Onsala Proposal

Rivilla 0108.F-9308

Is phosphine (PH3) the main carrier of Phosphorus in molecular clouds?

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

Abstract

We propose to detect phosphine (PH3) for the first time in the interstellar medium performing deep APEX observations of the G+0.693-0.027 molecular cloud located in the Galactic Center. PH3 is expected to be formed very efficiently on the surfaces of grains through hydrogenation of atomic phosphorus, according to theoretical calculations and chemical models. The cloud G+0.693-0.027 is the best source to detect PH3 because it presents a very rich chemistry due to dust grain sputtering induced by large-scale molecular shocks. While other P-bearing species, such as PO and PN, have been already detected, PH3 has not been reported yet. Based on the predictions of our chemical models, and on radiative transfer calculations (LTE and non-LTE), we argue that this project will confirm whether PH3 is the main carrier of phosphorus in the ISM. The derived abundance of PH3 in the case of detection, and even the upper limit if it is not detected, will impose strong constraints on the still poorly understood chemistry of interstellar phosphorus.

Applicants

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Is this a long term proposal: No

Overall scheduling requirements

none

Observing runs

run	telescope	instrument	time request (minimal)	frequency (GHz)	weather (pwv)	LST range	comments/constraints
A	APEX	nFLASH230 (200-270 GHz)	14h (14h)	266.944	1-2 mm	13-22	

Targets

Source	RA	Dec	Epoch	Vlsr (km/s)	Duration (min)	Runs	Comments
G0.693	17:47:21.90	-28:21:27.2	J2000	69.0	864	A	

1 Scientific Rationale: Phosphine in the ISM?

The detection of molecules related to prebiotic chemistry in molecular clouds allows us to better understand how the building blocks of life could originate in the interstellar medium (ISM). Among life's key elements (CHNOPS), phosphorus (P) is the least understood. It plays a central role in the formation of macromolecules such as DNA and RNA (genetic information), ATP (energy currency in cells) or phospholipids (structural components of cell membranes). P has a low cosmic abundance, P/H$\sim 3\times 10^{-7}$ (Asplund et al. 2009), which makes the detection of P-bearing molecules in the gas phase very challenging. In the last years, considerable advances in understanding the interstellar chemistry of P have been made. PN, and more recently PO, have been detected in several massive star-forming regions (Fontani et al. 2016, 2019, Rivilla et al. 2020a, Mininni et al 2018, Bernal et al. 2021), low-mass star-forming regions (Lefloch et al. 2016, Bergner et al. 2019), and Galactic Center molecular clouds (Rivilla et al. 2018; see Fig. 1). These works have shown that P is much less depleted on grains (depletion factor $\sim$100) than previously thought, and that the abundance of PN is correlated with that of SiO, a well-known shock-tracer. These results suggest that shocks are able to sputter dust grains and release to the gas phase significant amounts of P-bearing species that were locked on grains. The PO/PN ratios found (1.5$-$8) in different sources indicates that PO is more abundant than PN. However, the details of the chemistry remain largely unknown. *Are PO and PN the main reservoirs of P in the ISM, or alternatively most of the P is in another species?*

In particular, there is a key piece that is still missing: **phosphine (PH_3) has never been detected in the ISM**. This species has only been reported in the circumstellar envelope of an evolved star (Agundez et al. 2014), and towards the atmospheres of Jupiter and Saturn (Bregman et al. 1975; Ridgway et al. 1976). The non detection in the ISM is puzzling because chemical models show that PH_3 should be formed very efficiently on the surfaces of grains through hydrogenation of atomic P (Jimenez-Serra et al. 2018), in agreement with recent quantum theoretical studies (Molpeceres et al. 2021). The results of chemical models of shocked material developed by our group (Jimenez-Serra et al. 2018) shows that after the shock passage the PH_3 abundance is at least a factor of 5 higher than that of PO and PN. This indicates that PH_3 should be the main reservoir of P in gas enriched by freshly-sputtered icy mantles. Then, *why phosphine has not been detected yet?* This could be due to several reasons. First, only the J=1$-$0 transition of PH_3 at 266.944 GHz is observable from the ground in a reasonable observing time. Secondly, the PH_3 J=1$-$0 transition can be contaminated by other species: i) the SiS v=4 (15$-$14) transition, as observed in the envelope of the evolved star IRC+10216 (Agundez et al. 2014); ii) the SO_2 $30_{9,21}-31_{8,24}$ transition at 266.943 GHz which has been proposed as the responsible of the weak absorption line recently detected in the Venus's atmosphere close to the PH_3 J=1$-$0 frequency (Villanueva et al. 2021); and iii) the $12_{3,9}$-$11_{1,10}$ transition of methyl formate (CH_3OCHO) at 266.9337 GHz. Therefore, to successfully detect PH_3 in the ISM for the first time, we should search for it towards a source in which significant amounts of P are present in the gas-phase (thanks to shock-induced grain sputtering), and where there is not severe blending from the possible contaminants. The target that best fullfills these conditions is the molecular cloud G+0.693-0.027.

2 This project: Detection of PH_3 towards the G+0.693 molecular cloud

We propose to detect the PH_3(1$-$0) transition towards the G+0.693-0.027 molecular cloud (hereafter G+0.693) located in the Galactic Center. This cloud, although does not show any sign of active star formation such as H_2O masers, HII regions or dust continuum sources, exhibits an extremely rich chemistry. Our deep spectral survey towards this source has detected more than 120 molecules, including several first detections in the ISM, such as hydroxylamine (NH_2OH; Rivilla et al. 2020b), propargylimine (HCCCHNH, Bizzocchi et al. 2020), the Z-isomer of cyanomethanimine (Z-HNCHCN, Rivilla et al. 2019b), or thioformic acid (HCOSH; Rodríguez-Almeida et al. 2021). The chemical richness of this molecular cloud is thought to be mainly due to dust grain sputtering induced by large-scale molecular shocks related with a cloud-cloud collision (Zeng et al. 2020). Therefore, **the G+0.693 molecular cloud is an excellent source to study the freshly sputtered material from the icy mantles, and in particular, of phosphorus-bearing species.** This has been already confirmed by the previous detections of PN and PO (see Fig. 1), reported by Rivilla et. (2018), with a PO/PN ratio of ∼1.5. Moreover, G+0.693 presents another important advantage for the detection of PH_3. Since the gas densities are relatively low (n ∼10^{4-5} cm^{-3}; Zeng et al. 2020), all the molecules are sub-thermally excited, which results in low excitation temperatures of T_{ex}=5−20 K, well below the kinetic temperature of the gas (50−100 K; Zeng et al. 2020). For the case of PN, the three transitions detected are well fitted, assuming Local Thermodynamic Equilibrium (LTE) conditions, with T_{ex}=5 K (Fig. 1; Rivilla et al. 2018). Thus, only the lowest energy levels of the molecules are excited (E_{up} < 30 K), which produces a spectrum with significantly less blending problems.

• **Feasibility, line intensity and observing time estimates:** We have simulated the expected line emission of the PH_3(1−0) transition toward G+0.693, and have conservatively assumed a column density similar to that measured for PO toward this source (N =8.5×10^{12} cm^{-2}). We have assumed the T_{ex}=5 K and the $FWHM$=24 km s^{-1} derived for the fit of the several transitions of PN (Fig. 1), and the column density derived for PO (more abundant than PN) of N =8.5×10^{12} cm^{-2}. The predicted line intensity is ∼9 mK, as shown in Fig. 2 (dark blue). We thus request an rms of 1 mK, which will allow us to detect the PH_3(1−0) transitions at 9σ level if PH_3 is as abundant as PO. Since collisional coefficients of PH_3 have become recently available (Badri et al. 2020), we have also estimated the line intensity using non-LTE excitation with RADEX (van der Tak et al. 2007). The results are shown in Fig. 2 (right). For T_{kin}=50−150 K and n ∼10^{4-5} cm^{-3}, derived towards G+0.693 by Zeng et al. 2020, we expect lines intensities >20 mK, assuming the same column density and linewidth as in the LTE case. Therefore, the predicted LTE line intensity is conservative. To check that the line is not blended with other species, we have also predicted the contribution of the three possible contaminants (SO_2, SiS v=4, and CH_3OCHO), from the fits derived from our G+0.693 spectral survey. As expected, the high-energy transitions of the two former species (E_{up}=4342 and 625 K, respectively) are completely negligible in G+0.693. In the case of the CH_3OCHO transition (E_{up}=53.2 K), whose LTE best fit is shown in Fig. 3 (N =(5.8±0.4)×10^{14} cm^{-2}, T_{ex}=13±1 K, $FWHM$=20 km s^{-1}), the predicted line intensity is lower than the requested rms, and does not produce significant contamination to the PH_3 line, as shown in Fig. 2 (left). We have used the ON-OFF observing time calculator APEX V7.3 to estimate the total time needed to achieve our goal. Using NFLASH230 tuned to 266.944 GHz in the USB, selecting a spectral resolution of 3 km s^{-1} (enough to resolve the expected linewidths of ≥20 km s^{-1}), and assuming a typical source elevation of 45 deg and a typical PWV of 2 mm, we obtain a noise of 1 mK[Ta*] in **14.4 hours** (including telescope and calibration overheads). We stress that APEX is the only instrument that can carry this project in a reasonable amount of time: to achieve the same sensitivity using the IRAM 30m we would need more than 300/80 hr under average/good conditions (4mm/2mm pwv), and ALMA will filter out most of the extended emission from this cloud.

• **Scientific outcome:** This project aims to provide the first detection of PH_3 in the ISM. **If detected, we will confirm that PH_3 is equally or more abundant than PO and PN, and thus we will be able to establish if PH_3 is the main carrier of P in the ISM**. We note that even in the case of non detection, the 3σ upper limit will imply that PH_3/PO<1/4, which would clearly show than PH_3 is not the main carrier of P, and will suggest that this species is rapidly destroyed in gas phase. Therefore, *whatever the result of the observations is, it will impose important constraints to our current understanding of the P chemistry in the ISM.* We will derive the abundances of the three species using LTE and non-LTE analysis (the latter already used in Rivilla et al. 2020a for PO and PN in a star-forming region; and in this proposal for PH_3, Fig. 2), and we will compare them with the predictions of the chemical models that our group has already developed (Jimenez-Serra et al. 2018).

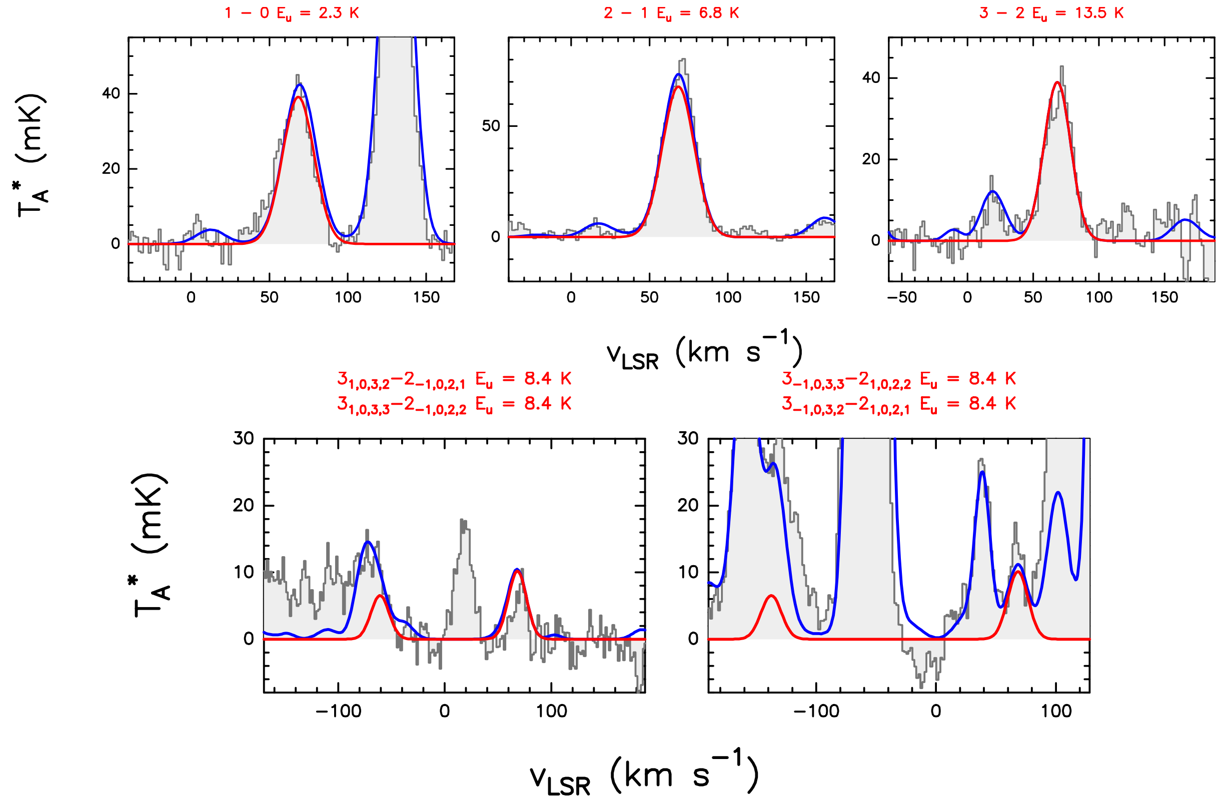

Figure 1: Detections of PN (upper) and PO (lower) towards the G+0.693 molecular cloud. The red curve indicates the best LTE fit for the P-bearing molecules, while the blue line indicates the contribution of all the molecules identified so far towards the cloud. The parameters of the best fits are: N =6.6×10^{12} cm^{-2}, $T_{\rm ex}$=5 K, $v_{\rm LSR}$=68.4 km s^{-1}, and $FWHM$=24 km s^{-1} (for PN); and N =8.5×10^{12} cm^{-2}, $T_{\rm ex}$=5 K, $v_{\rm LSR}$=68.2 km s^{-1}, and $FWHM$=20 km s^{-1} (for PO). The quantum numbers and upper energies of the transitions are indicated above each panel.

References • Agundez et al. 2014, ApJL, 790, L27 • Aplund et al. 2009, ARA&A, 47, 481 • Badri et al. 2020, MNRAS, 499, 1578 • Bergner et al. 2019, ApJ, 884, 36 • Bernal et al. 2021, ApJ, 906, 55 • Bizzocchi et al. (2020), A&A, 640, A98 • Bregman et al., 1975, ApJ, 202, L55 • Codella et al. 2018, MNRAS, 474, 5694 • Fontani et al. 2016, ApJ, 822, 30 • Fontani et al. 2019, MNRAS, 489, 4530 • Jimenez-Serra et al., 2018, ApJ, 862, 128 • Jiménez-Serra et al. 2020, Astrobiology, 1048-1066 • Lefloch, B. et al. 2016, ApJ, 462, 3937 • Molpeceres et al. (2021), ApJ, 910, 55 • Mininni et al. 2018, MNRAS, 476, L39 • Ridgway et al., 1976, ApJ, 207, 1002 • Rivilla et al. 2016, ApJ, 826, 161 • Rivilla et al. 2018, MNRAS, 475, L30 • Van der Tak et al (2007), A&A 468, 627 • Requena-Torres et al. 2008, ApJ, 672, 352 • Rivilla et al. 2019b, MNRAS, 483, L114 • Rivilla et al. 2020b, ApJL 899 L28 • Rodríguez-Almeida et al. 2021, ApJL, 912, L11 • Van der Tak et al (2007), A&A 468, 627 • Villanueva et al. (2021), arXiv:2010.14305 • Zeng et al. 2018, MNRAS, 478, 2962 • Zeng et al. 2020, MNRAS, 497, 4896

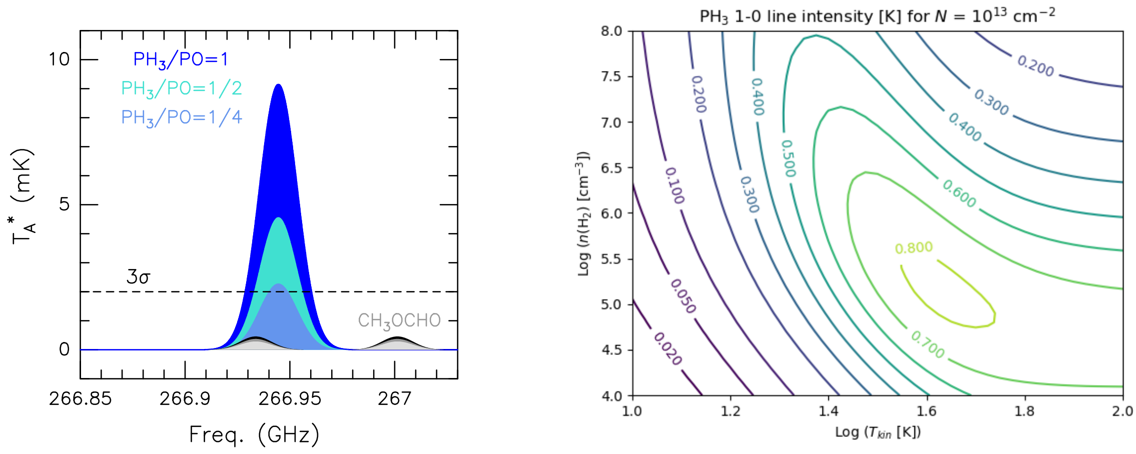

Figure 2: *Left:* Predicted line intensity of the $PH_3(1-0)$ transition towards G+0.693. We have assumed LTE excitation, using the temperature derived from the fit of PN shown in Fig. 1 (T_{ex}=5 K). We have considered three values for the PH_3 column density: equally abundant to PO (dark blue), less abundant by a factor of 2 and 4 (turquoise and cyan, repectively). The contribution of CH_3OCHO, calculated from the LTE fit shown in Fig. 3, is also shown. The gray curve shows the best LTE fit, while light gray and black show the minimum and maximum lines intensities, respectively, considering the uncertainties of the fit. The 3σ level of the proposed observations is denoted with a dashed black horizontal line. *Right:* Non-LTE calculations for the line intensity of $PH_3(1-0)$ assuming a column density of N=10^{13} cm^{-2}, $FHWH$=1 km s^{-1}, as a function of the volume gas density n and the kinetic temperature $T_{\rm kin}$. We have generated the plot using RADEX with the collisional rates from Badri et al. (2020). The colored lines show to the line intensity of the $PH_3(1-0)$ transition indicated in the labels (in K). Note that to estimate the expected line intensity towards G+0.693 the line intensities should be divided by the $FWHM$ of this cloud, which is ∼20-24 km s^{-1}, and scaled by the column density assumed.

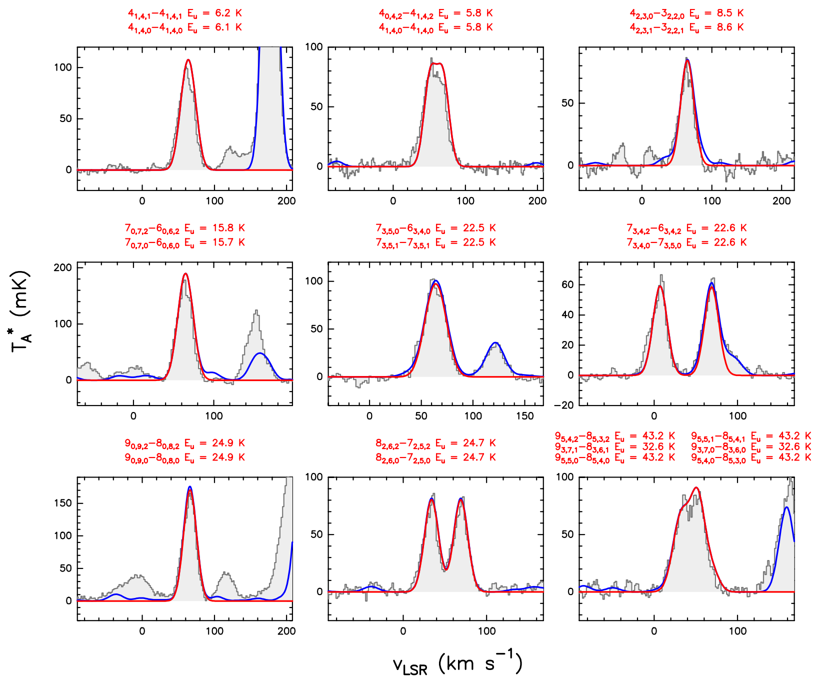

Figure 3: Selected transitions of methyl formate (CH_3OCHO) detected towards G+0.693. The red curve indicates the best LTE fit for CH_3OCHO, while the blue line indicates the contribution of all the molecules identified so far towards the cloud. The quantum numbers and upper energies of the transitions are indicated above each panel. The parameters of the best fit are: N = (5.8±0.4)×10^{14} cm^{-2}, T_{ex}=13±1 K, $v_{\rm LSR}$=69 km s^{-1}, and $FWHM$=20 km s^{-1}.

No PhD Students involved

Linked proposal submitted to this TAC: No

Linked proposal submitted to other TACs: No

Relevant previous Allocations: No

Additional remarks

ESO=<rivilla>

Observing run info :

Run: A backup strategy: The estimated observing time has been obtained for average weather conditions (2mm), however we note that NFLASH can be also used in less favourable conditions and that slightly worse PWV values (< 3mm) during the observations will not affect the project outcome.