

Supporting Information for “Intramolecular Halogen–Halogen Bonds?”

Mikael P. Johansson^{1,2*} and Marcel Swart^{1,3*}

¹ Institut de Química Computacional i Catàlisi and Departament de Química, Universitat de Girona,
Campus Montilivi, ES-17071 Girona, Spain

² Laboratory for Instruction in Swedish, Department of Chemistry, University of Helsinki, FI-00014
Helsinki, Finland

³ Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain

* *mikael.johansson@iki.fi, marcel.swart@icrea.cat*

12 Apr 2013

Cartesian coordinates (in Ångströms) for the ethanes

C₂H₆

C	0.00000	0.00000	-0.76700
H	0.00000	1.03833	-1.16558
H	0.89922	-0.51916	-1.16558
H	-0.89922	-0.51916	-1.16558
C	0.00000	0.00000	0.76700
H	0.00000	-1.03833	1.16558
H	0.89922	0.51916	1.16558
H	-0.89922	0.51916	1.16558

C₂F₆

C	0.00000	0.00000	-0.77250
F	0.00000	1.24839	-1.21949
F	1.08114	-0.62420	-1.21949
F	-1.08114	-0.62420	-1.21949
C	0.00000	0.00000	0.77250
F	0.00000	-1.24839	1.21949
F	1.08114	0.62420	1.21949
F	-1.08114	0.62420	1.21949

CF₃CCl₃

C	0.00000	0.00000	1.15944
F	0.00000	-1.24760	1.62212
F	1.08045	0.62380	1.62212
F	-1.08045	0.62380	1.62212
C	0.00000	0.00000	-0.39188
Cl	0.00000	1.67080	-0.94907
Cl	1.44696	-0.83540	-0.94907
Cl	-1.44696	-0.83540	-0.94907

C₂Cl₆

C	0.00000	0.00000	-0.78200
Cl	0.00000	1.66232	-1.38703
Cl	1.43961	-0.83116	-1.38703
Cl	-1.43961	-0.83116	-1.38703
C	0.00000	0.00000	0.78200
Cl	0.00000	-1.66232	1.38703
Cl	1.43961	0.83116	1.38703
Cl	-1.43961	0.83116	1.38703

C₂Cl₆ transition state

C	0.00000	0.00000	-0.82976
Cl	0.82237	1.42439	-1.47796
Cl	0.82237	-1.42439	-1.47796
Cl	-1.64474	0.00000	-1.47796
C	0.00000	0.00000	0.82976
Cl	0.82237	-1.42439	1.47796
Cl	0.82237	1.42439	1.47796
Cl	-1.64474	0.00000	1.47796

CH₃CCl₃

C	0.00000	0.00000	-0.85011
H	-0.51355	-0.88949	-1.20597
H	-0.51355	0.88949	-1.20597
H	1.02709	0.00000	-1.20597
C	0.00000	0.00000	0.66198
Cl	0.83436	1.44516	1.26869
Cl	-1.66872	0.00000	1.26869
Cl	0.83436	-1.44516	1.26869

Rotating view of the NCI regions in C₂Cl₆

Available as a separate file: C2Cl6-NCI .mpg