

Supplementary Material

Paper ref.: B712565H

Title: Two-Dimensional Free Energy Surface on Exchange Reaction of Alkyl
Chloride/Chloride Using QM/MM-MC Method

Listed below are the coordinates and the total energies of the reactant/product and the TS structure along the gas-phase IRC for each of Cl/Cl exchange reactions of R-Cl ((a) R=Me, (b) *t*-Bu) in Fig.1 at the theoretical level of HF/6-31G*.

(a) R=Me

(a-1) reactant/product (C_{3v}) Total Energy = -958.635496420a.u.

C	0.000000	0.000000	0.000000
H	0.000000	1.020361	0.331661
H	-0.883659	-0.510181	0.331661
H	0.883659	-0.510181	0.331661
Cl	0.000000	0.000000	3.265616
Cl	0.000000	0.000000	-1.827737

(a-2) TS (D_{3h}) Total Energy = -958.613461467a.u.

C	0.000000	0.000000	0.000000
H	0.000000	1.061242	0.000000
H	0.919063	-0.530621	0.000000
H	-0.919063	-0.530621	0.000000
Cl	0.000000	0.000000	2.382389
Cl	0.000000	0.000000	-2.382389

(b) R=*t*-Bu

(b-1) reactant/product (C _{3v})	Total Energy = -1075.75273062a.u.		
C	0.000000	0.000000	0.000000
C	0.000000	1.453080	0.448628
C	-1.258404	-0.726540	0.448628
C	1.258404	-0.726540	0.448628
H	0.000000	1.467016	1.533605
H	0.880186	1.971590	0.083919
H	-0.880186	1.971590	0.083919
H	-1.270473	-0.733508	1.533605
H	-2.147541	-0.223532	0.083919
H	-1.267354	-1.748059	0.083919
H	1.270473	-0.733508	1.533605
H	1.267354	-1.748059	0.083919
H	2.147541	-0.223532	0.083919
Cl	0.000000	0.000000	-1.877779
Cl	0.000000	0.000000	4.008340

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(b-2) C _{3h} structure		Total Energy = -1075.71663073a.u.	
C	0.000000	0.000000	0.000000
C	0.020047	0.000000	1.484338
C	1.275451	0.000000	-0.759530
C	-1.295498	0.000000	-0.724808
H	1.027422	0.000000	1.874587
H	-0.501871	0.888624	1.813169
H	-0.501871	-0.888624	1.813169
H	1.109729	0.000000	-1.827067
H	1.821186	0.888624	-0.471951
H	1.821186	-0.888624	-0.471951
H	-2.137151	0.000000	-0.047520
H	-1.319315	0.888624	-1.341218
H	-1.319315	-0.888624	-1.341218
Cl	0.000000	-2.985943	0.000000
Cl	0.000000	2.985943	0.000000