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Models for the atmospheres of distant comets: application to the detectability of carbon monoxide.

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Summary

We review the volatile molecules which might be responsible for cometary activity at large heliocentric distances. From our present knowledge, carbon monoxide is a likely candidate for remote sensing searches. After a short review of the physical conditions pertaining to the atmopheres of distant comets, we present a model of excitation of the emission lines of CO in these extreme conditions. We compute the signal intensities and compare them with the sensitivity of the best available facilities (IRAM mm-telescope, ISO, HST). The search for the CO lowest rotational lines appears to be the most promising. The CO J(2-1) line at 230 GHz might have been detectable with the IRAM telescope if the observation had been performed just after the recent outburst of P/Halley.

1. Volatiles responsible for distant cometary activity

Spectroscopic clues to the molecular content of distant comets are very sparse. The spectrum of P/Schwassmann-Wachmann 1 revealed CO^+, CN, and an unidentified band at 390.8 nm (Cochran & Cochran 1991). The CN band was detected in Chiron (Bus et al. 1991). No feature could be detected in the spectrum of P/Halley after its recent outburst (West et al. 1991).

Table 1 gives a list of volatile molecules that might be present in cometary nuclei, ordered by sublimation temperatures. This table is taken from Yamamoto (1985) and extended by Crovisier et al. (1992). Exotic species such as ions or radicals are not considered here. The listed temperatures are those of a pure species in equilibrium with its own vapour. They should be interpreted with caution, since cometary ices are complex mixtures.

The equilibrium temperatures in the Solar System are 125 K at 6 AU (P/Schwassmann-Wachmann 1), 85 K at 10 AU (Chiron), and 73 K at 14 AU (P/Haley during its recent outburst). The CN band detected in Chiron can difficultly be explained by the dissociation of HCN, which has an equilibrium sublimation temperature of 95 K. The presence of CO^+ in P/Schwassmann-Wachmann 1 is also a puzzle, due to the slow photoionization rate of CO at that heliocentric distance.

Highly polar molecules such as H_2S, OCS or NH_3 are likely to be trapped by water ice and to have their sublimation linked to that of water. Therefore, the most likely candidates in Table 1 for outgassing at large heliocentric distances are CO, N_2 and CH_4. Among these, only CO has been detected with significant abundances in comets. It has allowed vibrational and rotational transitions (although its electric dipole moment is relatively small: 0.1 D). The symmetric N_2 molecule has no allowed rotational nor vibrational transitions. CH_4 has only vibrational transitions. It thus seems encouraging to investigate the possibility to observe CO in distant comets.

Table 1: Sublimation temperatures

Molecule	log [X]/[H]	$T_{subl.}$	Reference
H_2O	**-4**	**152**	**Y**
H_2O_2	-7	128	HPC (S)
HCOOH	-7	112	Y
CH_3COOH	-8	106	HPC (S)
C_2H_5OH	-8	105	HPC (L)
CH_3OH	**-8**	**99**	**Y**
HCN	**-7**	**95**	**Y**
CH_3OHCO	-8	95	HPC (L)
SO_2	-8	83	Y
NH_3	-7	78	Y
HC_3N	-8	74	Y
C_3O_2	-8	73	HPC (L)
CH_3CHO	-8	73	HPC (L)
CO_2	**-5**	**72**	**Y**
CH_3CCH	-8	65	Y
H_2CO	**-8**	**64**	**Y**
CH_3OCH_3	-8	60	HPC (L)
N_2O	-7	59	HCP (S)
H_2S	**-7**	**57**	**Y**
OCS	-8	57	HPC (L)
CH_4	-4.5	31	Y
CO	**-5**	**24**	**Y**
N_2	-4	22	Y
H_2	0	5	Y

For a density of 10^{13} cm^{-3}. Detected molecules are in boldface.
Y: Yamamoto (1985); HPC: from Handbook of Chemistry and Physics, solid(S) or liquid (L) phase.

2. Physical conditions in the atmospheres of distant comets

Basically, the physical processes in distant comets are the same as those pertaining to comets in the inner Solar System, but with different scales.

Photolytic rates, which are proportionnal to r_h^{-2}, are excessively slow. Thus, photolytic heating is completely inefficient. Radiative cooling, which is an efficient process when water is abundant, can be neglected in distant comets whose atmospheres contain esssentially non-polar molecules or molecules with weak rotational lines. A more detailed analysis of radiative cooling is given in the Appendix.

The volatiles are no longer dominated by water, and the different composition leads to different hydrodynamics. Ip (1983) has analysed the hydronamics of a coma dominated by CO, but only for r_h = 1 AU. More important are the initial conditions at the surface: the smaller equilibrium temperature leads to significantly smaller expansion velocities.

The large size of some objects (Chiron) may lead to specific effects not included in present models of nearby comets. Gravity has to be considered, especially for dust. Geometry effects may be different: in a spherically symmetric model, the distance to nucleus centre may not be approximated to the distance to the surface; the expanding gas stays a longer time in a region of nearly constant density.

We will not further comment on such models. See Luu & Jewitt 1990, Meech & Belton 1990 and Boice & Huebner 1992 for more details.

3. The detectability of CO in distant comets

3.1 Models for molecular emission

3.1.1 Geometrical parameters

Assuming CO is a parent molecule sublimating from the nucleus, its density distribution is governed by the photodissociation rate and the expansion velocity.

With a photodissociation rate of 6.5 10^{-7} s^{-1} at 1 AU the CO lifetime is 18 days at 1 AU, and 10 years at 14 AU ! (As commented by M.C. Festou at this worshop, the CO lifetimes based from recent UV absorption spectra may be shorter by a factor of 2-3. This will not affect much our conclusions, however.)

The expansion velocity v_{exp} is somewhat larger than the sound velocity at the nucleus surface $v_c = (\gamma k T / m)^{1/2}$. At 1 AU, where sublimation is governed by water at 185 K, v_c = 0.34 km s^{-1} and v_{exp} is about 0.8 km s^{-1}, as shown both by measurements and hydrodynamical models. At 14 AU, if sublimation is governed by CO at 30 K, v_c = 0.11 km s^{-1} and we will assume that v_{exp} = 0.25 km s^{-1}.

3.1.2 Parameters of the excitation model

The ro-vibrational lines in the IR and the electronic bands of the 4th positive system of CO in the UV are emitting through fluorescence excited by the Sun. Fluorescence rates are thus proportional to r_h^{-2}, which gives excessively small rates at 14 AU. These rates are independent of the rotational distribution (i.e. of collisional rates or of temperature).

Rotational emissions in the millimetre and sub-millimetre regions depend upon the rotational distribution. At 1 AU, this distribution is ruled by the competition between collisions in the inner coma, and radiative excitation which tends to establish *fluorescence equilibrium* in the outer coma. We have modelled the evolution of the rotational population distribution as a function of distance to nucleus (Crovisier 1987). A 14 AU, radiative excitation can be neglected. We will assume that the initial T_{rot} at the surface is 30 K. When escaping from the nucleus, this temperature may become cooler, due to adiabatic expansion. It may also get warmer, due to heating by dust (Boice et al., *this workshop*). In our model, we will assume that either T_{rot} is constant (30 K), or that the rotational distribution is evolving from an initial T_{rot} = 30 K through spontaneous decay. The two cases lead to only small differences, because the Einstein coefficients A_{ij} for the first rotational lines of CO are very small ($A_{ij}(1\text{-}0)$ = 7 10^{-8} s^{-1}).

3.2 Sensitivity of available facilities

3.2.1 Radio: the IRAM 30-m telescope

The IRAM 30-m radio telescope can observe the *J(1-0)* CO line at 15 GHz or the *(2-1)* line at 230 GHz. The second one is more favourable (see below), but can only be observed by good weather. The *J(3-2)* line is only accessible by smaller telescopes at very good sites. From our experience of the observation of the 3_{12}-2_{11} line of formaldehyde at 225 GHz in various comets (Colom et al. 1992), we estimate that a conservative 5-σ upper limit on the *J(2-1)* CO line area is 0.1 K km s^{-1} for a few hours of integration.

One may wonder why this line has not yet been detected in comets: It was unsuccessfully searched for in P/Halley; at that time, the IRAM telescope was not equipped with a low-noise receiver at the frequency of the CO *J(2-1)* line. When we observed comets Austin 1990 V and Levy 1990 XX, during our limited alloted observing time, we gave a higher priority to the study of the HCN and H_2CO lines with the 1.3 mm receiver than to the CO line. If that line were searched for, we estimate that it could have been easily detected (Crovisier et al. 1992).

3.2.2 Infrared: the ISO photometer (ISOPHT-S)

We surmise that the most sensitive instrument to look for CO ro-vibrational lines will be the ISO satellite, to be launched in 1994.

One of the instruments of the ISO payload, the photometer, has a very efficient low-resolution spectrometer (ISOPHT-S). It is equipped with a grating and can observe the 2.5-5 μm region with 64 detectors in parallel, with a resolution of 0.04 μm. Its field of view has a diameter of 24", and its nominal sensitivity is 0.29 Jy per spectral element for 100 s integration and a S/N of 10 (ESA 1991). For a band 0.12 μm wide and 15 min integration, the 5-σ sensitivity level thus corresponds to 5.8 10^{-16} W m^{-2}.

3.2.3 Ultraviolet: the HST

The CO fourth-positive system at 154 nm was detected in several comets using rockets and the IUE satellite, but a more sensitive instrument is now the Faint Object Spectrograph of the Hubble Space Telescope. We will assume that the recent observations of comets P/Hartley 2 1991t and Shoemaker-Levy 1991a1, as reported by Weaver et al. (1992), are representative of what can be achieved with the HST. Both comets were at $r_h = \Delta = 1$ AU. A CO production rate of 1.5 10^{27} s^{-1} was observed in comet Shoemaker-Levy, and an upper limit of the same value was set up for P/Hartley 2.

3.3 Expected signals and detectability

We have evaluated the CO signals expected for two hypothetical comets, one at $r_h = \Delta = 1$ AU, the other at $r_h = \Delta = 14$ AU, both with the same CO production rate of 10^{27} s^{-1}. The evaluations are based upon the models described in Section 3.1 and the results are summarized in Table 2.

The most promising rotational line is the *J(2-1)* (although stronger, the *J(3-2)* line is more difficult to observe). Surprisingly, the signal is almost insensitive to the distance distance. At large heliocentric distances, the unfavourable large geocentric distance is counterbalanced by the smaller expansion velocity, the longer lifetime, and above all, the rotational distribution which is concentrated on low *J* levels.

Table 2: Expected signals for Q[CO] = 10^{27} s^{-1}.

	frequency	1 AU	14 AU	
radio (IRAM):				
J(1-0)	115 GHz	8.1 10^{-4}	1.6 10^{-3}	K km s^{-1}
J(2-1)	230	6.5 10^{-3}	7.9 10^{-2}	
J(3-2)	345	2.1 10^{-2}		
infrared (ISO):				
v(1-0)	4150 cm^{-1}	6.7 10^{-16}	7.7 10^{-19}	W m^{-2}

For the infrared v(1-0) band, the signal at 14 AU is about 1000 times smaller than at 1 AU. We have not made any evaluation for the UV signal, but since the geometrical factors and the fluorescence rates behave in the same way for UV and IR bands, we expect that the same scaling law applies as for the IR. The corresponding limits on the CO production rates are listed in Table 3.

Table 3: Expected observational limits (5-σ) for Q[CO].

Technique	1 AU	14 AU
Radio (230 GHz): IRAM 30-m	1.5 10^{28}	1.3 10^{28}
IR (4150 cm^{-1}): ISO PHT-S	0.9 10^{27}	0.7 10^{30}
UV (150 nm): HST FOS	1.0 10^{27}	1.0 10^{30}

4. Conclusion

Radio spectroscopy is thus the most sensitive technique to observe CO in distant comets, since it could detect a CO production rate of the order of 10^{28} s^{-1} at 14 AU. Such a large production rate may seem unlikely, since it is comparable to the water production rate of "standard" comets at 1 AU. However, according to the sublimation rate Z = 3.7 10^{16} molec. cm^{-2} s^{-1} estimated by Sekanina et al (1992) for pure CO ice at 14 AU, this production correponds to a surface of 35 km^2 of exposed CO ice, or 5% of the surface of a 7.5 km diameter body.

Instead of a constant gas production, another approach is to consider outgassing due to a short outburst. At 14 AU, CO molecules ejected at 0.25 km s^{-1} remain in the IRAM beam (12" at 230 GHz) during about two days. Sekanina et al. (1992) estimated that P/Halley ejected 10^{12} g of dust during its outburst. The gas-to-dust ratio is a very uncertain parameter. If we assume it is close to 1, the ejected dust corresponds to 2 10^{34} molec. of CO (if this species is the main volatile) and to a column density of 2.5 10^{14} cm^{-2} as long as the ejected CO is in the IRAM beam. This corresponds to the column density of a steady-state Q[CO] = 6 10^{28} s^{-1}, which, as computed above, should be readily detectable. Several facts, however, may affect the validity of this estimation: the outburst may last more than 2 days; the expansion velocity of CO may be larger than 0.25 km s^{-1} for an outburst ; the CO rotational distribution may equilibrate at a temperature larger than 30 K in such a process; and last but not least, the observation must be performed just after the outburst !

The gas production rates advanced at this workshop for Chiron and P/Schwassmann-Wachmann 1 during an activity period are insufficient to permit a radio detection of CO, even if this species alone is responsible for activity. If the CN radical detected in Chiron were due to the photodissociation of HCN (which is doubtful; see Section 1), the production rate of hydrogen cyanide would be about 1.4 10^{27} s^{-1} (Bus et al. 1991). Such a rate would be enormous, comparable to what was observed in P/Halley near perihelion. It does not correspond to a signal detectable in radio, however.

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Appendix: radiative cooling rates

Radiative cooling is due to the emission of rotational lines (vibrational or electronic transitions, which cannot be excited by collisions in cometary conditions, are not efficient for cooling). The cooling rate L of a molecular species is:

$$L(T) = \Sigma_i P_i (T) \Sigma_j A_{ij} h \nu_{ij},$$

where the summation is made over the rotational relative populations P_i (assumed to be Boltzmannian) and over the rotational lines of Einstein coefficients A_{ij} and frequencies ν_{ij}. For the strong lines of abundant species (like water; see Crovisier 1984), radiative transfer must be taken into account. Cooling is only effective when collisions are frequent enough to ensure exchange between translational and rotational energy.

The cooling rates have been evaluated as a function of temperature for several molecules. They are presented in Figure 1; Note that non-polar molecules such as N_2, CO_2 or CH_4 cannot cool. Cooling is increasing with temperature, thus tending to ensure a thermostating effect. Cooling is higher for molecules with large electric dipole moments. Cooling by H_2O is the strongest. NH_3 is second. CO, which has a small dipole moment, is not an efficient cooler.

We conclude that in the atmosphere of distant comets, which are presumably composed of CO or non-polar molecules, radiative cooling is inefficient.

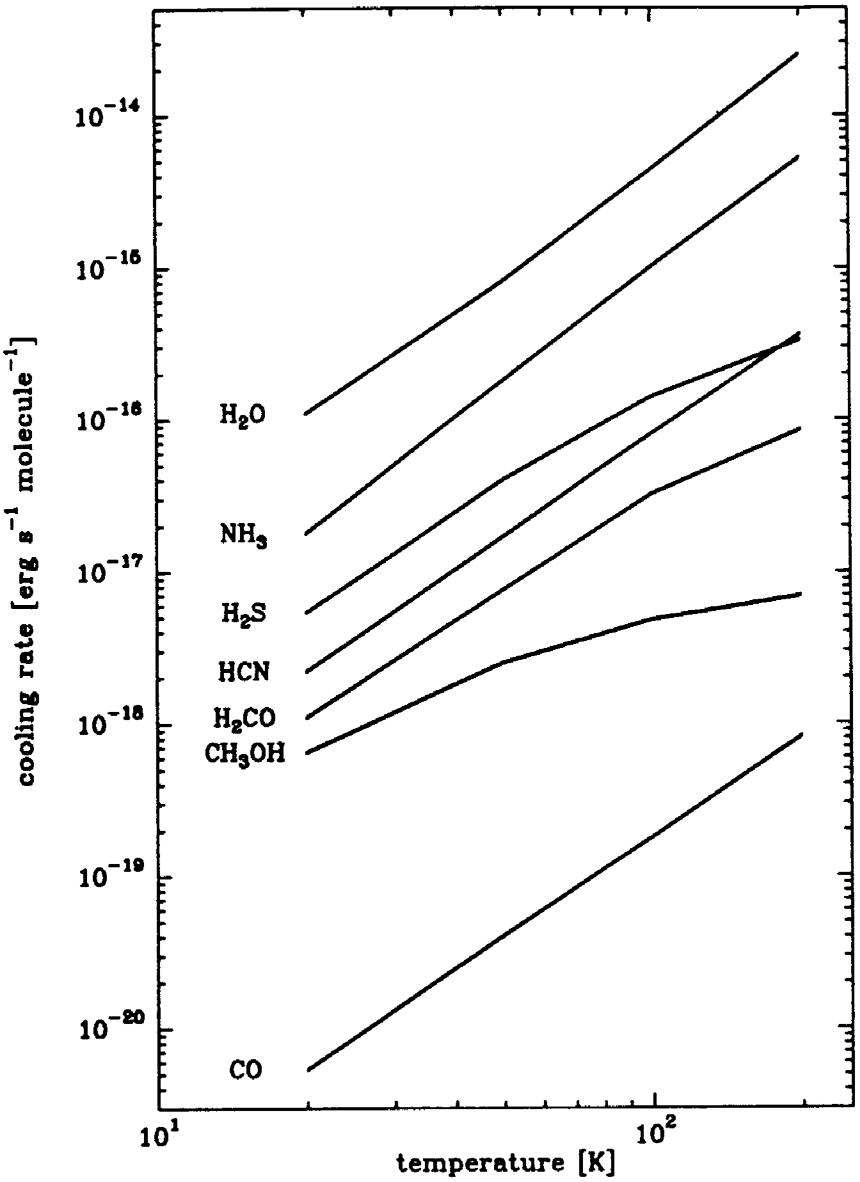

Figure 1: Radiative cooling rates as a function of temperature for various molecules (radiative trapping is neglected).