

ELECTRONIC SUPPLEMENTARY INFORMATION

Parameter free evaluation of S_N2 reactions rates for the substitution of halides to halomethanes

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Table 1 Coordinates (expressed in Å) of the investigated halides and halomethanes.
Level of theory is COSMO-ZORA-OLYP/(A)TZ

CH₃F				I	0.0000	0.0000	2.7034
E = -0.8612 Ha				I	0.0000	0.0000	-2.7034
F	0.0000	0.0000	-2.4252	C	0.0000	0.0000	0.0000
C	0.0000	0.0000	-1.0110	H	-0.5383	0.9323	0.0000
H	-0.5191	0.8992	-0.6699	H	-0.5383	-0.9323	0.0000
H	-0.5191	-0.8992	-0.6699	H	1.0766	0.0000	0.0000
H	1.0383	0.0000	-0.6699	TS3 [Cl---CH₃---Br]⁻			
CH₃Cl				E = -1.0014 Ha			
E = -0.7981 Ha				Nimag = -436.45 cm ⁻¹			
Cl	0.0000	0.0000	-2.7313	Cl	0.0000	0.0000	2.0563
C	0.0000	0.0000	-0.9302	Br	0.0000	0.0000	-2.7909
H	-0.5179	0.8971	-0.5947	C	0.0000	0.0000	-0.2975
H	-0.5179	-0.8971	-0.5947	H	-0.5380	0.9319	-0.3034
H	1.0359	0.0000	-0.5947	H	-0.5380	-0.9319	-0.3034
CH₃Br				H	1.0761	0.0000	-0.3034
E = -0.7759 Ha				TS4 [Cl---CH₃---I]⁻			
Br	0.0000	0.0000	-2.8529	E = -0.9804 Ha			
C	0.0000	0.0000	-0.8902	Nimag = -419.90 cm ⁻¹			
H	-0.5193	0.8994	-0.5675	Cl	0.0000	0.0000	2.0967
H	-0.5193	-0.8994	-0.5675	I	0.0000	0.0000	-2.9650
H	1.0386	0.0000	-0.5675	C	0.0000	0.0000	-0.2518
CH₃I				H	-0.5381	0.9320	-0.2741
E = -0.7555 Ha				H	-0.5381	-0.9320	-0.2741
I	0.0000	0.0000	-3.0090	H	1.0762	0.0000	-0.2741
C	0.0000	0.0000	-0.8486	TS5 [F---CH₃---Br]⁻			
H	-0.5197	0.9002	-0.5294	E = -1.0540 Ha			
H	-0.5197	-0.9002	-0.5294	Nimag = -466.33 cm ⁻¹			
H	1.0395	0.0000	-0.5294	F	0.0000	0.0000	1.7254
TS1 [I---CH₃---Br]⁻				Br	0.0000	0.0000	-2.6703
E = -0.9627 Ha				C	0.0000	0.0000	-0.2704
Nimag = -393.64 cm ⁻¹				H	-0.5379	0.9316	-0.2424
Br	0.0000	0.0000	2.2121	H	-0.5379	-0.9316	-0.2424
I	0.0000	0.0000	-2.9894	H	1.0757	0.0000	-0.2424
C	0.0000	0.0000	-0.2809	TS6 [F---CH₃---Cl]⁻			
H	-0.5382	0.9321	-0.2947	E = -1.0730 Ha			
H	-0.5382	-0.9321	-0.2947	Nimag = -492.13 cm ⁻¹			
H	1.0763	0.0000	-0.2947	F	0.0000	0.0000	1.6900
TS2 [I---CH₃---I]⁻				Cl	0.0000	0.0000	-2.5509
E = -0.9424 Ha				C	0.0000	0.0000	-0.2937
Nimag = -379.92 cm ⁻¹				H	-0.5378	0.9315	-0.2626
				H	-0.5378	-0.9315	-0.2626
				H	1.0756	0.0000	-0.2626