

Translucent Clouds as Testbeds of Basic Chemical Networks

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Abstract. We have developed comprehensive models, based on the New Standard Model reaction dataset, for the gas-phase chemistry of translucent clouds. These models predict satisfactorily the abundances of 34 of the 38 molecular species observed in both translucent and cold dense clouds. With 3 additional reactions, the models also appear able to explain diffuse cloud abundances.

1. Introduction

Translucent clouds (total extinction $\sim 2\text{--}5$ mag) are ideal objects for the study of quiescent astrochemistry because, unlike diffuse clouds, they have large enough column densities to exhibit a rich chemistry, and unlike cold dense clouds, their physical properties appear simple and well understood, as is necessary to derive reliable molecular abundances. We have been studying an ensemble of 38 translucent objects, established via maps in the $J=1\text{--}0$ and $2\text{--}1$ lines of C^{18}O and ^{13}CO to be spatially resolved, quiescent, and not clumped. These observations, together with a detailed chemistry model of the CO isotopomers, permit the derivation of detailed physical models of all 38 objects. In terms of specified functions $n(r)$ and $T(r)$, one obtains self-consistent models described by central quantities n_0 , T_0 , the extinction A_v , the mean external radiation field I_{UV} , and the electron distribution $X_r(e)$ (see Turner 1993, 1994 for details). With these models, we have derived fractional abundances for 38 species which include all the major chemical groups.

Our translucent cloud abundances, at $A_v=4$ mag are the same as those in TMC-1 within a factor of 4 for 33 of the 38 species, and within a factor of 10 for all 38 species.

2. Chemical Models

We have used the new standard gas-phase chemical model (NSM; Lee et al. 1996) slightly modified for translucent cloud conditions. Results of chemical models are highly sensitive to input conditions: elemental abundances, the C/O ratio, I_{UV} , the cosmic ray ionization rate for H_2 , and the epoch (early time vs. steady state). From simplest to most complex, we may categorize chemical models in terms of the range of A_v tested, and the range of parameter space included, as follows: (i) Most models to date are of TMC-1 type, and include only $A_v = \infty$ (no photochemistry) and elemental depletions restricted to those of high- and

low-metals (Lee et al. 1996). Depletion factors are defined as $d = n(X)_0/n(X)$ where $n(X)_0$ is defined as the mean diffuse cloud value for element X, i.e., a factor ~ 2 down from the solar value. The NSM has traditionally used $d(N,C,O)=1$ with high metals ($d(M)=1$; HM) or low metals ($d(M)=100$; LM). Recently models with higher $d(C,O)$ values have been applied to TMC-1 (Caselli et al. 1998; Terzieva & Herbst 1998). (ii) Our translucent cloud models include a range of A_v from ~ 0.5 to 10 mag, thus modeling the transition range from diffuse to dense clouds, and testing the dependence of photochemistry on A_v . Our published work so far has included the standard HM and LM abundances with $d(C,O)=1$, and a range of C/O from 0.4 (diffuse cloud value) to 1.1. (iii) In the present work, we expand category (ii) to include $d(C,O)$ and $d(S)$ as variables, retaining the HM and LM values of $d(M)$ for metals other than sulfur. The result is a “global” chemical model that simultaneously matches the observed and model abundances of all species studied with a single set of parameters that apply to both TMC-1 and the translucent clouds. (iv) Although the abundance determinations rest on multi-zone models of the clouds with physical conditions varying with radius, all current chemical models have uniform physical conditions. In reality, as the extinction of a cloud increases inward, the physical conditions, and also $d(C,O)$, $d(M)$, and the C/O ratio will be functions of radius. Important chemical gradients are expected, such as a concentration of hydrocarbons to the center and some sulfur species to the outer regions. Chemical models must be developed that include the radial dependence of all important parameters.

3. Comparison of Chemical Models with $d(C,O)=1$ and $d(C,O) > 1$

Our previous studies of translucent clouds, all with $d(C,O)=1$, included several individual species, and later focused independently on several groups: the sulfur family; the “acetylenic” group; the “heterogeneous” group (species containing O and N atoms as well as C); and the hydrocarbon family (C_nH_m). These studies have revealed that, under steady-state (SS) with $d(C,O)=1$, orthogonal sets of parameters are required to explain S-O species at one extreme (C/O=0.4; HM) and hydrocarbons at the other (C/O ≥ 0.7 ; LM). Other species are intermediate but with a preference for LM. A general problem is that steady-state chemical models with $d=1$ underproduce several species. Early-time (ET) conditions also underproduce the S-O and hydrocarbon species for C/O as small as 0.5. Even when ET models do match observed abundances, the specific ET epoch is not the same for every species. Further, ET actually overproduces CS and C₂S. A possible solution to the general $d(C,O)=1$ problem is that $d(M)$ and C/O both increase with decreasing radius (increasing extinction) within the clouds, although the details have not been worked out.

The other possibility to solve the S-O/hydrocarbon dichotomy is $d(C,O) > 1$. This requires LM. The way this works is that, for LM, both C⁺ and *e* are of low abundance and linked, so that decreasing C decreases both C⁺ and *e*. Electrons are the major species working against buildup of complex hydrocarbons. Similarly, O is a major destroyer of neutral hydrocarbons. The effect is dramatic. For cold dense clouds ($A_v = \infty$), Caselli et al. (1998) found that use of $d(C,O) = 3-5$ under SS conditions provided an alternative to ET to explain the very high abundances of C-rich species observed in TMC-1 and concluded that the high

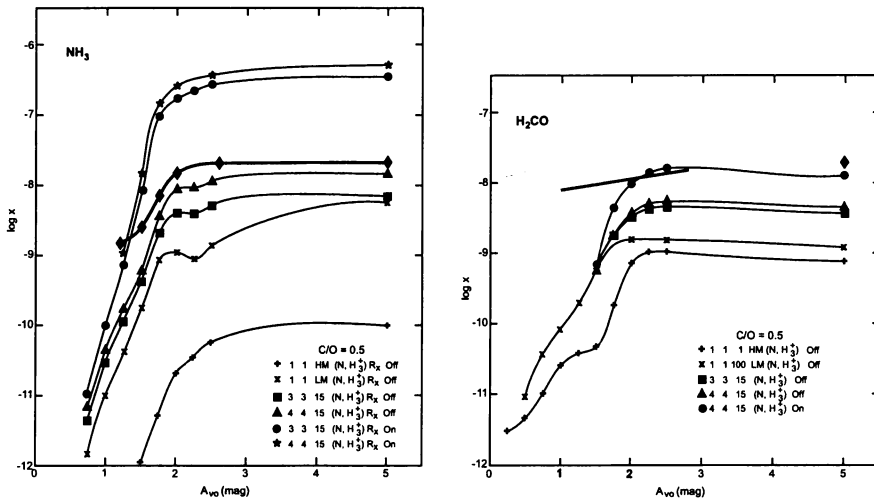


Figure 1. Observed and model abundances of NH_3 and H_2CO as a function of A_{v0} . See text for explanation.

$d(\text{C},\text{O})$ alternative was preferred in many of the dense cores if not in TMC-1 itself. In what follows, we discuss both SS and E/T models we have made of translucent clouds in which $d(\text{C},\text{O})$, $d(\text{S})$, $d(\text{M})$ and C/O are independent variables. The models have $n = 2000 \text{ cm}^{-3}$, $T_0 = T_0(A_{v0})$ as given by Turner (1993), and are run for $A_{v0} = 0.25$ to 5.0 in steps of 0.25 mag .

4. Comparison of Models and Observations for Selected Species

In the figures the observations are shown as straight line segments except for NH_3 where they are shown by the curve with diamond symbols. The diamond symbol at $A_{v0} = 5$ represents the observed value for TMC-1. Models are shown for $\text{C}/\text{O} = 0.5$. Models with $d(\text{C},\text{O}) > 1$ are denoted as $(d(\text{C}), d(\text{O}), d(\text{S})) \text{ Rx ON}$ or OFF . We also show $d(\text{C},\text{O}) = 1$ models for which $d(\text{M}) = 1$ for HM, 100 for LM. ‘Rx’ refers to the process $\text{N} + \text{H}_3^+ \rightarrow \text{NH}_2^+$ leading to NH_3 , whose status has recently reverted from active to inactive; we consider the matter unsettled.

4.1. Species relatively insensitive to $d(\text{C},\text{O})$: NH_3 , H_2CO , HCN

Figure 1 shows the case for NH_3 , typical of this group. For all three species, models with $d=1$, HM give the lowest abundance because destruction is by the abundant S^+ and Si^+ ions which are undepleted. Models with $d=1$, LM are next, where destruction is mainly by C^+ , of lower abundance. The various $d=3$ models produce higher abundances because C^+ has yet lower abundance. In each case, the Rx (N, H_3^+) produces the highest abundance: it forms NH_3 “directly”, HCN via $\text{C}^+ + \text{NH}_3$, and enhances H_2CO by decreasing the C^+ abundance. These species are best fit (see NH_3) by the models with $d = 4 \ 4 \ 15 \ \text{OFF}$.

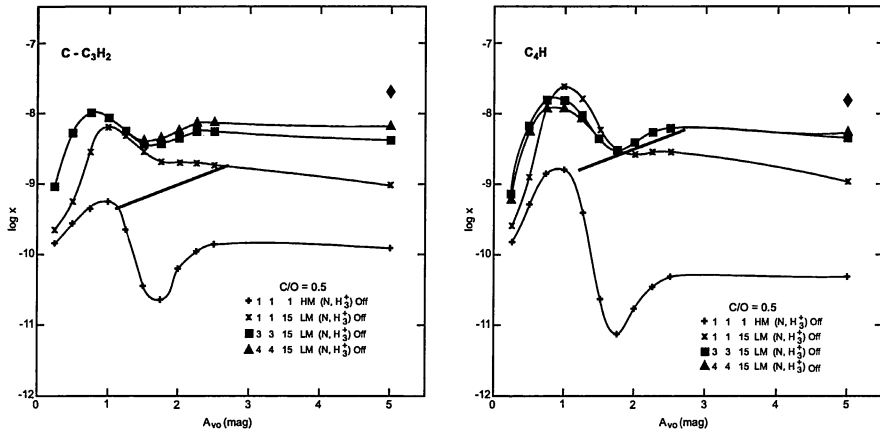


Figure 2. Observed and model abundances of $c\text{-C}_3\text{H}_2$ and C_4H as a function of A_{v0} .

4.2. Hydrocarbons

As mentioned earlier, hydrocarbons under SS generally require LM and $\text{C/O} > 0.7$ when $d(\text{C,O})=1$. Actually, C_2H is equally well fit with HM and LM, but as the number of C-atoms increases the requirement for LM becomes rapidly stronger, so that for HM, C_4H is underproduced by a factor > 100 at $A_{v0}=5$ mag (Fig. 2) and C_6H by a factor $\sim 10^4$. Models with $d=1$, LM, and $\text{C/O}=0.5$ reproduce observed abundances for hydrocarbons up to C_4H , but also fail (by smaller factors) at higher C-number. Models with $d=3, 4$ produce good fits for C_5H and C_6H_2 but C_6H is underproduced by a factor of 60. The key point, however, is that models with $d=3, 4$ can continue to produce large enough abundances to satisfy observations for C_5H and higher order, and for $\text{C/O}=0.5$, the latter being low enough to satisfy the S-O species.

4.3. The S-O species (SO , SO_2)

As Figure 3 shows, the role of HM and LM in $d=1$ models is reversed from that pertaining to all other species. The reason is that SO is formed via $\text{S} + \text{OH} \rightarrow \text{SO} + \text{H}$, and SO_2 by $\text{SO} + \text{OH} \rightarrow \text{SO}_2 + \text{H}$. SO and SO_2 are both removed primarily by C^+ . HM produces lots of SO and SO_2 mostly because $d(\text{S})=1$, while LM models badly underproduce SO and SO_2 because $d(\text{S})=100$. Even though a purely HM model predicts the observed abundance for SO , our goal of a single global model to fit all species means we must insure that the models with $d=(4\ 4\ 15\ \text{LM})$ and $\text{C/O}=0.5$ are also satisfactory. We remind the reader that the $d=4$ model is needed to augment the higher-order hydrocarbons which are otherwise optimized with $\text{C/O} > 0.7$, whereas we impose $\text{C/O}=0.5$ to increase the formation rates of SO and SO_2 , so as to avoid requiring too small a value for $d(\text{S})$. We see in Fig. 3 that the $d=4$ models closely mimic the purely HM models despite having $d(\text{S})=15$ rather than 1. The reason is that C^+ is reduced by a factor of 4 in the $d=4$ models. This increases OH , which increases the formation rate and reduces the destruction rate of SO . By reducing C^+ , the

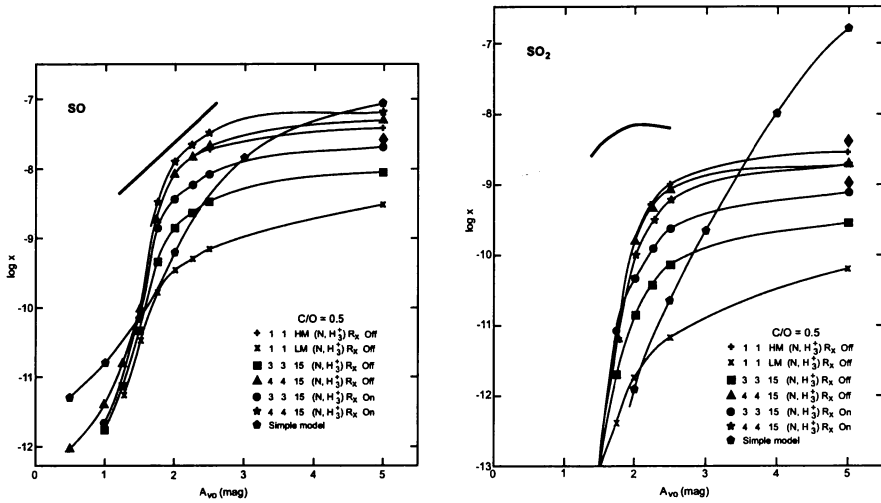


Figure 3. Observed and model abundances of SO and SO₂ of a function A_{v0}.

formation rate of SO₂ is increased even more because both SO and OH are involved in its formation. Production of both SO and SO₂ is enhanced if (N, H₃⁺) operates, presumably because it reduces C⁺ somewhat. This simple chemistry has the property that SO and SO₂ abundances are roughly linearly dependent on *d*(S). SO₂ could be better fit simply by decreasing *d*(S) from 15, but CS is then overproduced. At the high-A_v end of the transition region SO₂ is underproduced by a factor of 6, and much more at smaller A_v.

The large (observed/model) abundance ratio for SO₂ at smaller A_v is seen to occur for several other species (SO, H₂CO, HCN), all of which are detected recently in diffuse clouds at levels much higher than predicted by the NSM (but which we explain by simple modifications in Sec. 5).

4.4. Statistical comparisons of models

Figure 4 shows the log(obs/model) ratios for 33 species, for our “best” model (*d* = 4 4 15 100; C/O = 0.5). Omitted are the four species H₂S, CH₃OH, CH₃CHO and VyCN, which are not fit by gas phase models, and C₅H₄ (seen only in TMC-1). Figure 4 compares SS and ET models (epoch 3.2 × 10⁵ yr), with (N, H₃⁺) OFF. We see that SS abundances are lower than ET abundances for all species except the ions. We emphasize that the differences between SS and ET are small compared with the differences between SS models with *d* = 1 (which seriously underproduce many species for C/O = 0.5) and *d* = 4 models. Table 1 gives a formal statistical summary of the results shown in Fig. 4. Here, models A and B refer to the reaction (N, H₃⁺) OFF and ON respectively. For the preferred model 4 with (N, H₃⁺) OFF, we see that, averaged over the 33 species, the SS model underproduces by a factor of 2.2 and the ET model overproduces by a factor of 1.6. If (N, H₃⁺) is ON, the factors are 1.0 and 2.1 respectively, i.e. in this case the SS model is perfectly balanced. The variances for SS and ET models

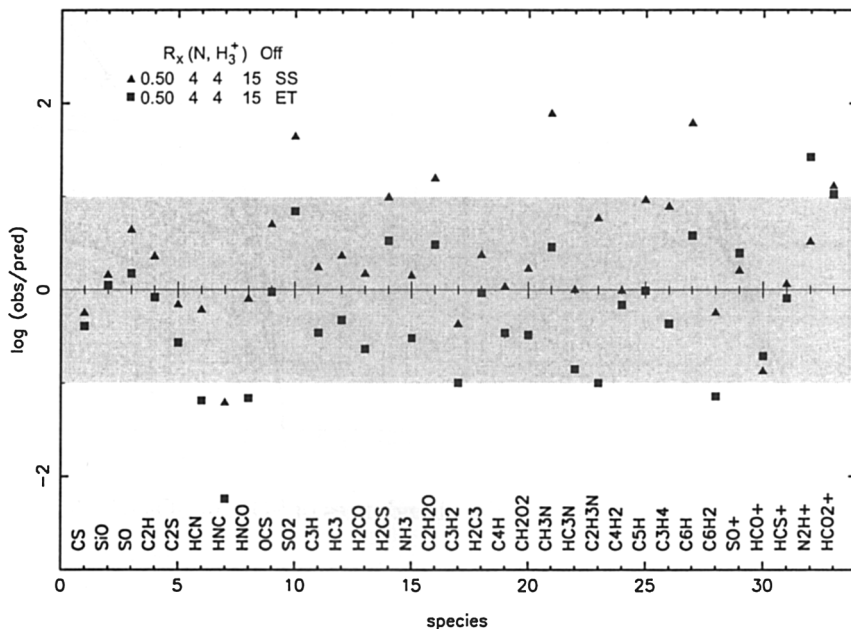


Figure 4. The ratio of observed to predicted abundances for 33 species.

Observed/Model Abundance Ratios for Steady-state Models								
Model	Parameters				Mean Ratio		Variance of Ratio	
	C/O	d(C)	d(O)	d(S)	Model A	Model B	Model A	Model B
1	0.41	3	3	15	4.45		8.1	
2	0.41	4	4	15	3.06		7.0	
3	0.50	3	3	15	3.19	1.19	6.9	5.8
4	0.50	4	4	15	2.25	0.99	6.1	6.0
5	0.50	4	4	5	2.30	0.95	7.0	6.5
6	0.68	3	3	15	1.81		6.8	
7	0.68	4	4	15	1.29		5.9	

Observed/Model Abundance Ratios for ET Models								
Model	Parameters				Mean Ratio		Variance of Ratio	
	C/O	d(C)	d(O)	d(S)	Model A	Model B	Model A	Model B
1	0.41	3	3	15	0.76		5.5	
2	0.41	4	4	15	0.75		5.6	
3	0.50	3	3	15	0.54	0.41	5.8	6.4
4	0.50	4	4	15	0.61	0.48	5.7	6.6
5	0.50	4	4	5	0.60	0.41	5.6	6.3
6	0.68	3	3	15	0.40		6.6	
7	0.68	4	4	15	0.47		6.4	

are indistinguishable. To decide the best model, i.e. SS vs. ET, and (N, H_3^+) OFF vs. ON on, it is necessary to look at the details. Within the shaded area the predicted and observed abundances are the same within a factor of 10. The number of points lying outside this area is 6 for SS (OFF), 5 for ET (OFF), 4 for SS (ON), and 10 for ET (ON). We reject the last model not only on this basis, but also because it seriously overproduces HNC. The SS (ON) model has the merit of fitting SO_2 but also overproduces HNC. Thus we consider the (N, H_3^+) OFF models to be more acceptable. In this case, the ET model still severely overproduces HNC and has problems with HCN as well, while the SS model underproduces SO_2 , although by a smaller factor. We attach low weight to the other deviant SS species (CH_2NH and C_6H) because we consider their chemistry to be poorly understood but easily correctable.

4.5. Summary of NSM Results for Translucent Clouds

- gas phase chemistry (NSM) has been successful over a wide range of species types, and appears to fit the dense cloud TMC-1 (single A_v) equally well.
- observed abundances can all be fit with SS and $d=4$. Only a subset of complex C-species can be fit with ET and $d=1$, and less well than SS with $d=4$. For models with $d=4$, ET produces only minor differences relative to SS.
- the 4 species that cannot be fit have observed/model abundance ratios > 100 for all gas-phase models. These species, H_2S , CH_3OH , CH_3CHO , VycN , are all reasonable candidates for grain chemistry.
- these conclusions are consistent with those for dense clouds (Caselli et al. 1998; Terzieva & Herbst 1998).

5. Diffuse Cloud Chemistry

Over several years Lucas & Liszt (e.g. 1997) have been studying several molecular species in anonymous galactic clouds seen in absorption against extragalactic continuum sources. These species include OH, CO, CN, HCN, HNC, NH_3 , H_2CO , C_2H , C_3H_2 , HCO^+ , CS, and SO. The estimated properties of these clouds are $n \lesssim 200 \text{ cm}^{-3}$, $T=60 \text{ K}$, and $A_v \lesssim 1 \text{ mag}$. The authors obtain column densities on the assumption that T_{ex} equals 2.7 K, and plots of these for pairs of species over all sources establish proportionalities between column densities. We have scaled these to a fractional abundance of OH of 1(-7). Remarkably, these abundances in all cases except SO are well within a factor of 10 of the translucent and cold dense cloud abundances.

For extinctions of $\sim 2 \text{ mag}$ (translucent clouds), the abundances produced by the NSM are insensitive to density down to 200 cm^{-3} . For $A_v=1 \text{ mag}$, however, we find that the NSM produces abundances well below those observed. This shortfall has been noted by others (Spaans 1995; Federman 1996; Hogerheijde et al. 1995; Joulain et al. 1998) who have invoked turbulence-driven enhancements of certain endothermic reactions to achieve higher abundances. We have included several of these reactions in the NSM, using the $d=(4,4,15,100, \text{C/O}=0.5)$ preferred model. These reactions and their effects are as follows: 1)

$O + H^+ \rightarrow O^+ + H$ (at $T=60$ K, augments OH, HCO^+); 2) $C^+ + H_2 \rightarrow CH^+ + H$: fits HCO^+ , CO, CN, CS, C_2H , C_3H_2 ; 3) $N + H_2 \rightarrow NH + H$: fits HCN, HNC; 4) $O + H_2 \rightarrow OH + H$: fits OH, HCO^+ .

Nine of the 12 species observed by Lucas & Liszt are fit, all within a factor 10 of the observed abundances. H_2CO , NH_3 , and SO remain underproduced by the model, by factors of 100 to 1000. H_2CO and NH_3 can be fit if n is as high as 1000 cm^{-3} .

The $d=4$ model may be criticized as overly depleted for the diffuse cloud regime. We have also run models with $C/O=0.5$ and $d = (1,1,15,100; \text{LM})$, and $d = (1,1,1,1; \text{HM})$. Results are very similar for all three models, and for SS and ET in each case. Omitting the poorly fit SO and H_2CO , the mean value of the (observed/model) ratios for the SS models are 1.7, 0.86, 1.2 for $d=4$, $d=1$ (LM) and $d=1$ (HM) respectively. For the ET models, the corresponding mean values are 1.3, 0.65, and 0.9.

The diffuse cloud model can be extended down to $A_v=0.5$ mag if the rates of $C^+ + H_2 \rightarrow CH^+$ and $N + H_2 \rightarrow NH$ are increased by a factor of 2. Only the C_3H_2 abundance declines somewhat.

To summarize, models without turbulence fit the observations for translucent cloud conditions ($A_v \geq 1.2$ mag, $n=2000 \text{ cm}^{-3}$), while turbulence-driven models fit diffuse cloud conditions ($A_v = 0.5$ to 1 mag, $n=200 \text{ cm}^{-3}$). The turbulence enhancement of rates is thought to onset at $A_v \sim 1$ and increase as A_v decreases, thus balancing the demands of the increasing photodestruction rates. Reasonably constant abundances throughout the diffuse and translucent ranges may therefore be expected, as observed.

6. Conclusions

1. The observed abundances are remarkably similar for cold dense clouds, translucent clouds, and diffuse clouds.
2. Gas-phase chemical models (NSM) are highly successful in predicting observed abundances in translucent clouds, in cold dense clouds, and now apparently also in diffuse clouds
3. Translucent clouds:
 - (a) 34 of 38 observed species are well modelled at either SS or ET with $d(C,O)=3-4$; $d(S) \sim 15$; $d(M)=100$.
 - (b) Is such a model "universal"? An alternative model with species favoring HM and low C/O ratio (SO, SO_2) in the outer regions and species requiring LM and high C/O ratio (esp. hydrocarbons) in the central regions, may be more realistic.
 - (c) ET is not needed and not superior to SS models with $d=3-4$.
4. Diffuse clouds:
 - (a) NSM models require addition of 3 key turbulent-driven (endothermic) reactions

- (b) Models explain abundances of 8 of 11 observed species within a factor of 3, and 9 species within a factor 5.
 - (c) All modeled abundances are similar over the complete range of depletions ($d=1$ (HM), $d=1$ (LM), $d=4$). Thus, expected diffuse cloud depletions are included in the models.
5. Questions remaining:
- (a) If abundances are similar in translucent and cold dense clouds, are their physical conditions more similar than we think? Are cold dense clouds filled with PDRs and penetrating UV so that effective extinctions are similar?
 - (b) Models require different physical conditions in diffuse clouds. Why are their abundances so similar to translucent and dense cloud abundances?
 - (c) Are we seeing clumped gas in all three regimes, with similar densities and similar (high) depletions? There are arguments against this possibility for translucent clouds (Turner 1993).
 - (d) The success of the gas-phase models is likely to be compromised by any significant contribution from catalytic grain processes. Yet such processes are needed for some species. How can we resolve this seeming contradiction?

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Discussion

M. Walmsley: You mentioned that the abundance distribution of different species in diffuse clouds, translucent clouds, and dense clouds are identical. You said also that one explanation might be clumping. Could you expand on that?

B. E. Turner: Simply, if most of the emission arises in clumps with $n \sim 10^4 \text{ cm}^{-3}$ or greater, with these clumps providing a sufficient beam filling factor to explain observed line intensities, then the 'effective' physical conditions would be similar in all three regimes. However there are a number of arguments based on observed line widths and derived physical parameters of translucent clouds, that make the presence of such clumps unlikely, at least in the translucent objects. See Turner (1993, ApJ) for an account of these arguments. Also, it is hard to see how the absorption studies of Lucas & Liszt for diffuse clouds could consistently miss seeing the presence of such clumps.