X-RAY FLARE DRIVEN CHEMISTRY IN PROTOPLANETARY DISKS

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Abstract: Planet formation begins within dusty and gaseous disks surrounding young stars. These disks, known as protoplanetary disks, are chemically rich, where light emitted by the young central star drives the formation of more complex (and pre-biological) molecules. In this work, we explore how large 'bursts' of X-ray photons, or flares, impact the chemical evolution in a protoplanetary disk. Chemical disk models indicate that the cumulative effect of thousands of flares over hundreds of years can increase chemical complexity, specifically in carbon-, oxygen-, and sulphur-bearing species. Additionally, this work presents observational evidence of flare driven chemistry in HCO^+ and $H^{13}CO^+$ using the Submillimeter Array (SMA) and Atacama Large Millimeter Array (ALMA).

1. BACKGROUND AND MOTIVATION

Protoplanetary disks are formed after a molecular cloud gravitationally collapses, forming a pre-main sequence (PMS) star surrounded by a chemically rich (Aikawa et al., 2002, 2003; Öberg et al., 2015; Walsh et al., 2016) and physically dynamic (Ardila et al., 2002) disk where planet formation occurs (Figure 1). To understand not only the formation of planets, but also the chemical compositions of the planets' terrain and atmosphere, we must be able to accurately model the chemical and physical processes that occur in the protoplanetary disk's complex environment (Lynden-Bell and Pringle, 1974; Bergin et al., 2007).

1.1. Chemical and Physical Structure

A typical protoplanetary disk has a radius of tens of astronomical units (au) with a total mass of ~ 0.04 $M_\odot$ (Williams and Cieza, 2011), but larger disks can span hundreds of au with masses up to ~ 0.04 $M_\odot$ (Cleeves et al., 2016). Studies from the from the Disk Substructure at High Angular Resolution Project (DSHARP) and Moleculars with ALMA at Planet forming Scales (MAPS) have shown that disks can, and are likely to, have substructure, such as rings or gaps, spiral arms, and misaligned rings (e.g., Andrews et al., 2018; Öberg and Bergin, 2021b). This complex physical structure results in the presence of a broad range of molecular and atomic species. The physical and chemical structure of a disk is described by three layers: i. the photon- dominated region, the outermost layer that is rich in atomic and ionic species, *ii.* the warm molecular layer, the middle layer that is dominated by gaseous molecular and radical species (Aikawa et al., 2002), and *iii.* the mid-plane, the innermost layer composed primarily of dust grains and molecular and atomic ices. The majority of observed species are small and simple molecules, such as CO, HCO^+, CN, H_2O, OH, CO_2, HCN, CS, C_2H, and N_2H^+; however, a number of more complex molecules, such as formaldehyde, methanol, and methyl

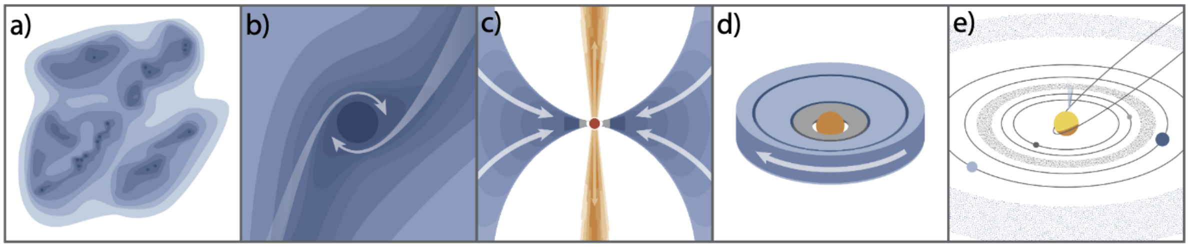

Figure 1: Figure taken from Öberg and Bergin (2021a). Planet formation begins with the collapse of a molecular cloud (a), which forms a pre-stellar core (b). Over time, a protostar and Class I disk with a molecular envelope forms (c). As the star fully develops, the envelope dissipates forming a Class II disk, or protoplanetary disk, where planet formation occurs (d), and eventually a planetary system forms (e). This work focuses on the protoplanetary disk phase.

cyanide have also been detected (Aikawa et al., 2003; Öberg et al., 2015; Walsh et al., 2016). McGuire (2022) provides a census of all detected molecules as of 2021. Historically, chemistry is thought to evolve slowly, over the lifetime of the disk (millions of years, Glassgold et al., 1997; Strom et al., 1989; Haisch et al., 2001; Fedele et al., 2010), but short-term (days to years) chemical evolution has been relatively unexplored. As detection methods and telescopes are becoming more efficient at detecting larger molecules and relatively less abundant species at higher resolutions, we must determine whether it is accurate to assume chemistry is constant over observational time scales, or if it is possible for external factors, such as radiation, to drive dynamic chemistry.

1.2. Central Star

Perhaps one of the most important features of a protoplanetary disk is the central PMS star. T Tauri stars are a typical PMS star studied in protoplanetary disks, as they are common and follow the same evolutionary track as the Sun. T Tauri stars are highly variable in the X-ray regime due to X-ray flaring produced by magnetic reconnention events on roughly a weekly basis (e.g., Wolk et al., 2005). On the stellar surface, magnetic loops can be as large as several stellar radii (Favata et al., 2005) and can trap hot ionized gas, which radiates X-ray photons at nearly a constant rate defined as the characteristic, or baseline, X-ray luminosity (L_{char}). When two magnetic loops undergo magnetic reconnection, the gas is heated up to millions of Kelvin, resulting in a burst of X-ray radiation known as an X-ray flare. As a star ages, the stellar dynamo stabilizes and magnetic fields are thought to become less intense and frequent, so the star experiences less intense X-ray radiation (Güdel, 2004, and citations therein). In order to best understand the earliest stages of our Solar System, we must first understand how the highly variable radiation of "young Suns," like T Tauri stars, affects the protoplanetary disk environment.

1.3. Influence of Stellar Radiation on Chemistry

The high levels of radiation emitted by T Tauri stars are known to shape the disk temperature and density distribution through low energy emission (Calvet et al., 1991) (e.g. IR and optical) and to drive disk chemistry through ionization by high energy emission (e.g. UV and X-rays). X-ray emission is of particular interest, as X-ray photons are capable of penetrating the inner layers of the disk, while UV photons are absorbed along the disk surface. Thus, X-rays have the potential to drive chemistry at greater disk depths (Glassgold et al., 2005). X-ray ionization occurs via the ionization of H_2 (Maloney et al., 1996), which results in the formation of H and H_3^+, both of which are essential in the formation of more complex molecules. Currently, it is considered typical for protoplanetary disk models to include a single characteristic X-ray ionization rate. However, a time variable X-ray ionization rate, as caused by X-ray flaring events, is still relatively unexplored.

2. PREVIOUS WORK

Waggoner and Cleeves (2019) and Waggoner and Cleeves (2022, hereby W22) present the most in-depth exploration of flare driven chemistry in protoplanetary disks to date. In these papers, we have used chemical disk models to show that X-ray flares drive a diverse range of chemical responses, as demonstrated in Figure 2. This figure, and the results presented in W22, model chemical evolution in response to flares for 500 years at 4 hour time step resolution. X-ray flares are modeled using a new X-ray light curve generator, or XGEN, which simulates a light curve based on an observed flare frequency and energy distribution. For the purpose of this work, XGEN uses observed statistics of solar mass stars (Wolk et al., 2005) from the Chandra Orion Ultra-deep Project (*COUP,* Getman et al., 2005). W22 have shown that flares are capable of causing rapid variability in small, gas-phase molecules (Figure 2b), while some species are gradually impacted over hundreds of years (Figure 2c), and many chemical species exhibit a combination response trends (Figure 2d). A.R.W. is currently in the process of upgrading both XGEN and the chemical disk model to more realistically represent the flaring events and the protoplanetary disk environment, as described in Sec 4.1. This will allow us to more accurately predict the flare driven chemistry in planet forming disks.

In addition to theoretical modeling, we explore observational evidence of flare driven chemistry to better constrain the implications of variable gas-phase cations. Atacama Large Millimeter Array (ALMA) observations of $H^{13}CO^+$ ($J = 3 - 2$) in the IM Lup protoplanetary disk have shown the first evidence of flare driven chemistry Cleeves et al. (2017). Cleeves et al. (2017) reported significant enhancement of $H^{13}CO^+$ flux (4σ) on one observation day compared to two others, while the continuum emission remained constant across all three epochs. Cleeves et al. (2017) were able to rule out the possibility of variability in the phase calibrator or an event that would have increased the disk temperature, such as an FU Ori outburst. Indeed, the most likely explanation for $H^{13}CO^+$ enhancement was a genuine increase in abundance driven by a flaring event. This project will search for further evidence of flare driven chemical variability in protoplanetary disks, as described in Sec 4.2.

3. RELEVANCE TO NASA AND VSGC

The results from W22 indicate that X-ray flares may contribute to several astronomical questions concerning the origins of life. In general, we find that X-ray flares tend to drive the production of more complex species. This result has direct complications to mapping out the planet formation process and origins of biologically sustaining planets. For example, observations have been unable to account for all of the sulphur in disks (e.g. Ruffle et al., 1999; Kama et al., 2019; Le Gal et al., 2019). Previous studies have suggested that this 'missing sulphur' problem could be explained by sulphur being locked up in (at this time) non-detecable organosulphides (Laas and Caselli, 2019; Shingledecker et al., 2020). Additionally, spectroscopy of comets 67P/Churyumov-Gerasimenko and 1P/Halley have shown that comets form with

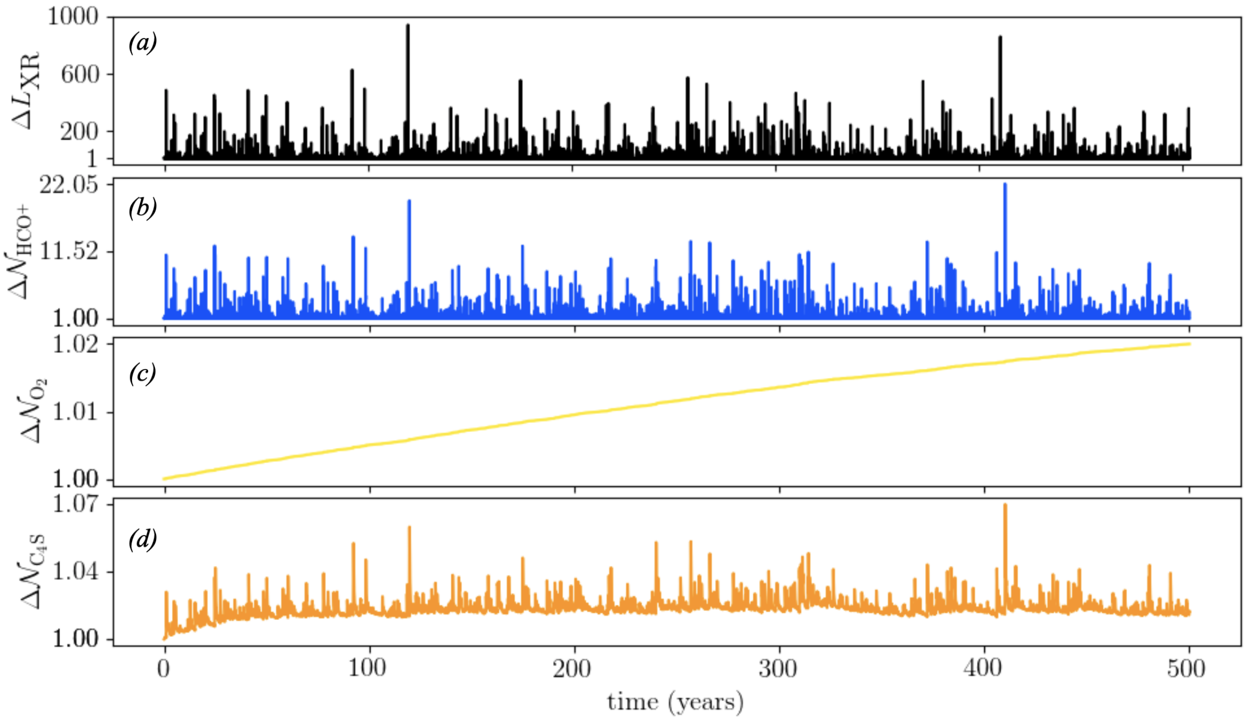

Figure 2: *(a):* A typical X-ray flare light curve for a T Tauri star simulated by XGEN, where ΔL_{XR} is the relative change in X-ray luminosity when there is a flare, compared to when there is not a flare. *(b-d)*: Relative change in disk integrated abundance of indicated species ($\Delta\mathcal{N}$). Models suggest a broad range of chemical responses to flares.

higher levels of O_2 predicted by current chemical disk models (Taquet et al., 2016; Eistrup and Walsh, 2019). The X-ray flare model predicts that flares may contribute to both of these conundrums, as we see that flares increase production rates of O_2 from O (Figure 2b), and flares aid in the conversion of atomic sulphur to organosulphides, such as C_4S (Figure 2c). Ultimately, this project is directly related to the NASA astrophysics division which seeks to "explore the origin and evolution of galaxies, stars, and planets that make up our universe*," because we are exploring a new interdisciplinary field that will aid in understanding the chemical history of life sustaining molecules.

4. CURRENT AND FUTURE WORK

4.1. Theoretical Projects

4.1.1. X-ray Hardening While XGEN has achieved the desired energy distribution and average flare frequency of T Tauri stars (as reported by Wolk et al., 2005), the current version of XGEN assumes that flares uniformly increase the X-ray spectrum.

In reality, flares disproportionally increase the number of hard X-ray photons ($>$ 1keV) emitted compared to soft photons ($\leq$ 1keV). This effect, known as hardening, increases the X-ray penetration depth, since hard photons have a lower scattering probability than soft photons. This likely means that hardening will drive X-ray photons closer to the disk mid-plane, and therefore to the chemicals available for planet formation.

Even though the current X-ray and chemical disk models do not include hardening, W22 find that flares drive chemistry to a more

*NASA Science Plan 2014, Sec 4.4 Astrophysics, page 74

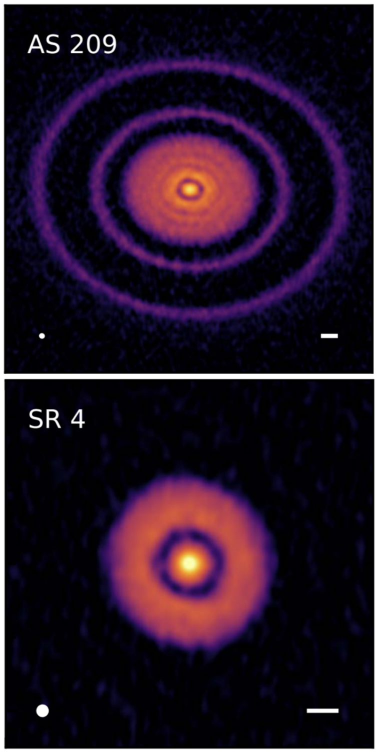

Figure 3: Modified from Andrews et al. (2018). This image shows the 240 GHz continuum for AS 209 and SR 4. Beam size and a 10 au scale are shown in the bottom left and right corners.

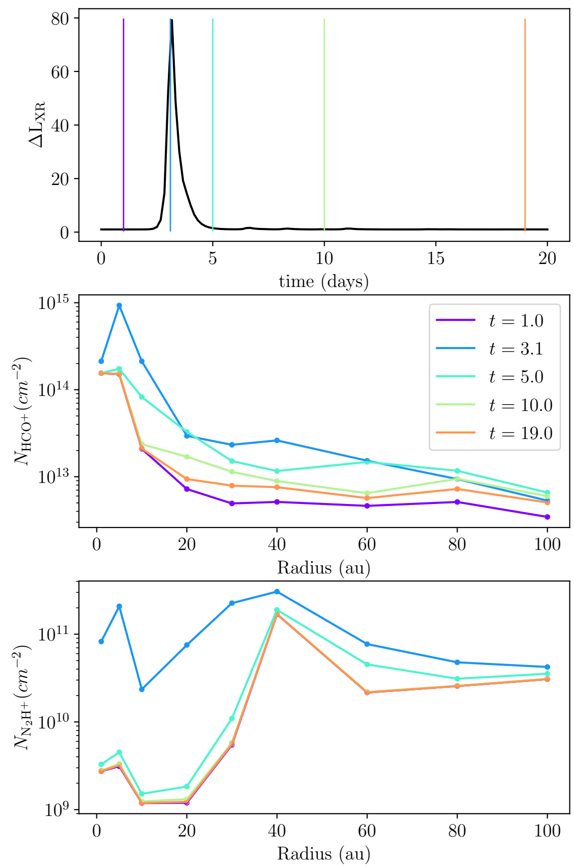

Figure 4: *Top:* X-ray flare with a peak that increases the characteristic luminosity by a factor of 80. *Middle and Bottom:* Column density (N) of HCO^+ and N_2H^+ before, during, and after a flare. Note that the flare increases N of both species by over an order of magnitude within 40 au.

complex state within the water snow line. Once X-ray hardening has been incorporated into the model, we anticipate that this affect will heighten. This project will proceed by adding a post processing script to XGEN that allows the user to create a time dependent X-ray spectrum. Currently, flares are simulated in the chemical model by including an X-ray ionization rate that scales directly with the relative changes in X-ray luminosity (i.e. uniformly increasing the X-ray spectrum). To include hardening, the time dependent spectrum created by XGEN can instead be incorporated into the chemical disk model, using the frequency dependent ionization rate calculations provided in Bethell and Bergin (2011). This will allow the model to accurately calculate a realistic time variable X-ray ionization rate at each modeled location in the disk. This project will be incorporated into structured disk model paper described in the next section.

4.1.2. Disk Substructure: Traditionally, disks have been modeled as a smooth, exponential drop off of gas and dust with increasing radius. However, observations have shown that disks exhibit a range of complex substructures including rings and gaps (Andrews et al., 2018; Öberg et al., 2021), as demonstrated by Figure 3. Previously the IM Lup protoplanetary disk was used to model the disk environment. However, IM Lup is considered a massive disk ($\log_{10} M_{disk}/M_* = -0.8$, Cleeves et al., 2016) compared to a typical disk mass ($\log_{10} M_{disk}/M_* \sim -1.5$, Andrews et al., 2013). In this project, three additional disks will be modeled using the commonly used code TORUS (Harries, 2000; Harries et al., 2004; Kurosawa et al., 2004; Pinte et al., 2009). These disks will be modeled after AS 209 (rings, Öberg et al., 2021), SR 4 (gaps, Andrews et al., 2018), and CX Tau (low mass, $\log_{10} M_{\rm disk}/M_* = -3.1$, Piétu et al., 2014) to develop a comprehensive view of flare driven chemistry in a range of known disk environments.

4.2. Observational Projects:

The observational projects will use radio and X-ray data obtained from the Sumbillimeter Array (SMA), the Atacama Large Milimeter Array (ALMA), Swift, and *Chandra*. All data for these projects has been completed and is currently accessible to A.R.W.

4.2.1. Observed Variability of $H^{13}CO^+$: As described in Sec 2, $H^{13}CO^+$ ($J = 3-2$) was observed to be in an enhanced state by Cleeves et al. (2017). Unfortunately, $H^{13}CO^+$ ($J = 3-2$) had not been re-observed in IM Lup since the observed enhancement in the third and final epoch of the project. Because of this, it is unclear if the enhancement was short lived, as the flare model predicts, or if the enhancement was actually long-lived.

To determine if the $H^{13}CO^+$ enhancement was short-lived, A.R.W. led a follow up observation of $H^{13}CO^+$ ($J = 3-2$) in IM Lup using the SMA (project code 2020B-S041). $H^{13}CO^+$ was observed on May 15, 2021 and June 13, 2021, and a preliminary analysis reveals that $H^{13}CO^+$ has returned to the pre-enhanced state. Using the same methods used by Cleeves et al. (2017), we will be able to rule out any artificial variability caused by the phase calibrator and/or temperature fluctuations.

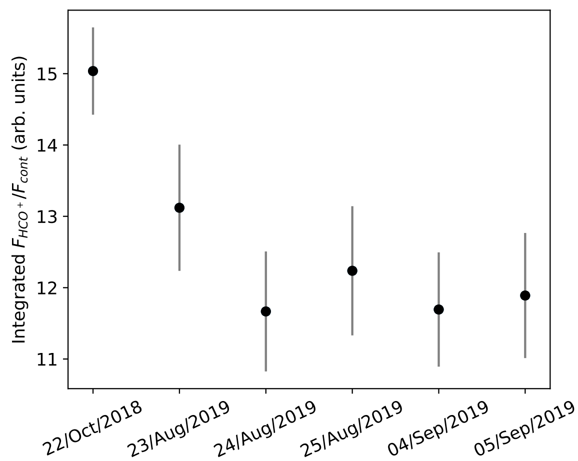

Figure 5: HD 163296 normalized flux of HCO^+ ($J = 1-0$) normalized to the continuum flux across six epochs.

4.2.2. Analysis with MAPS: The variable $H^{13}CO^+$ emission detected in IM Lup has led to the question: can variability be detected in other disks? Unfortunately, a large number of observations over several weeks (or longer) is the most likely observation set up to detect variability. This project uses ALMA observations of the most thorough radio observations of molecules in disks to date. The survey, Molecules with ALMA at Planet forming Scales (MAPS Öberg et al., 2021), observed five disks, IM Lup, AS 209, HD 163296, MWC 480, and GM Aur, a minimum of four times each between Oct 2018 and Sep 2019.

A.R.W. has completed the pipeline necessary to image line and continuum flux for each observation day. Preliminary results from HD 163296 indicate that HCO^+ ($J = 1-0$) was enhanced on 22/Oct/2021 with significant variability (4σ, Figure 5). This enhancement is attributed to a genuine increase in HCO^+ abundance, as the continuum flux remained constant. We have ensured that the increase in flux is not artificially introduced by varying telescope configures by ensuring that there is overlap in the probed UV space.

This project will continue to use the established pipeline to search for variability in the remaining four MAPS disks. We also plan on investigating other gas-phase cations, such as $H^{13}CO^+$ and N_2H^+, in disks with a strong enough detection to do so. In addition to using the MAPS data, the ALMA archive can be searched for previous observations of these disks. This project is anticipated to result in one paper highlighting variability (or the lack of) of gas-phase cations in disks.

4.2.3. Radio and X-ray Observations: While the variability detected in IM Lup and HD 163296 are best explained by an X-ray flaring event, we are unable to confirm that variability was caused by flares, because we have not yet observed a flaring event right before an observed HCO^+ enhancement. This project will seek to do so by analyzing data from a survey of protoplanetary disks in the Orion star forming cluster (PI: Cleeves). This survey observed 10 disks in both radio light (ALMA) and X-ray light (*Chandra* and Swift). These observations occurred several times throughout a week, and statistically determined that at least one flare in one disk should have been seen.

In this project we will search for variability in HCO^+ and analyze the X-ray luminosity and spectrum over the observation week. This project could provide the first direct observational evidence of flare induced chemistry, thus supporting the X-ray flare theory. It is important to note that if a strong level of variability is not detected (in X-ray or HCO^+), this project is still vital to the progression of the X-ray flare theory. For example, if the X-ray flux is observed to be quiescent, but HCO^+ emission increases, then this is evidence that a more complex phenomena than the flare theory is occurring.

5. SUMMARY

X-ray flares are known to drive chemistry and physics in all stages of the planet formation process. However, it is still uncertain the extent at which flares impact chemistry in protoplanetary disks. This research will combine theoretical models and observational astronomy spanning radio to X-ray wavelengths to constrain the implications of flare driven chemistry in planet forming disks.

6. ACKNOWLEDGEMENTS

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