and returns after the bandhead to the bluer wavelengths. The first three  ${}^PQ_{12}$  and  ${}^RQ_{21}$  satellite lines are also plotted above (vertical black bars at about 3910 Å), their intensity being negligible compared to the P or R lines for higher values of N. This figure is published in Rousselot et al. (2022).

their Einstein coefficients  $A_{v'J' \rightarrow v''J''}$  and  $B_{v''J'' \rightarrow v'J\rho_{\nu}}$ ; Each of these transitions has an associated lifetime  $\tau_i = 1/C_i$  in s, where  $C_i$  can be either  $B_{ji}\rho_{\nu}$  or  $A_{ij}$ .

- 2. For each transition, we generate a random time  $t_i$  so that  $t_i = -\tau_i \ln R_i$  with  $0 < R_i < 1$ .  $R_i$  is random for each transition. We choose the smallest  $t_i$  and add it to the simulation time, so that we are now at  $t = t_0 + t_i$ .
- 3. If this new  $t > t_f$ , where  $t_f$  the time we chose to inspect the population, the simulation ends, and we add 1 to the initial population; else, the simulation continues until it reaches  $t_f$ , but from each successive level *i* the particle transitions to.

This process is then repeated as long as necessary. From these relative populations it is easy to compute the relative populations of the upper levels by writing:

$$\sum_{j=1}^{N_X} B_{ji} \rho_{\nu} = \sum_{j=1}^{N_X} A_{ij} x_i$$
(4.37)

with  $N_X$  being the number of considered levels in the ground electronic state  $X^2\Sigma_g^+$ , *i* and *j* corresponding to the *i*<sup>th</sup> and *j*<sup>th</sup> levels. We considered the first three vibrational levels (v = 0, 1, 2) both the  $X^2\Sigma_g^+$  and  $B^2\Sigma_u^+$ , each of them with all the levels from N = 0 to 40.

Because our observational spectra are in units of erg s<sup>-1</sup> cm<sup>-2</sup> Å<sup>-1</sup>we must multiply the intensity by  $h\nu$  so as to obtain units of energy. The observed intensity is then the product of this luminosity per molecule by the number of molecules along the line of sight. The resulting model is shown in figure 4.7.

## 4.4 New Fluorescence Efficiencies

So far the only g factors published for  $N_2^+$  were computed by Lutz et al. (1993). Their computation corresponds to an approximation for the whole band. Their value for the (0,0) band is slightly higher than our computed value ( $g(0,0) = 7 \times 10^{-2}$  photon s<sup>-1</sup> ion<sup>-1</sup> for 1 au). Our method of computation, that takes into account all the lines, one by one, and confronted to an observational spectrum, is more accurate. A good test is to compute the ratio of the fluorescence efficiencies of the (1,1) band to the (0,0) band. From the fluorescence efficiencies published by (Lutz et al., 1993) this ratio is  $5.1 \times 10^{-3}/7.0 \times 10^{-2} = 0.0728$ . From our results it is close to 0.15 (either by using data for 1 au and 0 km s<sup>-1</sup> or by using the data computed for C/2016 R2), i.e. twice the ratio computed by (Lutz et al., 1993). Fig. 4.7 clearly shows that the ratio computed in this work is very close to the observed spectrum, a ratio twice

**Table 4.3** – Fluorescence efficiency (g factor), in photons  $s^{-1}$  ion<sup>-1</sup>, computed for comet C/2016 R2 at the time of observations (heliocentric distance of 2.76 au and heliocentric velocity of -5.99 km s<sup>-1</sup>) and for any comet at 1 au and an heliocentric velocity equal to 0.0 km s<sup>-1</sup>) (Rousselot et al., 2022).

band (v',v")	g (for C/2016 R2)	g (computed for 1 au)
(0,0)	$6.26\times10^{-3}$	$4.90\times10^{-2}$
(0,0)[3885.5–3915 Å]]	$5.41 \times 10^{-3}$	
(0,1)	$2.05\times10^{-3}$	$1.59\times10^{-2}$
(0,2)	$4.22\times10^{-4}$	$3.31 \times 10^{-3}$
(1,0)	$1.43 \times 10^{-3}$	$1.08 \times 10^{-2}$
(1,1)	$9.65 \times 10^{-4}$	$7.24 \times 10^{-3}$
(1,2)	$1.02 \times 10^{-3}$	$7.67 \times 10^{-3}$
(2,0)	$1.67  imes 10^{-4}$	$1.24\times10^{-3}$
(2,1)	$1.39 \times 10^{-3}$	$1.04\times10^{-2}$
(2,2)	$1.58 \times 10^{-4}$	$1.18 \times 10^{-3}$

smaller being, obviously, far from the observed intensity ratio. The resulting values computed for C/2016 R2 at the time of our observations are presented in Table 4.3. The same values at this heliocentric distance and an heliocentric velocity equal to  $0 \text{ km.s}^{-1}$  for all the bands taken into account by our model are presented in Table 4.4.

We must now update the values of the N<sub>2</sub>/CO ratio of comets, since they were based on the *g* factor from Lutz et al. (1993). With the newly calculated *g* of  $g = 4.90 \times 10^{-2}$  photons.s<sup>-1</sup>.molecule<sup>-1</sup> for the entire band, prior measurements of the N<sub>2</sub><sup>+</sup> production rate are recalculated and shown in table 4.5.

$\dot{r}_h$ (km s $^{-1}$ )	(0,0)	(1,1)
-20	$4.64 \times 10^{-2}$	$6.98 \times 10^{-3}$
-18	$4.60\times 10^{-2}$	$6.66 \times 10^{-3}$
-16	$4.76\times 10^{-2}$	$6.88 \times 10^{-3}$
-14	$4.79\times10^{-2}$	$7.11 \times 10^{-3}$
-12	$4.76\times10^{-2}$	$7.24 \times 10^{-3}$
-10	$4.64\times10^{-2}$	$7.31 \times 10^{-3}$
-8	$4.62\times10^{-2}$	$7.41 \times 10^{-3}$
-6	$4.72\times 10^{-2}$	$7.60  imes 10^{-3}$
-4	$4.77\times10^{-2}$	$7.85  imes 10^{-3}$
-2	$4.84\times10^{-2}$	$7.39  imes 10^{-3}$
0	$4.90\times10^{-2}$	$7.24 \times 10^{-3}$
+2	$4.95\times10^{-2}$	$7.27 \times 10^{-3}$
+4	$4.97\times10^{-2}$	$7.40 \times 10^{-3}$
+6	$4.93\times10^{-2}$	$7.57 \times 10^{-3}$
+8	$4.88\times10^{-2}$	$7.67 \times 10^{-3}$
+10	$4.79\times10^{-2}$	$7.65  imes 10^{-3}$
+12	$4.73\times10^{-2}$	$7.59  imes 10^{-3}$
+14	$4.68\times10^{-2}$	$7.53 \times 10^{-3}$
+16	$4.63\times10^{-2}$	$7.56 \times 10^{-3}$
+18	$4.62\times 10^{-2}$	$7.67 \times 10^{-3}$
+20	$4.62\times 10^{-2}$	$7.77 \times 10^{-3}$

**Table 4.4** – Fluorescence efficiency (g factor), in photons s<sup>-1</sup> ion<sup>-1</sup>, computed for 1 au and different heliocentric velocities  $\dot{r}_h$  (Rousselot et al., 2022).

Comet Designation	Old N <sub>2</sub> /CO	Updated N <sub>2</sub> /CO	Reference
C/1908 R1	≥0.06	0.085	Cochran et al. (2000)
C/1940 R2	≥0.04	0.057	Cochran et al. (2000)
C/1947 S1	0.05-0.09	0.071-0.125	Cochran et al. (2000)
C/1956 R1	>0.09	0.125	Cochran et al. (2000)
C/1957 R1	0.02	0.028	Cochran et al. (2000)
C/1961 R1	0.02-0.03	0.028-0.043	Cochran et al. (2000)
C/1969 T1	≤0.03	0.043	Cochran et al. (2000)
C/1969 Y1	0.03	0.043	Cochran et al. (2000)
C/1973 E1	0.07	0.100	Cochran et al. (2000)
C/1986 P1	0.07	0.100	Cochran et al. (2000)
C/1987 P1	0.02	0.028	Lutz et al. (1993)
C/2001 Q4	0.03	0.043	Feldman (2015)
C/2002 VQ94	0.06	0.085	Korsun et al. (2014)
C/2016 R2	0.06	0.085	Opitom et al. (2019)
1P	0.005	0.007	Wyckoff et al. (1991)
29P	0.01	0.014	Ivanova et al. (2016)
67P	0.03	0.043	Rubin et al. (2020)

**Table 4.5** – Orbital elements along with  $H_2O/CO$ ,  $N_2/CO$  abundance ratios of comets with peculiar  $N_2$ - rich and/or  $H_2O$ -poor compositions.

# 5 Calculating the N<sub>2</sub><sup>+</sup> Production Rate

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WE CAN NOW IDENTIFY the  $N_2^+$  emission lines in the spectra of C/2016 R2 so as to determine the quantity of  $N_2^+$  being produced. We do this through the Haser model, used to determine the number of molecules responsible for the intensity of the observed emission. This will give us new scale lengths determining the lifetime of the  $N_2$  molecules and  $N_2^+$  ions in the coma of C/2016 R2, which can be used for future comets presenting high quantities of  $N_2^+$ . This approach allows us to determine how much  $N_2^+$ , thus  $N_2$ , is being produced by the active surface of the comet's nucleus.

This chapter is the basis of Anderson et al. 2022.

# 5.1 Identifying the N<sub>2</sub><sup>+</sup> spectral lines

Using the new  $N_2^+$  model described in Chapter 4, shown in Fig. 5.1, we are now able to identify  $N_2^+$  lines in the spectrum of C/2016 R2. The  $N_2^+$  lines are then identified using the fluorescence model and summed for each pixel of the spectrometer using the synthetic model as a 'mask': for wavelengths Where the intensity of the  $N_2^+$  model is null, we ignore the intensity of the comet's spectrum. For each wavelength for which the  $N_2^+$  spectra is non-null, we have identified a potential match. We use the High-Resolution Spectral Atlas of list of 12,219 identified and 4,055 unidentified spectral lines in 122P/de Vico (Cochran & Cochran, 2002) in order to identify which lines belong to other identified species. In some cases, there is overlap of multiple species, which both could produce the observed intensity. In this case, the intensity is not measured, in order to ensure no contamination. We tested whether taking a fraction of this flux that was reflective of the contribution from each species, but the result was negligible as this was only a minor contribution overall (< 5% of the total flux). We also limit the identification process to the 3885.5 Å to 3915.0 Å interval in order to extract only the lines of the (0,0) band and further avoid contamination by the CN emission lines as well as the  $N_2^+$  (1,1) band. The



**Figure 5.1** – Spectrum of C2016/R2 on 14/02, near the nucleus, showing the (0,0) band of  $N_2^+$  at 3914 Å. This same process of identification is repeated for every day and every spectrum along the slit. Here we also see how the  $N_2^+$  (0,0) band is mixed with (1,1) band below 3885 Åand, in some cases the lines are superimposed. In order to avoid contamination from these lines, we only searched for  $N_2^+$  above 3885 Å. The *g* factor was also computed separately for the lines of the (0,0) band above 3885 Å.



**Figure 5.2** – Sum of  $N_2^+$  ray intensity for each spectra along the slit for each day of observation in units of flux in erg.s<sup>-1</sup>.cm<sup>-2</sup>/Å. The nights of 15/02 and 16/02 have been re-centered on the nucleus.

identified lines are separated from the spectra and integrated over the wavelength in order to remove the wavelength dependency for the units of flux. The final sum of the intensity of these  $N_2^+$  lines represent the total flux per pixel along the spectroscopic slit. For each day of observation 11, 13, and 14 Feb, we have 30 pixels, centered on the nucleus.

We average the flux for each pixel from the observations of these three days. The resulting averaged intensity profile is shown in black in figure 5.2. We observe that the intensities calculated from the observations of 15/02 and 16/02 are noisier than those of 11/02, 13/02 and 14/02, as well as off center. This is due to the different settings used on the last two days, as well as the shorter exposure time and limiting atmospheric conditions. The setting used for these first three dates being of better quality than that of the last two, an average of the intensities is therefore made with the spectra of 11/02, 13/02, and 14/02. This average almost completely aligns with the observations of 11/02, which were made under clear sky conditions, and was used for the study of Opitom et al. (2019). The total flux measured for N<sub>2</sub><sup>+</sup> over the entire spectrograph for 11, 13, and 14 February was 1.0, 0.8, and 1.2 ×10<sup>-14</sup> erg.s<sup>-1</sup>.cm<sup>-2</sup>.

This profile is essential to determining the production rate of  $N_2^+$  by the comet nucleus, as its shape is influenced by the quantity and activity of the  $N_2$  molecules



**Figure 5.3** – Line of sight and variables used for integration. The origin of our coordinates is the location at which *R* is minimum.

as they are photoionized by UV solar radiation. The most effective way to analyze this profile is by applying the Haser model.

# 5.2 New Scale Lengths for N<sub>2</sub><sup>+</sup>

#### 5.2.1 The Haser Model

In order to determine the production rate of  $N_2^+$  in C/2016 R2, we first need to estimate the true number of molecules that were measured during the observations. We have at our disposal a reliable model known as the Haser model (Haser, 1957), which has been used for decades to reliably describe the density distribution of cometary comae. More specifically, it allows us to find an analytical solution to the column density of parent- and daughter-molecules in the coma along the line of sight. While the model is theoretical, it serves as a sound estimate of this density and provides a basis for comparison with other comets.

First, we suppose that the medium is optically thin. In this situation, the intensity of the coma observed at a distance  $\rho$  from the nucleus is proportional to the number of molecules along the line of sight that produce it. Thus, if we can determine what proportion of that intensity is due to a specific molecule (or ion) then we can infer how much of said species is present in the coma at that specific cometocentric distance.

In order for this model to be properly applied to our observation, certain hypothesis need to be made:

- The comet's nucleus is spherical, with a radius of  $r_0$ . As the nucleus of C/2016 R2 is already assumed to be nearly isotropic (Wierzchos & Womack, 2018), this hypothesis should fit;
- The parent-molecules directly produced by the surface of the nucleus are expelled isotropically with a radial velocity *v*<sub>p</sub>;
- The parent-molecules are then disintegrated in a one-step process by photodissociation with the solar radiation following the law n = n<sub>0</sub>e<sup>-t/τ<sub>p</sub></sup> to form daughter species, with n<sub>0</sub> the number of parent-molecules at t = 0 and τ<sub>p</sub> the average lifetime of a parent molecule. Each daughter species corresponds to only one parent molecule;
- The daughter-molecules produced from the photo-dissociation of the parentmolecules are ejected radially with a velocity of v<sub>d</sub> from the nucleus. This is another simplification of what happens in reality, as there is no particular reason for the ejection to be perfectly radial after the photodissociation;
- On top of this, we also suppose that 100% of parent-molecules are being photodissociated into  $N_2^+$ , even if it is less in reality.

At a distance *R* from the nucleus, the molecular density n(R) (in molecules.cm<sup>-3</sup>) is given by:

$$n(R) = n(r_0) \cdot \left(\frac{r_0}{R}\right)^2 \cdot e^{-\frac{t-t_0}{\tau_p}}$$
(5.1)

where  $n(r_0)$  is the molecular density at the surface of the nucleus  $r_0$ . We have the dilution factor  $1/R^2$  and the disintegration factor  $e^{-\frac{t-t_0}{\tau_p}}$ . When we substitute  $t = R/v_p$ , we have:

$$n(R) = n(r_0) \cdot \left(\frac{r_0}{R}\right)^2 \cdot e^{-\frac{R-r_0}{v_p \tau_p}}$$
(5.2)

so long as  $R \ge r_0$ .

In the case of fluorescence as the emission mechanism, n(R) can be interpreted as the number of quanta emitted per unit of time and volume at a specific wavelength. This is particularly useful for us, as N<sub>2</sub><sup>+</sup> is produced through the fluorescence of the first negative group (B<sup>2</sup> $\Sigma_u^+$  - X<sup>2</sup> $\Sigma_g^+$ ). The photo-dissociation lifetime,  $\tau_p$ , is an important factor in the behavior of the parent and daughter species. We use the relationship  $l_{p,d} = \tau_{p,d}v_{p,d}$  which determines the scale length of the parent or daughter species, respectively. If we call  $Q = n(r_0) \cdot 4\pi r_0^2 v_p$  the production rate (in molecules.s<sup>-1</sup>) of a given parent molecule and n(R) the volume density of the parent molecules at distance R from the nucleus (of radius  $r_0$ ), we have:

$$n(R) = \frac{Q}{4\pi v_p R^2} \cdot e^{-\frac{R-r_0}{l_p}}$$
(5.3)

As we are interested in the column density, therefore in the number of integrated molecules on the line of sight of the spectrometer, it is necessary to integrate along the line of sight the different values of n(r) to get  $N(\rho)$ .

$$N(\rho) = \int_{-\infty}^{+\infty} n(R) \mathrm{d}z \tag{5.4}$$

where *z* is the coordinate of a point situated on the line of sight, at a distance R from the nucleus (see Fig. 5.3). In order to simplify this integration, we use the angle  $\alpha$  since  $\rho = R \cos{(\alpha)}$ . This gives us:

$$n(\alpha) = \frac{Q}{4\pi v_p \rho^2} e^{\frac{r_0}{l_p}} \cos^2(\alpha) \cdot e^{\frac{-\rho}{l_p \cos \alpha}}$$
(5.5)

In addition, we have the relationship  $dl = dz \cos(\alpha)$  and  $\tan(d\alpha) = dl/R \sim d\alpha$ since  $d\alpha$  is very small. As a result,  $dl = Rd\alpha$  and  $dz = \rho d\alpha / \cos^2(\alpha)$ . This allows us to do a variable change:

$$N(\rho) = e^{\frac{r_0}{l_p}} \cdot \frac{Q}{4\pi v_p \rho^2} \int_{-\pi/2}^{+\pi/2} \cos^2(\alpha) e^{-\frac{\rho}{l_p \cos \alpha}} \frac{\rho}{\cos^2 \alpha} d\alpha$$
(5.6)

Since this function is even, we can simplify it further:

$$N(\rho) = e^{\frac{r_0}{l_p}} \cdot \frac{Q}{2\pi v_p \rho} \int_0^{+\pi/2} e^{\frac{-\rho}{l_p \cos \alpha}} d\alpha$$
(5.7)

This gives us a fair assessment of the number of parent molecules at a chosen distance from the nucleus of the comet. However, is  $N_2^+$  a daughter species: we need to take into account the photo-dissociation of the parent molecule at each cometo-centric distance in order to determine the quantity of molecules being produced by successive disintegrations of the parent molecule.

The total number of parent molecules crossing a sphere of radius R is given by:

$$n(R) \cdot 4\pi v_p R^2 = Q \cdot e^{-\frac{R-r_0}{l_p}}$$
 (5.8)

from which we can determine the formation rate of the daughter species, the products of this disintegration:

$$-d[n(R)4\pi v_p R^2]\frac{1}{dR} = \frac{Q}{l_p} e^{-\frac{R-r_0}{l_p}}$$
(5.9)

When the molecules produced at a distance  $r_0$  from the nucleus reach the distance R, their number is reduced by a factor of  $e^{\frac{R-r_0}{v_d\tau_d}} = e^{\frac{R-r_0}{l_d}}$ . If we position ourselves at a radius  $R_1$ , where  $R_1$  is greater than R, we can determine that the total number of daughter particles arriving per second is:

$$\frac{Q}{l_p} e^{-\frac{r_0}{l_p}} \int_{r_0}^{R_1} e^{-\frac{R}{l_p}} e^{-\frac{R-r_0}{l_d}} dR$$
(5.10)

Knowing that the daughter species expand outwards at a rate of  $v_d$  km.s<sup>-1</sup>, the number of particles arriving per cm<sup>2</sup> at a distance  $R_1$  is therefore:

$$n(R_1)\pi R_1^2 = \frac{Q}{l_p} e^{-\frac{R-r_0}{l_p}} \int_{r_0}^{R_1} e^{-\frac{R-r_0}{l_d}} dR$$
(5.11)

We integrate this equation and find:

$$n(R_1) = \frac{Q}{4\pi v_d R_1^2} \frac{l_d}{l_p - l_d} \left( e^{\frac{r_0 - R_1}{l_p}} - e^{\frac{r_0 - R_1}{l_d}} \right)$$
(5.12)

This density will always be positive  $(n(R_1) > 0)$  so long as the scale length of the daughter species  $l_d \neq l_p$ . We'll integrate along the line of sight in order to obtain the number of molecules present at each successive distance from the nucleus.

From here, to obtain the distribution of observable intensity, we use the projection of the radial distribution onto the celestial sphere along the line of sight using the same method as for the parent molecule (See equations 5.3-5.7).

$$N(\rho) = \frac{Q}{2\pi v_d \rho} \frac{l_d}{l_p - l_d} \int_0^{+\pi/2} e^{\frac{1}{l_p}(r_0 - \frac{\rho}{\cos(\alpha)})} - e^{\frac{1}{l_d}(r_0 - \frac{\rho}{\cos(\alpha)})} d\alpha$$
(5.13)

This integration is the basis of our numerical model. It can be applied to any known disintegration process. Once we have the associated molecular distribution profile, we can compare with the intensity distribution obtained by observation of our comet's spectra in order to determine the relevant physical parameters. Since the flux is proportional to the column density, we can fit the parent and daughter scale lengths without yet knowing Q.

Other models also exist, such as the Festou Vectorial model (Festou, 1981), which, while taking into account the collisions in the inner coma which can produce a

non- radial motion of the molecules, has more free parameters, which are usually poorly determined and may be a major source of uncertainty in the determination of the gas-production rates. The Haser model is still a prominent model used by the majority of cometary spectroscopists. In this work, we decided to use this model to compute the production rates in order to compare our results with others.

#### 5.2.2 Applying the model to the CN molecule

Since the N<sub>2</sub><sup>+</sup> ion had not been identified in comets before we do not have an estimate of the magnitude of the scale lengths of parent- and daughter-molecules of this species. However, we need to know if the application of the Haser model is possible on the observed spectra before we apply this method of identification to N<sub>2</sub><sup>+</sup>. There is the distinct possibility that there is too much dust present in the coma for the dinitrogen to be properly quantified, though our main challenge is that most Haser model fits are done over large cometocentric ranges,  $> 10^4$  km. In order to determine if the spectrum is clean enough to be useful, we will test the Haser model on an already known molecule: that of CN, whose lines have already been identified in the coma of C/2016 R2.

One of the unique features of C/2016 R2 is the lack of strong CN band at 3880 Å, which may account for slight differences between our findings and the literature.

The CN lines are first identified and summed along the spectrometer in the same way as with  $N_2^+$  (see sec. 5.1). This allows us to draw an intensity profile on either side of the comet's nucleus. The resulting intensity profiles are shown for all five days in fig. 5.5. Once again, the setting used for these first three dates being of better quality than that of the last two, we will focus on the observations of 11, 13, and 14 February, as they were made under clear sky conditions.

Unfortunately, the N<sub>2</sub><sup>+</sup> band partially overlaps with the CN(0,0) band. If in the instance where a specific spectral line could be interpreted as one or the other, I chose not to take it for either. As with N<sub>2</sub><sup>+</sup>, I attempted to find ways to take only a small percentage of flux pertaining only to the relative contribution of CN. This only had a minimal effect on the final intensity. The total flux measured for N<sub>2</sub><sup>+</sup> over the entire spectrograph for 11, 13, and 14 February was 2.31, 2.01, and  $2.01 \times 10^{-15}$  erg.s<sup>-1</sup>.cm<sup>-2</sup>, respectively. The total flux measured for CN over the entire spectrograph averaged for the three days was  $F_{\text{TOT}}(\text{CN} = (2.1 \pm 0.1) \times 10^{15}$ erg.s<sup>-1</sup>.cm<sup>-2</sup>.Å<sup>-1</sup>. The flux intensities are then averaged over their cometocentric distances so as to allow for a proper fit of the Haser model. The final intensity profile is a 1D profile starting from the nucleus of the comet and sweeping outwards along the coma ending at a distance of  $R = 6.5 \times 10^3$  km.



**Figure 5.4** – Spectra of C2016/R2 on 14/02, near the nucleus, showing the (0,0) band of CN at 3883 Å. This same process of identification is repeated for every day and every spectrum along the slit.



**Figure 5.5** – Summed Flux of the identified CN lines for the night of February 11, 13, 14, 15, and 16. We move forward using the average of February 11, 13, and 14.

**Table 5.1** – Parent and daughter Haser scale lengths  $l_p$  and  $l_d$  at 1 au for the CN molecule found in literature, collected by Rauer, H. et al. (2003). This gives us an upper and lower limit of what to expect to find in C/2016 R2. The values of the daughter scale lengths are not proportional to the parent scale lengths. These are strictly valid only in the range  $r_h \ge 3$  au.

Reference	$l_p$ (km)	$l_d$ (km)
A'Hearn et al. (1995)	$1.3 \times 10^{4}$	$2.2 \times 10^{5}$
Cochran et al. (1992)	$1.4 \times 10^{4}$	$3.0 \times 10^{5}$
Randall (1992)	$1.5 \times 10^4$	$1.9 \times 10^{5}$
Wyckoff et al. (1998)	$1.6 \times 10^{4}$	$3.3 \times 10^{5}$
Newburn & Spinrad (1989)	$1.8 \times 10^{4}$	$4.2 \times 10^{5}$
Womack et al. (1994)	$2.5 \times 10^4$	$1.9 \times 10^{5}$
Fink et al. (1991)	$2.8 \times 10^4$	$3.2 \times 10^5$

The Haser model can now be fitted to our intensity profile. We could convert the scale to column density, but since the number of molecules is proportional to the study, this does not change the fit of the model.

The parameters we seek to determine are the scale lengths of the parent-molecule and the daughter-molecule producing this intensity profile,  $l_p$  and  $l_d$ , respectively. CN is the daughter molecule produced by photo-dissociation of HCN, so we integrate the daughter Haser equation (eq. 5.13). These values are known in literature, but are in no way certain as of today: multiple pairs of parent and daughter species scale lengths have been calculated and vary from study to study, and even from day to day of observation (See Table 5.1). They do give us a good idea of the order of magnitude for our starting parameters. In order to compare them, these parameters are brought to their value at 1 au. They scale as  $r_h^2$ . This will also allow us to compare our results with others who have used the Haser model, as similar values are used throughout.

These parameters are linked to the lifetimes of the molecules by the simple relation  $l = \tau v$ . These values were given in A'Hearn et al. (1995) for previous TRAPPIST data analysis and this homogeneity allows us to compare our results with theirs, as they provide the largest sample analyzed and published so far.

The actual size of the radius of the nucleus, as well as its shape, are unknown; a reasonable approximation must be used. The following results are based on calculations using a 5 km radius. The effects of nucleus size on the resulting scale lengths will be discussed in section 5.4.2.

For each parent-daughter scale length pair, we create a Haser profile spanning 0-6500 km from the nucleus. We also must take into consideration the modulation



**Figure 5.6** – Contours showing the results of the  $\chi^2$  test to find the optimal values of the parent and daughter scale lengths. The white lines indicate the value at which minimum  $\chi^2$  was obtained (values given in  $10^{-16}$  erg.s<sup>-1</sup>.cm<sup>-2</sup>). There are more than one possible solutions to our fit. An identical optimal fit is obtained for parent-daughter pairs in the black zone.



**Figure 5.7** – Best fit of the Haser model (blue) to the observed CN intensity profile of the three night average (black). We find the best scale lengths to be  $l_p = 1.3 \times 10^4$  km and  $l_d = 2.8 \times 10^5$  km.

of the observed spectra as it passed through the atmosphere, as we were using ground based telescopes to obtain them. The theoretical intensity profile must be convoluted by the seeing value in order to be properly modeled. Usually this plays little because the profile is obtained over several tens of arc seconds. In the case of an 8" slit, or 4" for our cometocentric model, this effect will be small, but no less significant. For the three observational nights we have chosen to use, the seeing was 0.95", 1.1", and 0.94". We therefore must convolve the obtained Haser profile by a Gaussian of 1" FWHM.

Once the profile is calculated and convolved, it is then scaled to the observed data that we are attempting to fit before we can verify this fit. The scaling can be done one of two ways: by normalizing to a certain point (for example, r = 300km) or by using python's integrated curvefit function. This curvefit function takes as input parameters both scale lengths and the Haser model equation and attempts to find the ideal scalar for the theoretical data to match the observed data. Since the convolution function is applied outside of the coded Haser model function, the curve can only be fit outside of the scope of the convolution's influence and hence cannot be fit optimally across the whole curve. By choosing a scaling parameter first by normalizing the model to a point of the observed data, we can already encourage the curvefit function to search for a value near it, and ultimately the fit is good.

A  $\chi^2$  test is then implemented in order to estimate the quality of each fit by comparing the resulting curve made with each pair of parent-daughter species scale lengths to the averaged profile obtained by summing the CN intensity lines:

$$\chi^2 = \sum \frac{(O_i - E_i)^2}{E_i}$$
(5.14)

where  $O_i$  is the observed value, i.e. our observed intensity profile, and  $E_i$  the expected value, or our resultant Haser fit. A smaller  $\chi^2$  value represents a better fit.

We fix these parameters and explore a large phase space determined from the literature. We explore  $l_p$  from  $l_p = 1 \times 10^3$  to  $l_p = 1 \times 10^5$  by increments of  $1 \times 10^3$ , and  $l_d$  from  $l_p = 1 \times 10^4$  to  $l_p = 1 \times 10^6$  by increments of  $1 \times 10^4$ . We then refine this phase space as we approach the ideal combination, as seen in fig. 5.6. Here, we see the best pairs of parent- and daughter- scale lengths are located in this narrow black band. While we have a 'best' pair, there is no unique solution for our Haser model scale lengths. Instead, we get a 'family' of solutions which fit the observed intensity profile. Multiple combinations result in a similarly good fit and could equally be the best pair.

The smallest  $\chi^2$  had for result a scale length of HCN of  $l_p = 1.3 \times 10^4$  km while the scale length of CN, the daughter-molecule, was determined to be  $l_d = 2.8 \times 10^5$  km.

**Table 5.2** – CN parent- and daughter- scale lengths with similar quality fit for our Haser model. This 'family' of scale length pairs make up our result.

$l_p$ (km)	$l_d$ (km)	$\chi^2 \times 10^{-16}$
$1.2 \times 10^4$	$4.8 \ge 10^5$	5.703
$1.3 \ge 10^4$	$2.8 \times 10^5$	5.692
$1.4 \ge 10^4$	$1.8 \ge 10^5$	5.694
$1.5 \ge 10^4$	$1.2 \ge 10^5$	5.693
1.6 x 10 <sup>4</sup>	$1.0 \ge 10^5$	5.693

Both values have been scaled to 1 au using the  $r_h^2$  law. Equally likely pairs are presented in table 5.2.

Our best fitting scale length pair is incredibly similar to those calculated by A'Hearn et al. (1995) who found  $l_p = 1.3 \times 10^4$  km and  $l_d = 2.2 \times 10^5$  km for comet 1P/Halley at or near perihelion. As seen in figure 5.8, when compared to other scale length pairs from literature, our measurement both fits the observation best while comparing seamlessly with the others.



**Figure 5.8** – Our best fit of the Haser model (purple) on the observed flux of CN (black) with scale lengths from literature. The observed CN flux is from 11-13-14 Feb, averaged again over cometocentric distance in dashed lines, with the left and right arms of the flux quantities in solid lines. The scale lengths given in literature fit our observations well.

$l_p$ (km)	$l_d$ (km)	$\chi^2 \times 10^{-16}$
$1.8 \ge 10^{6}$	$1.2 \ge 10^{6}$	5.693
$2.4 \ge 10^6$	$4.6 \ge 10^6$	5.693
$2.8 \ge 10^6$	$3.8 \times 10^{6}$	3.693
$3.0 \ge 10^6$	$3.4 \times 10^{6}$	5.693
$3.6 \ge 10^6$	$3.4 \times 10^{6}$	5.693
$4.2 \ge 10^{6}$	$2.6 \ge 10^6$	5.693

**Table 5.3** – Parent- and daughter- scale lengths with similar quality fit for our Haser model. This 'family' of scale length pairs make up our result.

# 5.2.3 Application to the N<sub>2</sub><sup>+</sup> ion

 $N_2^+$  is produced in the coma of C/2016 R2 via photon and electron impact ionization of  $N_2$ . Unlike CN, no benchmark has been made for  $N_2^+$  scale lengths in comets. There is no literature to compare these values to, but since our results with CN were promising, it is safe to apply our methods to  $N_2^+$ .

One of the limitations of the Haser model for computing the profile of a ionic species like  $N_2^+$  is that it considers neutral products (like OH,  $C_2$ , CN...) not affected by electric forces due to the solar wind particles (or any other ionic species present in the coma). This work being restricted, nevertheless, to the inner coma (projected distance inferior to 8000 km), this limit effects of electric forces on the dynamic of this ion and the physical hypothesis of the Haser model are still valid. (Raghuram



**Figure 5.9** – Summed flux of the identified  $N_2^+$  lines for February 11,13, and 14.



**Figure 5.10** – Contours of our results of the  $\chi^2$  test to find the optimal values of the parent and daughter scale lengths. There are more than one possible solutions to our fit. An identical optimal fit is obtained for parent-daughter pairs in the black band.



**Figure 5.11** – Best fit of the Haser model (blue) on the observed flux of  $N_2^+$  (black). The observed  $N_2^+$  flux is from 11-13-14 February, averaged over cometocentric distance. We find the best scale lengths to be  $l_p = 2.8 \times 10^6$  km and  $l_d = 3.8 \times 10^6$  km.

et al., 2021) computed that the dominant process for creating  $N_2^+$  ions in C/2016 R2 is the photoionization process due to solar UV photons, the ionization process due to electrons inside the coma representing only a few percents relative to photoionization. The validity of using a Haser modeling is also confirmed by the quality of our fit (see Fig. 5.11).

Our intensity profiles can be used to get an independent determination of the scale lengths both for the parent molecule and the daughter species.  $N_2^+$  is the daughter ion produced by photoionization of  $N_2$ , so we apply the daughter Haser model (see eq.5.13). We use the same parameters as those in our fit of the Haser model to the CN intensity profile. The Haser model is then fitted with the same methods as CN presented in section 5.2.2 as it was shown to be effective.

From the synthetic fluorescence spectrum computed in Chapter 4 we determined the line wavelengths of  $N_2^+$  and the corresponding lines in our observational spectra. This allows us to draw an intensity profile on either side of the comet's nucleus for the averaged observations of 11-13-14 Feb. In some cases, there is overlap of multiple species, which both could produce the observed intensity. No flux is taken for wavelengths were the  $N_2^+$  model overlaps with the spectral Atlas of Cochran & Cochran (2002) in order to avoid contamination from other species present. Here, we limit the identification process to the 3885.5 Å to 3915.0 Å interval in order to extract only the lines of the (0,0) band outside the CN emission lines region. The Haser model is then fit to our observations using the same methods as presented in section 5.2.2. The final intensity profile is a 1D profile starting from the nucleus of the comet and sweeping outwards along the coma ending at a distance of  $R = 6.5 \times 10^3$  km, shown in Fig. 5.9.

We first explore this interval with the  $\chi^2$  test in order to estimate the quality of each fit by comparing the resulting curve made with each pair of parent-daughter species scale lengths to the intensity profile. We once again start with a large phase space of 100 x 100 parent-daughter scale lengths. We explore  $l_p$  from  $l_p = 1.0 \times 10^3$  to  $l_p = 1.0 \times 10^5$  by increments of  $1.0 \times 10^3$ , and  $l_d$  from  $l_p = 1.0 \times 10^4$  to  $l_p = 1.0 \times 10^6$ by increments of  $1.0 \times 10^4$ . We then refine this phase space as we approach the ideal combination. However, the  $\chi^2$  test does not converge in this phase space: I was forced to enlarge the test until I was testing scale lengths for both mother and daughter species in the order of  $10^6$  km.

We can estimate the value of  $l_p$  from the inverse of the rate coefficients given by Huebner et al. (1992) for both quiet and active Sun. Unlike CN,  $N_2^+$  is not the only product of its parent-molecule. N<sub>2</sub> can produce:

$$\begin{split} \mathbf{N}_2 + h\nu &\rightarrow \mathbf{N} + \mathbf{N} \\ &\rightarrow \mathbf{N}_2^+ + \mathbf{e}^- \\ &\rightarrow \mathbf{N} + \mathbf{N}^+ + \mathbf{e}^- \end{split}$$

by photodissociation, photoionization, and dissociative photoionization, in descending order. When we take into account the branching ratio, only a small fraction of N<sub>2</sub> molecules is ionized to N<sub>2</sub><sup>+</sup>, most of them being photodissociated. To estimate the scale length of N<sub>2</sub>, we follow the law  $l_{p,d} = \tau_{p,d}v_{p,d}$ . The rate coefficient  $\tau_{p,d}$ would be the sum of the rate coefficients of the three processes. For quiet sun, the rate of photodissociation is  $6.61 \times 10^{-7} \text{ s}^{-1}$ ,  $3.52 \times 10^{-7} \text{ s}^{-1}$ for photoionization, and  $1.50 \times 10^{-8} \text{ s}^{-1}$ for the dissociative photoionization for a total of  $1.03 \times 10^{-6} \text{ s}^{-1}$ . Assuming the radial velocity v is 1 km/s at  $r_h$ , this gives us an  $l_{p,d}$  of  $9.71 \times 10^5$  km. For active sun, the rate of photodissociation is  $1.56 \times 10^{-6} \text{ s}^{-1}$ ,  $9.11 \times 10^{-7} \text{ s}^{-1}$ for photoionization, and  $5.47 \times 10^{-8} \text{ s}^{-1}$ for the dissociative photoionization for a total of  $2.53 \times 10^{-6} \text{ s}^{-1}$ , gives us an  $l_{p,d}$  of  $3.95 \times 10^5$  km. The scale length should be in the order of  $10^6$  km since we were in a period of quiet solar activity.

Similarly, Raghuram et al. (2021) calculate that the rate of production and loss reactions of N<sub>2</sub><sup>+</sup> in C/2016 R2 may be in the order of  $6.95 \times 10^{-7}$  s<sup>-1</sup>, suggesting that the scale length of the parent molecule would be  $1.44 \times 10^{6}$  km. Wyckoff & Wehinger (1976)'s rate coefficients give us an upper limit of  $5.55 \times 10^{6}$  km. However, these rates are only for photoionization.

The final  $\chi^2$  test reveals the best pair of scale lengths to be  $l_p = (2.8 \pm 1.0) \times 10^6$  km and  $l_d = (3.8 \pm 1.0) \times 10^6$  km. This fit is shown in figure 5.11 after having been convolved by the average seeing of the three nights. These values are within the expected range estimated from the rate coefficients. However, at this scale, multiple pairs of scale lengths could be selected for N<sub>2</sub><sup>+</sup> with an almost equally good fit, each dependent on the selection criteria we impose. The difference between the fit of different scale length pairs is incredibly small and the effect on the slope is almost imperceptible. We understand our intensity profile presents a certain degree of noise, and a slight alteration in the selection criteria would give an alternate best fit profile.

## 5.3 Calculating the production rates

The column density is linked to the flux per solid angle unit by:

$$N(\rho) = \frac{4\pi F}{g\Omega} \tag{5.15}$$

where N( $\rho$ ) is still the column density in molecules.cm<sup>-2</sup> for a solid angle  $\Omega$  defined by this surface, *F* the observed flux at each radial distance from the nucleus in erg.s<sup>-1</sup>.cm<sup>-2</sup>, and *g* the fluorescence factor in photons.molecules<sup>-1</sup>.s<sup>-1</sup>.

We take into account the geocentric distance  $\Delta$  converted to cm which gives us:

$$N(\rho) = \frac{4\pi F \Delta^2}{g} \tag{5.16}$$

At this stage, we are finally able to combine both the result of our Haser model fit and the observed intensity profile. Using the best fit from section 5.2.3, we can integrate the area under the curve and calculate  $N_{\text{tot}}$  the total number of molecules in the spectroscopic slit for a production rate of 1 molecule.s<sup>-1</sup>. We apply this value to the relationship:

$$N_{\rm tot}Q = \frac{4\pi F_{\rm tot}\Delta^2}{g} \tag{5.17}$$

with Q the production rate of the of the parent molecule in molecules/s. If we make the hypothesis that 100% of the parent molecules are photo-dissociated into daughter species, and  $F_{tot}$  the total flux observed through the slit, we could determine that:

$$Q = \frac{4\pi F_{\text{tot}}\Delta^2}{gN_{\text{tot}}}$$
(5.18)

The observed flux is in units of erg.s<sup>-1</sup>.cm<sup>-2</sup>.Å<sup>-1</sup>and thus must first be integrated along the wavelengths to remove the dependence, which we have done when we made the intensity profile. It then must also be integrated for the area of the spectroscopic slit in order to remove any pixel or arcsec dependence. Similarly, the fluorescence factor *g* needs to be converted into erg.molecule<sup>-1</sup>.s<sup>-1</sup>by means of  $E = hc/\lambda$  where  $\lambda = 3910$ Å is the wavelength of the bandhead for N<sub>2</sub><sup>+</sup> and  $\lambda = 3883$ Å the wavelength of the bandhead for CN. Our *g* values then must also be scaled by  $r_h^{-2}$ .

This corresponds to the simple case where all 100% of the parent species photodissociate into the same daughter species. If this is not the case the branching ratio (i.e. the fraction of daughter species produced compared to all the destruction processes) must be taken into account. The production rate given by the equation 5.18 must be divided by this branching ratio.

#### 5.3.1 Estimating the production rate of CN

We start by determining the production rate of CN. The fluorescence efficiencies g taken from Schleicher (2010)<sup>1</sup> gives us a g-factor of  $g = 3.52 \times 10^{-2}$  photons. s<sup>-1</sup>. molecule<sup>-1</sup>at 2.882 au, which, brought to the distance of our comet at 2.76 au and converted so as to be compatible with our flux, gives us a g-factor of  $g = 1.7 \times 10^{-13}$  erg. s<sup>-1</sup>. cm<sup>-2</sup>. The branching ratio for CN produced by HCN is nearly equal to one (Huebner et al., 1992), meaning ~100% of all HCN is photodissociated into CN.

The daughter velocity  $v_d$  is given an arbitrary value so as to compare with other comets estimations via the Haser model. Hence, we need to investigate the effect of higher velocities on the final production rate. Since the value of N<sub>TOT</sub> scales with  $v_d$  (see 5.18), Q is scaled inversely to  $v_d$ . Setting an upper value of  $v_d$  to to 1 km.s<sup>-1</sup> is a reasonable estimate for comets at  $\sim$ 1 au based on the results from space probes. However Cochran & Schleicher (1993) discuss the variability of this parameter both with heliocentric distance and production rate. The production rate seems to influence this parameter only for very active comets, which is not the case for C/2016 R2. The heliocentric distance influences significantly the gas expansion radial velocity inside the coma. This effect cannot be neglected in our case because of the large heliocentric distance of C/2016 R2 at the time of our observations (2.76 au). Cochran & Schleicher (1993) conclude their discussion by using the law  $v_d = 850 \times r_h^{-0.5}$  with  $v_d$  expressed in m.s<sup>-1</sup>. Such a law provides  $v_d = 511 \text{ m.s}^{-1}$ . As a result, we use 0.5 km.s<sup>-1</sup>, which is also the value used by Raghuram et al. (2021). It is important to keep in mind, nevertheless, that such a law is based on observations of comets with coma dominated by water molecules. In the case of C/2016 R2 the coma is dominated by CO, which may have an influence on this parameter. This influence being difficult to quantify the above mentioned value seems the best approximation that we can use. Others consider scale lengths varying as  $r_h^2$ , such as the velocity is constant with heliocentric distance and only the variation of lifetime with heliocentric distance.

With all these considerations, we calculate a production value of  $Q_{CN} \sim 5 \times 10^{24}$ molecules.s<sup>-1</sup>

The production rate of  $(3.0 \pm 1) \times 10^{24}$  molecules.s<sup>-1</sup>found by Opitom et al. (2019) has since been reviewed and an error was found. After correction, it agrees with

<sup>&</sup>lt;sup>1</sup>Schleicher's website, while practical, does not include his latest values. It gives us gives us a *g*-factor of  $g = 4.67 \times 10^{-14} \text{ erg.s}^{-1} \text{.cm}^{-2} \text{.Å}^{-1}$  for our comet at 2.76 au, which can account for differences in production rates. https://asteroid.lowell.edu/comet/cover\_ghq.html.

our revised CN production rate, having measured the same total flux, and using the scale lengths given by (A'Hearn et al., 1995), which our  $\chi^2$  approaches.

#### 5.3.2 Estimating the production rate of N<sub>2</sub>

We apply this same calculation to the observed N<sub>2</sub><sup>+</sup> flux, using the scale lengths calculated in section 5.2.3. The fluorescence factor *g* estimated by Rousselot et al. (2022) for the (0,0) band in the 3885.5 Å to 3915.0 Å interval is  $5.41 \times 10^{-3}$  photon.s<sup>-1</sup>.ion<sup>-1</sup> at  $r_h$ .

From the rate coefficients provided by Huebner et al. (1992) (see Section 5.2.3), we compute that the branching ratio (ratio of molecules of N<sub>2</sub> which are ionized to the total) forming the N<sub>2</sub><sup>+</sup> ion is 0.34 for a quiet Sun, while Wyckoff & Wehinger (1976) find significantly rate coefficients with a branching ratio of 0.42. Like Huebner et al. (1992) there is a large uncertainty on their values. The photodissociation rate is sensitive to the uncertainties on the cross sections and the fact that a predissociation line has a similar wavelength to the solar Lyman  $\gamma$  line (highly variable with solar activity and that could be Doppler shifted). We use 0.38, the average of these two branching ratios, meaning 38% of N<sub>2</sub> will be photodissociated into N<sub>2</sub><sup>+</sup>.

The fluorescence factor g estimated by Rousselot et al. (2022) for the (0,0) band in the 3885.5 Å to 3915.0 Å interval is  $5.41 \times 10^{-3}$  photon.s<sup>-1</sup>.ion<sup>-1</sup> at  $r_h = 2.76$  au. Using this value of g, the measured total integrated flux  $F_{tot} = 1.0 \times 10^{-14}$  erg.s<sup>-1</sup>.cm<sup>-2</sup>, a branching ratio of 0.38, and a velocity  $v_d$  of 0.5 km.s<sup>-1</sup>at  $r_h$  (see Sec.5.3.1) we estimate a N<sub>2</sub> production rate of  $\sim 1.0 \times 10^{28}$  molecules.s<sup>-1</sup>. When compared to a CO production rate of Q(CO)  $\sim 1.1 \times 10^{29}$  molecules.s<sup>-1</sup>, we find a N<sub>2</sub>/CO ratio of 0.09.

These new calculations of the *g* factor from Rousselot et al. (2022) force us to update former results, as the relative ratio was determined using a *g* factor of  $7 \times 10^{-2}$  photons.s<sup>-1</sup>.molecule<sup>-1</sup> from Lutz et al. (1993) scaled to 1 au. Using  $g = 4.90 \times 10^{-2}$  photons.s<sup>-1</sup>.molecule<sup>-1</sup>for the entire band, prior measurements of the N<sub>2</sub><sup>+</sup> production rate become  $Q(N_2) = 4.6 \times 10^{27}$  molecules.s<sup>-1</sup> for Wierzchos & Womack (2018),  $Q(N_2) = 8.0 \times 10^{27}$  molecules.s<sup>-1</sup> for McKay et al. (2019), and  $Q(N_2) = 1.4 \times 10^{28}$  molecules.s<sup>-1</sup> for Biver et al. (2018), giving us the upper and lower values of the expected production rate. These results are shown in Table 5.4. Our N<sub>2</sub> production rate, consequently, is right within the adjusted production rates found using relative ratios. It is, nevertheless, the first direct estimate of this production, independent from any assumption about the CO production rate.

This value is possible with our absolute best fit of the parent and daughter scale lengths. However, different fits are equally likely and give a different result. While our results are perfectly in line with part estimates, the narrow difference between

**Table 5.4** – Updated values of  $Q(N_2)$  based on the new *g* factor of  $g = 4.90 \times 10^{-2}$  calculated by Rousselot et al. (2022) (since these were using the entire N<sub>2</sub><sup>+</sup> (0,0) band). Values not given in the article referenced but inferred based on other data published are shown in **bold**.

Reference	Q(CO) (mols.sec <sup>-1</sup> )	New $Q(N_2)$ (mols.sec <sup>-1</sup> )	N <sub>2</sub> /CO	New N <sub>2</sub> /CO
Wierzchos & Womack (2018) Biver et al. (2018) McKay et al. (2019)	$\begin{array}{c} \textbf{4.6}\times10^{28}\\ \textbf{1.1}\times10^{29}\\ \textbf{9.5}\times10^{28} \end{array}$	$\begin{array}{c} 2.8\!\times\!10^{27} \\ 8.4\!\times\!10^{27} \\ 4.8\!\times\!10^{27} \end{array}$	<b>0.06</b> 0.08 0.05	0.10 0.13 0.08

**Table 5.5** – Best fit parent- and daughter-scale lengths for CN depending on the radius of C/2016 R2's nucleus. With a larger radius, while the parent scale length remains the same, the daughter scale length shrinks.

Radius Size (km)	1.7	5	10	15
$l_p(\times 10^3 \text{ km})$	12	13	13	13
$l_d( imes 10^3 \text{ km})$	220	280	160	120
$Q(CN)(\times 10^{24} \text{ molecules.s}^{-1})$	6.25	4.89	4.98	5.04

each of the possible best fits causes concern. We must consider the problem from every angle as there are many sources of uncertainty.

# 5.4 Considerations for Uncertainty

## 5.4.1 Errors on previous estimations

There is a distinct possibility that our measurements of the flux itself differs from those of our colleagues. Possible explanations for this difference could be the fact we only relied on the (0,0) band for our model, but the other bands are not likely to add much to the observed flux.

Another possibility could be a very different  $N_2^+/CO^+$  ratio from  $Q(N_2)/Q(CO)$ . This is possible if the probability of ionization of CO into CO<sup>+</sup> from CO<sub>2</sub> is significantly lower than that of  $N_2$  into  $N_2^+$ . This would account for a lot of CO produced but, comparatively, little CO<sup>+</sup> visible in the slit.

## 5.4.2 Influence of the Nucleus Size

As there are many parameters we must set beforehand, it is worth estimating what kind of influence they might have on the resulting scale length. One of the unfortunate unknowns in this situation is the size of C/2016 R2's nucleus, which cannot be seen through the bright coma.



**Figure 5.12** – Results of the  $\chi^2$  test to find the optimal values of the parent and daughter scale lengths for CN with different nucleus radii, at 1.5, 5, 10, and 15 km. The  $\chi^2$  is in  $10^{-16}$  erg.s<sup>-1</sup>.cm<sup>-2</sup>.



**Figure 5.13** – Results of the  $\chi^2$  test to find the optimal values of the parent and daughter scale lengths for N<sub>2</sub><sup>+</sup> with different nucleus radii, at 1.5, 5, 10, and 15 km. The  $\chi^2$  is in 10<sup>-16</sup> erg.s<sup>-1</sup>.cm<sup>-2</sup>.



**Figure 5.14** – Best fit of the Haser model for CN with different nucleus radii, at 1.5, 5, 10, and 15 km. The  $\chi^2$  test would seem to indicate a better fit for r = 15 km.



**Figure 5.15** – Best fit of the Haser model for  $N_2^+$  with different nucleus radii, at 1.5, 5, 10, and 15 km. The  $\chi^2$  test would seem to indicate a better fit for r = 5 km.
Radius Size (km)	1.5	5	10	15
$l_p(\times 10^3 \text{ km})$	2600	2800	2400	2400
$l_d(\times 10^3 \text{ km})$	7200	3800	3200	2500
$Q(N_2^+)(\times 10^{28} \text{ molecules.s}^{-1})$	1.0	1.1	0.98	0.99

**Table 5.6** – Best fit parent- and daughter-scale lengths for  $N_2$  depending on the radius of C/2016 R2's nucleus. Here we see how delicate the fit truly is.

Biver et al. (2018) suggest the massive production of CO of C/2016 R2 could be related to the size of its nucleus. Given the pure CO ice sublimation rate at 2.8 au based on Sekanina (1991), they estimate that the outgassing rate of C/2016 R2 could be supplied by a pure CO ice object of 3 km in diameter. This should be our minimum limit.

However, as there is more than just CO present, the true nucleus size could be anywhere upwards of that, and potentially very large. Other comets with known nucleus size show us that there can be a lot of variation amid the small bodies. The nucleus of comet Hale-Bopp has a radius estimated to  $r_n \sim 37$  km (Altenhoff et al., 1999), making this comet one of the largest ever observed. Distant comet 29P/Schwassmann-Wachmann 1, which also shows a large CO production on its circular 6-au orbit (~ 4 × 10<sup>28</sup> molecules.s<sup>-1</sup>), has a radius of ~ 23 km (Stansberry et al., 2004). Recently, C/2014 UN271 (Bernardinelli-Bernstein) was estimated to have a nucleus of >119 km(Hui et al., 2022).

Nevertheless, Wierzchos & Womack (2018) suggest that if C/2016 R2's CO output is proportional to surface area of the nucleus, then the radius need not exceed  $\sim 15$  km in order to explain the measured CO production rate. Thus, C/2016 R2 may be larger-than-average in size, but need not be a giant comet in order to explain the measured CO production rates.

Using eq. 3.2, this gives us a potential radius of  $(17.5 \pm 7 \text{ km})$ , hence a nucleus of  $(35 \pm 14 \text{ km})$  in diameter, which is near the approximation made by Wierzchos & Womack (2018). It is worth noting that this is the magnitude of the comet's nucleus cross section, meaning it could be longer, or shorter, if we had observed it from a different angle. However, this is a robust estimate of the radius for the purposes of our study.

Now that we have an estimate of the range of the nucleus radius, we run the  $\chi^2$  test again, this time for multiple values of  $r_0$ : 1.5, 5, 10, and 15 km. The results for CN are presented in Fig. 5.12 and Table 5.5 and for N<sub>2</sub><sup>+</sup> in Fig. 5.13 and Table 5.6.

In the case of CN, as the radius expands, the parent scale length remains the same as the daughter scale length retracts. The best fit of all four scale length pairs is in the case of r = 15 km, as the  $\chi^2$  results are 7.184, 5.692, 5.354, and 4.689  $\times 10^{-16}$  erg.s<sup>-1</sup>.cm<sup>-2</sup>respectively. The resulting difference in Q is of 0.02% between the

one calculated at  $r_0 = 5$  km and the one with the newly calculated best fit pair at  $r_0 = 15$  km.

In the case of N<sub>2</sub>, the best fitting pair sees a lower  $l_p$  and lower  $l_d$  for each higher value of  $r_0$ . We still remain in the  $l_p \pm .5 \times 10^6$  km range, well within the anticipated values. This is due to the sensitivity of our fit at this scale, as the difference in  $\chi^2$  is much smaller. Plotting the best fitting scale lengths at identical radius gives us a plot with all Haser profiles superimposed, with variations too slight to see with the naked eye. Knowing that our intensity profile must contain some degree of noise, the  $\chi^2$  test can only guide our research but is not likely to have given us a truly perfect fit, as evidenced by these fluctuations. These ideal pairs are fit dependent and will not be able to be refined further without a perfect noise-free intensity profile. These fits are shown in Fig. 5.15.

Detailed thermal and structural modeling is necessary to provide valuable constraints on the nucleus size from the CO production rate. We are left with having to chose a safe value for the radius: We continue to use 5 km for the rest of this study, in order for us to compare results with others who have tested the Haser model on different comets.

#### 5.4.3 Alternative scale lengths based on other observation days

Another important result from our work concerns the variability of  $N_2$  production rate between observation dates. The production rate given above corresponds to the average of our three observing nights but, as shown Figure 5.2, the observed intensity significantly changes from one night to another. Having access to other days of observation, even those done in less optimal sky conditions, gives us the opportunity to see other possible results for our fits. Here, we attempt to fit the Haser model to the days of 11/02, 13/02, 14/02, and to the averaged flux of the three days. These results are presented in table 5.7 and the best fits are shown in figures 5.16 (CN) and 5.17 ( $N_2^+$ ).

It is interesting just how much variation we have for the best fit when comparing the different days of observation. We can clearly see how the noise influences the model of CN when it is not averaged out. The fits do their best, but are not exceptional, as seen in figure 5.16. The model for 11/02 pushes the upper limit of our testing window, while the model for 13/02 pushes the lower limit. The fit for 14/02 seems close to that of our three day average. However, it is clear that much of our CN is disrupted by noise.

The bright emission of  $N_2^+$  benefits us greatly when it comes to our fit. As seen in the intensity profile, figure 5.9, the observations of 11/02 line up with our three day average, and as a result our best fit is almost the same as our final fit on the

	Date	$l_p$ (×10 <sup>3</sup> km)	$l_d$ (×10 <sup>3</sup> km)	$F_{TOT}$ (×10 <sup>-15</sup> erg.s <sup>-1</sup> .cm <sup>-2</sup> )	Q (molecules.s <sup>1</sup> )
CN	11/02 13/02 14/02 Average	29 10 11 13	140 100 280 280	2.31 2.01 2.01 2.11	$\begin{array}{c} 7.9\times 10^{24}\\ 3.6\times 10^{24}\\ 4.1\times 10^{24}\\ 5.0\times 10^{24} \end{array}$
N <sub>2</sub>	11/02 13/02 14/02 Average	2600 1100 4800 2800	3800 1000 8800 3800	10.38 8.00 12.12 10.16	$9.5 \times 10^{27}$ $3.6 \times 10^{27}$ $1.9 \times 10^{28}$ $1.1 \times 10^{28}$

**Table 5.7** – Best pair of parent-daughter scale lengths as a result of our Haser day for each individual day of observation. The variation of Flux is shown along with the resulting production rate.

averaged days. Meanwhile the observations of 13/02 push the lower limit of our testing window (as with CN) as it is more faint and our observations of 14/02 push the higher limit as it is much noisier. Through discussion with the observers, it was clear that the C/2016 R2 has a rapidly changing morphology. These strong variations of  $N_2^+$  could be due to the rapid variations of the ion streams through the slit from one day to the next due to unevenly distributed nucleus sublimation.

It is evident that fitting new Haser fits to our observational data will not ameliorate our results. If we compute N<sub>2</sub> production rates separately for these three nights with the same scale lengths as with the average of the three nights, we find a  $Q(N_2)$ , respectively for 11, 12 and 13 Feb.:  $1.0 \times 10^{28}$ ,  $8.0 \times 10^{27}$ , and  $1.2 \times 10^{28}$ . Such rapid changes in the N<sub>2</sub> line intensities are not an instrumental effect because CN profiles do not reveal any similar change ( $F_{tot} = 2.31, 2.01, 2.01 \times 10^{-15}$  erg.s<sup>-1</sup>.cm<sup>-2</sup> for  $Q(CN) = 5.4, 4.7, 4.7 \times 10^{24}$  molecules.s<sup>-1</sup> on Feb 11, 13, and 14, respectively).

#### 5.4.4 Error Bars

There are unfortunately many sources of uncertainty in our calculation. We assume the uncertainty on  $\Delta$  and  $r_h$  to be insignificant at these distances. Errors arise from our estimation of the total flux  $F_{\text{TOT}}$ : Our selection criteria on the emission lines can be more restrictive or permissive. However, this only has an effect of  $\pm 0.1$ erg.s<sup>-1</sup>.cm<sup>-2</sup>. Our greatest uncertainty is on  $N_{\text{TOT}}$ , as we have seen above the lack of information on the parameters  $r_0$ ,  $v_d$ ,  $l_p$ , and  $l_d$ , can have a significant effect on our final production rate. Just the velocity  $v_d$  alone can reduce the production rate in half. It must also be kept in mind that photodestruction of N<sub>2</sub> is strongly dependent



**Figure 5.16** – Best fit of the Haser model (red) on the observed flux of CN (black) for each day of observation, as well as the fit for the averaged intensity for the three days.



**Figure 5.17** – Best fit of the Haser model (red) on the observed flux of  $N_2^+$  (black) for each day of observation, as well as the fit for the averaged intensity for the three days. The observations of 13/02 are faint, resulting in shorter scale lengths. The observations of 14/02 are much noisier than the other days, making the fit difficult, and inadequate.

of solar activity, our estimate of  $l_p$  corresponds to a low solar activity and could be significantly different for comets observed during maxima of solar activity.

### 5.5 Summary and Conclusions

We investigated the CO-dominated and water-poor comet C/2016 R2 (PanSTARRS) using the Haser model in order to determine the  $N_2$  production rate. The intensity of the  $N_2^+$  lines is truly incomparable to what has been seen in comets so far, confirming the rarity of this type of comet. We determined the following characteristics:

- Parent (HCN) and daughter (CN) scale lengths of  $l_p = 1.3 \times 10^4$  km and  $l_d = 2.8 \times 10^5$  km respectively (scaled to 1 au using  $r_h^2$ ), consistent with the literature;
- A CN production rate of  $Q(CN) \sim 5 \times 10^{24}$  molecules.s<sup>-1</sup>, lower than usually observed in cometary spectra at similar heliocentric distances but consistent with other estimates for this comet;
- Parent (N<sub>2</sub>) and daughter (N<sub>2</sub><sup>+</sup>) scale lengths of  $l_p = 2.8 \times 10^6$  km and  $l_d = 3.8 \times 10^6$  km respectively (for 1 au, when using a scaling with  $r_h^2$ ).
- A N<sub>2</sub> production rate of  $Q(N_2) \sim 10^{28}$  molecules.s<sup>-1</sup>, exceptionally high, within the values estimated by other teams from the ratio N<sub>2</sub><sup>+</sup>/CO<sup>+</sup>;
- When compared to a CO production rate of Q(CO) ~ 1.1 × 10<sup>29</sup> molecules.s<sup>-1</sup>, we find a N<sub>2</sub>/CO ratio of 0.09, which is consistent with observed intensity ratios. This is the highest of such ratios observed for any comet so far with high resolution spectroscopy;
- Some large variations of N<sub>2</sub> production rates over the course of the three observing nights, the N<sub>2</sub> production rate given above being the average of these values. The production rate computed with the same parameters varies between  $8.0 \times 10^{27}$  and  $1.2 \times 10^{28}$  molecules.s<sup>-1</sup>.

These results are summarized in Table 5.8.

Large uncertainties still remain, and as it is so far the only comet of this kind to ever be observed, we are lacking a point of comparison. A detailed observation of C/2016 R2 at high heliocentric distances could still be possible, as CO would continue to sublimate under 40 au, and would provide further detail of the nucleus while inactive, in order to create a detailed thermal and structural model of this peculiar comet.

	$l_p( imes 10^3 \text{ km})$	$l_d( imes 10^3 \text{ km})$	Q (molecules.s <sup>-1</sup> )
CN	13	280	$5 \times 10^{24}$
$N_2^{+}$	2800	3800	$1 \times 10^{28}$

**Table 5.8** – Parent and daughter scale lengths calculated for CN and  $N_2^+$  (at 1 au, scaled with  $r_h^2$ ) and the resulting production rates for their parent species.

# 5.6 Identifying N<sub>2</sub><sup>+</sup> in Historic Comets

#### 5.6.1 Comet C/1908 R1 (Morehouse)

From the descriptions given of comet C/1908 R1 (Morehouse)'s behavior, it seems similar in morphology and composition to C/2016 R2. Sadly, its singular passage in 1908 was long before the use of high resolution spectroscopy. We believe we can improve on the estimates of N<sub>2</sub><sup>+</sup> in comet C/1908 R1. A scan of the October 18t<sup>th</sup> plate (Plate VI) from de La Baume Pluvinel & Baldet (1911) is available to us. Using JPL horizons, we calculate that the observation was made at an  $r_h = 1.35$  au and  $\Delta = 1.03$  au. From this, we attempted to extract the intensities of the band using MATLAB's IMSHOW function. This determines the intensity of an image based on pixel values and creates a 1D intensity profile.

I use Plate VII (Fig. 5.18) in order to align the image with the wavelength scale. On Plate VI I draw two vertical 1-pixel wide black lines down each edge of each spectra at 3500 Å and 5000 Å so as to create a digital signpost for the spectra, as pure black indicates saturation of the image, and a maximum value for the extracted intensity: this allows me to convert pixel distances into wavelengths. From here I extract the 1D intensity profile from the plate (Fig. 5.19). As is clear with Plate VII, The scaling is not linear, but the authors displayed laboratory spectra of other gases



**Figure 5.18** – Plate VII of de La Baume Pluvinel & Baldet (1911). This was used by the authors to align and display the spectrum from Plate VI on October 18.



**Figure 5.19** – Extracted spectrum (blue) from Plate VI of de La Baume Pluvinel & Baldet (1911). The laboratory spectrum of  $N_2^+$  is shown in orange and that of Cyanogen in green. We can clearly see strong peaks of the  $N_2^+$  (0,0) band  $\sim 3914$  Å and the CO<sup>+</sup> (2,0) band  $\sim 4250$  Å, though they appear  $\sim 4350$  Å due to poor scaling.

which aid in the alignment. Using a simple python code, I take the intensity of the  $N_2^+(0,0)$  peak at ~ 3914 Å and the intensity of the CO<sup>+</sup>(2,0) peaks at ~ 4252 Å and ~ 4273Å, in order to produce a proper comparison with Opitom et al. (2019). I once again use eq. 3.1 and calculate a  $N_2^+/CO^+$  value of 0.06, the same as with C/2016 R2.

However, non-uniformity in plate response and possible vignetting of the spectrograph slit cause difficulty interpreting these spectra. We cannot be sure they are properly calibrated. The units of flux are also unknown, but will be valuable to our estimates of relative ratios. Further study should help elucidate these results. We are in communication with the library of Meudon to see if scanning the archived plates could provide a workable resolution.

#### 5.6.2 Comet C/1961 R1 (Humason)

A scan of the grating spectra from which these intensities were calculated was provided in the same 1962 paper (Greenstein, 1962). From this, we once again attempted to extract the intensities of the band using MATLAB's IMSHOW function. The spectrum from August 2<sup>nd</sup>, N1702, is divided into 20 equal horizontal slices, from which I will make individual intensity profiles (see Fig. 5.20). I draw two vertical 3 pixel wide black lines down each edge of each spectra at 3188 Å and 5015Å



**Figure 5.20** – Division of the N1702 spectrum of C/1961 R1 Humason from August 2<sup>nd</sup> 1962 as observed by Greenstein (1962). Each red line indicates where an intensity profile was taken along the slit. It measures  $4 \times 1$  arcmin, a total width of  $5 \times 10^6$  km, centered on the nucleus.



**Figure 5.21** – Intensity of  $N_2^+$  in the coma of C/1961 R1 Humason (arbitrary units). These are traced over cometocentric distance (left) and then averaged over cometocentric distance (right). The solar continuum has not been removed. The scope of the spectum is too large for an accurate Haser model fit as the  $N_2^+$  ion would be interacting with UV solar radiation.

so as to align the spectra, as pure black indicates saturation of the image, and a maximum value for the extracted intensity. This also allows me to convert pixel values into wavelengths.

The resulting intensity profile displays remarkably strong lines of  $CO^+$  and  $N_2^+$ , from which we can now extract more accurate intensity levels. For each pixel, the result is the same:  $N_2/CO = 0.005$ , or half as much as we estimated using Greenstein (1962)'s intensity table.

I then identify the intensity of  $N_2^+$  for each of the 20 slits, and calculate their cometocentric distance. This gives us a cometocentric  $N_2^+$  intensity profile. However, the units of flux are also unknown. They will be valuable to our estimates of relative ratios but we could not calculate production rates from these results.



**Figure 5.22** – Spectrum of comet C/2001 Q4 (NEAT) with the solar continuum subtracted (red) on May 7<sup>th</sup> 2004. The  $N_2^+$  fluorescence model is superimposed (black). The identified  $N_2^+$  is in blue. It is much weaker than in C/2016 R2.

#### 5.6.3 Comet C/2001 Q4 (NEAT)

Feldman (2015) found a N<sub>2</sub><sup>+</sup>/CO<sup>+</sup> ratio of 0.027 by using the N<sub>2</sub> (0,0) band of the Carroll-Yoshino ( $c_4'^1\Sigma_u^+ - X^1\Sigma_g^+$ ) system at 958 Å, while Cochran et al. (2000) and Cochran & Cochran (2002) could not find any N<sub>2</sub><sup>+</sup>, and placed an upper limit of N<sub>2</sub>/CO $\leq 5 \times 10^4$ . We will see if our new fluorescence model can identify the N<sub>2</sub><sup>+</sup> (0,0) band and refine this value, using the UVES spectrum of C/2001 QA from May 7<sup>th</sup> 2004.

As shown in figure 5.22, the  $N_2^+$  (0,0) is much weaker than what we found in C/2016 R2, and is mostly hidden in noise. One way to extract a signal from a noisy spectrum is to stack the intensities of each line: when we did this, the noise was overwhelming and no clear  $N_2^+$  lines could be extracted. Thus, we were unable to find the  $N_2^+$  (0,0) band in C/2001 Q4.

#### **PART III**

# TOWARDS A RESERVOIR OF N<sub>2</sub> COMETS

*Comets are like cats: they have tails, and they do precisely what they want.* 

David H. Levy, Comets: Creators and Destroyers, 1998

# 6 The Dynamical History of N<sub>2</sub>-rich comets

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# 6.1 The Dynamical History of C/2016 R2

#### 6.1.1 The N-body Problem

Understanding the motion of celestial bodies has long been one of the core drivers of astronomy. Isaac Newton's<sup>1</sup> work with classical mechanics determined that every point mass attracts every single other point mass by a force acting along the line

<sup>&</sup>lt;sup>1</sup>The subject of plagiarism arises on the subject of the laws of gravitation. It is known that Robert Hooke indeed wrote to Newton about his hypothesis concerning orbital motion, but both claimed they were the first to have proven the inverse-square law. Newton produced *De motu corporum in gyrum* ('On the motion of bodies in an orbit') in which he derives Kepler's laws of planetary motion while Hooke refused to produce his proofs. The classic anecdote of his discovery having been sparked by a falling apple during the plague year of 1665 was most likely great marketing on

intersecting both points. The force is proportional to the product of the two masses and inversely proportional to the square of the distance between them. The equation is the following:

$$\mathbf{F} = \mathcal{G} \frac{m_1 m_2}{r^2} \mathbf{r} \tag{6.1}$$

where *F* is the force,  $m_1$  and  $m_2$  are the masses of the objects interacting, *r* is the distance between the centers of the masses and *G* is the gravitational constant  $(6.6743 \times 10^{-11} \text{ m}^3 \text{.kg}^{-1} \text{.s}^{-2})$ . This simple law is the cornerstone of our dynamical models. It rests on a set of postulates which are 'approximately true', in that they describe the observable with a precision enough to be useful.

However, the Solar System is a much more complex system, comprised of the Sun and (at least) eight planets, along with countless dwarf planets, asteroids, etc. In order to calculate the motion of a body through this system, its interaction with each of these bodies needs to be evaluated. Using a heliocentric equatorial coordinate system ( $P_{\odot}$ , x, y, z), the motion of a body h through the Solar System can be described as:

$$\frac{\mathrm{d}^{2}\mathbf{r}_{\mathbf{h}}}{\mathrm{d}t^{2}} = \underbrace{-\mathcal{G}M_{\odot}\frac{\mathbf{r}_{\mathbf{h}}}{\|\mathbf{r}_{\mathbf{h}}\|^{3}}}_{\text{Keplerian Term}} + \underbrace{\sum_{i=1}^{N}\mathcal{G}m_{i}\left(\begin{array}{c} \overbrace{\mathbf{r}_{i}-\mathbf{r}_{\mathbf{h}}}^{\text{Direct Perturbation}} & \text{Indirect Perturbation}\\ \left\|\mathbf{r}_{\mathbf{i}}-\mathbf{r}_{\mathbf{h}}\right\|^{3}} & - \underbrace{\overbrace{\mathbf{r}_{i}}^{\mathbf{r}_{i}}}_{\text{Perturbation}}\right)$$
(6.2)

where  $\mathbf{r_h}$  position vector of body h,  $M_{\odot}$  the mass of the Sun, N the number of i bodies,  $m_i$  the mass of body i,  $\mathbf{r_h}$  position vector of body i. The Keplerian term represents the interaction of body h with the Sun, the direct perturbation the interaction with planet i, and the indirect perturbation the gravitational action of body i on the Sun.

This only accounts for the purely gravitational forces acting on the body. In the case of a comet, it can be subjected to other forces depending on its orbit. If it passes too close to the Sun, we need to take into account the relativistic effects; it will also be subjected to non-gravitational forces due to the physical effects of the sublimation of its ices as they approach the Sun. If the nucleus was not rotating, the sublimation of its surface ices would produce a nearly-constant jet that will push it in the anti-solar direction as a result of the reaction force. In this case, the non-gravitational forces would not affect the period of a periodic-comet, since it experiences the same force with each perihelion passage. However, if the nucleus is rotating, then these forces accelerate or decelerate the comet. If the comet is rotating in the opposite direction as its orbit around the Sun, the reaction force will push in

his part (Gribbin & Gribbin, 2017). Even the great Isaac Newton exaggerated what he accomplished during his plague year.

the negative direction, and slow the comet down; if instead the comet is rotating in the same direction as its orbit, then the reaction to the sublimation will 'spin up' the comet and it will arrive at perihelion sooner than if acting under gravitational forces alone<sup>2</sup>. Additionally, comet surfaces are unevenly heated due to the distribution of their active or inactive surface areas, creating patches where the ices sublimate more or less efficiently; their nuclei are rarely spherical, and not always symmetrical. This results in an uneven outgassing of the nucleus. With this in mind, equation 6.2 becomes:

$$\frac{\mathrm{d}^{2}\mathbf{r}_{\mathbf{h}}}{\mathrm{d}t^{2}} = -\mathcal{G}M_{\odot}\frac{\mathbf{r}_{\mathbf{h}}}{\|\mathbf{r}_{\mathbf{h}}\|^{3}} + \sum_{i=1}^{N}\mathcal{G}m_{i}\left(\frac{\mathbf{r}_{i}-\mathbf{r}_{\mathbf{h}}}{\|\mathbf{r}_{i}-\mathbf{r}_{\mathbf{h}}\|^{3}} - \frac{\mathbf{r}_{i}}{\|\mathbf{r}_{i}\|^{3}}\right) + \mathbf{R} + \mathbf{A}_{\mathbf{NG}}$$
(6.3)

where  $\mathbf{R}$  the relativistic forces and  $\mathbf{A}_{\mathbf{NG}}$  the non-gravitational forces.

In the cases we study here, none of the comets have a perihelion small enough to warrant the use of relativistic forces. These are only interesting if a comet goes under  $\sim 0.5$  au, around the orbit of Mercury. While some of the comets on our list enter within the orbit of Earth, none get close enough for us to need these forces. For the comets added from the list from Cochran et al. (2000), which we will not have time to simulate, we will base our results on other databases.

Calculating the non-gravitational forces is not within the scope of this study. They are sometimes available to us through the *JPL Small Body Database*, meaning they will be used automatically for simulations using REBOUND.

The gravitational effects of the galactic tides are not available to us. On the large scale, these galactic tides are caused by the gravitational pull of our own galaxy on our Solar System. They can be enhanced by events such as distant galactic collisions or the disruption of dwarf or satellite galaxies. Perturbations can also be caused by the passage of a nearby star. These tidal forces are experienced by objects loosely bound by our Sun's gravitational pull: at a high enough heliocentric distance, galactic tides may dominate over the force of the Sun's attraction. Oort cloud objects hang in the balance in this transitional region, at > 10<sup>4</sup> au, and even a small perturbation can be enough to place Oort cloud comets on orbits that lead into the inner Solar System (Fouchard et al., 2006).

There are many integration methods which can be used to determine the trajectory of bodies from eq. 6.2, as we only need a first-order numerical procedure for solving ordinary differential equations (ODEs) with a given initial value. While I created my own program and tested different integration methods (Euler-backwards,

<sup>&</sup>lt;sup>2</sup>This was discovered by Encke in 1819, as he studied the comet that now carries his name. This comet only had a period of 3.3 years, and notoriously arrives 2h30 early to each perihelion passage, which could not be explained by gravitational forces alone. Due to its inclination and shape, however, this it now only arrives five minutes early. Non gravitational forces are a complex problem.

Runge-Kutta 4th order...), it is slow and struggles to handle the large number of bodies over such a large timescale: I need to turn to already optimized dynamical tools.

#### 6.1.2 Numerical N-body Integrators

In order to compute equation 6.3, we have at our disposal a plethora of numerical integrators. These software packages can integrate the motion of particles (stars, planets, moons, dust...) in a gravitational field. Some have been optimized to handle the relativistic and non-gravitational forces as well. The ones we chose to use for this study are:

- MERCURY: a general-purpose software package for carrying out N-body orbital integrations for problems in solar-system dynamics, created by John E. Chambers, with some subroutines supplied by Hal Levison and Martin Duncan (Chambers, 1999, 2012). It is designed to calculate the orbital evolution of objects moving in the gravitational field of a large central body. It is run in Fortran 77, making it quite fast. It is incredibly versatile and easy to use, as it requires only a few files as input —one file for the 'active' particles, which contribute to the force in the gravity calculation (planets, significant mass), and one for the test particles, which do not influence any other particle (comets and clones, where the mass is negligible) —using yes/no commands to determine which forces need to be taken into account. Mercury is able to monitor and output details of close encounters, Sungrazing events, ejections and collisions between objects.
- REBOUND is a commonly used N-body integrator, popular for its simple interface and efficient integrators (Rein & Liu, 2012). It is renowned for its flexibility and customizability and has gained incredible popularity in the astronomical community in the past few years. Since all the computationally expensive parts of REBOUND are written in C, but can be controlled either in python or C, it is quick and efficient even for long integrations. It allows the user multiple choices of integrators, from the symplectic integrators such as WHFast, WHFastHelio, SEI, or LEAPFROG, to the High accuracy non-symplectic integrator with adaptive timestepping (IAS15), which is what we chose to use. REBOUND is also able to download the orbits or any body in the JPL *Horizons* database (JPL DE 431).

Using hybrid integrators, we can save much integration time, as they have an adaptive timestep. We require the timestep to be small enough to handle the close

encounters with giant planets, but once the comet is far from the inner Solar System, its trajectory will be unchanged, and position will thus be much quicker to calculate using a larger timestep.

#### 6.1.3 Generating Comet Clones

Despite the high precision of modern telescopes, our knowledge of the orbital elements still contains uncertainties: our observation arcs are short, due to the limited amount of time the comet is visible. These remain quite small (see Table 3.1) but, as we will see, can have a great impact on the dynamical evolution of comets. In order to take these uncertainties into account, we compute the dynamical evolution not only of our comet, but also of its 'clones', massless facsimiles generated within these uncertainties. These are potential alternative initial conditions for the comet we wish to study. The resulting dynamical history will then be evaluated based on the dispersion of these clones, which provides a statistical model of the potential histories.

We take the orbital elements provided by the *JPL Small Body Database*, shown here in Tab. 3.1, along with the orbital covariance matrix<sup>3</sup>. This matrix represents the covariance between each pair of orbital elements: eccentricity, perihelion distance, time of perihelion passage, longitude of the ascending node, argument of perihelion, and inclination.

We then generate 1000 clones using a multivariate normal distribution with the object's orbital elements as the mean. This allows us to have a thousand more potential starting points for our comet before we send it on its dynamical journey. If all the trajectories follow the same trend, we can be certain of a comet's dynamical history; if they diverge, then it is clear we will not be able to retrieve the trajectory.

# 6.2 The Dynamical History of Comet C/2016 R2

We begin with MERCURY, with C/2016 R2's orbital elements from epoch 2458267.5 (2018-May-29.0) as the mean, solution date: 2019-Apr-15 23:33:5 (Reference: JPL 43, heliocentric IAU76/J2000 ecliptic). The planets' orbits are also generated on this date from the JPL Horizons database. We select an integration step of 0.1 year, without gravitation effects or galactic tides<sup>4</sup>. The positions of the eight planets and

<sup>&</sup>lt;sup>3</sup>This used to be readily available in the visual SBD Lookup tool, but has since been removed when the update of September 2021. They're now available on the SBD API in a machine readable form.

<sup>&</sup>lt;sup>4</sup>At the time we did our simulations, the non-gravitational forces were unknown: now, both A1 and A2 are available on the SBD. REBOUND will use these automatically.



**Figure 6.1** – The dynamical evolution of comet C/2016 R2 (PanSTARRS) one million years in the past (orange) and the future (blue) from October 4<sup>th</sup> 2019. It would seem it was once an Oort cloud comet, but is on a shorter orbit after having been pushed towards the inner Solar System. It will pass near the Sun multiple times before returning to its former home.

each C/2016 R2 clone are calculated at each time-step. The integration is conducted with the *hybrid* integrator in heliocentric Cartesian coordinates. The results both forward and backward in time are shown in Fig. 6.1. They are in agreement with the JPL database. We see that C/2016 R2 is not dynamically new, that it once was an Oort cloud object, pushed on a trajectory that makes it orbit the Sun ~10 times before returning to the Oort cloud. After a few more journeys into the inner Solar System, it will eventually return to the Oort Cloud.



Figure 6.2 – Final distribution of C/2016 R2 clones.



**Figure 6.3** – The dynamical history of comet C/2016 R2 (black) as estimated with 1000 clones. Clones lost to the numerical integrator are shown in green. Those with e < 1 at the end of the 1 Myr are shown in orange and those with e > 1 are shown in blue.



**Figure 6.4** – Recent dynamical history of comet C/2016 R2 (black) as estimated with 1000 clones (colored). Here, we see that the clones are in agreement as to its last passage at perihelion.



**Figure 6.5** – Evolution of eccentricity *e* (top) and semi-major axis *a* (middle) for 1000 clones (color) of C/2016 R2 (black). The scattering occurs during the close encounters of with Jupiter (blue) and Saturn (red) the last time it passed through the inner Solar System (bottom). The moment of closest approach is shown the gray. This encounter  $\sim$  3 au from Jupiter was enough to set the comets on a chaotic orbit, as seen in the the scattering of the orbital elements of the clones.

In order to determine the statistical accuracy of this dynamical history, we generate the clones from the covariance matrix of the same solution date. The positions of the planets and each individual C/2016 R2 clone are calculated at each time-step. The clones are seen as independent test particles and do not interact with each other. We run the integration over 1 Myr in negative time.

The clones unfortunately do not converge towards a single result: the final clones are split almost in half, with 43% of clones ending the simulation with e > 1 and 53% with e < 1 (Fig. 6.2). We also lose 45 clones during the simulation: this may be due to collisions with the larger planets or numerical error.

As shown in Figure 6.3, the clones share the same trajectory for a single orbit, or  $\sim$  19000 years. This is due to the fact that C/2016 R2 is subjected to close encounters with the giant planets (see Fig. 6.5), where the clones passed on average 1.1 au from Jupiter. For such a small object, mass-less in our simulations, even approaching <2 au of the giant planets will affect the trajectory greatly. This past close encounter is very sensitive to the initial conditions, and with the small variations in our clones, they are scattered on many possible orbits. For this reason, it is impossible to determine the trajectory of a comet with any close encounter in its dynamical past. Our knowledge of C/2016 R2's past is only certain for this 19000 year window: beyond this, its behavior is chaotic.

In order to gain further insight, we now use REBOUND. We now have our disposal an updated table of orbital elements and covariance matrix, at solution Date: 2021-Apr-15 23:33:5, Reference: JPL 43 (heliocentric IAU76/J2000 ecliptic). C/2016 R2's updated orbital elements at Epoch 2458267.5 (2018-May-29.0) are the mean for generating our clones. REBOUND could download the position of C/2016R2 for us, but we lock in our values manually, as the SBD continues to update, and we need to be sure of our sources. We find that REBOUND has a much longer runtime over such a large timescale, despite its adaptive timestep IAS15 integrator, though a positive is that it has no clone loss. When we look at the first orbit of C/2016 R2 (Fig. 6.4), we see that the same close encounter occurs, and we can not improve on the dynamical history by changing integrators. It would see that no matter what we do, the uncertainties on the comet combined with the limitations of our numerical integrators mean that we will never see C/2016 R2's history before this close encounter. The integration is thus stopped at 250 kyr to avoid wasting computing time. At this point, the nature of the comet is already a 50-50 split of fully-hyperbolic or nearly-hyperbolic.

## 6.3 The Dynamical History of N<sub>2</sub><sup>+</sup>-rich Comets

#### 6.3.1 C/1908 R1 (Morehouse)

We did not expect clear results with comet Morehouse, as its century-old orbital elements have large uncertainties due to the limits of the limits of precision of astrometric observations at the time, as well as the detectibility of the comet, limiting the duration of the observation arc. One of the best accounts we have was made in Greenwich, which suffered from the usual English fall weather. There were also no telescopes powerful enough to observe the comet from the southern



Figure 6.6 – Final distribution of C/1908 R1 clones.



**Figure 6.7** – The dynamical history of comet C/1908 R1 (Morehouse) (black) as estimated with 1000 clones. Clones lost to the numerical integrator are shown in green. Those with e < 1 at the end of the 1 Myr are shown in orange and those with e > 1 are shown in blue.



**Figure 6.8** – Distribution of the final orbital elements of comet C/1908 R1 Morehouse at the end of the 1 Myr. The average eccentricity exceeds 1, meaning this comet very likely had a hyperbolic orbit.



**Figure 6.9** – The dynamical history of comet C/1908 R1 Morehouse (black) as estimated with 1000 clones using the REBOUND integrator. Clones with e < 1 at the end of the 1 Myr are shown in orange and those with e > 1 are shown in blue.

hemisphere, removing any certainty December onward. To give an idea of the scale, the uncertainty on the semi-major axis was  $\pm 15\%$ , compared to  $\pm 0.05\%$  today.

Unlike our experience with comet C/2016 R2, C/1908 R1 has a clear dynamical past. In the 1 Myr simulation time with MERCURY, only five out of the 1000 clones we launched have orbited the Sun before, none passing < 10 au, and only three 'originating' <  $10^4$  au from the Sun. These results are coherent with comet Morehouse having traveled in the distant Oort cloud ~  $10^5$  au from the Sun. This is surprising, as with an older comet, the uncertainties on the initial orbital conditions are much larger, yet the results clearly converge (see Fig.6.6): With 88% of clones having a hyperbolic orbit combined with a semi-major axis >  $10^4$  au, this comet is clearly an Oort cloud object and dynamically new. As a result it may be the most pristine remnant of our early Solar System found to date.

The average eccentricity is 1.15. This alone is not enough to determine if the comet is interstellar in nature, as we expect much higher eccentricities (> 3) though interstellar object 1I/'Oumuamua had an eccentricity of e = 1.2. It may suggest C/1908 R1 was loosely bound to our Solar System, as its final heliocentric distance is on average 8.6 ×10<sup>4</sup> au, or 1.4 ly. At this distance it would be subjected to the interstellar regime, and galactic tidal forces dominate.

With such promising results, we decide to run the simulation again, this time with REBOUND. We generated a new batch of clones with the same initial orbital elements from the covariance matrix and run the simulation again. The results are shown in Fig. 6.9. Each comet completed on average 0.03 orbits through the inner Solar System <10 au; the final average eccentricity is 1 (0.9999...) and the average final distance is  $7.3 \times 10^4$  au, similar to the result with MERCURY. However, the final clones are more dispersed: 80% of all clones have an e > 1 compared to 88%. This is likely due to the non-identical batches of clones, which were generated independently. Since there were no close encounters with Jupiter, the integrators will have computed both evolutions the same way; thus, the results should be seen together as a 2,000 clone evolution.

We may be tempted to say that this is the first passage of C/1908 R1 back in the inner Solar System since it was placed in the Oort cloud billions of years ago. However, we must accept the fact that, due to the nature of the galactic tides, we do not know if it once completed a similar orbit once —or more —before. This is unlikely, as the odds of an Oort Cloud object doing two independent trips to the inner Solar System are infinitesimally low.

#### 6.3.2 C/1947 S1 (Bester)

Comet C/1947 S1 Bester is not as clear cut as comet C/1908 R1. At -1 Myr, almost half or 42% of clones have a hyperbolic orbit, with an average of e = 1.01, while the other half are nearly-parabolic. The statistics are shown in Fig. 6.10. Its average final distance is  $2.4 \times 10^4$  au, with a peculiar split population (see Fig. 6.12), with a peak at 500 au and a peak over > 1600 au. The reason for this cliff is unknown and may be the result of a numerical error.



Figure 6.10 – Final distribution of C/1947 S1 clones.



**Figure 6.11** – The dynamical history of comet C/1947 S1 (Bester) (black) as estimated with 1000 clones. Clones lost to the numerical integrator are shown in green. Those with e < 1 at the end of the 1 Myr are shown in orange and those with e > 1 are shown in blue.



**Figure 6.12** – Distribution of the final orbital elements of comet C/1947 S1 (Bester) at the end of the 1 Myr. The grouping around e = 1 shows the comet very likely had a hyperbolic or near-parabolic orbit.

#### 6.3.3 C/1961 R1 (Humason)

In the 1 Myr simulation time with MERCURY, only 22% of C/1961 R1 clones were 'injected', while 78% are bound to the Sun. There were no losses in this run. The average eccentricity 1 Myr ago was ~ 1, and the average heliocentric distance was  $1.2 \times 10^4$  au. The final average eccentricity is >1 at 1.07. On average, the clones made 34 passes < 10 au each: this comet is not dynamically new.



Figure 6.13 – Final distribution of C/1961 R1 clones.

#### 6.3.4 C/1987 P1 (Bradfield)

Comet C/1987 P1 (Bradfield) is much like C/1961 R1, with the caveat that a third of clones were lost before reaching simulation's end. With MERCURY the average final eccentricity of the clones was 1.07, as is customary with these near-parabolic orbits. With 43 average passes < 10 au per clone, this comet is not dynamically new. Unfortunately it has too many numerical losses to be any stronger, more reliable statistics.



**Figure 6.14** – Final distribution of C/1987 P1 clones.

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**Figure 6.15** – The dynamical history of comet C/1961 R1 (Humason) (black) as estimated with 1000 clones. Clones lost to the numerical integrator are shown in green. Those with e < 1 at the end of the 1 Myr are shown in orange and those with e > 1 are shown in blue.



**Figure 6.16** – Distribution of the final orbital elements of comet C/1961 R1 (Humason) at the end of the 1 Myr. The grouping around e = 1 shows the comet very likely had a hyperbolic or near-parabolic orbit.



**Figure 6.17** – The dynamical history of comet C/1987 P1 (Bradfield) (black) as estimated with 1000 clones. Clones lost to the numerical integrator are shown in green. Those with e < 1 at the end of the 1 Myr are shown in orange and those with e > 1 are shown in blue.



**Figure 6.18** – Distribution of the final orbital elements of comet C/1987 P1 (Bradfield) at the end of the 1 Myr.

#### 6.3.5 C/2001 Q4 (NEAT)

Comet C/2001 Q4 (NEAT) is interesting as it seems to be a returning comet, though its last passage at perihelion was over  $9 \times 10^5$  years ago. No comets were lost during the integration, and the comets seem split down the middle of whether they will pass the e = 1 threshold. In fact, as we see in Fig. 6.22, every comet clone remains e < 1, with an average of e = 0.998. Despite these similar eccentricities, the dispersion of semi-major axes is much more widespread.



Figure 6.19 – Final distribution of C/2001 Q4 clones.

#### 6.3.6 C/2002 VQ94 (LINEAR)

Unlike the others comets in this study, C/2002 VQ94 (LINEAR) is the only one which remains clearly in our Solar System, with only 18 clones exceeding e = 1 with MERCURY. The eccentricity remains 0.989 on average, slightly lower than most near-parabolic comets. On average, each comet makes 25 passes < 10 au, though the perihelion remains ~ 10 au, thus it may not be outgassing. There seems to be a dual distribution for the average final heliocentric distance, with a population at 350 au and one at 650 au, seen in Fig.6.24.



Figure 6.20 – Final distribution of C/2002 VQ94 clones.



**Figure 6.21** – The dynamical history of comet C/2001 Q4 (NEAT) (black) as estimated with 1000 clones. Clones lost to the numerical integrator are shown in green. Those with e < 1 at the end of the 1 Myr are shown in orange and those with e > 1 are shown in blue.



**Figure 6.22** – Distribution of the final orbital elements of comet C/2001 Q4 (NEAT) at the end of the 1 Myr. The average eccentricity exceeds 1, meaning this comet very likely had a hyperbolic orbit.



**Figure 6.23** – The dynamical history of comet C/2002 VQ94 (LINEAR) (black) as estimated with 1000 clones. Clones with an eccentricity < 1 at the end of the 1 Myr are shown in orange and those with an eccentricity > 1 are shown in blue.



**Figure 6.24** – Distribution of the final orbital elements of comet C/2002 VQ94 (LINEAR) at the end of the 1 Myr. We see two groupings of the final heliocentric distribution, at 350 au and 650 au.

#### 6.3.7 29P/Schwassmann-Wachmann 1

We can only look at a short period comets on a small timescale, especially one such as 29P, which has a period of only 14.6 years, and an eccentricity of 0.04. This quasi-circular orbit lies between Jupiter and Saturn which means it must have come quite close to Jupiter to indeed be captured. Its perihelion is at 5.7 au, meaning its volatiles continue to sublimate rapidly, so it must have happened relatively recently, though with its large nucleus of 60 km (Schambeau et al., 2015), it may have been even larger at the moment of capture.

Due to its close proximity to Jupiter, 29P's orbit evolves significantly on short timescales. As a result, we were able to use both MERCURY and REBOUND to evaluate the dynamical history. Rather than show the heliocentric distance, as this comet was much closer, I show the evolution of the semi-major axis in Fig. 6.25. It would appear 29P' orbit undergoes semi-major axis and eccentricity changes when it comes to conjunction with Jupiter every ~50 yr, but these are relatively predictable. We see that for MERCURY there was a moment of dispersal around the year ~1700, while for REBOUND, this occurred around the year ~1500.

Much work has been done by others on the subject of 29P's peculiar orbit. (Sarid et al., 2019) estimate that its that present day, very-low-eccentricity orbit (e = 0.043) was established after a 1975 conjunction and will continue until a 2038 Jupiter conjunction nearly doubles its eccentricity and pushes its semi-major axis out to its current aphelion  $\sim$ 7 au, causing 29P to experience much wider variations in solar heating. Their clones diverge too much past  $\sim$ 700 yrs. They believe it is a new visitor to the Gateway region<sup>5</sup>, rather than a return visitor that had ever spent any significant time in the inner Solar System as indicated by its current low-inclination orbit (< 10°), high activity at high heliocentric distance, and the lack of a historical record of a short-period "super-comet." Estimates show this comet was likely a captured OC object (Neslušan et al., 2017).

<sup>&</sup>lt;sup>5</sup>Describe this region's criteria



**Figure 6.25** – Dynamical history of comet 29P/Schwassmann-Wachmann as estimated by 1000 clones by MERCURY (above) and REBOUND (below).

# 6.4 Oort Cloud Comet Classes

Not all comets in our sample were able to be analyzed using our integration methods as they were added at the last minute. The comets identified by Cochran et al. (2000) which are missing from our dynamical study are C/1940 R2, C/1956 R1, C/1957 R1, C/1969 T1, C/1969 Y1, C/1973 E1, and C/1986 P1. We would like to attempt to classify them as well, despite our time limitation. Based on Fouchard et al. (2018) and Fouchard et al. (2020), who search for a record of the Oort cloud formation process in the orbital distribution of currently observable long-periodic comets, we can split Oort cloud comets into Jumpers (q > 10 au) and creepers (q < 10 au). When the original orbital energy z = -1/a has increased over  $10^{-5}$  au<sup>-1</sup>over the last orbital period, the comet is called a Kaib–Quinn comet (KQ) (Kaib & Quinn, 2009). This splits the comets into four classes: jumpers, KQ-jumpers, creepers, and KQ-creepers.



**Figure 6.26** – The Fouchard Classification of Oort Cloud Comets (Fouchard et al., 2018, 2020)

To find the orbital elements of these comets, we use the Warsaw catalog of cometary orbits, known as the CODE catalog (Królikowska, 2014). This is available on the VizieR database<sup>6</sup> as well as on the website<sup>7</sup>. As of July 2022, the original orbital elements of 279 comets are available with  $1\sigma$  uncertainties, including also their previous, current, next, and future orbits, and the values at r = 250 au, which are a good indicator for these comets' elements while in the Oort cloud.

<sup>&</sup>lt;sup>6</sup>https://vizier.u-strasbg.fr/

<sup>&</sup>lt;sup>7</sup>https://pad2.astro.amu.edu.pl/comets/

Comet	$a_p$	$\Delta z (10^{-5} \mathrm{au}^{-1})$	$q_p$ (au)	Dynamical status	Class
C/1908 R1	-	-	-	-	
C/1940 R2	31806.62	2.01	2.588	Uncertain	KQ-jumper
C/1947 S1	18811.14	0.017	0.315	Definitely dynamically old	Creeper
C/1956 R1	13007.28	0.089	0.784	Most probably dynamically old	Creeper
C/1957 R1	-	-	-	-	
C/1961 R1	-	-	-	-	
C/1969 T1	-	-	-	-	
C/1969 Y1	-	-	-	-	
C/1973 E1	54614.96	2.46	42.046	Definitely dynamically new	KQ-jumper
C/1986 P1	23854.96	0.008	5.12	Most probably dynamically old	Creeper
C/1987 P1	-	-	-	-	-
C/2001 Q4	33795.20	0.017	52.036	Definitely dynamically new	Jumper
C/2002 VQ94	-	-	-	-	-
C/2016 R2	-	-	-	-	

Table 6.1 – Orbital elements from the CODE catalog for the previous orbit of each comet.

Of the six comets of our sample that can be found in the catalog, four are comets we did not have time to investigate with our numerical integrators. We are in agreement with the CODE catalog when it comes to C/1947 S1 as we both find it is dynamically old, though they consider C/2001 Q4 to be dynamically new when we found it to be returning. In any case, were we to use the Fouchard et al. (2018) classification of Oort cloud comets, based solely on their semi-major *a*, C/1973 E1 would be considered a jumper, C/1940 R2 and C/2001 Q4 are KQ-jumpers, C/1986 P1 is a KQ-creeper, and C/1947 S1 and C/1956 R1 are creepers. Once again, these objects do not have a clear concordant dynamical history.

#### 6.5 Summary and Discussion

The results are, unfortunately, inconclusive. There appears to be no correlation between the comets in our study, save that they have highly eccentric orbits. Whether or not the comet's eccentricity was < or > 1 before the simulation does not influence the final e: some nearly-hyperbolic comets were more statistically likely to have had hyperbolic orbits before passage in the inner Solar System, and vice versa.

Each time a comet crosses the orbit of a giant planet, it receives a small 'kick' causing its eccentricity and semi-major axes to increase, while the perihelion distance remains constant. Once the eccentricity of an asteroid is  $e \ge 0.998$  and its semi-major axis is  $\ge 20\ 000$  au, the Galactic tidal field starts to dominate. As soon as the perihelion distance exceeds the semi-major axis of the giant planet  $q > a_P$ , the eccentricity of the planetesimal's orbit continues to be reduced until the Galaxy starts damping its eccentricity and randomizing the inclination. In this case, the

Comet	P (Yrs)	q (AU)	e	$inc(deg^{\circ})$	N <sub>2</sub> /CO	Av. Nb. Orb.	Av. e.
C/1908 R1	-	0.945	1.0009	140.17	0.06	0.00	1.15
C/1947 S1	-	0.368	1.0005	49.89	0.04	0.26	1.01
C/1961 R1	2944	2.133	0.9896	153.28	0.01	34	1.01
C/1987 P1	2122	0.869	0.9947	34.00	0.02	43	1.07
C/2001 Q4	-	0.962	1.0007	99.64	0.027	0.01	0.998
C/2002 VQ94	2863	6.797	0.9663	70.52	0.06	25	0.989
C/2016 R2	18709	2.602	0.9963	58.22	0.06	8	1.04

**Table 6.2** – Orbital elements along with  $N_2/CO$  abundance ratios of comets for which  $N_2$  has been detected, before and after our simulation. Periodic comets are not shown.

object would be considered bound to the Sun and part of the OC. Its final orbit entirely depends on the last interaction it had with a giant planet. What is clear is that we cannot quantify when the last interaction occurred, as each successive interaction erases the memory of the last one.

We investigated whether the passage these comets within the inner Solar System can be traced back to the passage of a single star. We traced the angle of elevation  $\alpha$ of our comets as a function of azimuth angle  $\delta$  centered on the Sun; if these objects were destabilized by a star, they should be seen arriving from the same place in the sky. If they were destabilized by a distant object orbiting the Sun, they would fit a sine function with a 24h period in  $\alpha$ . Unfortunately, this is not the case. In an attempt to identify if the passage of a nearby star could have forced a comet shower,



**Figure 6.27** – The final x,y, coordinates of all the clones in our study. There is no shared origin point, and no C/2016 R2-type orbit.



**Figure 6.28** – Evolution of the percentage of dynamically new clones (solid lines) and returning clones (dashed lines) over time on the total number of clones for each individual comet. The number of clones with  $T_J > 2$  was too small to represent. Dynamically new comets are defined as  $T_J < 2$  and  $a > 10^4$  au while returning comets have  $a < 10^4$  au. The further back in time we go, the more likely the comet was dynamically new. The moment the comet was likely injected into the inner Solar System would be when these two lines intersect as it represents the moment the comet was more likely to be returning than new. Comet C/1908 R1 is the only one for which each clone consistently fulfills this criterion. Comets C/1981 P1 and C/2016 R2 present similar dynamical histories and would have become returning long-period comets around the same time.


**Figure 6.29** – Position of all  $N_2$ -rich comets on the sky, from the perspective of the Sun. There is no shared sinusoidal function.

we examined the position of these clones projected in space, centered on the Sun (Fig. 6.29). If a large disruptor altered their trajectory, they would fit a sin-wave with a 24h period. This is not what we see here. It is unlikely a single event caused their influx.

We also investigated the possibility that C/2016 R2 could have resulted from a recent collision in the outer Solar System. In the case of collisional asteroids families, the orbital elements are similar. Unfortunately, none of our N<sub>2</sub>-rich comets share enough orbital elements to have come from a unique object. If we assume that C/2016 R2 was created via impact with a local TNO, possibly Pluto itself. We simulated the trajectory of 1000 clones of our six principle candidates over 15000 years and looked for possible close encounters with the 17 largest TNOs (Eris, Gonggong, Haumea, Makemake, Pluto, Quaoar, Sedna, 2002 MS4, Orcus, Salacia, 2014 EZ51, 2002 AW197, 2013 FY27, 2010 JO179, 2003 AZ84, Varda, and 1995 SM55) with over 700 km in diameter. We found the percentage of 'close' encounters to be so small that it would most likely be insignificant. While it's equally possible that a collision occurred much longer ago, our clones disperse too quickly for us to have any chance of tracking their path back reliably.

Knowing that volatiles would not have survived multiple passes near the Sun since the formation of the Solar System, it would seem a viable hypothesis to say that these objects are all or once were Oort Cloud objects captured by Jupiter as they visited the inner Solar System. We know from other studies that comets 1P, 29P, and 67P must have been captured Oort Cloud objects (Neslušan et al., 2017). All of comets in our study must have been stored in the Oort cloud for most of the time since they were formed in order for them to keep the volatile content we see today. Comet C/1908 R1 was clearly stored at the outer edge of the Oort Cloud, though further knowledge of the galactic tides must be evaluated in order to determine how stable its position there truly was. As we see in Fig. 6.28, it is the only comet for which each clone fits the criteria of dynamically new comets for the entire time of our simulation. An interesting observation is that there seems to be no link between the  $N_2/CO$  ratio and the dynamical history of the comet nor the average number of orbits within the inner Solar System: this would seem to indicate that these objects are not stratified and likely undifferentiated. There does not seem to be a baseline  $N_2/CO$  ratio from which these comets would have eroded down with each successive pass near the sun.

Unfortunately, we cannot determine precisely where in the Oort Cloud they were stored for the majority of the Solar System's lifetime. Some could be interstellar in nature, but none had a high enough e to be conclusive (C/1908 R1 is borderline). However, comets would not have formed in the Oort cloud: these comets were once part of the PPD. We need a completely different approach to identify their true, pre-OC origins, whether they formed in our own Solar System... or in a neighboring one.

# 7 Hypotheses for R2's Origin

#### Contents

7.1	Interstellar Visitor
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MULTIPLE HYPOTHESES HAVE ALREADY been suggested to explain comet C/2016 R2's peculiar composition: this comet could be a fragment of a differentiated object (Biver et al., 2018; Desch & Jackson, 2021; Jackson & Desch, 2021); it could represent a particular formation region in our Solar System (Mousis et al., 2021; Price et al., 2021); or perhaps a different Solar System altogether. It could even be a combination of these hypotheses, as represented in table 7.1. Here we compare these hypotheses and weigh the likelyhood of their accuracy.

	Interstellar Comet	Locally Formed Comet		
Differentiated Comet	Exo-Pluto fragment	Pluto(-like) fragment		
Undifferentiated Comet	Representative of neighbor-	Formed in peculiar area of		
	ing disk	our disk		

Table 7.1 – Possible hypotheses for C/2016 R2's origin.

### 7.1 Interstellar Visitor

Despite the lack of strong conclusion from our dynamical simulations, the similarities between the composition of C/2016 R2 and 2I/Borisov raise the possibility that C/2016 R2 may have an interstellar history. As discussed in previous sections and shown in figure 7.1, 2I/Borisov shares C/2016 R2's water depletion. However, 2I/Borisov is clearly an interstellar object: with an eccentricity of e = 3.4, there is absolutely no doubt it originated outside our Solar System. Could it be possible that comet C/2016 R2 was formed in a Solar System like the one that formed 2I/Borisov, only to somehow have been captured by the Opik-Oort Cloud?

Based on observations of long-period comets, there should be  $N_B \simeq 7.6 \pm 3.3 \times 10^{10}$  bound Oort Cloud objects with diameter ~ 2.3 km (Brasser & Morbidelli, 2013;



**Figure 7.1** – A comparison of the average composition of comets with C/2016 R2 (McKay et al., 2019), 1I/'Oumuamua as suggested by Jackson & Desch (2021), and 2I/Borisov estimated on the values given by Bodewits et al. (2020) and Cordiner et al. (2020).

Rickman et al., 2017). Siraj & Loeb (2021a) suggest that the existence of 2I/Borisov implies a number density of distant Borisov-like objects of  $9 \times 10^{-3}/au^3$ , consistent with the number density implied by 11/'Oumuamua (Jewitt et al., 2020), which would indicate there should be  $6 \times 10^{14}$  Borisov-like objects per star. Using the values  $r_B = 0.7$  km and q = 3 au, the number density of interstellar objects far from the Sun exceeds significantly that of similarly sized bound Oort cloud objects. In essence, they predict that interstellar objects may outnumber Solar System objects in the OC. Based on their results, nearly 1% of the carbon and oxygen contained in stars and the ISM should be locked in interstellar objects, which is comparable to the metals budget required for the minimum mass Solar nebula model to form the planets (Desch, 2007). Thus, if these objects formed in protoplanetary disks, a significant proportion of protoplanetary material is ejected during the planetary formation process. These objects may also have a finite lifetime, which would imply a larger mass budget. Portegies Zwart (2021) predicts that only 0.98% to 2.6% of these planetesimals remain bound to their parent star while the others are ejected and become free floating in the Galactic potential. Since our OC is expected to have formed from the depletion of planetesimals between Uranus and Neptune, the giant planets appear to be insufficiently efficient to explain the currently anticipated mass of the Oort cloud, as the retention rate would be several orders of magnitude too low. This suggests that more than 90% of the OC is likely to have come from elsewhere. They suggest that while the orbits of captured planetesimals could be rather distinct from those scattered outwards by our own PPD, Galactic tidal field would isotropize the orbital inclinations on a timescale of a only few hundred million years. This would imply that most of our OC population would not be representative of our Solar System, as a large majority would have formed elsewhere. Levison et al. (2010) suggest that  $\sim 90\%$  of OC comets resulted from exchange with the comets of other stars in the Sun's natal cluster. Unfortunately, there would be no way of knowing which of these objects were local or external, as they would be entirely mixed within the OC and any extra-Solar dynamical history erased.

#### 7.2 C/2016 R2 as a fragment of a Differentiated Object

Biver et al. (2018) suggest that C/2016 R2 may be a fragment of a differentiated Kuiper Belt body in order to explain the large observed hypervolatile abundances. This same theory could be applied to 2I/Borisov as suggested by Cordiner et al. (2020). De Sanctis et al. (2001) found that CO and other volatiles could almost be completely absent in the upper layers of a hypothetical differentiated comet: In that case, these two comets could be pieces of the cores of such differentiated comets.

The composition of Pluto's Sputnic Planitia is remarkably similar to that of C/2016 R2 — despite the presence of CH<sub>4</sub>, which would not have been observed on C/2016 R2 since it was outside the scope of the spectroscope — and stands out as the one region of Pluto's encounter hemisphere where CO, CH<sub>4</sub> and N<sub>2</sub> ices coexist, though it is mostly N<sub>2</sub>-CO ice. This region has been interpreted as a cold trap where volatile ices have accumulated in a topographic low, possibly originating as an impact basin. The red color and spectral slope of 'Oumuamua also were a good match to Pluto's surface. However, though similar, the relative abundances of CO, CH<sub>4</sub>, and N<sub>2</sub> we observe for C/2016 R2 do not match surface spectra of Pluto, though the relationship between the surface composition and interior of large KBO has yet to be thoroughly understood (Protopapa et al., 2008).

As seen in Chapter 6, it would seem unlikely that C/2016 R2 could have resulted from a (recent) impact with Pluto itself: if not from impact, C/2016 R2 could have at the very least formed from the same primordial grains as Pluto, and perhaps even Triton. We can however conclude that C/2016 R2 did not form from a recent collision with a TNO.

Along those same lines, a possible explanation for C/2016 R2's composition was presented by Desch & Jackson (2021), who suggest that C/2016 R2 is a nitrogen iceberg, a fragment of a differentiated KBO surface that was created during the period of energetic impacts during the 2:1 Jupiter:Saturn resonance epoch. 1I/'Oumuamua may be an N<sub>2</sub> iceberg chipped off from the surface of an ex-Pluto by an impact during a period of dynamical instability. Since no dust production or outgassing was detected during the passage of 1I, its true composition could not be determined, but the trajectory demanded a non-gravitational force directed away from the Sun varying roughly as  $1/r^2$ , consistent with cometary outgassing, albeit at a slightly higher magnitude than is typical for comets. They found that these unusual properties could be explained if 'Oumuamua is composed of N<sub>2</sub> ice like that found on the surface of Pluto, suggesting that N<sub>2</sub> ice could provide the non-gravitational acceleration necessary to match observations at either a low albedo  $\sim 0.1$ , or a high albedo ~0.64, the latter matching the albedos of the  $N_2$ -covered surfaces of outer Solar System bodies like Pluto and Triton. This predicted composition is shown in Fig. 7.1.

However, Siraj & Loeb (2021b) study this theory by examining the mass budget in exo-Pluto planets necessary to produce a population of  $N_2$  icebergs that would explain the detection of 'Oumuamua and find that stars would have to have a mass of heavy elements exceeding our knowledge of their composition. Only a small fraction of the mass of stars ends in exo-Plutos, making this scenario unlikely. They also give an estimate for the erosion of interstellar nitrogen icebergs by cosmic rays, based on the research of Phan et al. (2021). The cosmic-ray heating might destroy icy interstellar objects very efficiently such that the initial size of an  $N_2$  fragment as suggested by Jackson & Desch (2021) to explain the composition of 'Oumuamua should be at least 10 km in size in order to survive the interstellar journey. However, if C/2016 R2 had truly formed in our own Solar System, these constraints would be lifted.

It would be interesting to examine the possibility of collisional fragments of differentiated objects being a source of comets. We would need to estimate the likelihood of forming a differentiated KBO, establishing the size of the population; then the odds of collisionally fragmenting this KBO; then the processes which would transport this object to the OC, or remove them from the Solar System. This would be an interesting, long-term project.

# 7.3 Could Iceline Enrichment Produce C/2016 R2-like Comets?

Another possibility is that C/2016 R2's particular composition arises from where it formed in the PSN, first proposed by Bodewits et al. (2020). The hypothesis stipulated that this PPD could evolve over time to create 'exotic' compositions at different disk locations in unique proportions, in special comet forming zones, and a comet's particular composition comes from where it formed in this planetforming disk. Could there be a region of the protosolar disk where CO and N<sub>2</sub> are not efficiently processed into more complex species in order to account for the strong enhancement of these species in C/2016 R2? Two studies have independently estimated the possible origin of this comet from building blocks formed in a peculiar region in the PSN, near the ice line of CO and N<sub>2</sub>.

The ice line (also iceline, snowline, frostline, or simply condensation line) is defined as the radius where the temperature of the PSN is equal to the sublimation/condensation temperature of water- ice (or any species of interest) in the protosolar- and circumplanetary- disk. Inside the snowline, water-ice will be evaporated into water vapor. Outside the snowline, ice is present due to the condensation of vapor, though the motion of particles within the disk would allow for solids to exist in front of this line as well as some vapors to exist beyond. While the vaporous grains would contribute to the formation of the Sun, the remaining solid dust would be the building blocks of various planets, the leftover planetesimals contributing to the formation of comets and asteroids. Being able to physically determine the ice line allows us to understand under what form the species are at each radius, essentially giving us the available building blocks for each planet, and thus for

peculiar comets as well. However, this line is not fixed, and moves inward in time as the disk cools. Today, the water ice line is  $\sim 2.5$ au

Price et al. (2021) investigate if these comets could form in a pocket of CO-rich material in an otherwise H<sub>2</sub>O-rich disk as a result of dust transport, and under what conditions such pockets could form. To form CO-rich comets, we need a mechanism that can both create enhanced CO to H<sub>2</sub>O ratios compared to interstellar or disk-averaged CO/H<sub>2</sub>O abundance ratios and create a spread of CO to H<sub>2</sub>O within a disk like our solar nebula. Iro et al. (2003) suggests that at low H<sub>2</sub>O/H<sub>2</sub> ratios, the CO/H<sub>2</sub>O ratio first rapidly increases when the amount of water ice increases. They find that most of their disk models readily produce a region where CO ice is more abundant than H<sub>2</sub>O ice, no matter the initial conditions. This pocket would be between between 20 and 100 au. In some conditions this pocket can be as far inward as 10 au. They also suggest the reason interstellar comets could be more likely to have this composition is because they are more easily ejected due to being weakly gravitationally bound to their host star, which would explain the composition of 21/Borisov. However, this would seem to indicate that more CO rich comets should exist than have previously been observed. N<sub>2</sub> was not a part of their study.







**Figure 7.3** – Radial profiles of the N<sub>2</sub>/CO and H<sub>2</sub>O ratios relative to their initial abundance, for viscosity  $\alpha = 10^{-4}$ , from Mousis et al. (2021).

Mousis et al. (2021) run a similar simulation, based on the same disk model proposed by Birnstiel et al. (2012), taking into account the contribution of  $N_2$ . The focus is less on dust transport and more on the agglomeration of clathrates: H<sub>2</sub>O must be abundant enough to trap the clathrates, but that contradicts the low water abundance in C/2016 R2. The dust transport model is much more promising (just as for (Price et al., 2021)). They show that  $N_2/CO$  ratios reproducing the value estimated in comet C/2016 R2 can be found in dust formed in the vicinity of the CO and N<sub>2</sub> icelines, i.e. within the 10–15 au region of the PSN, depending on the adopted viscosity parameter  $\alpha$  of the disk (See Fig. 7.3). Meanwhile, extensively high  $CO/H_2O$  ratios, i.e. up to more than 200 times the value derived from a protosolar gaseous mixture, can be found in dust formed in the vicinity of the CO iceline ( $\sim 10$ au), the extent of which also depending on the adopted viscosity parameter. If the building blocks of a comet assembled from grains formed close to the CO iceline in the PSN, they should present  $N_2/CO$  and  $CO/H_2O$  ratios consistent with the measurements made in comet C/2016 R2's coma. This is lower than what Price et al. (2021) found, but the values are similar, and much depend on the disk parameters chosen at the beginning of the simulation - especially the  $\alpha$ , the viscosity parameter. In either case, the agglomeration of C/2016 R2 from dust condensed in the region of the CO iceline indicates that this comet formed at a greater heliocentric distance than a H<sub>2</sub>O-rich comet formed from clathrates. The formation temperatures of N<sub>2</sub>and CO-rich clathrates are always higher than those of the pure condensates at PSN conditions (Mousis et al., 2021).

They proceeded to investigate this further by examining the interplay of clathrate hydrates with the disk. They examine two scenarios in which the PSN is fed only



**Figure 7.4** – Results of the pure condensate scenario (above) and amorphous ice pebbles scenario (below). From (Schneeberger et al, Citation TK). The pure condensate scenario is more likely to produce a peak of CO-enrichment corresponding to C/2016 R2's composition.



**Figure 7.5** – A representation of the percentage of total disk composition per heliocentric distance With data from Schneeberger et al (Citation TK), in the pure condensate scenario at 1 Myr.

with pure condensates or fed only with volatiles trapped in amorphous ice pebbles. They find that both scenarios readily allow for formation zones that deplete H<sub>2</sub>O compared to CO and those that enrich N<sub>2</sub>. Certain locations would allow for both processes to occur, but they were incredibly slim, < 1 au wide. These are shown in Fig. 7.4. This would be ~8 au in the pure condensate scenario, and ~9 au in the volatiles trapped in amorphous ice pebbles scenario, if the peak of CO could enrich more.

If this comet did indeed form from a unique location in the PSN, we will likely not be able to estimate the exact location, since heliocentric distances for the different icelines are model- dependent. However, the 'Sweet Spot' would indeed be quite narrow, and near the CO and  $N_2$  ice lines. Based on the results shown in Fig. 7.5, this formation zone would be between 7.8 and 8.3 au, approximately, and only 0.5 au wide. These results are of course model dependent, but clearly show that an R2-like comet could form at some narrow point in time and space in our Solar System.

## 8 A Dynamical Model of the Early Solar System

#### Contents

8.1	The Nice Model
8.2	Integration Method
8.3	Results and Discussion
8.4	Conclusions of our Model

HERE WE EXPLORE THE potential fates of comets formed from these building blocks using a numerical simulation of early Solar System. By examining the dynamical evolution of only the objects formed in the small exotic pockets, or Sweet Spot, of the PSN which allows for peculiar-composition comets to form, we hope to understand why so few are observed today. This chapter is the basis of the article Anderson et al. 2022 (Citation TK).

#### 8.1 The Nice Model

At the moment the gas was removed from the PPD, the giant planets of the Solar System did not yet occupy their current orbits. This is clear in that Uranus and Neptune should not have formed at their current orbits, as the composition of the disk was not dense enough for planet formation, and should have formed nearer Jupiter and Saturn where building blocks were abundant. In order to reach the modern day structure, they must have migrated all while interacting with the remaining planetesimal disk (Fernández & Ip, 1984).

In 2005, Gomes, Tsiganis, Morbidelli, and Levison, suggested that the giant planets were formed in a much more compact region, surrounded by a a disk of leftover planetesimals (Gomes et al., 2005; Morbidelli et al., 2005; Tsiganis et al., 2005). Jupiter would have formed around 5.45 au, with Saturn slightly interior to its 2:1 mean motion resonance (MMR), interior to 8.65 au (compared to 5.2 and 9.5 au today, respectively). The semi-major axis of Uranus would have been between 11 and 13 au while that of Neptune would have been between 13.5 and 17 au (compared



**Figure 8.1** – Evolution of the early Solar System in the Nice model. Left: early configuration, before Jupiter and Saturn reach a 2:1 resonance. Middle: scattering of planetesimals into the inner Solar System after the orbital shift of Neptune (dark blue) and Uranus (light blue). Right: after ejection of planetesimals by planets (Gomes et al., 2005).

to their modern day orbits of 19.2 and 31.1 au, respectively). These planets would have been surrounded by a disk of leftover planetesimals with a mass of  $\sim 35 M_{\oplus}$ , between 16 and 30 au.

The planetesimals at the inner edge of this disk would frequently have their orbits altered by interaction with the planets. These scattered objects would exchange angular momentum with the planets, elongating their semi-major axis and drawing them outwards. This is referred to as planetesimal driven migration. These planetesimals traveled inward far enough to interact with Jupiter, which increased their eccentricity while pushing the giant planet inwards. After millions of years (500-600 Myr), this is enough to move Jupiter into 2:1 MMR with Saturn, which destabilized the entire system in a relatively short timeframe. Jupiter shifts Saturn out towards its present position, causing the latter to interact with the two ice giants, which propelling them onto much more eccentric orbits with higher semi-major axes. They plow into the disk, scattering the planetesimals further, removing 99% of the disk's total mass. Uranus and Neptune may even have swapped orbits during this period. Some of these planetesimals are thrown outwards towards the OC, while the others are thrown into the inner Solar System. This may have been responsible for the period of Late Heavy Bombardment (a period evidenced by the massive cratering on the M-bodies in the Solar System, along with many of the giant planets' moons). The process only abated when the giant planets reached their current orbits, and dynamical friction with the remaining planetesimal disk damped their eccentricities and circularized their orbits once again. This is known as the Nice model, for the Observatoire de la Côte d'Azur where the team was based.

Later, they suggested the evolution of Jupiter's semi-major axis was not through a smooth series of resonances, but rather through short jumps. This is known as the Jumping Jupiter scenario (Brasser et al., 2009). Jupiter would then encounter an ice giant, causing it to migrate away from Saturn much faster than if migration is driven solely by encounters with planetesimals. This ice giant is occasionally ejected from simulations, positing the existence of a fifth ice giant which was removed from the Solar System during this period of instability (Nesvorný, 2011). Jupiter and Saturn would begin in a 3:2 MMR because it allows their gaps in the protoplanetary gas disk to overlap, refraining Jupiter from migrating close to the Sun and forming a hot Jupiter instead.

In order to constrain this migration, we look for clues in the orbital elements of the Solar System Belts: the asteroid belt and the EKB. The objects that occupy these belts have peculiar configurations that act as fingerprints of this early giant planet sculpting. One of these would be the difference between the populations of dynamically hot and the dynamically cold populations in the classical EKB. The composition of both asteroids and KBOs can impose further constraints on how and when these planetesimals were transported through the disk. By testing different initial configurations of the gas and ice giants and simulating the evolutions of planetesimals in these disk, we can compare the resulting EKB structure with observation in order to determine which is the most valid. In order to reproduce the observed ratio between the resonant and non-resonant Kuiper Belt populations, the planetesimal-driven migration of Neptune should have been characterized by several small amplitude jumps, similar to the jumps undergone by Jupiter, and should have migrated to  $\sim 28$  au before the onset of planetary instability. (Nesvorný, 2015; Nesvorný & Vokrouhlický, 2016). This could have been caused by a population of 1000-4000 Pluto-size objects in the disk.

Deienno et al. (2017) implemented this new constraint to Neptune's evolution (27 au  $\ge a_N \ge$  29 au at the time of the instability) in order to investigate the resonant configurations that would create the EKB as we observe it today. They found that an 3:2, 3:2, 2:1, 3:2 multi-resonance configuration was the only one successful in fulfilling all the requirements: only four giant planets remain at the end, with orbits similar to their present ones; Jupiter's eccentricity is at least half is current values; the probability of the jump occurring evolves between 2.1 and 2.3 in less than 1 Myr, and finally the  $a_N$  constraint.

#### 8.2 Integration Method

We employ the Jumping Neptune scenario from Nesvorný (2015), with five initial giant planets: Jupiter, Saturn, and three ice giants of comparable mass, as described by Deienno et al. (2017). This third ice giant, henceforth I1, undergoes a series of encounters with Jupiter and Saturn which causes a divergent jump in their semi-



**Figure 8.2** – Dynamical evolution of the five planets' semi-major axes as a function of simulation time, with Scenarios 1-5 in descending order. Planets are represented with Jupiter in purple, Saturn in blue, Ice1 in turquoise, Uranus in green, and Neptune in yellow. These scenarios are only shown up to t = 25 Myr, as they remain in stable orbits after this time. The removal of Ice1 occurs at different times in each scenario.

major axes before inducing a jump in Neptune's orbit as well. Finally, it is ejected onto a hyperbolic orbit, leaving the remaining four planets near their current orbits. This model is described in section 8.1.

We have selected the simulations which best satisfy the criteria of similarity with the Solar System today, consistent with the current orbital structure of the trans-Neptunian population, in line with Deienno et al. (2017), which were all from the 3:2, 3:2, 2:1, 3:2 multi-resonance configuration, with a disk of 40  $M_{\oplus}$ . The initial multi-resonant configurations we choose for Jupiter, Saturn, Uranus, Neptune, and I1, along with parameters for the location and mass of disk begin in a 3:2, 3:2, 2:1, 3:2 resonance, as Baguet et al. (2019) find it is able to place a secular tilt resonance in the area of the cold EKB (between 39 and 48 au). We tested several alternative simulations varying the multi-resonance configurations: the distance from the last planet to the inner edge of the disk (1 or 2 au), the mass of the disk (20 or 40  $M_{\oplus}$ ), as well as the inclination of the disk in relation to the plane of the planets. This provides us with five scenarios to explore, as defined in Tab. 8.1, all requiring the existence of a fifth giant planet, with a mass comparable to those of Uranus or Neptune, which was eventually ejected during the instability. This ice planet would have formed within the volatile rich zone identified by Mousis et al. (2021).

**Table 8.1** – Initial conditions for the five scenarios explored in this study. The multiresonance configuration is the 3:2, 3:2, 2:1, 3:2, with the outermost planet at 20.18 au from the Sun. In all cases studied here, we used a disk of 40  $M_{\oplus}$ . a. Distance of Inner Bound of Disk (au), b. Inclination of disk with respect to invariable plane (°), c. Node of Disk (°), and d. Running Number. The running number corresponds to the generations used to test the configuration.

	a.	b.	с.	d.
Scenario 1	1	1	100.2	08
Scenario 2	1	0	0	02
Scenario 3	2	0	0	04
Scenario 4	2	1	100.2	01
Scenario 5	2	1	100.2	05

The current day Edgeworth–Kuiper belt extends from the orbit of Neptune at 30 au to approximately 50 au from the Sun. However, most of the small bodies of the outer Solar System originated from the region between Jupiter and ~30 au. With this in mind, we chose to limit our simulations to planetesimals formed in the 4 - 50 au range. This allows us to neglect the influence of the inner planets, which, having small orbits, require smaller integration intervals  $\delta t$ , more integration steps, and longer calculations for each of simulations. While the CO-rich comet forming zone could extend to 100 au (Price et al., 2021), the mass depletion of the classical belt is already well explored. This allows us to limit our computation time.

For this simulation, we chose the SWIFT numerical integrator. This is yet another N-body integrator, written by Levison & Duncan (1994), originally written in Fortran 77, which is why we did not use it for the dynamical simulations presented in Chapter 6. However, it is particularly well adapted for this set of integrations, namely because we have access to a pre-recorded evolution of the giant planets (Petit et al., 1999) of our system over 100 Myr, in which the previously calculated evolution of the planets is recorded every 1000 yr or less and the positions of the planets are interpolated at each time-step necessary for the integration of the motion of the test particles. This model was chosen because the pre-recorded evolutions are shown to produce the modern day Edgeworth-Kuiper Belt and will save us additional computation time. This ensures that each simulation for a given planetary evolution will use exactly the same planetary evolution track, avoiding divergence due to the intrinsic chaotic nature of planetary motion. Thus our final planetary system is sure to correctly reproduce the structure of the present-day Solar System. An additional benefit is another reduction to our computation time, as the positions of the planets do not need to be computed at each time step.

For each scenario, we run 50 sets of 1000 massless planetesimals. By running the simulations in independent sets, we were able to save additional computation

time, as we can run them in parallel on the local server cluster. Each clone has randomly generated orbital elements setting them on the same plane as the disk with varying semi-major axes between 4 au to avoid the inner Solar System, and 50 au. We thus have a total of 250,000 planetesimals for our 5 scenarios. Our simulations count a particle as lost if it reaches beyond 10,000 au as we don't yet have the ability to estimate the effects of the galactic tidal forces. It is considered ejected if its eccentricity e > 1, meaning it is on a hyperbolic trajectory. If a clone moves under 0.5 au from the sun, or in collision with a planet, it is also removed from the integration, as it is most likely destroyed and used to form the larger body.

#### 8.3 Results and Discussion

Based on the ranges proposed by Price et al. (2021) and Mousis et al. (2021), we chose to examine different formation zones. Price et al. (2021) suggest a wide range, arguing that the CO/H<sub>2</sub>O ice enrichment zone is likely between 20-100 au and could make up for 40% of the disk mass. They do not investigate a  $N_2/CO$  ice enrichment zone, though seeing as how both CO and N<sub>2</sub> have similar sublimation temperatures, the two ice lines should be near each other and make the 20-30 au annulus an area to explore. However, the  $CO/H_2O$  ice enrichment zone evolves over time, and without seeing how N<sub>2</sub> would evolve in their simulations, we cannot determine where a specific C/2016 R2 formation zone could occur. Meanwhile, the results of Mousis et al. (2021) would indicate a narrow area, as they find a  $CO/H_2O$  ice enrichment zone of  $\sim$ 1-2 au wide, near 10 au. Their N<sub>2</sub>/CO ice enrichment zone is narrower still, seemingly less than 1 au wide. The overlapping formation zone for an C/2016 R2-like comet would thus be incredibly thin. While the overlap between the formation annulus of N<sub>2</sub>-enriched and CO-enriched planetesimals is likely  $< \sim 1$  au in width, we examine a wider zone as we acknowledge the model-dependence of these ice lines. We examine both a wide C/2016 R2 forming annulus between 8-20 au; a narrow one, between 8-11 au, the ideal formation location of N<sub>2</sub>-rich, H<sub>2</sub>O-poor comets, as identified by Mousis et al. (2012); and the slimmest one between 10-11 au, or the 'Sweet Spot'. Interestingly, I1 is initialized and subsequently ejected from this narrow zone as well.

We examine the final orbital elements of each clone, identified by its formation location (initial semi-major axis). A snapshot of the first 1000 planetesimals in our first scenario is shown in Fig. 8.3 with their first and final positions. Each clone is color-coded for the moment it is lost, with earlier losses in purple and those which remain in the end shown in yellow. We see within the first 5 Myr, over a third of all planetesimals are ejected from the Solar System. This number rises to nearly half







**Figure 8.4** – Dynamical evolution of the planets and 1000 comet clones in Scenario 1 with eccentricity as a function of semi-major axis in log scale. Planets are represented in black, with Jupiter, Saturn, Ice 1, Uranus, and Neptune, respectively, from left to right. Blue indicates comets formed between 4-8 au. Turquoise indicates comets formed between 8-12 au. Green indicates comets formed between 12-20 au. Yellow indicates comets formed between 20-50 au. After 100 Myr, the area around the giant planets is entirely cleared. Comets formed between 4-12 au are the first to be ejected, and by 1 Myr almost none remain. Comets formed between 12-20 au population.

**Table 8.2** – Statistical loss outcomes of each of the scenarios after 100 Myr for each formation zone. planetesimals are considered lost if they enter into collision with a planet or if their semi-major axis a > 10,000 au. The number of collisions with major planets is insignificant (< 0.1%).

	Total Loss	8-10 au	10 <b>-</b> 11 au	8-20 au	20-30 au
S1	73%	97%	96%	88%	76%
S2	<b>79</b> %	97%	96%	90%	80%
S3	75%	98%	96%	91%	79%
S4	77%	97%	96%	90%	79%
S5	73%	97%	96%	89%	76%

**Table 8.3** – Statistical ejection outcomes of each of the scenarios after 100 Myr for each formation zone. An object is considered ejected if e > 1.

	Total Loss	8-10 au	10 <b>-</b> 11 au	8-20 au	20-30 au
S1	58%	81%	79%	70%	57%
S2	63%	80%	81%	72%	61%
S3	60%	81%	<b>79</b> %	71%	61%
S4	61%	80%	80%	72%	61%
S5	57%	79%	80%	70%	57%

after 10 Myr and to over half after 15 Myr. Meanwhile, while those formed over 40 au barely move from formation location over the course of our 100 Myr. The major loss of planetesimals occurs even before Jumping Neptune at ~10 Myr: after this time, the area around the giant planets is entirely cleared. With Saturn's final aphelion at 10.5 au, it continues to destabilize the narrow Sweet Spot until nothing remains. It is important to note here that if we had used a four planet model, based on current planetary orbits, Saturn would play the role of I1 and clear this narrow formation zone. This ejection zone exists no matter which model we select, and coincides perfectly with the location of our Sweet Spot.

We examine more closely the percentage of planetesimals ejected in our simulations for each 1 au annulus from 4 au to 50 au, as shown in Fig. 8.5. We see that for every 1 au annulus between 4 and 10 au, over 95% of the planetesimals are ejected before the end of the 100 Myr in each scenario. This number dips to 90% around 12 au. Then, between 12 and 20 au, each scenario still loses at least 80% of their planetesimals within the simulation time. In comparison, annuli beyond 40 au —the current location of the Classical Edgeworth–Kuiper Belt —only lose half their planetesimals, showing a zone that is relatively stable, containing objects that do not move far from where they are formed. The behavior of these clone sets is consistent between scenarios, as is seen in Fig. 8.5.

The resulting statistics are shown in Tab. 8.2. On average, each simulation loses 75% of their planetesimals by 100 Myr, losing 90% of all planetesimals formed in the



**Figure 8.5** – Percentage of planetesimals lost per formation location for each of the five scenarios. The gray zone indicates the limitation of our simulation. The blue zone indicates the  $N_2/CO$  enrichment zone as predicted by Mousis et al. (2021), while the overlaid green zone indicates the location of the ideal CO/H<sub>2</sub>O enrichment zone.



**Figure 8.6** – Percentage of planetesimals formed between 8 and 11 au lost over the 100 Myr simulation time, with time given in log scale. The greatest period of loss occurs in the first 1 Myr. This behavior is consistent for all five scenarios.



**Figure 8.7** – Final semi-major axes and eccentricities of all planetesimals from all simulations remaining after 100 Myr. Comets formed in the 8-11 au zone are shown in black. A majority of these remaining Sweet-Spot comets have higher eccentricities than average.



**Figure 8.8** – Final semi-major axes and perihelion distances of all planetesimals from all simulations remaining after 100 Myr. Comets formed in the 8-11 au zone are shown in black. Any object with a perihelion under 35 au will remain under the dynamic influence of Neptune, and likely be sent to the Oort Cloud by Neptune, or will lose their hypervolatile majority ices to vacuum via insolation heating (Lisse et al., 2022).

8-20 au range, 97% of all planetesimals formed in the 8-10 au range, and  $\sim 80\%$  in the 20-30 range. Consistently they lose 96% of all comets formed between 10-11 au. If we examine the region of planetesimals initialized between 8–20 au, we find that half the planetesimals are already removed from the inner Solar System by 5 Myr, with two thirds of planetesimals removed after 15 Myr. If we narrow that region further to 8 - 11 au, we find that 60% of planetesimals formed in this region are removed in the first 1 Myr and 90% after 10 Myr, shown in Fig. 8.6.

A handful of planetesimals ( $\sim 0.1\%$ ) are lost to collisions with the giant planets. Depending on the chronology, these could help account for the delivery of the building blocks of the Galilean and Saturnian satellites necessary for their formation (Ronnet et al., 2018; Anderson et al., 2021).

In each simulation, no matter the scenario, only <150 remained from the initial 8-11 au population. This averaged to be  $\sim$ 1% of all surviving planetesimals. These few remaining planetesimals, shown in black in Fig. 8.7, will find themselves either on highly eccentric orbits, be absorbed into the EKB, or anything in between. They seem to be evenly distributed within the population of remaining comets. The 10-11 au population makes up only 0.4% of all surviving planetesimals: if these are not sent towards the OC soon, they will likely sublimate as such low heliocentric distances and will not survive.

In order to determine if the planetesimals were captured by the OC or ejected from the Solar System entirely, we look at the energy E of each clone after they are r > 250 au from the Sun. We can use the Energy  $E = 1/a_{r=250}$  as a proxi (Oort, 1950), as this will be the semi-major axis a it will retain until its next passage in the inner Solar System (if that is ever to occur). If the energy is positive (E > 0), the comet is considered unbound from the Solar System. This in short returns to using the eccentricity e to determine if the object's orbit is hyperbolic and ejected or elliptical. The results of this statistical analysis are presented in table 8.3. We see that most comets formed in the 8-11 au zone, 80% on average, are ejected from the Solar System.

Interestingly, the distance the remaining comets traveled before finding a stable orbit is inversely proportional to its initial semi-major axis: that is to say, comets formed ahead of the EKB will find themselves behind the EKB, as if the belt were flipped inside out, or as if they had leapfrogged over these stable objects.

#### 8.4 Conclusions of our Model

We find that the majority of planetesimals formed between Saturn and the  $N_2$  iceline are ejected early in the simulation, so that even by the time the Jumping Neptune

scenario occurs, the planetesimals are already gone. This could explain the lack of  $N_2$ -, CO-rich, and  $H_2O$  depleted comets: they were formed in a very narrow region, which would account for their limited number, and this region empties rapidly due to the influence of giant planets, quickly stripping this already small population. This number could be further attenuated by the pressure bumps in the early Solar System, though enrichment at the icelines would account for the existence of specific populations. We also do not know the exact lifetime of this region, which may not have had time to produce many planetesimals of this peculiar composition.

With only on average ~0.4% of the total remaining comet population having formed in the narrow Sweet Spot, the odds of observing one are incredibly low. As of March 2022 there are 4397 known comets, though approximately 3000 of them are Kreutz Sungrazers (*Minor Planet Center*): based on our results, of the 1000 remaining comets, at least 5 N<sub>2</sub>-, CO-rich, and H<sub>2</sub>O depleted comets should have been observed, and many more CO-rich H<sub>2</sub>O depleted comets. One possible explanation for this lack of observation could be that our instruments have greatly improved in the last half century, only now enabling us not only to spot these relatively faint objects, but also to quantify their composition through spectroscopy.

However we should consider the possibility that many of these comets may have lost their bulk hypervolatile species in the billions of years since their formation, or even within the timeframe of our simulation. Pure hypervolatile ices are only stables on Gyr timescales beyond a heliocentric distance of 100 au Lisse et al. (2021). If this ejection period were to take place at the same time as the 'sublimative period' of the Edgeworth–Kuiper Belt (Lisse et al., 2021; Steckloff et al., 2021), then they only have  $\sim 20$  Myr to be placed on a trajectory towards the Oort Cloud before they lose their hypervolatile majority ices to vacuum via insolation heating Lisse et al. (2022). When looking at both the sublimation chronology and the Oort Cloud formation chronology together, we have a small window of only  $\sim 10$  Myr in which an object could be ejected from the giant planet region and inserted into the Oort Cloud. There, objects with a nucleus larger than 5 km could survive thousands of orbits and hypervolatile loss upon possible perihelion passage. This would indicate that C/2016 R2 would represent one of the first Oort Cloud objects, which could provide a direct measurement of CO/N<sub>2</sub>/CH<sub>4</sub> ratios in the PSN (Steckloff et al., 2021; Davidsson, 2021; Prialnik, 2021; Lisse et al., 2022), and would explain why so few N<sub>2</sub>-, CO-rich, and H<sub>2</sub>O-depleted comets have been observed today. Our results are in line with Lisse et al. (2022)'s hypothesis that interstellar object 2I/Borisov was ejected early from its parent system.

Further numerical simulations are required in order to investigate the behavior of these comets beyond the 10,000 au cutoff. As we have not accounted for the galactic tidal forces in our simulations, we unfortunately cannot quantify how many hyperbolic comets are truly ejected from the Solar System, and how many are recaptured and integrated into the Oort Cloud. Our estimates of the quantity of hyperbolic planetesimals can give us a good idea of this ejected population, but the true number depends on the chronology of Solar System formation events, i.e. the sublimative period of the Kuiper Belt compared to Neptune's jump compared to the exit of the Sun from its birth cluster.

These results are coherent with our current understanding of the chronology of Oort Cloud formation (Portegies Zwart et al., 2021). They call this procession of comet ejections from the 5-11 au zone the 'Conveyor Belt', which aptly describes the phenomenon we see here (See Fig.8.9). Objects formed in this region would be ejected early from the Solar System, in less than ~10 Myr, and unlikely to 'brake' enough to join the Oort Cloud. Thus, if N<sub>2</sub>-, CO-rich, and H<sub>2</sub>O depleted comets were to have formed under 11 au, ~90% of this population would have been ejected from the Solar System without having been captured by the Oort Cloud. The chronology depends on the moment the Sun leaves its birth cluster: So long as the Sun is a cluster member, planetesimals with an eccentricity of e > 0.98 with a semi-major



**Figure 8.9** – Evolution of planetesimals simulated by Portegies Zwart et al. (2021). The black line indicates planetesimals that are ejected from the Solar System on a relatively short timescale ( $\leq 10$  Myr). This corresponds to the R2 formation zone indicated by Mousis et al. (2021).

axis of a > 2400 au (q > 50 au) are vulnerable to being stripped from by the cluster potential or by passing stars.

We see a trend of long-period comets having formed between 15 and 40 au, despite being lost to our simulation after 80 Myr. Portegies Zwart et al. (2021) estimate that the bulk or 70% of the Oort Cloud material originates from this zone. This 15-40 au formation zone for Oort Cloud objects overlaps with the formation zone of CO-rich/H<sub>2</sub>O-depleted planetesimals predicted by Price et al. (2021). They find that objects formed in this zone would account for 40% of the disk mass, but is much higher than what has been observed today. It is possible these objects would have sublimated before being placed on OC trajectories. However, this would seem to lend credence to the validity of Mousis et al. (2021)'s model with a CO iceline at smaller heliocentric distances, as we do not observe such a high quantity of CO-rich,  $H_2O$ -depleted comets.

Raymond & Izidoro (2017) investigate how these planetesimals migrate into the inner Solar System, how they can be deposited onto stable orbits interior to Jupiter's, forming the asteroid belt, and and supplying water to the terrestrial planets. While the smallest comets were too strongly-coupled to the gaseous disk to be scattered out to the OC and were instead trapped in exterior resonance with giant planets, large comets with D > 20km were more easily unbound. While we are examining a period after the gas of the PPD has depleted, the resulting chaotic zone remains the same. This would indicate that the objects that were fortunate to be captured by the OC were larger than average sized. We see in the size distribution of our N<sub>2</sub> comets that they are larger than usual, with D > 30 km for those whose nucleus size has been estimated. Most of the comets in our sample have larger than average nuclei. It would be interesting to further investigate how this timelime of planetary migration coincides with the timeline of planetary formation, as it would reveal important clues to the availability of species within the disk, the timeline of planetesimal formation, and their ejection from the Solar System.

This is a promising lead for the formation zone of comets with R2-like composition. It would explain their size, placement in the OC, and rarity. This also allows for the existence of possible exotic comets, with peculiar enrichments stemming from unique composition pockets in the disk. Hypothetically, each species' ice line would create a small enrichment zone producing small bodies dominated by this species rather than  $H_2O$ : By examining the ice lines of the volatiles, we can estimate the odds of finding comets with each composition. It would be interesting to investigate what other types of comets could be formed under peculiar conditions.

#### **PART IV**

## **CONCLUSIONS AND OUTLOOK**

*Comets giveth and comets taketh away.* 

11

11

Carl Sagan, Comet, 1997

*I* I have worn myself thin trying to find out about this comet, and I know very little now in the matter.

Maria Mitchell, Comet, 1896

## Conclusions

THE GOAL OF THIS research was to investigate origins of N<sub>2</sub>-rich comets through the nature of comet C/2016 R2 (PanSTARRS) in order to create a new baseline for N<sub>2</sub><sup>+</sup> and N<sub>2</sub> study in cometary science: both with a spectroscopic approach, through the creation of a new fluorescence model and estimates of the scale lengths for future spectroscopic study, and via a dynamical approach, in reconstructing the dynamical history of comet C/2016 R2 and similar comets in order to identify a shared formation reservoir.

#### **Conclusions of Spectroscopic Model**

We created a new fluorescence model for N<sub>2</sub><sup>+</sup> in cometary spectra. Using the new fluorescence factors, I then re-estimated the N<sub>2</sub>/CO ratios of N<sub>2</sub>-rich comets. My estimate of the new scale lengths of the parent (N<sub>2</sub>) and daughter (N<sub>2</sub><sup>+</sup>) species gives  $l_p = 2.8 \times 10^6$  km and  $l_d = 3.8 \times 10^6$  km respectively (for 1 au, when using a scaling with  $r_h^2$ ). This provides an N<sub>2</sub> production rate of  $Q(N_2) \sim 10^{28}$  molecules.s<sup>-1</sup>, exceptionally high, within the values estimated by other teams from the ratio N<sub>2</sub><sup>+</sup>/CO<sup>+</sup>. When compared to a CO production rate of  $Q(CO) \sim 1.1 \times 10^{29}$  molecules.s<sup>-1</sup>, I find a N<sub>2</sub>/CO ratio of 0.09, which is consistent with observed intensity ratios. This is the highest of such ratios observed for any comet so far with high resolution spectroscopy. There is also a strong variability over the course of the three observing nights, likely due to the non-uniform distribution of N<sub>2</sub> rich active areas on the surface of the nucleus.

### **Conclusions of Dynamical Study**

I investigated whether the comets in our study had a shared dynamical history which could point to a particular formation region, or at the very least, a shared origin point which could help identify their original formation zone. The results are, unfortunately, inconclusive. There appears to be no correlation between the comets in our study, save that they have highly eccentric orbits. It is clear that each successive interaction with the giant planets erases the memory of the last one. I also investigated whether the passage of these comets within the inner Solar System can be traced back to the movement of a single star. We did not find a shared event that could have caused their influx. We found the odds of a recent collision to be so small that it would most likely be insignificant.

It would seem a viable hypothesis to say that these objects are all or once were Oort Cloud objects captured as they visited the inner Solar System, though we cannot determine precisely where in the Oort Cloud they were stored for the majority of the Solar System's lifetime. There seems to be no link between the N<sub>2</sub>/CO ratio and the dynamical history of the comet nor the average number of orbits within the inner Solar System: there does not seem to be a baseline N<sub>2</sub>/CO ratio from which these comets would have eroded down with each successive pass near the Sun, which would indicate that a comet's volatile content is heterogeneously distributed. Like snowflakes, they are quite simply unique.

By using an already established model of Edgeworth-Kuiper Belt formation, along with estimates of possible C/2016 R2 formation zones, I investigated the fates of objects formed in these regions (8-11 au). They objects are almost entirely ejected from the Solar System in astronomically short time frames. If these objects did indeed form in a narrow formation region in our own Solar System, they would have been ejected, which could explain why we do not see these comets today.

#### Outlook

During World War II, the loss of aircraft and their pilots was crushing. Materials were scarce, and aircraft needed to remain light and agile, thus added defense would be limited. Statistical Research Group (SRG) at Columbia University was put to the task of deciding where this re-enforcement would go by examining returning aircraft shot down in the line of fire and counting the bullet holes and creating a statistical estimate of their distribution. It would appear that the bullet holes clustered around the wingtips and the fuselage, sparing the engines. Abraham Wald, a statistician, realized that these bullet holes did not represent where the aircraft were more likely to be shot, but that they represented the areas in which a shot aircraft could limp home. The areas where bullet holes were not present, the engines, were representative of strikes which could take the aircraft down entirely, leaving no remains to be studied.

Just as Wald realized the value of understanding where bullets are *not*, I believe there may be more to learn from the comets that we *don't* observe rather than the ones that we do. Before the discovery of C/2016 R2 PanSTARRS, such a depletion of  $H_2O$  in comets was unthinkable. After all, it is the most important component of

cometary ices and in the very definition of comets. This forces us to examine the possibility of other comets, like C/2016 R2, that we have not — yet — observed, comets with exotic compositions such as enrichment in noble gases or other volatile ices, due to formations in narrow reservoirs around their icelines with peaks of abundance. Understanding why these comets have not been observed will be key to revealing the structure of our early Solar System and its dynamical evolution.

### Appendix

$\overline{v}$	N	F	$X^2\Sigma_q^+$	$B^2\Sigma_u^+$	v	N	F	$X^2\Sigma_q^+$	$B^2\Sigma_u^+$
0	0	1	1099.556	26665.617	0	21	2	1986.048	27622.441
0	1	2	1103.400	26669.764	0	21	1	1986.381	27622.957
0	1	1	1103.400	26669.763	0	22	2	2070.597	27713.200
0	2	2	1111.089	26678.066	0	22	1	2070.807	27713.857
0	2	1	1111.088	26678.066	0	23	2	2158.483	27808.545
0	3	2	1122.627	26690.509	0	23	1	2158.830	27809.073
0	3	1	1122.627	26690.508	0	24	2	2250.654	27907.508
0	4	2	1138.000	26707.108	0	24	1	2250.865	27908.212
0	4	1	1138.069	26707.108	0	25	2	2346.135	28011.062
0	5	2	1157.223	26727.847	0	25	1	2346.519	28011.619
0	5	1	1157.223	26727.916	0	26	2	2445.910	28118.220
0	6	2	1180.291	26752.707	0	26	1	2446.134	28118.965
0	6	1	1180.360	26752.773	0	27	2	2548.973	28229.970
0	7	2	1207.160	26781.737	0	27	1	2549.388	28230.564
0	7	1	1207.226	26781.895	0	28	2	2656.339	28345.319
0	8	2	1237.948	26814.862	0	28	1	2656.590	28346.109
0	8	1	1238.026	26815.052	0	29	2	2766.988	28465.239
0	9	2	1272.498	26852.235	0	29	1	2767.430	28465.873
0	9	1	1272.572	26852.435	0	30	2	2881.909	28588.766
0	10	2	1310.956	26893.644	0	30	1	2882.181	28589.562
0	10	1	1311.049	26893.880	0	31	2	3000.125	28716.844
0	11	2	1353.143	26939.278	0	31	1	3000.579	28717.492
0	11	1	1353.298	26939.547	0	32	2	3122.612	28848.380
0	12	2	1399.321	26988.952	0	32	1	3122.902	28849.327
0	12	1	1399.434	26989.292	0	33	2	3248.246	28984.715
0	13	2	1449.136	27042.903	0	33	1	3248.832	28985.374
0	13	1	1449.335	27043.223	0	34	2	3378.393	29124.318
0	14	2	1502.946	27100.803	0	34	1	3378.692	29125.312
0	14	1	1503.110	27101.219	0	35	2	3511.522	29268.723
0	15	2	1560.302	27162.996	0	35	1	3512.138	29269.434
0	15	1	1560.637	27163.400	0	36	2	3649.207	29415.208
0	16	2	1621.938	27229.030	0	36	1	3649.529	29417.372
0	16	1	1622.121	27229.616	0	37	2	3789.974	29569.350
0	17	2	1686.937	27299.651	0	37	1	3790.594	29569.391
0	17	1	1687.252	27300.099	0	38	2	3935.075	29724.989
0	18	2	1756.219	27373.935	0	38	1	3935.395	29724.651
0	18	1	1756.415	27374.529	0	39	2	4083.316	29884.197
0	19	2	1828.858	27452.806	0	39	1	4083.936	29892.282
0	19	1	1829.177	27453.291	0	40	2	4235.890	30051.562
0	20	2	1905.777	27535.335	0	40	1	4236.210	30052.573
0	20	1	1905.981	27535.954					

**Table 8.4** – Energy levels for v = 0 and  $N = 0 \rightarrow 40$ . Energy levels are given in cm<sup>-1</sup>.
v	N	F	$X^2\Sigma_q^+$	$B^2\Sigma_u^+$	v	N	F	$X^2\Sigma_a^+$	$B^2\Sigma_u^+$
1	0	1	3274.297	29037.059	1	21	2	4152.008	29983.596
1	1	2	3278.107	29041.229	1	21	1	4152.34	29984.72
1	1	1	3278.107	29041.328	1	22	2	4235.735	30073.329
1	2	2	3285.754	29049.494	1	22	1	4235.924	30074.574
1	2	1	3285.706	29049.687	1	23	2	4322.74	30167.61
1	3	2	3297.183	29061.799	1	23	1	4323.099	30168.677
1	3	1	3297.117	29062.085	1	24	2	4413.997	30265.464
1	4	2	3312.414	29078.258	1	24	1	4414.204	30266.683
1	4	1	3312.396	29078.436	1	25	2	4508.529	30367.888
1	5	2	3331.427	29098.782	1	25	1	4508.914	30368.904
1	5	1	3331.385	29098.978	1	26	2	4607.311	30473.826
1	6	2	3354.254	29123.465	1	26	1	4607.543	30475.045
1	6	1	3354.295	29123.515	1	27	2	4709.364	30584.326
1	7	2	3380.853	29152.163	1	27	1	4709.781	30585.359
1	7	1	3380.903	29152.204	1	28	2	4815.652	30698.395
1	8	2	3411.353	29184.911	1	28	1	4815.909	30699.586
1	8	1	3411.394	29184.898	1	29	2	4925.216	30816.967
1	9	2	3445.545	29221.891	1	29	1	4925.629	30817.999
1	9	1	3445.607	29221.708	1	30	2	5038.994	30938.989
1	10	2	3483.623	29262.812	1	30	1	5039.263	30940
1	10	1	3483.702	29262.584	1	31	2	5155.909	31065.755
1	11	2	3525.399	29308.025	1	31	1	5156.473	31066.79
1	11	1	3525.537	29307.273	1	32	2	5277.3	31195.772
1	12	2	3571.115	29357.140	1	32	1	5277.58	31197.128
1	12	1	3571.216	29355.627	1	33	2	5401.632	31330.599
1	13	2	3620.437	29410.415	1	33	1	5402.266	31331.667
1	13	1	3620.624	29406.460	1	34	2	5530.526	31469.243
1	14	2	3673.712	29475.534	1	34	1	5530.823	31470.243
1	14	1	3673.871	29471.779	1	35	2	5662.338	31611.668
1	15	2	3738.487	29529.244	1	35	1	5662.979	31612.668
1	15	1	3730.819	29531.616	1	36	2	5798.631	31758.096
1	16	2	3791.514	29594.537	1	36	1	5798.961	31759.096
1	16	1	3791.692	29596.459	1	37	2	5938.099	31908.522
1	17	2	3855.862	29664.387	1	37	1	5938.592	31909.522
1	17	1	3856.170	29665.898	1	38	2	6081.666	32062.939
1	18	2	3924.463	29737.829	1	38	1	6081.957	32063.939
1	18	1	3924.651	29739.242	1	39	2	6228.538	32221.341
1	19	2	3996.379	29815.831	1	39	1	6329.012	32222.341
1	19	1	3996.694	29817.091	1	40	2	6379.447	32383.723
1	20	2	4072.539	29897.422	1	40	1	6379.756	32384.723
1	20	1	4072.737	29898.756					

**Table 8.5** – Energy levels for v = 1 and  $N = 0 \rightarrow 40$ . Energy levels are given in cm<sup>-1</sup>.

v	N	F	$X^2\Sigma_q^+$	$\mathbf{B}^2 \Sigma_u^+$	v	N	F	$X^2\Sigma_q^+$	$B^2\Sigma_u^+$
2	0	1	5416.534	31356.191	2	21	2	6285.795	32290.695
2	1	2	5420.303	31360.243	2	21	1	6285.795	32290.695
2	1	1	5420.303	31360.243	2	22	2	6368.449	32379.546
2	2	2	5427.84	31368.346	2	22	1	6368.449	32379.546
2	2	1	5427.84	31368.346	2	23	2	6454.835	32472.407
2	3	2	5439.145	31380.501	2	23	1	6454.835	32472.407
2	3	1	5439.145	31380.501	2	24	2	6544.949	32569.275
2	4	2	5454.217	31396.706	2	24	1	6544.949	32569.275
2	4	1	5454.217	31396.706	2	25	2	6638.79	32670.146
2	5	2	5473.057	31416.961	2	25	1	6638.79	32670.146
2	5	1	5473.057	31416.961	2	26	2	6736.352	32775.017
2	6	2	5495.663	31441.265	2	26	1	6736.352	32775.017
2	6	1	5495.663	31441.265	2	27	2	6837.632	32883.882
2	7	2	5522.035	31469.618	2	27	1	6837.632	32883.882
2	7	1	5522.035	31469.618	2	28	2	6942.626	32996.738
2	8	2	5552.172	31502.017	2	28	1	6942.626	32996.738
2	8	1	5552.172	31502.017	2	29	2	7051.331	33113.58
2	9	2	5586.071	31538.463	2	29	1	7051.331	33113.58
2	9	1	5586.071	31538.463	2	30	2	7163.741	33234.404
2	10	2	5623.733	31578.953	2	30	1	7163.741	33234.404
2	10	1	5623.733	31578.953	2	31	2	7279.854	33359.204
2	11	2	5665.155	31623.486	2	31	1	7279.854	33359.204
2	11	1	5665.155	31623.486	2	32	2	7399.664	33487.975
2	12	2	5710.337	31672.06	2	32	1	7399.664	33487.975
2	12	1	5710.337	31672.06	2	33	2	7523.166	33620.713
2	13	2	5759.275	31724.672	2	33	1	7523.166	33620.713
2	13	1	5759.275	31724.672	2	34	2	7650.357	33757.411
2	14	2	5811.97	31781.322	2	34	1	7650.357	33757.411
2	14	1	5811.97	31781.322	2	35	2	7781.23	33898.066
2	15	2	5868.417	31842.007	2	35	1	7781.23	33898.066
2	15	1	5868.417	31842.007	2	36	2	7915.782	34042.67
2	16	2	5928.616	31906.724	2	36	1	7915.782	34042.67
2	16	1	5928.616	31906.724	2	37	2	8054.006	34191.218
2	17	2	5992.564	31975.47	2	37	1	8054.006	34191.218
2	17	1	5992.564	31975.47	2	38	2	8195.898	34343.704
2	18	2	6060.259	32048.243	2	38	1	8195.898	34343.704
2	18	1	6060.259	32048.243	2	39	2	8341.452	34500.122
2	19	2	6131.697	32125.041	2	39	1	8341.452	34500.122
2	19	1	6131.697	32125.041	2	40	2	8490.663	34660.465
2	20	2	6206.877	32205.859	2	40	1	8490.663	34660.465
2	20	1	6206.877	32205.859					

**Table 8.6** – Energy levels for v = 2 and  $N = 0 \rightarrow 40$ . Energy levels are given in cm<sup>-1</sup>.

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