ADDITIONS AND CORRECTIONS

1994, Volume 98

Betsy M. Rice* and Cary F. Chabalowski: *Ab Initio* Potential Energy Surface for H + OCS Reactions: Extended Basis Sets and Correlation Treatment

Page 9488. In this article, the transition states labeled **k** and **m** were *assumed* to be barriers to the direct addition of hydrogen to OCS to form *trans*-HSCO or *trans*-HOCS. This assumption was not confirmed by intrinsic reaction coordinate (IRC) calculations, due to inadequate computational resources at that time.

Recent BLYP/6-311+G(2df,2p) IRC calculations[1] indicate transition states **k** and **m** are not barriers to these assumed hydrogen addition reactions, but are rather barriers to isomerization. We subsequently performed IRC calculations from transition states **k** and **m** at the UMP2/aug-cc-pVTZ level. The results confirmed that these transition states are barriers to *cis*–*trans* isomerization of the four-body complexes.

Traversing transition-state structures **k** and **m** result in the isomerization reactions *cis*-HSCO (**e**) → *trans*-HSCO (**f**) and *cis*-HOCS (**g**) → *trans*-HOCS (**h**). DFT/6-311+G(2df,2p) IRC calculations from all remaining saddle points indicate that all the other features of Figure 2 in this article have been interpreted correctly. Thus, the conclusions of the previous study are unchanged, including the determination that the low-energy path for the formation of products of (II) is

$$\mathrm{H} + \mathrm{OCS} \rightarrow \mathbf{l} \rightarrow cis\text{-}\mathrm{HSCO}\ (\mathbf{e}) \rightarrow \mathbf{s} \rightarrow \mathrm{SH} + \mathrm{CO}$$

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[1] Rice, B. M.; Pai, S. V.; Chabalowski, C. F. *J. Phys. Chem. A*, submitted for publication.

S1089-5639(98)01669-7 CCC: $15.00