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“Isolation of a 1,2-Dialuminacyclobut-3-ene”

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All the calculations were carried out with Gaussian98 package. The geometries of the interesting molecules (**4**, **5**, **6**, and **7**) were fully optimized by employing B3LYP/6-31G* method, and the nature of the stationary points were characterized by analytical frequency calculations. The results of the enthalpy change from **4** to **6** and **5** to **7**, and the detailed optimized geometries of **4**-**7** were outlined in Table 1, 2 and 3, respectively. Natural bond orbital method was used to do the charge density analysis (table 4). In order to do a detailed studying of the electronic properties of molecule **4**, the HOMO and LUMO energies were also calculated. The maps of the two orbitals of **4** were shown in Figure 2.

Table 1. The calculated dihedral angles of the Al_2C_2 rings and enthalpy changes from **4** to **6** and **5** to **7.**.

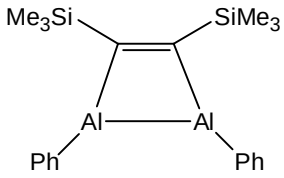
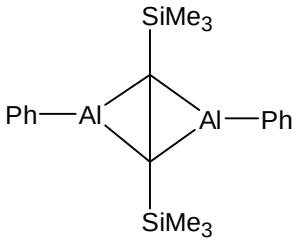
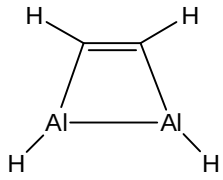
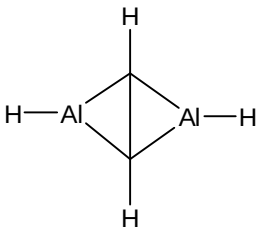
molecule	**4**		**6**
structure			
dihedral angle (º)	-27.60		131.40
H(hartree)	-1842.450146		-1842.424223
? ΔH (kcal/mol)[a]		H(**6**) – H(**4**) **=** 16.26	
molecule	**5**		**7**
structure			
dihedral angle (º)	0.03		-153.49
H(hartree)	-563.371051		-563.319828
? H (kcal/mol)[b]		H(**7**) – H(**5**) **=** 32.14	

Table 2. The detailed geometries of **4** calculated using B3LYP/6-31G* method**.**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.581929	0.842703	0.365592
2	6	0	0.581930	0.842705	-0.365594
3	13	0	-1.214178	-1.068431	0.208374
4	14	0	-1.553038	2.234483	1.210155
5	13	0	1.214178	-1.068430	-0.208382
6	6	0	-3.020345	-1.749068	-0.201580
7	14	0	1.553040	2.234489	-1.210146
8	6	0	-0.469746	3.624709	1.917003
9	6	0	-2.833640	2.968551	0.014447
10	6	0	-2.456960	1.445078	2.681030
11	6	0	3.020344	-1.749070	0.201571
12	6	0	-3.157999	-3.092465	-0.612065
13	6	0	-4.202774	-0.983973	-0.116043
14	6	0	2.456954	1.445100	-2.681035
15	6	0	0.469749	3.624726	-1.916977

16	6	0	2.833647	2.968539	-0.014434
17	1	0	0.029983	4.215251	1.142614
18	1	0	-1.084351	4.314459	2.509608
19	1	0	0.303858	3.221661	2.581406
20	1	0	-2.350031	3.511652	-0.804376
21	1	0	-3.464152	2.192112	-0.433752
22	1	0	-3.494131	3.671193	0.538242
23	1	0	-1.746315	0.998785	3.387844
24	1	0	-3.037977	2.195712	3.231383
25	1	0	-3.152466	0.655909	2.370518
26	6	0	-4.402676	-3.643330	-0.923435
27	6	0	-5.451528	-1.525463	-0.424947
28	6	0	4.202779	-0.983987	0.116002
29	6	0	3.157991	-3.092458	0.612089
30	1	0	-2.274777	-3.724867	-0.694760
31	1	0	-4.155179	0.056974	0.196551
32	1	0	3.152426	0.655895	-2.370540
33	1	0	1.746303	0.998858	-3.387874
34	1	0	3.038006	2.195732	-3.231355
35	1	0	1.084351	4.314472	-2.509590
36	1	0	-0.303867	3.221686	-2.581369
37	1	0	-0.029964	4.215272	-1.142580
38	1	0	2.350041	3.511593	0.804423
39	1	0	3.464189	2.192097	0.433718
40	1	0	3.494109	3.671221	-0.538211
41	6	0	-5.552986	-2.858141	-0.830063
42	6	0	5.451532	-1.525480	0.424906
43	6	0	4.402668	-3.643325	0.923461
44	1	0	-4.475778	-4.681623	-1.238213
45	1	0	-6.344822	-0.909744	-0.350829
46	1	0	4.155190	0.056952	-0.196619
47	1	0	2.274766	-3.724850	0.694809
48	6	0	5.552984	-2.858148	0.830056
49	1	0	-6.524571	-3.282321	-1.071191
50	1	0	6.344831	-0.909770	0.350762
51	1	0	4.475764	-4.681611	1.238264
52	1	0	6.524567	-3.282330	1.071184

Table 3. The detailed geometries of **6** calculated using B3LYP/6-31G* method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.000593	1.167376	0.171152
2	13	0	-1.382641	0.000101	-0.452195
3	13	0	1.381788	-0.000181	-0.453087
4	6	0	0.000176	-1.167181	0.171689
5	14	0	0.001583	2.420383	1.549611
6	14	0	-0.000810	-2.419664	1.550628
7	6	0	-3.189281	0.000069	-1.190291
8	6	0	3.188420	-0.000573	-1.191175
9	6	0	-1.477289	2.216977	2.725043
10	6	0	1.589415	2.361668	2.591784
11	6	0	-0.111446	4.131112	0.724689
12	6	0	-3.866425	1.205169	-1.470676
13	6	0	-3.866991	-1.204561	-1.471269
14	6	0	3.866427	1.203894	-1.472128
15	6	0	3.865370	-1.205836	-1.471322
16	6	0	1.479338	-2.216195	2.724480
17	6	0	-1.587556	-2.360351	2.594395

18	6	0	0.111182	-4.130573	0.725965
19	1	0	-2.431192	2.285469	2.187075
20	1	0	-1.453930	1.246228	3.235631
21	1	0	-1.479176	2.993993	3.500128
22	1	0	1.708888	1.391943	3.090872
23	1	0	2.480626	2.526737	1.973182
24	1	0	1.583042	3.132423	3.373113
25	1	0	-0.098525	4.925024	1.482499
26	1	0	0.729672	4.305278	0.043838
27	1	0	-1.035610	4.237428	0.144898
28	6	0	-5.156297	1.209244	-2.003979
29	6	0	-5.156856	-1.207754	-2.004578
30	6	0	5.156399	1.206777	-2.005184
31	6	0	5.155345	-1.210222	-2.004376
32	1	0	-3.380970	2.159146	-1.271853
33	1	0	-3.382035	-2.158872	-1.272910
34	1	0	3.381621	2.158316	-1.273938
35	1	0	3.379690	-2.159698	-1.272490
36	1	0	2.432668	-2.284321	2.185453
37	1	0	1.456331	-1.245640	3.235442
38	1	0	1.482219	-2.993493	3.499285
39	1	0	-1.706391	-1.390422	3.093239
40	1	0	-2.479355	-2.525463	1.976648
41	1	0	-1.580626	-3.130841	3.375972
42	1	0	1.033564	-4.236118	0.143204
43	1	0	0.101505	-4.924302	1.484012
44	1	0	-0.731953	-4.305742	0.047867
45	6	0	-5.803003	0.000967	-2.271446
46	6	0	5.802348	-0.002099	-2.271822
47	1	0	-5.656525	2.152113	-2.211045
48	1	0	-5.657556	-2.150273	-2.212088
49	1	0	5.657334	2.149175	-2.212675
50	1	0	5.655424	-2.153210	-2.211260
51	1	0	-6.807535	0.001305	-2.687158
52	1	0	6.806961	-0.002679	-2.687340

Table 4. The detailed geometries of **5** calculated using B3LYP/6-31G* method**.**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.262735	-0.647030	-0.000053
2	13	0	1.262811	-0.646964	0.000016
3	6	0	-0.686548	1.243906	-0.000278
4	1	0	-2.743477	-1.247616	0.001113
5	6	0	0.686397	1.243998	0.000302
6	1	0	2.743660	-1.247286	-0.000751
7	1	0	-1.232539	2.194622	-0.000654
8	1	0	1.232276	2.194782	0.000637

Table 5. The detailed geometries of **7** calculated using B3LYP/6-31G* method.

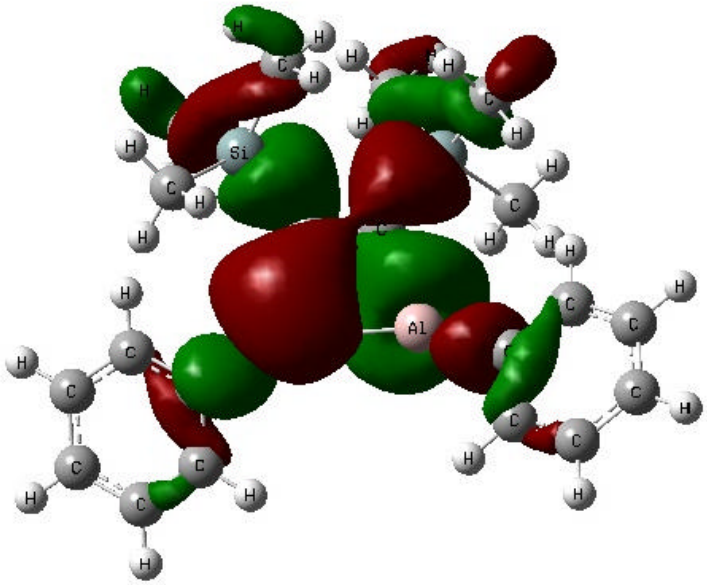
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

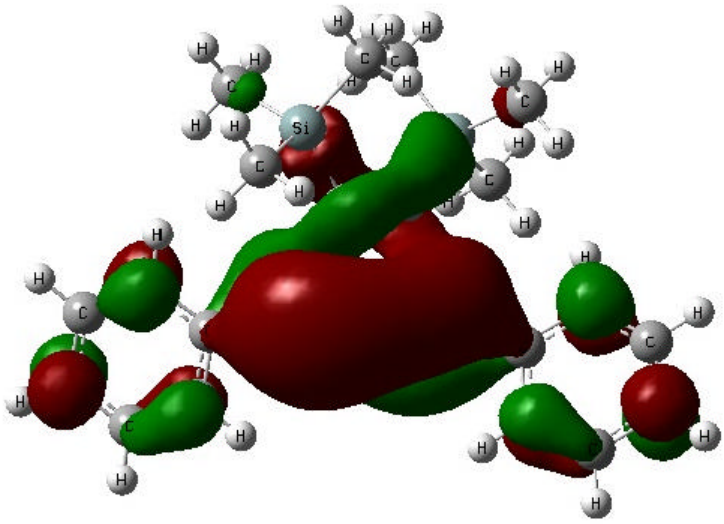
1	6	0	-0.000047	-1.289639	0.211678
2	13	0	-1.392789	-0.000087	-0.116445
3	6	0	-0.000129	1.289906	0.211454
4	13	0	1.392770	0.000159	-0.116585
5	1	0	0.000248	-2.244306	0.742605
6	1	0	-2.931030	-0.000425	-0.497676
7	1	0	0.000872	2.244390	0.742664
8	1	0	2.931224	-0.002205	-0.496999

Table 6. Natural charges of atoms in **4** calculated using B3LYP/6-31G* method.

atom	No	Natural charge	atom	No	Natural charge
C	1	-0.97665	C	27	-0.23775
C	2	-0.97665	C	28	-0.21243
Al	3	1.06907	C	29	-0.21085
Si	4	1.81242	H	30	0.23117
Al	5	1.06907	H	31	0.22384
C	6	-0.61289	H	32	0.24600
Si	7	1.81242	H	33	0.25108
C	8	-1.19240	H	34	0.25052
C	9	-1.18964	H	35	0.25073
C	10	-1.19500	H	36	0.25182
C	11	-0.61289	H	37	0.24372
C	12	-0.21085	H	38	0.25213
C	13	-0.21243	H	39	0.24765
C	14	-1.19500	H	40	0.24925
C	15	-1.19240	C	41	-0.21919
C	16	-1.18964	C	42	-0.23775
H	17	0.24372	C	43	-0.23837
H	18	0.25073	H	44	0.23529
H	19	0.25182	H	45	0.23506
H	20	0.25213	H	46	0.22384
H	21	0.24765	H	47	0.23117
H	22	0.24925	C	48	-0.21919
H	23	0.25108	H	49	0.23542
H	24	0.25052	H	50	0.23506
H	25	0.24600	H	51	0.23529
C	26	-0.23837	H	52	0.23542



HOMO (-0.1943 ev)



LUMO (-0.0547 ev)

Figure 2. The HOMO and LUMO maps of **4** calculated using B3LYP/6-31G* method.