Supplementary Material (ESI) for PCCP

Supplementary data

A theoretical study of the rearrangement processes of energized CCCB and CCCAl.

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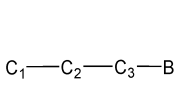
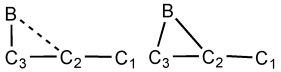
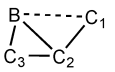
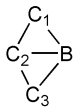
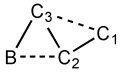
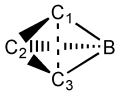
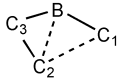
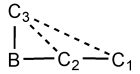
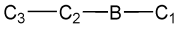
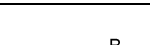
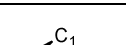
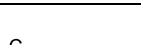
Tables 3-7 contain data concerning the geometries [UB3LYP/6-311+G(3df) level of theory] and single point energies [calculated at UCCSD(T)/aug-cc-pVTZ] of all minima and transition states shown in the appropriate Figures in the text. Energies (in hartree and kJ mol^{-1}) at the lower UCCSD(T)/aug-cc-pVDZ//UB3LYP/6-31+G(d) level of theory are indicated in parenthesis for comparison purposes. Geometric data are not included at this level of theory. Tables 8-9 contain data concerning the geometries [UX3LYP/cc-pVTZ or UBMK/cc-pVTZ levels of theory] and single point energies [calculated at UCCSD(T)/aug-cc-pVTZ] of selected minima. Relative energies obtained by subtraction of corrected hartree energies are recorded in kJ mol^{-1} units in all tables. Standard enthalpies of formation [UCCSD(T)/aug-cc-pVTZ//UB3LYP/6-311+G(3df) level] are contained in Table 10, and charge distributions of selected C_3B and C_3Al isomers are contained in Table 11 and 12.

Table 3. Minima and Transition Structures on the Quartet C_3B Surface Calculated at the UB3LYP/6-311+G(3df) Level of Theory, with Single Point Energies (Including Zero-Point Energy Correction) Calculated at UCCSD(T)/aug-cc-pVTZ

											
	^4A	TS $^4A/^4D$	^4D	TS $^4D/^4H$	^4H	TS $^4A/^4G$	TS $^4H/^4G$	^4G	TS $^4H/^4B$	TS $^4G/^4B$	^4B
State	$^4\Sigma$	^4A	$^4A''$	$^4A''$	$^4A''$	$^4A''$	^4A	$^4A''$	$^4A''$	$^4A''$	^4A
Symmetry	$C_{\infty V}$	C_1	C_S	C_S	C_S	C_S	C_1	C_{2V}	C_S	C_S	$C_{\infty V}$
Energy (Hartree)	-138.55013 (-138.44884)[a]	-138.51650 (-138.41617)	-138.51885 (-138.41808)	-138.51807 (-138.41732)	-138.53817 (-138.43526)	-138.49098 (-138.39043)	-138.50209 (-138.40399)	-138.51868 (-138.41549)	-138.47976 (-138.38057)	-138.45362 (-138.35582)	-138.51861 (-138.42170)
Energy Relative to ^4A (kJ mol^{-1})	0	88.3 (85.7)	82.0 (80.7)	84.1 (82.8)	31.4 (35.5)	155.2 (153.0)	126.0 (117.5)	81.5 (87.4)	184.7 (178.9)	253.5 (244.1)	82.8 (71.1)
Dipole Moment (Debye)	3.9473	3.2388	2.5327	1.5085	0.1897	1.9949	0.3350	0.0986	2.2269	3.1030	4.2137
Bond Lengths (Å)											
C1C2	1.301	1.319	1.324	1.312	1.355	1.302	1.438	1.374	2.170	1.299	
C2C3	1.283	1.330	1.347	1.358	1.355	1.485	1.316	1.374	1.303	2.050	1.278
C3B	1.380	1.397	1.412	1.443	1.517	1.436	1.616	1.501	1.428	1.391	
C1C3						1.920		1.476		3.081	
C1B				2.187	1.518		1.458		1.420		1.418
C2B		1.924	1.711	1.653	1.589	1.549			1.676	1.439	1.385
Bond Angles (°)											
C1C2C3	180.0	179.8	176.8	150.6	122.9	86.8	102.5	64.9		132.6	
C1C3C2						42.6		57.5		18.1	
C1C2B		133.6	129.8	94.4	61.5				40.9	18.1	
C1BC2				36.7	51.7				88.6		180.0
C1C3B								60.6			
C1BC3					103.3		88.5	58.9			
C2C1C3						50.6				29.3	
C2C1B				48.9	66.9		79.2	118.1	50.6		
C2C3B	180.0	89.7	76.6	72.3	66.9	64.0	77.3		75.5	44.5	
C2BC3		43.7	50.0	51.5	51.7	59.5			48.9	92.8	
C3C2B		46.6	53.4	56.3	61.4	56.5				42.7	180.0
Dihedral Angles (°)											
BC3C2C1	—	180.0	180.0	0.0	0.0	180.0	26.9	180.0	0.0	180.0	—
C1C2BC3	—	180.0	180.0	180.0	180.0	0.0	-145.3	0.0	180.0	0.0	—

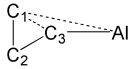
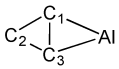
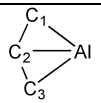
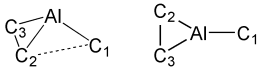
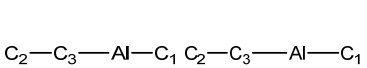
[a] Energy data in parentheses are calculated at CCSD(T)/aug-cc-pVDZ//B3LYP/6-31+G(d) level of theory.

Table 4. Minima and Transition Structures on the Doublet C_3B Surface Calculated at the UB3LYP/6-311+G(3df) Level of Theory, with Single Point Energies (Including Zero-Point Energy Correction) Calculated at UCCSD(T)/aug-cc-pVTZ

									
	^{2}A	**TS ^{2}A/^{2}H**	**^{2}H**	**TS ^{2}A/^{2}G**	**TS ^{2}H/^{2}G**	**^{2}G**	**TS ^{2}H/^{2}B**	**TS ^{2}G/^{2}B**	**^{2}B**
State	^{2}A	^{2}A	^{2}A'	^{2}A'	^{2}A	^{2}A'	^{2}A	^{2}A"	—
Symmetry	C_1	C_1	C_S	C_S	C_1	C_S	C_1	C_S	$C_{\infty V}$
Energy (Hartree)	-138.53113 (-138.43637)[a]	-138.51075 (-138.41421)	-138.55423 (-138.45111)	-138.49458 (-138.39310)	-138.51962 (-138.41518)	-138.56890 (-138.46675)	-138.50505 (-138.40882)	-138.48675 (-138.38023)	-138.51565 (-138.41846)
Energy Relative to ^{2}A (kJ mol^{-1})	0	53.5 (58.1)	-60.7 (-38.5)	95.8 (113.7)	30.1 (55.6)	-99.2 (-79.8)	68.6 (72.3)	116.3 (147.1)	40.6 (46.8)
Dipole Moment (Debye)	1.3307	1.7131	0.5529	1.0750	1.0679	2.4172	0.8293	2.5651	1.6581
Bond Lengths (Å)									
C1C2	1.316	1.324	1.361	1.349	1.318	1.435		1.717	
C2C3	1.268	1.312	1.361	1.364	1.491	1.435	1.274	1.310	1.284
C3B	1.503	1.603	1.574	1.564	1.533	1.482	1.516		
C1C3				1.435		1.492		2.886	
C1B		2.331	1.575	2.748	1.527	1.482	1.518	1.443	1.503
C2B		2.008	1.519				1.517	1.426	1.377
Bond Angles (°)									
C1C2C3	174.2	138.4	132.0	63.9	92.4	62.6		144.5	
C1C3C2				57.6	40.4	58.7		20.2	
C1C2B		86.2	66.0		50.1			53.7	
C1BC2		34.5	52.2		41.5		155.2	73.5	180.0
C1C3B				132.7	48.3	59.8			
C1BC3			104.3	22.6	83.1	60.4	155.1		
C2C1C3					47.2	58.7		15.3	
C2C1B		59.3			88.4	118.5		52.85	
C2C3B	150.7	86.5		169.7	82.3		65.2		
C2BC3		40.7			47.9		49.7		
C3C2B		52.8			49.8		65.1	161.8	180.0
Dihedral Angles (°)									
BC3C2C1	180.0	11.8	0.0	180.0	28.9	0.0	0.0	180.0	—
C1C2BC3	180.0	-172.2	180.0	0.0	-141.0	180.0	180.0	180.0	—

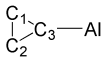
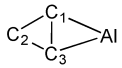
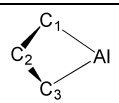
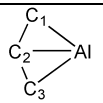
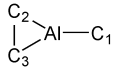
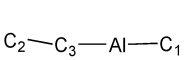
[a] Energy data in parentheses are calculated at CCSD(T)/aug-cc-pVDZ//B3LYP/6-31+G(d) level of theory.

Table 5. Minima and Transition Structures on the Doublet C_3Al Surface Calculated at the B3LYP/6-311+G(3df) Level of Theory, with Single Point Energies (Including Zero-Point Energy Correction) Calculated at UCCSD(T)/aug-cc-pVTZ

										
	^2A	TS $^2A/^2G$	^2G	TS $^2A/^2H$	TS $^2G/^2H$	^2H	TS $^2H/^2E$	^2E	TS $^2E/^2B$	^2B
State	$^2A''$	$^2B_2$	$^2A'$	$^2A'$	$^2A_2$	$^2A''$	$^2A'$	$^2B_2$	—	$^2A''$
Symmetry	C_S	C_{2v}	C_S	C_S	C_{2v}	C_S	C_S	C_{2v}	$C_{\infty v}$	C_S
Energy (Hartree)	-355.86101 (-355.75938)[a]	-355.81649 (-355.71539)	-355.86550 (-355.76184)	-355.85276 (-355.75215)	-355.84188 (-355.74031)	-355.85379 (-355.75299)	-355.73423 (-355.63634)	-355.74974 (-355.64623)	-355.71962 (-355.60162)	-355.72342 (-355.61101)
Energy Relative to ^2A (kJ mol^{-1})	0	115.5 (115.4)	-12.1 (-6.3)	21.8 (18.8)	50.2 (50.2)	18.8 (16.7)	333.0 (322.7)	289.0 (296.8)	371.1 (408.4)	361.0 (389.2)
Dipole Moment (Debye)	3.8556	3.2413	1.0615	1.7848	1.6006	1.2148	4.7498	3.4632	5.0387	2.4167
Bond Lengths (Å)										
C1C2	1.317	1.342	1.347	1.309	1.316	1.308	2.805			
C2C3	1.265	1.402	1.347	1.303		1.308	1.262	1.267	1.272	1.243
C3Al	2.017	2.056	2.141	2.194	2.190	2.327	1.878	1.892	1.788	1.820
C1C3			1.533							
C1Al		3.355	2.140	2.643		2.327	1.963	2.054	1.012	1.902
C2Al				2.347		2.310	1.935	1.892		
Bond Angles (°)										
C1C2C3	179.9	61.4	69.4	154.7	118.6	148.6	112.6			
C1C3C2		57.2	55.3							
C1C2Al				87.8		74.3	44.4			
C1AlC2				29.7		32.8	92.0	160.4		
C1C3Al		151.4	69.0							
C1AlC3		11.5	42.0	62.8	62.2	65.5	130.7		180.0	179.4
C2C1C3			55.3							
C2C1Al		78.5	124.3	62.6	89.6	72.9	43.6			
C2C3Al	179.4	151.4	124.3	79.9	89.6	72.9	73.2	70.4	180.0	179.5
C2AlC3				33.1			38.6	39.1		
C3C2Al						74.3	68.2			
Dihedral Angles (°)										
AlC3C2C1	0.0	180.0	180.0	0.0	0.0	0.0	0.0	0.0	—	0.0
C1C2AlC3	180.0	0.0	0.0	-180.0	180.0	-180.0	180.0	180.0	—	0.0

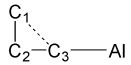
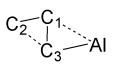
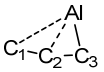
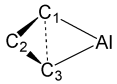
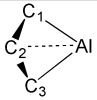
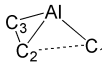
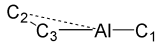
[a] The data in parentheses are calculated at CCSD(T)/aug-cc-pVDZ//B3LYP/6-31+G(d) level of theory.

Table 6. Minima Structures on the Quartet C_3Al Surface Calculated at the UB3LYP/6-311+G(3df) Level of Theory, with Single Point Energies (Including Zero-Point Energy Correction) Calculated at UCCSD(T)/aug-cc-pVTZ

							
	^{4}A	**^{4}C**	**^{4}G**	**^{4}F**	**^{4}H**	**^{4}E**	**^{4}B**
State	$^4\Sigma$	$^4A_2$	$^4A''$	$^4A''$	$^4A''$	$^4A_2$	$^4A''$
Symmetry	$C_{\infty V}$	C_{2V}	C_S	C_S	C_S	C_{2V}	C_S
Energy (Hartree)	-355.81666 (-355.71434)[a]	-355.77916 (-355.67690)	-355.79101 (-355.69359)	-355.78889 (-355.68203)	-355.82328 (-355.71459)	-355.77747 (-355.67386)	-355.74613 (-355.64647)
Energy Relative to ^{4}A (kJ mol^{-1})	0	98.3 (98.2)	62.8 (54.2)	72.8 (84.9)	-17.6 (-0.8)	102.9 (106.2)	185.4 (178.1)
Dipole Moment (Debye)	8.2012	3.6262	2.0958	3.9989	3.2751	3.5680	5.1272
Bond Lengths (Å)							
C1C2	1.30173	1.324	1.358	1.361	1.322		
C2C3	1.28410	1.415	1.358	1.361	1.322	1.265	1.256
C3Al	1.79564	1.919	1.951	1.926	1.992	1.886	1.785
C1C3		1.415	1.490				
C1Al			1.952	1.926	1.992	1.896	1.889
C2Al					1.980	1.886	
Bond Angles (°)							
C1C2C3	180.0	62.1	66.6	85.3	142.1		
C1C3C2		55.8	56.7				
C1C2Al					71.1		
C1AlC2					38.9	160.4	
C1C3Al		152.1	67.6				
C1AlC3			44.9	57.2	77.8		179.4
C2C1C3			56.7				
C2C1Al			124.3	97.9	70.0		
C2C3Al	180.0		124.3	97.9	70.0	70.4	173.6
C2AlC3					38.9	39.2	
C3C2Al					71.1		
Dihedral Angles (°)							
AlC3C2C1	—	180.0	0.0	38.4	0.0	0.0	0.0
C1C2AlC3	—	0.0	180.0	-125.6	180.0	180.0	180.0

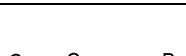
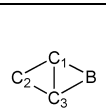
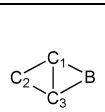
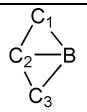
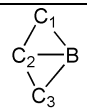
[a] Energy data in parentheses are calculated at CCSD(T)/aug-cc-pVDZ//B3LYP/6-31+G(d) level of theory.

Table 7. Transition Structures on the Quartet C_3Al Surface Calculated at the UB3LYP/6-311+G(3df) Level of Theory, with Single Point Energies (Including Zero-Point Energy Correction) Calculated at UCCSD(T)/aug-cc-pVTZ

							
	TS ^{4}A/^{4}C	**TS ^{4}C/^{4}G**	**TS ^{4}A/^{4}H**	**TS ^{4}G/^{4}F**	**TS ^{4}F/^{4}H**	**TS ^{4}H/^{4}E**	**TS ^{4}E/^{4}B**
State	^{4}A”	^{4}A”	^{4}A”	^{4}A	^{4}A	^{4}A”	^{4}A”
Symmetry	C_S	C_S	C_S	C_1	C_1	C_S	C_S
Energy (Hartree)	-355.77642 (-355.67512)[a]	-355.77889 (-355.67562)	-355.79972 (-355.69777)	-355.78268 (-355.67604)	-355.78163 (-355.67592)	-355.71507 (-355.61276)	-355.74490 (-355.64894)
Energy Relative to ^{4}A (kJ mol^{-1})	105.8 (102.8)	99.1 (101.6)	44.3 (43.5)	89.0 (100.3)	92.0 (100.7)	266.3 (266.3)	188.1 (171.4)
Dipole Moment (Debye)	5.4164	5.4211	5.6806	4.1200	3.4073	4.4521	5.1752
Bond Lengths (Å)							
C1C2	1.313	1.308	1.309	1.311	1.303	2.500	1.258
C2C3	1.342	1.913	1.322	1.412	1.425	1.277	1.782
C3Al	1.818	1.855	1.844	1.861	1.900	1.873	
C1C3	1.847	1.474					
C1Al		1.980	3.350	2.009	2.021	1.916	1.889
C2Al			2.397			2.006	2.958
Bond Angles (°)							
C1C2C3	88.2	50.3	176.607	77.8	106.8		
C1C3C2	45.3	43.0		48.5			
C1C2Al			126.852		61.9	48.8	
C1AlC2					34.7	79.2	
C1C3Al	134.4	72.0		68.3			
C1AlC3		45.0		52.4	34.7		179.8
C2C1C3	46.6	86.7		53.7			
C2C1Al			34.925	111.7	83.5	52.0	
C2C3Al			97.074	115.3	85.1	76.5	152.8
C2AlC3			33.171		38.6	38.3	11.2
C3C2Al					56.3	65.2	16.0
Dihedral Angles (°)							
AlC3C2C1	180.0	0.0	0.0	15.1	37.5	0.0	0.0
C1C2AlC3	0.0	180.0	180.0	-157.8	-138.6	180.0	180.0

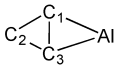
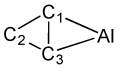
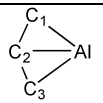
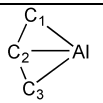
[a] Energy data in parentheses are calculated at CCSD(T)/aug-cc-pVDZ//B3LYP/6-31+G(d) level of theory.

Table 8. Selected Minima Structures of Doublet and Quartet C_3B Calculated Using UX3LYP and UBMK (in parentheses) Methods with cc-pVTZ Basis Set. Single Point Energies (Including Zero-Point Energy Correction) Calculated at UCCSD(T)/aug-cc-pVTZ

						
	^{2}A	**^{4}A**	**^{2}G**	**^{4}G**	**^{2}H**	**^{4}H**
State	^{2}A"	$^4\Sigma$	^{2}A'	^{4}B$_1$	^{2}A'	^{4}A"
Symmetry	C_S	$C_{\infty V}$	C_S	C_{2V}	C_{2V}	C_{2V}
Energy (Hartree)	-355.86080 (-355.86082)	-355.81663 (-355.81632)	-355.86546 (-355.86467)	-355.78159 (-355.78208)	-355.82519 (-355.78767)	-355.82340 (-355.82365)
Energy Relative to ^{2}G (kJ mol^{-1})	+12.2 (+10.1) [a]	+128.2 (+126.9)	0 (0)	+220.2 (+216.8)	+117.7 (+116.5)	+110.4 (+107.7)
Dipole Moment (Debye)	1.2576 (0.9320)	3.8682 (3.8931)	2.3755 (2.3998)	0.1446 (0.1109)	0.5205 (0.6491)	0.1521 (0.2241)
Bond Lengths (Å)						
C1C2	1.317 (1.321)	1.301 (1.300)	1.435 (1.458)	1.374 (1.389)	1.361 (1.360)	1.355 (1.355)
C2C3	1.267 (1.261)	1.283 (1.284)	1.435 (1.460)			
C3B	1.506 (1.520)	1.380 (1.379)	1.482 (1.492)	1.501 (1.509)	1.576 (1.586)	1.519 (1.523)
C1C3			1.492 (1.545)	1.476 (1.525)		
C1B			1.482 (1.491)			
C2B					1.519 (1.549)	1.590 (1.625)
Bond Angles (^{o})						
C1C2C3	174.5 (174.1)	180.0	62.6 (63.9)	64.9 (66.6)		122.93961
C1C3C2			58.7 (58.0)	57.5 (56.7)		
C1C2B					66.1 (65.7)	61.5 (60.7)
C1BC2					52.1 (51.4)	51.6 (50.9)
C1C3B			59.8 (58.8)	60.6 (59.6)		
C1BC3			60.4 (62.4)	58.9 (60.7)		
C2C1C3			58.7 (58.1)			
C2C1B						
C2C3B	151.4 (156.4)	180.0				
C2BC3						
C3C2B						
Dihedral Angles (^{o})						
BC3C2C1	180.0	—	0.0	0.0	0.0	0.0
C1C2BC3	180.0	—	180.0	180.0	180.0	180.0

[a] The relative energies shown in parentheses refer to the UCCSD(T)/aug-cc-pVTZ//UBMK/cc-pVTZ level of theory.

Table 9. Selected Minima Structures of Doublet and Quartet C_3Al Calculated Using UX3LYP and UBMK (in parentheses) Methods with cc-pVTZ Basis Set. Single Point Energies (Including Zero-Point Energy Correction) Calculated at UCCSD(T)/aug-cc-pVTZ

						
	^{2}A	**^{4}A**	**^{2}G**	**^{4}G**	**^{2}H**	**^{4}H**
State	^{2}A' (^{2}A)	$^4\Sigma$	^{2}A'	$^4B_1$ (^{4}A")	$^2B_2$ ($^2B_1$)	^{4}A"
Symmetry	$C_{\infty V}$	$C_{\infty V}$	C_S	C_{2V} (C_S)	C_{2V}	C_S (C_{2V})
Energy (Hartree)	-138.53081 (-138.53233)	-138.55005 (-138.54997)	-138.56887 (-138.57089)	-138.51861 (-138.52072)	-138.55430 (-138.55492)	-138.53818 (-138.53840)
Energy Relative to ^{2}G (kJ mol^{-1})	+99.9 (+101.2) [a]	+49.4 (+54.9)	0 (0)	+132.0 (+131.7)	+38.3 (+41.9)	+80.6 (+85.3)
Dipole Moment (Debye)	3.7527 (3.6932)	8.0248 (8.3278)	0.9845 (1.0238)	2.0212 (4.4468)	3.4060 (3.4231)	3.2172 (3.3155)
Bond Lengths (Å)						
C1C2	1.318 (1.322)	1.302 (1.303)	1.346 (1.351)	1.357 (1.362)	1.332 (1.340)	1.322 (1.331)
C2C3	1.264 (1.262)	1.284 (1.284)	1.346 (1.352)	1.357 (1.368)		1.322 (1.331)
C3Al	2.020 (2.011)	1.799 (1.784)	2.147 (2.136)	1.960 (1.917)	2.013 (2.000)	2.000 (1.990)
C1C3			1.532 (1.618)	1.491 (1.798)		
C1Al			2.147 (2.134)	1.960 (1.919)		2.000 (1.990)
C2Al					1.974 (1.965)	1.986 (1.972)
Bond Angles (°)						
C1C2C3	180.0	180.0	69.3 (73.5)	66.7 (82.4)		142.5 (142.2)
C1C3C2			55.3 (53.2)	56.7 (48.7)		
C1C2Al					72.1 (71.7)	71.2 (71.1)
C1AlC2					39.0 (39.5)	38.7 (39.2)
C1C3Al			69.1 (67.6)	67.6 (62.1)		
C1AlC3			41.8 (44.5)	44.7 (55.9)		
C2C1C3			55.3 (53.3)			
C2C1Al						70.0 (69.7)
C2C3Al	180.0	180.0				70.0 (69.7)
C2AlC3						38.7 (39.2)
C3C2Al						
Dihedral Angles (°)						
AlC3C2C1	—	—	0.0	0.0	0.0	0.0
C1C2AlC3	—	—	180.0	180.0	180.0	180.0

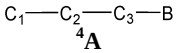
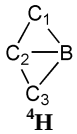
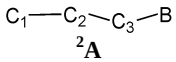
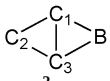
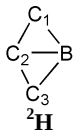
[a] The relative energies shown in parentheses refer to the UCCSD(T)/aug-cc-pVTZ//UBMK/cc-pVTZ level of theory.

Table 10. Standard enthalpies of formation [UCCSD(T)/aug-cc-pVTZ//UB3LYP/6-311+G(3df) level][a]

	Structure	$\Delta_f H^o$ (298K)	Structure	$\Delta_f H^o$ (298K)
	^{4}**A**	1120.5	^{2}**A**	1171.9
	^{4}**B**	1204.2	^{2}**B**	1212.9
C_3B	^{4}**D**	1202.9	^{2}**G**	1069.8
	^{4}**G**	1202.1	^{2}**H**	1108.3
	^{4}**H**	1149.8		
	^{2}**A**	909.2	^{4}**A**	1050.2
	^{2}**B**	1297.0	^{4}**B**	1237.6
	^{2}**E**	1226.7	^{4}**C**	1148.5
C_3Al	^{2}**G**	894.5	^{4}**E**	1153.5
	^{2}**H**	954.0	^{4}**F**	1121.7
			^{4}**G**	1117.1
			^{4}**H**	1030.9

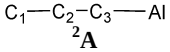
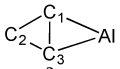
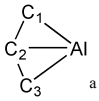
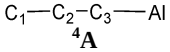
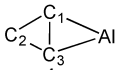
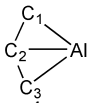
[a] For a definition of structures, see Supplementary Table 3-7. Enthalpies of formation $\Delta_f H^o$ (298K) in kJ mol^{-1}.

Table 11. Charge Distribution of selected C_3B isomers [Mulliken charge[1] (given in normal print), NBO charge[2] (given in bold print), and AIM charge[3] (given in italics print) are shown in the table respectively].[a]

	B	C_1	C_2	C_3
	0.423	-0.366	1.367	-1.424
^{4}**A**	**0.674**	**0.137**	**-0.273**	**-0.538**
	1.137	*0.123*	*-0.296*	*-1.011*
	0.326	-0.012	-0.303	-0.012
^{4}**G**	**0.322**	**-0.163**	**0.004**	**-0.163**
	1.194	*0.068*	*-0.705*	*0.172*
	0.605	-0.340	0.075	-0.340
^{4}**H**	**0.533**	**-0.183**	**-0.166**	**-0.184**
	1.585	*-0.862*	*0.432*	*-0.308*
	0.130	-0.625	0.989	-0.494
	**0.492**	**0.228**	**-0.322**	**-0.398**
^{2}**A**	*0.824*	*0.172*	*-0.261*	*-0.739*
	0.521	-0.079	-0.363	-0.079
^{2}**G**	**0.609**	**-0.322**	**0.034**	**-0.322**
	1.323	*-0.720*	*0.112*	*-0.720*
	0.598	-0.396	0.194	-0.396
^{2}**H**	**0.523**	**-0.109**	**-0.304**	**-0.110**
	1.523	*-0.961*	*0.399*	*-0.961*

[a] (1) R. S. Mulliken, *J. Chem. Phys.*, 1955, **23**, 1833-1840; I. G. Csizmadia, Theory and Practice of MO Calculations on Organic Molecules, Elsevier, Amsterdam, 1976; F.M. Bickelhaupt, N. J. R. van Eikema Hommes, C. Fonseca Guerra and E.J. Baerends. Organometallics, 1996, **15**, 2923-2931. (2) A. E. Reed, L. A. Curtiss, and F. Weinhold, *Chem. Rev.* 1988, **88**, 899-926; F. Weinhold and J. E. Carpenter, in, R. Naaman and Z. Vager (eds.), "The Structure of Small Molecules and Ions" (Plenum, New York, 1988), pp.227-236. J. M. Anglada and J. M. Bofill, *Theor. Chim. Acta.* 1995, **92**, 369-381. (3) R. F. W. Bader. Atoms in Molecules: A Quantum Theory; Clarendon Press, Oxford, 1990; R. Bader. Atoms in Molecules: A Quantum Theory, USA: Oxford University Press, 1994; R. Bader. *Chem. Rev.,* 1991, **91**, 893-928.

Table 12. Charge Distribution of selected C_3Al isomers [Mulliken charge (given in normal print), NBO charge (given in bold print), and AIM charge (given in italics print) are shown in the table respectively].

	Al	C_1	C_2	C_3
 ^{2}**A**	0.196	-0.592	0.645	-0.249
	0.753	**0.170**	**-0.461**	**-0.462**
	1.194	*-1.197*	*0.622*	*-0.619*
 ^{2}**G**	0.405	-0.135	-0.134	-0.136
	0.771	**-0.366**	**-0.366**	**-0.039**
	1.092	*0.091*	*-0.090*	*0.412*
 [a] ^{2}**H**	0.489	-0.436	0.383	-0.436
	0.757	**-0.055**	**-0.648**	**-0.055**
	0.849	*-0.164*	*-0.523*	*-0.164*
 ^{4}**A**	0.501	-0.645	0.554	-0.410
	1.084	**0.060**	**-0.370**	**-0.775**
	1.232	*0.053*	*-0.323*	*-0.966*
 ^{4}**G**	0.359	-0.112	-0.136	-0.112
	0.780	**-0.345**	**-0.074**	**-0.360**
	1.349	*0.111*	*-0.235*	*0.249*
 ^{4}**H**	0.656	-0.541	0.426	-0.541
	1.270	**-0.412**	**-0.442**	**-0.416**
	1.567	*-0.390*	*0.477*	*0.001*

[a]Mulliken charge distribution calculations for this structure have been reported previously at MP2/6-311G* and B3LYP/6-311G* levels of theory.[61] These results are comparable to those listed in this Table.