Onsala Proposal

Keyte 0108.F-9320

A Song of Ice and Fire: the quest for sulfur in planet-forming disks

Semester: may2021 **Science Cat.: ISM and star formation**

Abstract

Sulfur is important in astro-, geo-, and biochemistry. Its main reservoirs in star- and planet-forming environments have however eluded observations, which are missing >90% of gaseous sulfur. Of the main volatile sulfur carriers, CS and SO have received the most attention, while H2S -- which chemical models and cometary ices suggest is the most abundant -- has rarely been targeted. We recently found 89% of elemental sulfur in Herbig Ae/Be protoplanetary disks is locked as refractory minerals in dust (likely FeS), leaving 11% of all S nuclei for volatiles. We propose to target H2S to reveal volatile S in the warm HD 100546 disk. In this system, slow stellar mixing and a high disk accretion rate, along with a dust-poor inner disk cavity, allow us to predict with high confidence the amount of sulfur in the gas phase in the inner 13au of the disk. This observation would lead to the first complete accounting of all key sulfur reservoirs in a planet-forming disk, paving the way for new disk-planet composition links using sulfur species.

Applicants

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Is this a long term proposal: No

No overall scheduling requirements

Observing runs

run	telescope	instrument	time request (minimal)	frequency (GHz)	weather (pwv)	LST range	comments/constraints
A	APEX	SEPIA180 (159-211 GHz)	24h (8h)	168	1-2 mm		Targeting the o-H2S 1_1_0 - 1_0_1 line at 168.76276GHz

Targets

Source	RA	Dec	Epoch	Vlsr (km/s)	Duration (min)	Runs	Comments
HD100546	11:33:25.44	-70:11:41.2	J2000	6.0	367	A	

Executive summary

Sulfur is a bio-essential element, central to astro- and geochemisty, but poorly understood in the context of star and planetary formation. Leveraging previous observations and following our recent discovery that 89% of sulfur in Herbig Ae/Be disks is locked in refractory species, we propose to track down the elusive volatile component - 11% of total S/H - by observing the ortho-H_2S $1_{1,0}1_{0,1}$ transition at 168.7 GHz in the HD 100546 disk with APEX/SEPIA.

1 Introduction: the missing sulfur problem

Understanding sulfur's path from the interstellar medium through disks and into planets is of increasing importance, relevant to the study of planetary formation and the search for life. The sulfur abundance in the envelopes of giant planets may act as a diagnostic of their formation history, complementing the carbon-to-oxygen ratio (e.g. Öberg et al. 2011), while the FeS content in rocky planets affects the speed of differentation and core formation.

For decades, most of the sulfur in protostellar clouds and protoplanetary disks has eluded detection; the "missing sulfur problem". In the diffuse interstellar medium, over 99% of sulfur is in the gas phase (Savage & Sembach 1996), with an estimated cosmic abundance of S/H $= 1.3 \times 10^{-5}$. In dense, cold protostellar cores, a factor of $\sim$10 depletion is observed, i.e. $[S/H]_{gas} \leq 10^{-6}$ (e.g. Tieftrunk et al. 1994). It is unclear where the missing sulfur is, as the abundances of dominant gas- or ice-phase carriers such as CS, SO, SO_2, OCS, H_2S_2, HS_2, and S_2 are $\leq 10^{-7}$ (Boogert et al. 1997; Geballe et al. 1985; Martín-Doménech et al. 2016; Palumbo et al. 1995; Schöier et al. 2002; van der Tak et al. 2000). Models predict that S-atoms frozen onto dust grains preferentially interact to form H_2S (Charnley 1997), and indeed solid-phase H_2S has the highest inferred abundance, S/H $\sim 10^{-7} - 10^{-6}$ (Smith 1991; van Dishoeck & Blake 1998) - although still a factor of ≥ 10 below the total S/H.

The main carrier of volatile sulfur in protoplanetary disks is similarly unknown. Astrochemical models predict the dominant carriers of volatile sulfur in disks to be H_2S, SO, SO_2, and CS, while the main refractory component is iron sulfide, FeS (e.g. Pasek et al. 2005; Wakelam et al. 2004). The conversion from volatile molecules to FeS likely proceeds in the early stages of disk evolution when, it is hypothesized, gas-phase molecules react with warm, iron-rich dust grains (e.g. Lauretta et al. 1996). Members of our team recently measured the FeS abundance in a sample of disks to be 89% of the total sulfur (Kama et al. 2019), leaving 11% to be distributed to volatile molecules. Observations of disks such as AB Aur, DM Tau, and GG Tau A have found gas-phase CS, SO, and H_2S corresponding to $[S/H]_{gas}$ values that are factors of 10 to 1000 lower than the total elemental S/H (Blake et al. 1992; Dutrey et al. 2011; Fuente et al. 2010; Kastner et al. 2014; Phuong et al. 2018). A full accounting of sulfur has not yet been completed for any protoplanetary disk.

2 Target: HD 100546

HD 100546 is a well-characterized Herbig Ae/Be disk system (e.g. Booth et al. 2018; Bruderer et al. 2012; Kama et al. 2016; Walsh et al. 2014). It is one of the closest and brightest protoplanetary disks, situated at 108pc (Gaia Collaboration et al. 2018) around a luminous A0 star (Vioque et al. 2018). It is one of the few disks for which a well-constrained 2D structure model is available (Bruderer et al. 2012; Kama et al. 2016), constrained by the spectral energy distribution (Mulders et al. 2013), spatially resolved CO 3-2 emission (Walsh et al. 2014), and various lines of CO isotopologs and other species (Bruderer et al. 2012; Kama et al. 2016).

The disk has a warm (200 K), large (r=13 au), and dust-depleted inner cavity. Its outer edge acts as a filter, allowing only gas-phase volatiles and a small amount of refractory dust to pass onto the star (Figure 1). The host star has a radiative, slowly-mixing envelope, such that the elemental composition in the inner cavity is imprinted on the stellar photosphere. In effect, the photospheric composition provides a snapshot of the most recently accreted material, freshly arrived through the inner disk cavity. Using this indicator, the baseline prediction for the fractional amount of elemental sulfur in gas-phase species and small dust grains combined is $\approx 30\,\%$ for this disk (Kama et al. 2016). Volatile species carry $\approx 11\,\%$ of all sulfur in Herbig Ae/Be disks (Kama et al. 2019). Both numbers suggest a significant fraction of total sulfur is in the gas phase in the dust-poor inner cavity, providing a testable prediction for this proposal.

We have obtained upper limits for CS, SO, SO_2, and several minor sulfur-bearing species in HD 100546 with ALMA (2017.1.00885.S) and for H_2S with APEX (0104.F-9308). An incomplete execution within 2017.1.00885.S yielded an ACA detection of CS 7-6 (0.47 Jy beam^{-1} km s^{-1}). In totality, these data are consistent with an outer disk gas-phase sulfur depletion factor of 10^5 ($[S/H]_{gas} \approx \times 10^{-10}$ at >13 AU), but are insufficient to strongly constrain abundances within the disk cavity. By measuring the H_2S line emission we will complete the sulfur inventory for the disk of HD 100546.

An analysis of archival ALMA data yields a faint detection consistent with a full-disk molecular abundance of SO/H $\sim 10^{-7}$ to 10^{-6} (Booth et al. 2018). This is higher than we report above, but that work did not study cavity-dominated abundance distributions and used a simpler, less constrained physical model. Our comprehensive analysis will include findings from that work.

3 Modelling and analysis

Our analysis will utilize the DALI disk modelling code (Bruderer et al. 2012) which solves for radiative transfer, gas and dust thermal balance, and chemistry using the UMIST/Rate12 gas-phase chemical network (McElroy et al. 2013) which includes sulfur. We will adopt both forward-modelling and retrieval techniques. The H_2S abundance can be retrieved by varying the H_2S abundance to match observations. In forward-modelling, we will run a full chemical network on the physical disk structure, determining the total gas-phase S/H from the H_2S data, as illustrated in Figure 2.

We will quantify the H_2S abundance and it's role in the volatile sulfur budget. If it is as high as expected, the APEX data will complete the first-ever sulfur inventory in a protoplanetary disk. If it is low, we will have ruled out all "classical" candidate molecules as the main carriers of volatile sulfur in the inner disk. This could suggest an important role for small sulfur chains, S_n ($n \in [2, 8]$) which lie between H_2S and FeS in sublimation temperature, although high abundances are not predicted by laboratory work or chemical models (Druard & Wakelam 2012; Jiménez-Escobar & Muñoz Caro 2011).

Completing the inventory of sulfur in HD 100546 will allow us to contribute to an improved understanding of the sulfur content of all disks, and of planetary cores and atmospheres which are built up of solids and volatiles respectively. This will open new avenues beyond the C/O ratio to constrain the formation location of giant planets (Turrini et al. 2021) and late-stage volatile delivery, as JWST and ARIEL will be able to measure the H_2S abundance in Hot Jupiters.

4 Observation request

We request a total of 23.8 hours of time including overheads (6.1 hours on-source). This was calculated using our customised HD 100546 disk model, and the online observing time estimator V6.1.2, with a goal RMS of 1.1mK in $dv = 1$ km s^{-1} channels. Integrated across the expected FWHM of 35 km s^{-1}, this corresponds to a 3σ gas-phase sulfur abundance detection limit of $S/H = 10^{-7}$, or 0.01 of total elemental sulfur.

References

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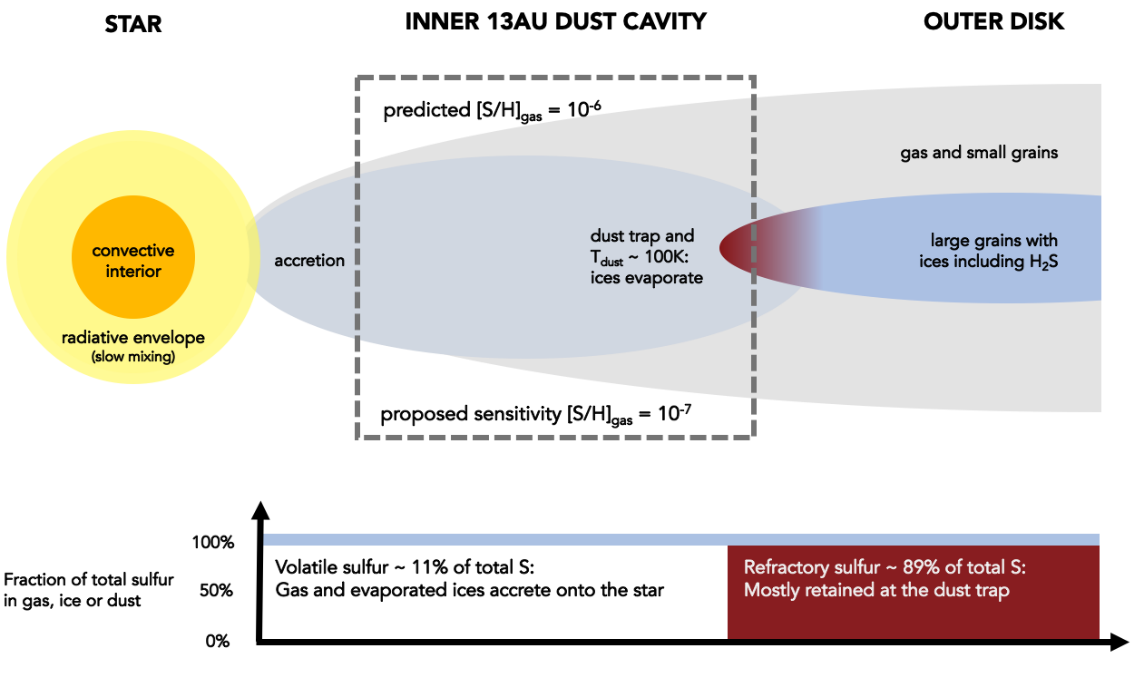

Figure 1: Gaseous sulfur in the warm, dust-depleted cavity of the HD 100546 disk. Our physical-chemical model, based on that in Kama et al. (2016), predicts most of the available gas-phase sulfur to be contained in H_2S molecules.

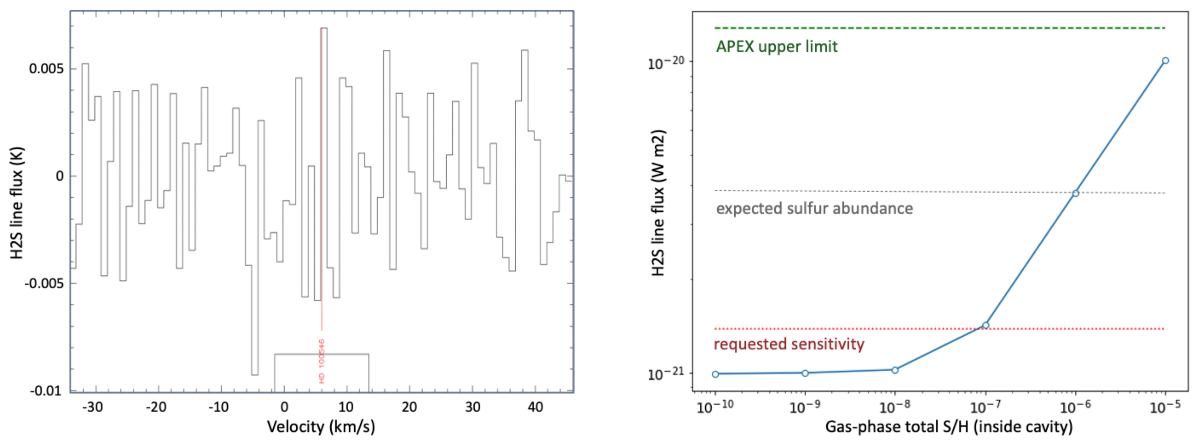

Figure 2: *Left-hand panel:* ortho-$H_2S\,1_{1,0}-1_{0,1}$ spectrum previously obtained with APEX, from which we infer an upper limit on the disk-integrated flux of $1.28\times10^{-20}\,\mathrm{W\,m^{-2}}$. *Right-hand panel:* Modelled disk-integrated line fluxes where $[\mathrm{S/H}]_{\mathrm{gas}}$ ranges from 10^{-5} to 10^{-10} in the inner cavity, and is always fixed at 10^{-10} outside (based on past data). Our requested RMS is sensitive down to an elemental abundance of $[\mathrm{S/H}]_{\mathrm{gas}}=10^{-7}$ in the cavity.

Students involved

Student	Level	Applicant	Supervisor	Applicant	Expected completion date	Data required
Mr Luke Keyte	Doctor	Yes	Dr. Mihkel Kama	Yes	2024/03	No

Linked proposal submitted to this TAC: No

Linked proposal submitted to other TACs: No

Relevant previous Allocations: Yes

0104.F-9308, 2h total, H2S upper limit factored into the preparation of this proposal

Additional remarks

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Observing run info :

Run: A backup strategy: To integrate as deep as possible. Any data will improve our signal-to-noise for this spectral line. We note that the minimum useful time represents a compromise to still retain sensitivity to very low sulfur abundance.