Remarks on a comment on Photodestruction of PAHs in the interstellar medium. I

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We clarify as follows Fig. 2 and the single paragraph of a 14 page article (Allain et al. 1996) which have been questioned by P. Boissel (1997) in his Comment. Fig. 2 of Allain et al. (1996) compares for a number of PAHs the calculated rates of loss of C_2H_2 (RRK theory) with PhotoThermoDissociation (PTD) (Léger et al. 1989) calculations of the rate of loss of C_2, using a value $D(-C_2) = 8$ eV and a pre- exponential factor 10^{17} s^{-1}.

PTD calculations require evaluation of vibrational energy level densities of the species whose dissociation rates are to be determined. Experimental data on the complete set of vibrational frequencies of a PAH are only incompletely or not at all available for most PAHs. In practice the necessary vibrational frequencies are estimated or approximated and statistical methods are used for the determination of approximate energy level densities required for PTD calculations using the Inverse Laplace Transform (ILT) method (Forst 1973; Léger et al. 1989). Thus, although the PTD-ILT and RRK methods both require experimental input, this input is made the basis for approximations inherent in the calculation methods used. It is thus premature to assert, as does Boissel in his Comment, that "if both calculations are based on experimental results, the ILT method becomes better...". This is asserted by Boissel to be the case "especially for the evolution of the rate near the dissociation threshold". Pathological behaviour of calculated rates near threshold can also occur in calculations using statistical methods to obtain a function from its average; this may have the correct average behaviour but not necessarily the correct behaviour at some particular energy (Forst 1973). In any case, dissociation rates in the threshold region are difficult to evaluate by any method, since in this region it is necessary to take into account more specific dynamic processes, such as those involving centrifugal effects in the fragmenting species.

We acknowledge textual cleaning-up negligence concerning the definition of E_0 mentioned in Boissel's footnote. Of course, the calculations in the whole of our paper were based on the correct definition of this quantity.

In our paper (Allain et al. 1996) the few lines devoted to a comparison of the PTD-ILT and RRK methods do not bear on the detailed results of our study on the photodestruction of PAHs in the interstellar medium. They serve only to emphasize, as clearly stated in our paper, that use of the semi-empirical RRK technique method, based on constants whose values are fixed by experimental results on the dissociation of PAH species (Jochims et al. 1994), is simpler than the PTD-ILT method and that it gives results that are satisfactory in the context of the study carried out.

References

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