A NEW MODEL FOR COMPLEX CHEMISTRY IN HOT CORES

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Gas phase ion-molecule reactions have long been thought to be the key formation mechanism for complex organic molecules in hot cores. However, recent theoretical calculations[a] have shown that these types of reactions are inefficient for the formation of methyl formate (CH_3OCHO), and so grain surface formation mechanisms may be important. To date hot core chemical models have included primarily single-atom addition grain surface reactions, but more complex grain surface chemistry involving simple radicals was suggested by Allen and Robinson[b]. Radicals such as OH, NH_2, CH_3, CH_3O, CH_2OH, and HCO can form from photolysis of simple grain surface species such as NH_3, CH_3OH, H_2O, and H_2CO. These radicals would become mobile on the grain surface during the warm up phase of a hot core and could react to form more complex species. Garrod & Herbst[c] showed that this type of formation mechanism is viable for methyl formate, formic acid (HCOOH), and dimethyl ether (CH_3OCH_3). The reaction network from this study has now been extended to include the full set of grain surface and gas phase reactions involving the radicals listed above as well as the products resulting from their combination on grain surfaces. A physical model including a warm-up phase from 10 to 200 K has been employed to investigate this chemical network for low-, intermediate-, and high-mass hot cores. The results have been compared to observational studies of hot cores, and the photolysis branching ratios and initial ice composition have been adjusted to produce final abundances that best match the observations.

[a] Horn et al. *Ap. J.* **611** (605), 2004.
[b] Allen & Robinson *Ap. J.* **212** (396), 1977.
[c] Garrod & Herbst *A. & A.* **457** (927), 2006.