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SUPPLEMENTARY MATERIAL

A Theoretical Study of the Astrochemical $^{13}C^{12}CS + H \rightarrow {}^{12}C^{13}CS + H$ Reaction

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The XYZ coordinates (in Angstroms) of the stationary points optimized on the $^{13}C^{12}CS + H \rightarrow {}^{12}C^{13}CS + H$ reaction pathways at the M06-2X/aug-cc-pVTZ level as well as the corresponding energies calculated at the RCCSD(T) level.

CCS

C 0.000000 0.000000 -0.027618
C 0.000000 0.000000 1.283229
S 0.000000 0.000000 2.844389
RCCSD(T)-FC/aug-cc-pVQZ energy: -473.6637325 a.u.

HCCS (min_1)

C 0.016521 0.000000 -0.100070
C 0.005612 0.000000 1.122980
S -0.008913 0.000000 2.740069
H 0.022378 0.000000 -1.162358
RCCSD(T)-FC/aug-cc-pVQZ energy: -474.3391788 a.u.

TS_{1-2}

C 0.000000 0.000000 0.000000
C 0.000000 0.000000 1.307769
S 1.128147 0.000000 2.569713
H -1.102824 -0.000050 1.475555
RCCSD(T)-FC/aug-cc-pVQZ energy: -474.2569816 a.u.

***c*-HCCS (min_2)**

C -0.008434 0.000000 0.038144
S -0.007059 0.000000 1.938033
C 1.155741 0.000000 0.677009
H 2.230322 0.000000 0.640683
RCCSD(T)-FC/aug-cc-pVQZ energy: -474.2944472 a.u.

TS_{2-2}

C 0.000000 0.000000 0.000000
C 0.000000 0.000000 1.356101
S 1.745154 0.000000 0.678636
H -0.383167 1.018246 0.677968
RCCSD(T)-FC/aug-cc-pVQZ energy: -474.2013334 a.u