Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Potential Energy Surface Stationary Points and Dynamics of the $F^- + CH_3I$ Double Inversion Mechanism

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Table 1. $S_o \rightarrow T_1$ Vertical Excitation Energies

	$S_o \rightarrow T_1$ Energy (ev)	
S_o Structure [a]	CCSD(T)[b]	MP2[b]
$F^- + CH_3I$	4.44	4.09
$FCH_3 + I^-$	3.84	3.95
$HF + CH_2I^-$	2.00	2.06
TS0	1.69	1.88
TS1	2.01	2.14
TS2	2.13	2.29
TS3	2.03	2.15
TS4	1.79	1.93
TS $[F--CH_3--I]^-$	4.24	4.85
TS$[F^--HCH_2--I]^-$	4.47	4.92
IM-A	4.23	5.12
IM-B	2.03	2.16
IM-C	2.18	2.31
IM-D	2.06	2.20
IM FCH_3---I^-	4.12	4.25
IM F^---CH_3I	4.75	4.96

a. The S_o structures for TS0 to TS4 are in Figure 2. The structures for the TSs $[F^--CH_3--I]^-$ and $[F--HCH_2--I]^-$ are in Figure 4. The structures for intermediates IM-A to IM-D are in Figure 2. The structures for the intermediates FCH_3---I^- and F^---CH_3I are in Figure 4. Figures 2 and 4 are in the article.

b. The ECP/d basis set was used.