

Role of Quantum Mechanical Tunneling on the γ – effect of Silicon on Carbenes in 3 - Trimethylsilylcyclobutylidene

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Supporting Information File

Available Information:

- Cartesian Coordinates for Optimized Structures and their Energies in Hartrees at M06-2X/6-311+G(d,p) level.
- Thermal Corrections and Zero – Point Energies.
- Harmonic Frequencies.
- CVT, CVT + SCT rate constants from 100 K – 600 K.
- Calculation Scheme for estimating Barrier Width (w).
- Cartesian Coordinates for Optimized Structures, Energies and Thermal Corrections and Zero – Point Energies in Hartrees at QCISD/TZVP level for **1** to **4** and their respective compliance matrixes.
- Complete Reference 20 and 21.

Cartesian Coordinates for Optimized Structures at M06-2X/6-311+G (d,p) :

1:

Atomic Numbers Coordinates (Angstroms)

X	Y	Z	
6	-0.307395	1.818789	1.110895
6	-0.974118	2.491737	0.000000
6	-0.307395	1.818789	-1.110895
1	-1.855374	0.524750	0.000000
6	-0.307395	-1.759416	1.546918
1	0.784337	1.743986	-1.161950
1	-0.791518	1.831650	-2.083533
1	0.784337	1.743986	1.161950
6	-0.307395	-1.759416	-1.546918
1	-0.791518	1.831650	2.083533
6	-0.800902	0.791342	0.000000
14	0.196025	-0.827978	0.000000
6	0.193339	-2.729885	1.598340
1	-1.385409	-1.936675	1.569012
1	-0.040051	-1.195733	2.444354
1	2.555843	-1.513360	0.000000
1	2.383865	0.001592	0.885354
1	2.383865	0.001592	-0.885354
1	0.193339	-2.729885	-1.598340
1	-0.040051	-1.195733	-2.444354
1	-1.385409	-1.936675	-1.569012

M06-2X /6-311+g(d, p) = -564.4853417 Hartree

Sum of electronic and zero-point Energies= -564.298176 Hartree

Sum of electronic and thermal Energies= -564.286719 Hartree

Sum of electronic and thermal Enthalpies= -564.285775 Hartree

Sum of electronic and thermal Free Energies= -564.336213 Hartree

Low frequencies (cm⁻¹): 5.6167 121.5136 157.1917 164.1658
179.1430 185.1157 190.8539 209.6206 217.5921 269.2462 .

2:

Atomic Numbers

Coordinates (Angstroms)

X	Y	Z			
6		-0.427940	1.951589	1.123957	
6		-1.365303	1.689487	0.000000	
6		-0.427940	1.951589	-1.123957	
1		-2.342596	1.232336	0.000000	
6		-0.427940	-1.537150	1.542612	
1		0.045575	2.930704	-1.186657	
1		-0.653371	1.490145	-2.080865	
1		0.045575	2.930704	1.186657	
6		-0.427940	-1.537150	-1.542612	
1		-0.653371	1.490145	2.080865	
6		-0.026486	1.026945	0.000000	
14		0.343164	-0.788333	0.000000	
6		2.193954	-1.104103	0.000000	
1		-0.285205	-2.620808	1.561769	
1		-1.502872	-1.340757	1.581817	
1		0.023702	-1.128147	2.450063	
1		2.411063	-2.175731	0.000000	
1		2.664574	-0.664731	0.882932	
1		2.664574	-0.664731	-0.882932	
1		-0.285205	-2.620808	-1.561769	
1		0.023702	-1.128147	-2.450063	
1		-1.502872	-1.340757	-1.581817	

M06-2X /6-311+g(d, p) = -564 .5626807 Hartree

Sum of electronic and zero-point Energies= -564.374101 Hartree

Sum of electronic and thermal Energies= -564.362640 Hartree

Sum of electronic and thermal Enthalpies= -564.361696 Hartree

Sum of electronic and thermal Free Energies= -564.411101 Hartree

Low frequencies (cm⁻¹): 31.7571 99.6513 106.9408 145.4726
160.9842 168.4996 188.7270 192.1142 207.3095 297.4430.

1-2 (TS):

Atomic Numbers Coordinates (Angstroms)

X	Y	Z		
6	-0.355962	1.953084	1.088661	
6	-1.375835	2.243869	0.000000	
6	-0.355962	1.953084	-1.088661	
1	-1.584409	0.761764	0.000000	
6	-0.355962	-1.735998	1.547558	
1	0.567700	2.524208	-1.066264	
1	-0.722322	1.715410	-2.082759	
1	0.567700	2.524208	1.066264	
6	-0.355962	-1.735998	-1.547558	
1	-0.722322	1.715410	2.082759	
6	-0.397371	0.878224	0.000000	
14	0.260042	-0.878868	0.000000	
6	2.129531	-0.761186	0.000000	
1	0.037780	-2.753699	1.612617	
1	-1.446998	-1.798172	1.559291	
1	-0.039035	-1.197753	2.444313	
1	2.584671	-1.755391	0.000000	
1	2.485024	-0.226344	0.884199	
1	2.485024	-0.226344	-0.884199	
1	0.037780	-2.753699	-1.612617	
1	-0.039035	-1.197753	-2.444313	
1	-1.446998	-1.798172	-1.559291	

M06-2X /6-311+g(d, p) = -564.4686923 Hartree

Sum of electronic and zero-point Energies= -564.284012 Hartree

Sum of electronic and thermal Energies= -564.272625 Hartree

Sum of electronic and thermal Enthalpies= -564.271681 Hartree

Sum of electronic and thermal Free Energies= -564.321014 Hartree

Low frequencies (cm-1): -731.0572 41.6640 92.5818 114.5807
119.3053 143.2913 149.1049 189.6598 195.5110 201.2483

3:

Atomic Numbers		Coordinates (Angstroms)		
X	Y	Z		
1		0.345980	-0.085443	2.085309
6		-0.122668	-0.272108	1.123952
6		0.726764	-0.595282	0.000000
6		-0.122668	0.882331	0.000000
6		-0.122668	-0.272108	-1.123952
1		0.345980	-0.085443	-2.085309
1		-1.163863	-0.607724	-1.193931
1		-1.163863	-0.607724	1.193931
1		-1.138297	1.264365	0.000000
1		0.621496	1.664970	0.000000

M06-2X /6-311+g(d, p) = -155.8418809 Hartree

Sum of electronic and zero-point Energies = -155.756716 Hartree

Sum of electronic and thermal Energies = -155.752738 Hartree

Sum of electronic and thermal Enthalpies = -155.751794 Hartree

Sum of electronic and thermal Free Energies = -155.782301 Hartree

Low frequencies (cm⁻¹): 428.8460 490.2809 519.9912 810.9376
871.2764 933.4985 953.7581 992.1776 1087.2808 1115.1361

4:

Atomic Numbers		Coordinates (Angstroms)		
X	Y	Z		
1		0.000000	2.077740	-0.211913
6		0.000000	1.129917	0.316072
6		0.739934	0.000000	-0.322125
6		-0.739934	0.000000	-0.322125
6		0.000000	-1.129917	0.316072

1	0.000000	-2.077740	-0.211913
1	0.000000	-1.209833	1.402636
1	0.000000	1.209833	1.402636
1	-1.422950	0.000000	-1.154407
1	1.422950	0.000000	-1.154407

M06-2X /6-311+g(d, p) = -155.9202199 Hartree

Sum of electronic and zero-point Energies = -155.833280 Hartree

Sum of electronic and thermal Energies = -155.829574 Hartree

Sum of electronic and thermal Enthalpies = -155.828630 Hartree

Sum of electronic and thermal Free Energies = -155.858016 Hartree

Low frequencies (cm⁻¹): 436.5349 702.0625 774.4755 870.7699
920.7011 938.4297 950.9319 1007.5061 1076.3262 1111.9316.

3-4 (TS):

Atomic Numbers Coordinates (Angstroms)

X	Y	Z	
1	0.162880	0.007754	2.078874
6	-0.197106	-0.240769	1.085674
6	0.842457	-0.529564	0.000000
6	-0.197106	0.818643	0.000000
6	-0.197106	-0.240769	-1.085674
1	0.162880	0.007754	-2.078874
1	-1.093262	-0.854684	-1.069580
1	-1.093262	-0.854684	1.069580
1	-0.607131	1.823140	0.000000
1	0.961055	1.025474	0.000000

M06-2X /6-311+g(d, p) = -155.8186012 Hartree

Sum of electronic and zero-point Energies= -155.735199 Hartree

Sum of electronic and thermal Energies= -155.731651 Hartree

Sum of electronic and thermal Enthalpies= -155.730707 Hartree
 Sum of electronic and thermal Free Energies= -155.760543 Hartree

Low frequencies (cm⁻¹): -823.0355 592.1897 710.1581 786.3592
 882.3994 891.3126 946.7664 965.1417 1081.9930
 1089.1001.

Table 1. CVT, CVT + SCT Rate Constants for 1 → 2 and CVT and CVT + SCT Rate Constants for 3 → 4 from 100K – 600K

T(K)	1→2		3→4	
	k _{CVT} (s ⁻¹)	k _{CVT+SCT} (s ⁻¹)	k _{CVT} (s ⁻¹)	k _{CVT+SCT} (s ⁻¹)
100	5.44E-008	1.36E-003	4.17E-018	7.19E-004
102	1.35E-007	1.94E-003	1.64E-017	7.43E-004
123	3.35E-004	9.00E-002	1.99E-012	1.18E-003
125	6.15E-004	1.29E-001	4.94E-012	1.25E-003
127	1.11E-003	1.84E-001	1.19E-011	1.33E-003
141	4.34E-002	2.01E+000	2.85E-009	2.25E-003
143	6.91E-002	2.77E+000	5.71E-009	2.47E-003
145	1.09E-001	3.82E+000	1.12E-008	2.72E-003
148	2.10E-001	6.10E+000	2.99E-008	3.16E-003
150	3.20E-001	8.30E+000	5.63E-008	3.51E-003
152	4.84E-001	1.12E+001	1.04E-007	3.93E-003
171	1.51E+001	1.57E+002	1.75E-005	1.47E-002
173	2.08E+001	2.02E+002	2.81E-005	1.74E-002
175	2.84E+001	2.59E+002	4.47E-005	2.06E-002
177	3.85E+001	3.31E+002	7.03E-005	2.46E-002
198	6.54E+002	3.40E+003	5.24E-003	2.01E-001
200	8.30E+002	4.16E+003	7.46E-003	2.53E-001
202	1.05E+003	5.07E+003	1.05E-002	3.17E-001
213	3.52E+003	1.42E+004	6.31E-002	1.11E+000
220	7.15E+003	2.61E+004	1.80E-001	2.44E+000
236	3.09E+004	9.33E+004	1.56E+000	1.35E+001
238	3.65E+004	1.08E+005	2.01E+000	1.66E+001
240	4.32E+004	1.25E+005	2.57E+000	2.03E+001
273	4.74E+005	1.06E+006	8.88E+001	4.16E+002
298	2.05E+006	3.97E+006	7.73E+002	2.82E+003
300	2.28E+006	4.38E+006	9.05E+002	3.25E+003
315	4.87E+006	8.74E+006	2.77E+003	8.90E+003
331	1.01E+007	1.71E+007	8.16E+003	2.37E+004
333	1.10E+007	1.85E+007	9.28E+003	2.67E+004
335	1.20E+007	2.01E+007	1.05E+004	2.99E+004
500	1.35E+009	1.66E+009	1.10E+007	1.90E+007
600	6.73E+009	7.64E+009	1.95E+006	2.43E+006

Table 2. CVT, CVT + SCT Rate Constants for 5→6 and CVT and CVT + SCTRate Constants for 7 → 8 from 100K – 600K

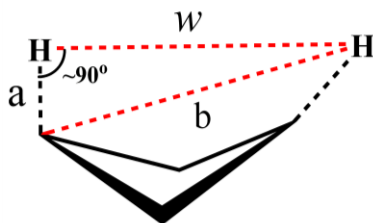
T(K)	5→6		7→8	
	$k_{\text{CVT}}(\text{s}^{-1})$	$k_{\text{CVT+SCT}}(\text{s}^{-1})$	$k_{\text{CVT}}(\text{s}^{-1})$	$k_{\text{CVT+SCT}}(\text{s}^{-1})$
100	6.75E-009	8.22E-005	1.12E-019	2.01E-008
102	1.75E-008	1.24E-004	4.44E-019	2.11E-008
123	6.19E-005	9.61E-003	5.51E-014	5.03E-008
125	1.17E-004	1.44E-002	1.37E-013	5.68E-008
127	2.17E-004	2.14E-002	3.32E-013	6.48E-008
141	1.00E-002	3.07E-001	7.96E-011	2.05E-007
8	1.63E-002	4.39E-001	1.60E-010	2.50E-007
145	2.62E-002	6.25E-001	3.14E-010	3.07E-007
148	5.20E-002	1.05E+000	8.36E-010	4.26E-007
150	8.10E-002	1.47E+000	1.57E-009	5.36E-007
152	1.25E-001	2.05E+000	2.91E-009	6.79E-007
171	4.57E+000	3.65E+001	4.87E-007	9.02E-006
173	6.38E+000	4.81E+001	7.82E-007	1.21E-005
175	8.84E+000	6.30E+001	1.24E-006	1.63E-005
177	1.22E+001	8.22E+001	1.95E-006	2.20E-005
198	2.35E+002	1.02E+003	1.30E-004	4.88E-004
200	3.02E+002	1.27E+003	1.85E-004	6.47E-004
202	3.86E+002	1.57E+003	2.61E-004	8.55E-004
213	1.37E+003	4.74E+003	1.56E-003	3.74E-003
220	2.87E+003	9.11E+003	4.44E-003	9.09E-003
236	1.33E+004	3.56E+004	3.83E-002	5.93E-002
238	1.58E+004	4.18E+004	4.91E-002	7.38E-002
240	1.88E+004	4.88E+004	6.27E-002	9.17E-002
273	2.31E+005	4.74E+005	2.11E+000	2.20E+000
298	1.07E+006	1.94E+006	1.79E+001	1.60E+001
300	1.20E+006	2.15E+006	2.10E+001	1.85E+001
315	2.64E+006	4.48E+006	6.33E+001	5.23E+001
331	5.68E+006	9.15E+006	1.84E+002	1.43E+002
333	6.22E+006	9.96E+006	2.09E+002	1.62E+002
335	6.80E+006	1.08E+007	2.37E+002	1.82E+002
350	1.29E+007	1.97E+007	5.76E+002	4.25E+002
400	7.71E+007	1.06E+008	6.88E+003	4.63E+003
500	9.49E+008	1.16E+009	2.21E+005	1.39E+005
600	5.06E+009	5.68E+009	2.25E+006	1.40E+006

Table 3. CVT, CVT + SCT Rate Constants for 9→10 and CVT and CVT + SCTRate Constants for 11 → 12 from 100K – 600K

T(K)	9→10		11→12	
	$k_{\text{CVT}}(\text{s}^{-1})$	$k_{\text{CVT+SCT}}(\text{s}^{-1})$	$k_{\text{CVT}}(\text{s}^{-1})$	$k_{\text{CVT+SCT}}(\text{s}^{-1})$
100.00	9.01E-09	2.29E-05	6.38E-21	6.25E-11
102.00	2.33E-08	3.72E-05	2.63E-20	7.09E-11
123.00	7.79E-05	5.24E-03	4.71E-15	4.77E-10
125.00	1.47E-04	8.15E-03	1.21E-14	6.07E-10
127.00	2.70E-04	1.26E-02	3.01E-14	7.82E-10
141.00	1.22E-02	2.17E-01	8.64E-12	6.34E-09
143.00	1.98E-02	3.16E-01	1.77E-11	8.93E-09
145.00	3.16E-02	4.58E-01	3.56E-11	1.27E-08
148.00	6.26E-02	7.88E-01	9.82E-11	2.19E-08
150.00	9.71E-02	1.12E+00	1.89E-10	3.17E-08
152.00	1.49E-01	1.59E+00	3.56E-10	4.62E-08
171.00	5.32E+00	3.10E+01	7.14E-08	1.79E-06
173.00	7.41E+00	4.11E+01	1.17E-07	2.60E-06
175.00	1.02E+01	5.41E+01	1.88E-07	3.78E-06
177.00	1.41E+01	7.10E+01	3.01E-07	5.46E-06
198.00	2.66E+02	9.22E+02	2.33E-05	1.98E-04
200.00	3.41E+02	1.15E+03	3.36E-05	2.71E-04
202.00	4.35E+02	1.42E+03	4.81E-05	3.69E-04
213.00	1.53E+03	4.37E+03	3.08E-04	1.85E-03
220.00	3.20E+03	8.46E+03	9.10E-04	4.82E-03
236.00	1.46E+04	3.35E+04	8.52E-03	3.56E-02
238.00	1.74E+04	3.93E+04	1.10E-02	4.49E-02
240.00	2.07E+04	4.60E+04	1.42E-02	5.65E-02
273.00	2.40E+05	4.34E+05	5.52E-01	1.58E+00
298.00	1.10E+06	1.79E+06	5.14E+00	1.24E+01
300.00	1.23E+06	1.99E+06	6.04E+00	1.45E+01
315.00	2.71E+06	4.16E+06	1.91E+01	4.23E+01
331.00	5.81E+06	8.53E+06	5.83E+01	1.20E+02
333.00	6.36E+06	9.29E+06	6.65E+01	1.35E+02
335.00	6.95E+06	1.01E+07	7.57E+01	1.53E+02
350.00	1.34E+07	1.90E+07	1.92E+02	3.65E+02
400.00	7.90E+07	1.02E+08	2.56E+03	4.20E+03
500.00	9.46E+08	1.10E+09	9.64E+04	1.33E+05
600.00	4.99E+09	5.41E+09	1.09E+06	1.35E+06

Calculation Scheme for Estimating Barrier Width (w):

From *Pythagoras Theorem*, for a right angle triangle: $b^2 = a^2 + w^2$
Where, b =hypotenuse, a =base and w = vertical height;



For, $1 \rightarrow 2$; $a= 1.09\text{\AA}$, $b=2.33\text{\AA}$, $w =2.06\text{\AA}$
 $3 \rightarrow 4$; $a=1.08\text{\AA}$, $b=2.32\text{\AA}$, $w =2.05\text{\AA}$

Cartesian Coordinates for Optimized Structures at QCISD/TZVP:

1:

Atomic Numbers Coordinates (Angstroms)

X	Y	Z		
	6	-0.31434600	1.84915400	1.09667000
	6	-0.97061700	2.58518000	0.00000000
	6	-0.31434600	1.84915400	-1.09667000
	1	-1.84068400	0.57995900	0.00000000
	6	-0.31434600	-1.79628600	1.55411800
	1	0.77723800	1.80309900	-1.14907400
	1	-0.78658600	1.86371700	-2.07519500
	1	0.77723800	1.80309900	1.14907400
	6	-0.31434600	-1.79628600	-1.55411800
	1	-0.78658600	1.86371700	2.07519500
	6	-0.77362300	0.79331200	0.00000000
	14	0.19115300	-0.84891900	0.00000000
	6	2.05819600	-0.56588000	0.00000000
	1	0.17709900	-2.77271400	1.58883400
	1	-1.39440200	-1.96284600	1.58026800
	1	-0.03508000	-1.24734900	2.45728500

1	2.56560900	-1.53564600	0.00000000
1	2.39148700	-0.01867700	0.88490100
1	2.39148700	-0.01867700	-0.88490100
1	0.17709900	-2.77271400	-1.58883400
1	-0.03508000	-1.24734900	-2.45728500
1	-1.39440200	-1.96284600	-1.58026800

QCISD/TZVP = -563.35323985 Hartree

Sum of electronic and zero-point Energies=	-563.164594Hartree
Sum of electronic and thermal Energies=	-563.153003Hartree
Sum of electronic and thermal Enthalpies=	-563.152059Hartree
Sum of electronic and thermal Free Energies=	-563.202020Hartree

2:

Atomic Numbers Coordinates (Angstroms)

X	Y	Z
---	---	---

6		-0.426588	1.966959	1.123485
6	6	-1.373405	1.724057	0.000000
6	6	-0.426588	1.966959	-1.123485
1	1	-2.357659	1.284681	0.000000
6	6	-0.426588	-1.568205	1.550684
1	1	0.062591	2.937899	-1.190163
1	1	-0.661029	1.514017	-2.082237
1	1	0.062591	2.937899	1.190163
6	6	-0.426588	-1.568205	-1.550684
1	1	-0.661029	1.514017	2.082237
6	6	-0.036557	1.031286	0.000000
14	14	0.338089	-0.797008	0.000000
6	6	2.206677	-1.087408	0.000000
1	1	-0.261752	-2.649301	1.565768
1	1	-1.505362	-1.393294	1.589189
1	1	0.016268	-1.151718	2.459392
1	1	2.442557	-2.155490	0.000000
1	1	2.669123	-0.639473	0.883669
1	1	2.669123	-0.639473	-0.883669
1	1	-0.261752	-2.649301	-1.565768
1	1	0.016268	-1.151718	-2.459392

1 -1.505362 -1.393294 -1.589189

QCISD/TZVP = -563.427084 Hartree
Sum of electronic and zero-point Energies= -563.237015 Hartree
Sum of electronic and thermal Energies= -563.225567 Hartree
Sum of electronic and thermal Enthalpies= -563.224623 Hartree
Sum of electronic and thermal Free Energies= -563.273959 Hartree

3:

Atomic Numbers		Coordinates (Angstroms)		
X	Y	Z		
	1	0.322727	-0.090260	2.071688
	6	-0.130194	-0.240852	1.096316
	6	0.734035	-0.715130	0.000000
	6	-0.130194	0.914125	0.000000
	6	-0.130194	-0.240852	-1.096316
	1	0.322727	-0.090260	-2.071688
	1	-1.168836	-0.577815	-1.156597
	1	-1.168836	-0.577815	1.156597
	1	-1.079633	1.437997	0.000000
	1	0.711129	1.594400	0.000000

QCISD/TZVP = -155.4589158 Hartree
Sum of electronic and zero-point Energies= -155.372924 Hartree
Sum of electronic and thermal Energies= -155.368902 Hartree
Sum of electronic and thermal Enthalpies= -155.367958 Hartree
Sum of electronic and thermal Free Energies= -155.398585 Hartree

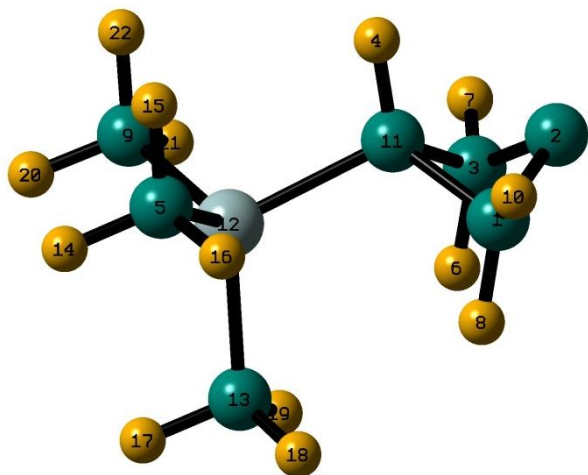
4:

Atomic Numbers		Coordinates (Angstroms)		
X	Y	Z		
1		0.000000	2.077893	-0.216345
6		0.000000	1.131213	0.314716
6		0.746577	0.000000	-0.319401
6		-0.746577	0.000000	-0.319401
6		0.000000	-1.131213	0.314716
1		0.000000	-2.077893	-0.216345
1		0.000000	-1.222782	1.399776
1		0.000000	1.222782	1.399776
1		-1.423907	0.000000	-1.155317
1		1.423907	0.000000	-1.155317

QCISD/TZVP = -155.5320571 Hartree
 Sum of electronic and zero-point Energies = -155.444432 Hatree
 Sum of electronic and thermal Energies = -155.440718 Hatree
 Sum of electronic and thermal Enthalpies = -155.439774 Hatree
 Sum of electronic and thermal Free Energies = -155.469183 Hatree

Compliance Matrixes at QCISD/TZVP and M06-2X/6-31+G(d,p) level:

1:



Molecule 1

a.

	2-4	2-11	4-11
2-4	1.697		
2-11	0.413	0.744	
4-11	0.087	0.015	0.184

b.

	2-11	2-12	11-12
2-11	0.744		
2-12	0.724	1.297	
11-12	-0.031	0.306	0.374

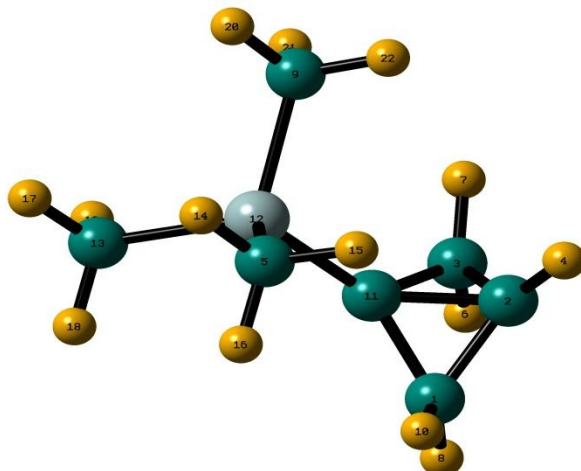
c.d.

	2-4	2-11	4-11
2-4	1.523		
2-11	0.198	0.550	
4-11	0.103	0.002	0.184

	2-11	2-12	11-12
2-11	0.550		
2-12	0.532	1.117	
11-12	-0.041	0.305	0.400

Compliance Matrixes for 1; a. with atom number 2-4-11 at QCISD/TZVP level, b. with atom number 2-11-12 at QCISD/TZVP level, c. with atom number 2-4-11 at M06-2X/6-311+G(d,p) level, d. with atom number 2-11-12 at M06-2X/6-311+G(d,p) level.

2:



Molecule2.

e.

	2-4	2-11	4-11
2-4	0.172		
2-11	-0.002	0.304	
4-11	0.144	0.138	0.856

f.

	2-11	2-12	11-12
2-11	0.304		
2-12	0.046	2.011	
11-12	0.000	0.264	0.320

g.

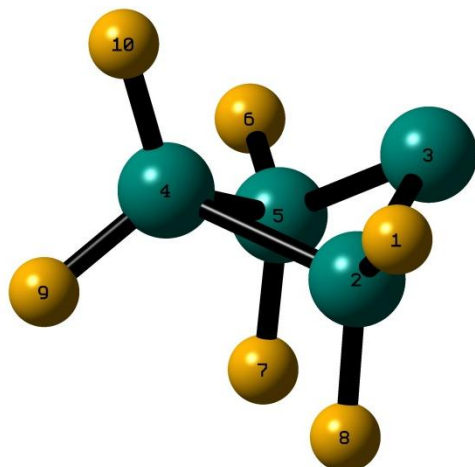
	2-4	2-11	4-11
2-4	0.177		
2-11	-0.002	0.252	
4-11	0.147	0.121	0.862

h.

	2-11	2-12	11-12
2-11	0.252		
2-12	0.043	2.104	
11-12	-0.001	0.249	0.317

Compliance Matrixes for 2; e. with atom number 2-4-11 at QCISD/TZVP level, f. with atom number 2-11-12 at QCISD/TZVP level, g. with atom number 2-4-11 at M06-2X/6-311+G(d,p) level, h. with atom number 2-11-12 at M06-2X/6-311+G(d,p) level.

3:



Molecule 3.

i.

	3-4	3-10	4-10
3-4	1.295		
3-10	0.703	1.732	
4-10	0.029	0.112	0.177

j.

	3-4	3-9	4-9
3-4	1.295		
3-9	1.529	2.307	
4-9	0.004	0.181	0.180

k.

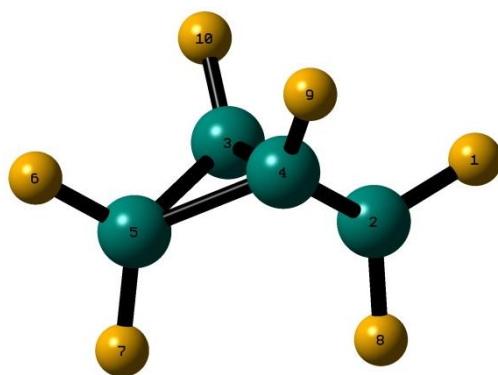
	3-4	3-10	4-10
3-4	0.652		
3-10	0.235	1.279	
4-10	-0.002	0.124	0.178

l.

	3-4	3-9	4-9
3-4	0.652		
3-9	0.774	1.471	
4-9	-0.019	0.144	0.183

Compliance Matrixes for 3; i. with atom number 3-4-10 at QCISD/TZVP level, j. with atom number 3-4-9 at QCISD/TZVP level, k. with atom number 3-4-10 at M06-2X/6-311+G(d,p) level, l. with atom number 3-4-9 at M06-2X/6-311+G(d,p) level.

4:



Molecule 4.

m.

	3-4	3-9	4-9
3-4	0.305		
3-9	0.105	.876	
4-9	-0.001	0.142	0.169

n.

	3-4	3-9	4-9
3-4	0.247		
3-9	0.097	0.866	
4-9	-0.001	0.143	0.172

Compliance Matrixes for 4; m. with atom number 3-4-9 at QCISD/TZVP level, n. with atom number 3-4-9 at M06-2X/6-311+G(d,p) level.

All the compliance constants are in cm/N unit.

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