Supporting information for:

$Al_2C_4H_2$ Isomers with the Planar Tetracoordinate Carbon (ptC)/Aluminum (ptAl)

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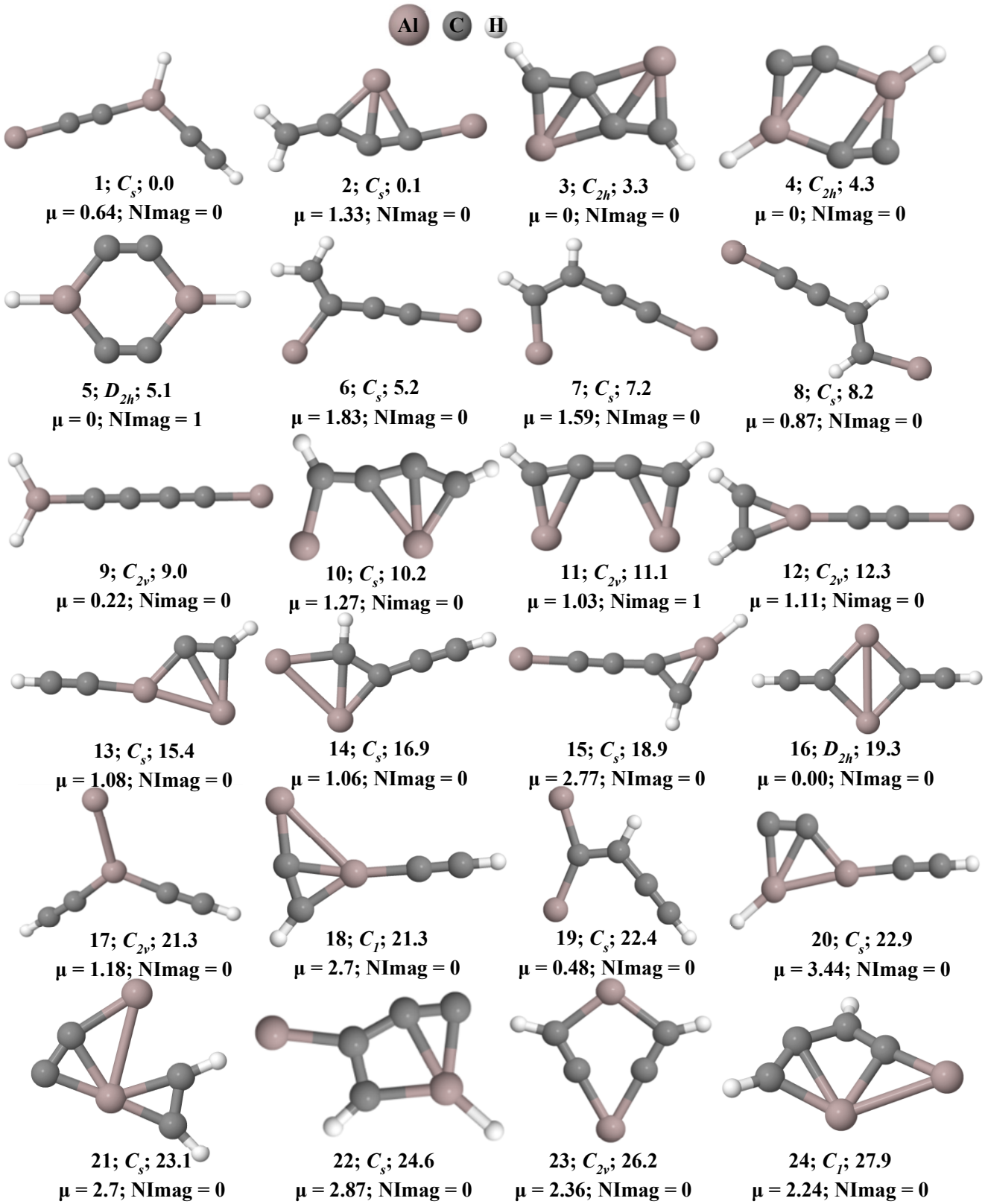
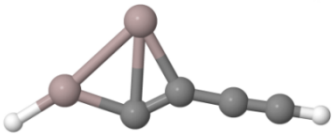
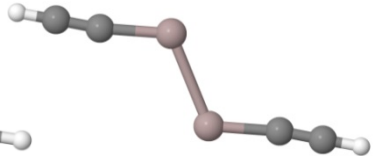
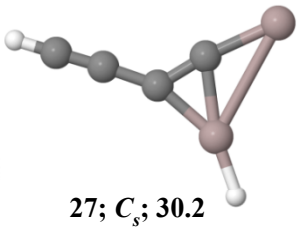

Al
C
H
1; C_s; 0.0
μ = 0.64; NImag = 0
2; C_s; 0.1
μ = 1.33; NImag = 0
3; C_{2h}; 3.3
μ = 0; NImag = 0
4; C_{2h}; 4.3
μ = 0; NImag = 0
5; D_{2h}; 5.1
μ = 0; NImag = 1
6; C_s; 5.2
μ = 1.83; NImag = 0
7; C_s; 7.2
μ = 1.59; NImag = 0
8; C_s; 8.2
μ = 0.87; NImag = 0
9; C_{2v}; 9.0
μ = 0.22; Nimag = 0
10; C_s; 10.2
μ = 1.27; Nimag = 0
11; C_{2v}; 11.1
μ = 1.03; Nimag = 1
12; C_{2v}; 12.3
μ = 1.11; Nimag = 0
13; C_s; 15.4
μ = 1.08; NImag = 0
14; C_s; 16.9
μ = 1.06; NImag = 0
15; C_s; 18.9
μ = 2.77; NImag = 0
16; D_{2h}; 19.3
μ = 0.00; NImag = 0
17; C_{2v}; 21.3
μ = 1.18; NImag = 0
18; C_1; 21.3
μ = 2.7; NImag = 0
19; C_s; 22.4
μ = 0.48; NImag = 0
20; C_s; 22.9
μ = 3.44; NImag = 0
21; C_s; 23.1
μ = 2.7; NImag = 0
22; C_s; 24.6
μ = 2.87; NImag = 0
23; C_{2v}; 26.2
μ = 2.36; NImag = 0
24; C_1; 27.9
μ = 2.24; NImag = 0



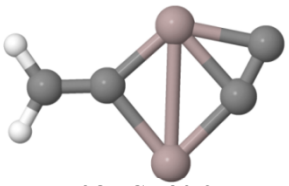
25; C_1; 28.0
μ = 0.96; NImag = 0



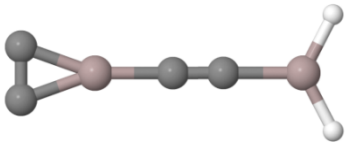
26; C_{2h}; 29.4
μ = 0.00; NImag = 0



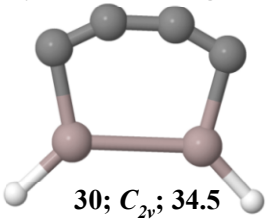
27; C_s; 30.2
μ = 2.09; NImag = 0



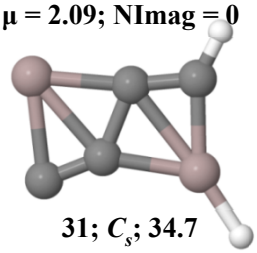
28; C_s; 30.9
μ = 4.18; NImag = 0



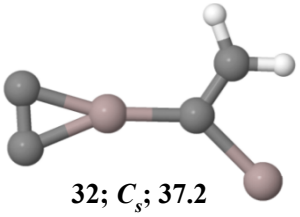
29; C_{2v}; 34.5
μ = 6.15; NImag = 1



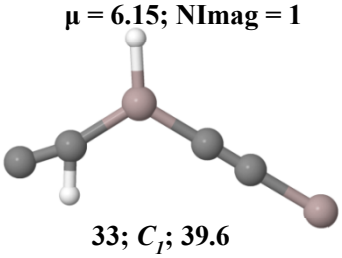
30; C_{2v}; 34.5
μ = 2.03; NImag = 0



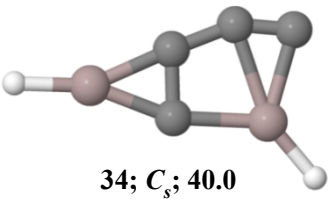
31; C_s; 34.7
μ = 4.13; NImag = 0



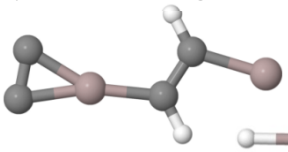
32; C_s; 37.2
μ = 6.03; NImag = 0



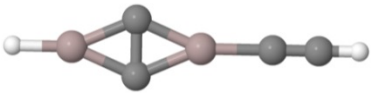
33; C_1; 39.6
μ = 3.24; NImag = 0



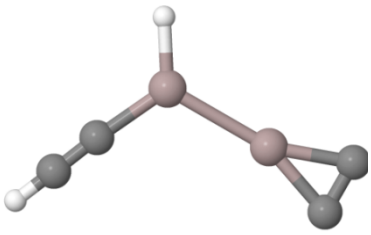
34; C_s; 40.0
μ = 4.41; NImag = 0



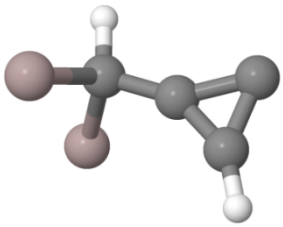
35; C_s; 40.1
μ = 5.85; NImag = 1



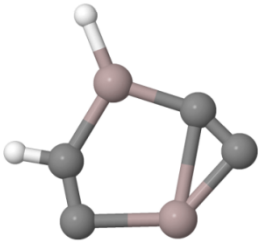
36; C_{2v}; 42.7
μ = 0.67; NImag = 0



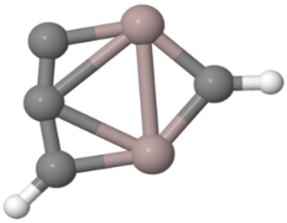
37; C_1; 43.3
μ = 6.39; NImag = 0



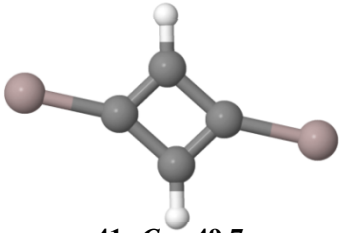
38; C_1; 45.8
μ = 4.38; NImag = 0



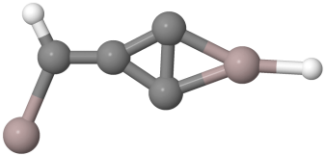
39; C_s; 46.6
μ = 1.54; NImag = 0



40; C_s; 49.7
μ = 3.07; NImag = 1

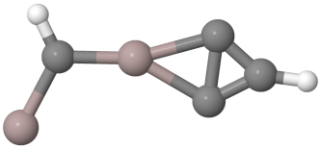


41; C_{2h}; 49.7
μ = 0; NImag = 0



42; C_s; 51.6
μ = 4.61; NImag = 0

43; C_1; 55.0
μ = 4.6; NImag = 0



44; C_s; 63.2
μ = 6.32; NImag = 0

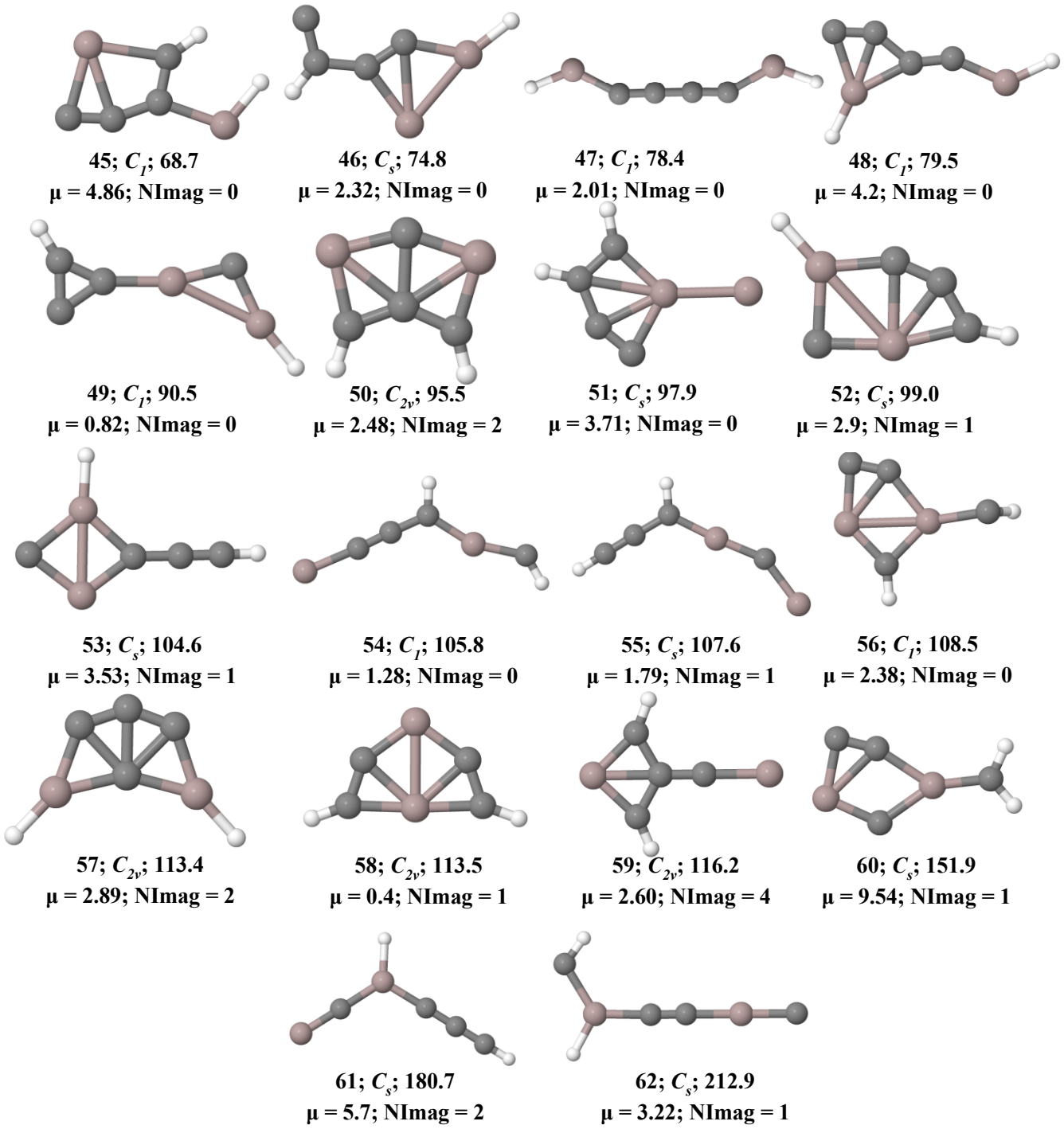
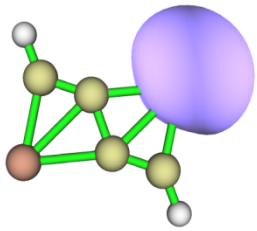
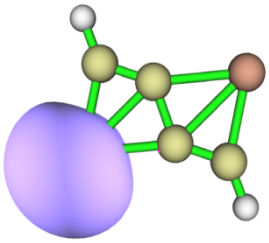


Figure S1. Isomers of $Al_2C_4H_2$ and their zero-point vibrational energy (ZPVE) corrected relative energies (in kcal mol^{-1}), dipole moments (in Debye), and number of imaginary frequencies (NImag) obtained at the ωB97XD/6-311++G(2d,2p) level of theory.

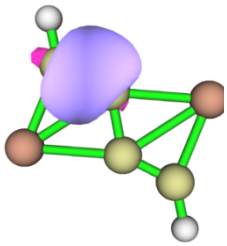
3



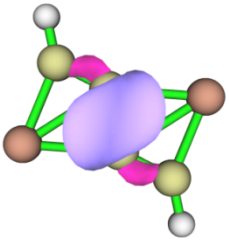
1c-2e lone pair
ON=1.80|e|



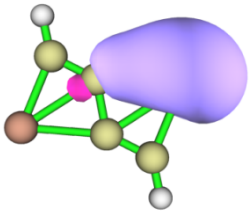
1c-2e lone pair
ON=1.80|e|



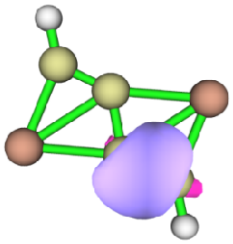
2c-2e σ bond
ON=1.99|e|



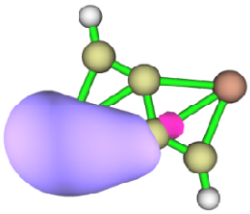
2c-2e σ bond
ON=1.98|e|



2c-2e σ bond
ON=1.99|e|

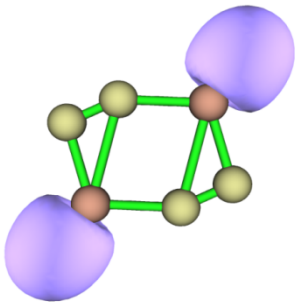


2c-2e σ bond
ON=1.99|e|



2c-2e σ bond
ON=1.99|e|

4



Two 2c-2e σ bond
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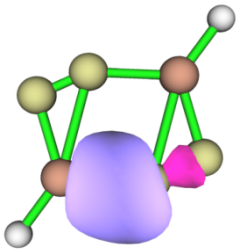
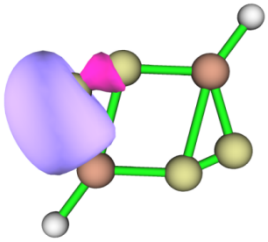
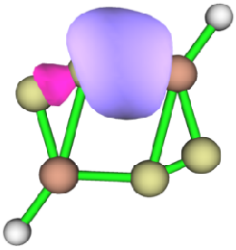


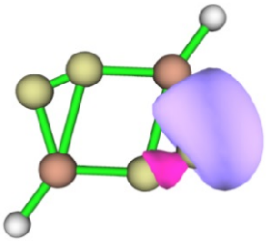
2c-2e σ bond
ON=1.98|e|



2c-2e σ bond
ON=1.99|e|



2c-2e σ bond
ON=1.98|e|



2c-2e σ bond
ON=1.99|e|

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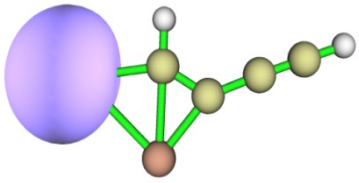
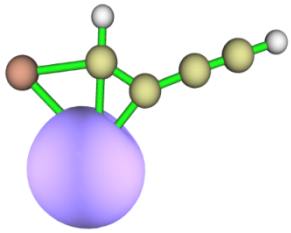


1c-2e lone pair
ON=1.97|e|



1c-2e lone pair
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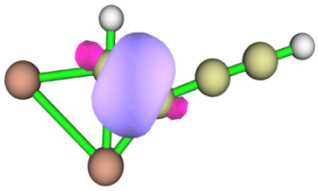

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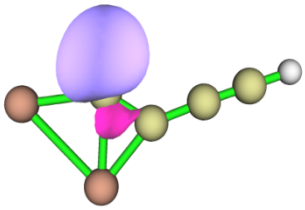
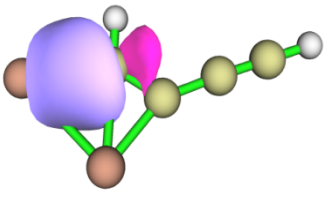
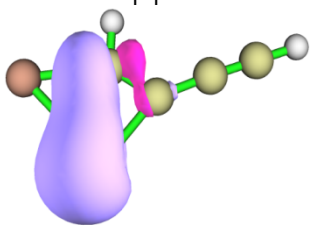


2c-2e σ bond
ON=1.97|e|



2c-2e σ bond
ON=1.86|e|



2c-2e σ bond
ON=1.73|e|

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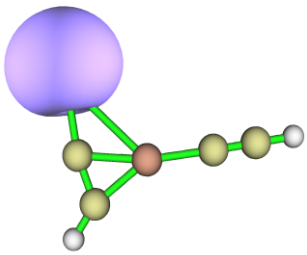
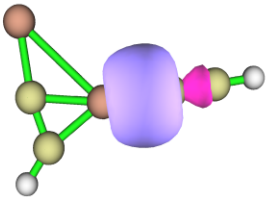


1c-2e lone pair
ON=1.97|e|



2c-2e σ bond
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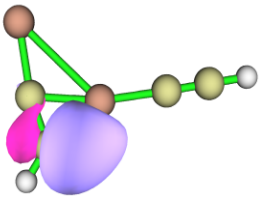

2c-2e σ bond
ON=1.94|e|

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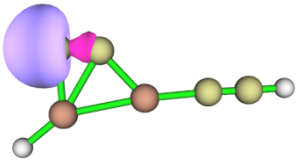

1c-2e lone pair
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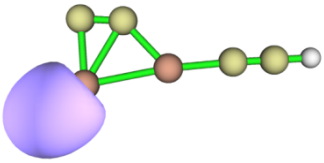

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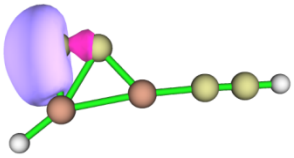

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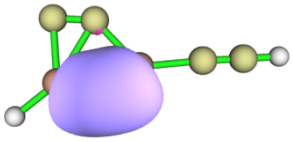

2c-2e σ bond
ON=1.99|e|

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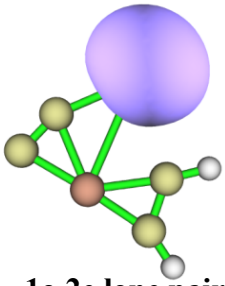
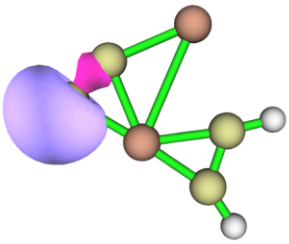
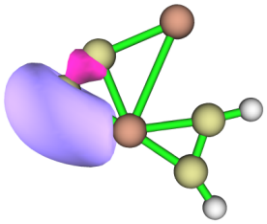


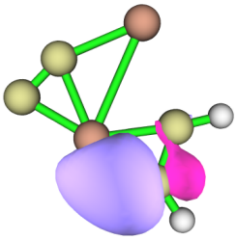
1c-2e lone pair
ON=1.97|e|



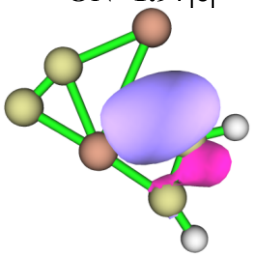
1c-2e lone pair
ON=1.72|e|



2c-2e σ bond
ON=1.99|e|

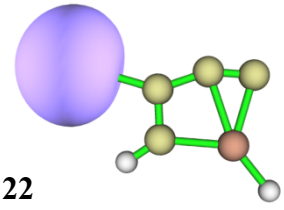


2c-2e σ bond
ON=1.95|e|

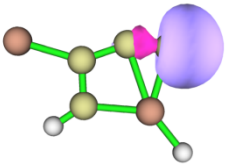


2c-2e σ bond
ON=1.80|e|

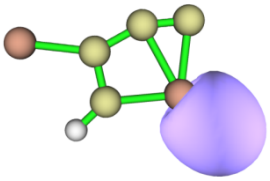
22



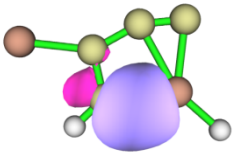
1c-2e lone pair
ON=1.99|e|



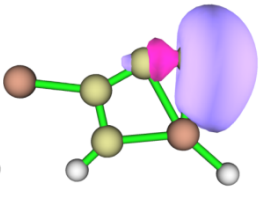
1c-2e lone pair
ON=1.79|e|



2c-2e σ bond
ON=1.99|e|



2c-2e σ bond
ON=1.97|e|



2c-2e σ bond
ON=1.97|e|

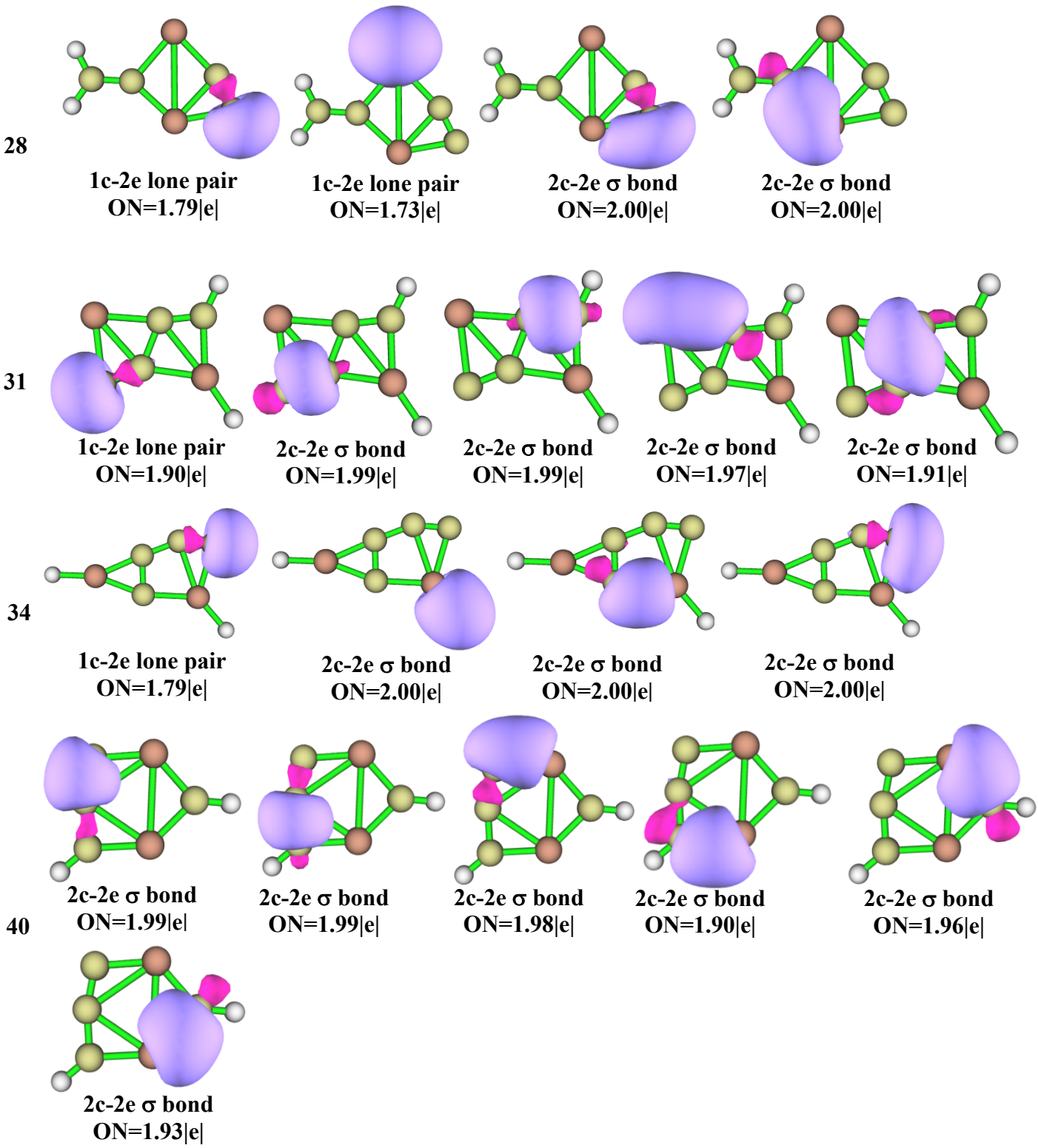


Figure S2. Lone pairs and 2c–2e bonds of $Al_2C_4H_2$ isomers **3**, **4**, **14**, **18**, **20**, **21**, **22**, **28**, **31**, **34**, **and 40** from AdNDP analysis at the ωB97XD/6-311++G(2d,2p) level of theory

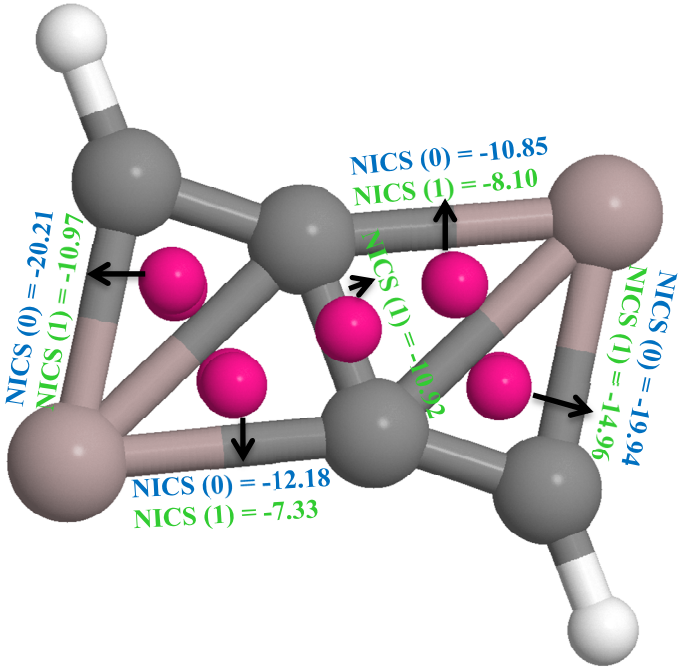


Figure S3. Nucleus independent chemical shifts (NICSs; in ppm) for isomer **3** at the ωB97XD/6-311++G(2d,2p) level. NICS (1) (green color) is calculated at 1 Å above the ring, whereas NICS(0) (blue color) refers to on the plane values.

Table S1. Total energy (in a.u), zero-point vibrational energy (ZPVE; in a.u), ZPVE corrected total energy (E+ZPVE; in a.u), relative energy (ΔE + ZPVE; in a.u and kcal mol^{-1}), and the number of imaginary frequencies (NImag) of various $Al_2C_4H_2$ isomers calculated at ωB97XD/6-311++G(2d,2p) level of theory.

ωB97XD/6−311++G(2d,2p)						
Isomer	**Energy (a.u)**	**ZPVE (a.u)**	**E+ZPVE (a.u)**	**ΔE+ZPVE (a.u)**	**ΔE+ZPVE (kcal mol^{-1})**	**NImag**
1	−638.33933	0.034904	−638.304485	0.00000	0.0	0
2	−638.34577	0.041396	−638.304375	0.00011	0.1	0
3	−638.34	0.040721	−638.299282	0.005203	3.3	0
4	−638.32969	0.032049	−638.297641	0.006844	4.3	0
5	−638.32823	0.031901	−638.296326	0.008159	5.1	1
6	−638.33736	0.041124	−638.29624	0.008245	5.2	0
7	−638.33417	0.041218	−638.292953	0.011532	7.2	0
8	−638.33256	0.041178	−638.291381	0.013104	8.2	0
9	−638.3234	0.033296	−638.290103	0.014382	9.0	0
10	−638.32825	0.040028	−638.28822	0.016265	10.2	0
11	−638.32642	0.039635	−638.28678	0.017705	11.1	1
12	−638.32415	0.039332	−638.28481	0.019675	12.3	0
13	−638.31841	0.038447	−638.27997	0.024515	15.4	0
14	−638.31741	0.039925	−638.27749	0.026995	16.9	0
15	−638.31146	0.037145	−638.27432	0.030165	18.9	0
16	−638.31069	0.03704	−638.27365	0.030835	19.3	0
17	−638.30849	0.037972	−638.27052	0.033965	21.3	0
18	−638.30936	0.038876	−638.27048	0.034005	21.3	0
19	−638.30877	0.040059	−638.26871	0.035775	22.4	0
20	−638.30298	0.034895	−638.26809	0.036395	22.8	0
21	−638.30687	0.039162	−638.26771	0.036775	23.1	0
22	−638.30239	0.037115	−638.26527	0.039215	24.6	0
23	−638.30095	0.038206	−638.26274	0.041745	26.2	0

24	−638.3002906	0.040188	−638.260103	0.044382	27.9	0
25	−638.29586	0.035974	−638.25988	0.044605	28.0	0
26	−638.29468	0.037012	−638.25767	0.046815	29.4	0
27	−638.29248	0.036156	−638.25632	0.048165	30.2	0
28	−638.29478	0.039585	−638.2552	0.049285	30.9	0
29	−638.28012	0.030584	−638.24954	0.054945	34.5	1
30	−638.28222	0.032735	−638.24949	0.054995	34.5	0
31	−638.28511	0.036001	−638.24911	0.055375	34.7	0
32	−638.28403	0.038894	−638.24513	0.059355	37.2	0
33	−638.27218	0.030762	−638.24142	0.063065	39.6	0
34	−638.27429	0.033607	−638.24068	0.063805	40.0	0
35	−638.27924	0.038636	−638.24061	0.063875	40.1	1
36	−638.27216	0.03574	−638.23642	0.068065	42.7	0
37	−638.26937	0.033958	−638.23542	0.069065	43.3	0
38	−638.27069	0.039196	−638.2315	0.072985	45.8	0
39	−638.26371	0.033442	−638.23027	0.074215	46.6	0
40	−638.2646625	0.039315	−638.225347	0.079138	49.7	1
41	−638.26645	0.041203	−638.22525	0.079235	49.7	0
42	−638.2589114	0.036795	−638.22218	0.082305	51.6	0
43	−638.25339	0.036659	−638.21673	0.087755	55.1	0
44	−638.2413584	0.037617	−638.20374	0.100745	63.2	0
45	−638.22934	0.03434	−638.195	0.109485	68.7	0
46	−638.21958	0.034218	−638.18536	0.119125	74.8	0
47	−638.21013	0.030555	−638.17958	0.124905	78.4	0
48	−638.20931	0.031457	−638.17785	0.126635	79.5	0
49	−638.19497	0.03467	−638.1603	0.144185	90.5	0
50	−638.19081	0.038467	−638.15234	0.152145	95.5	2
51	−638.19079	0.042244	−638.14854	0.155945	97.9	0
52	−638.18194	0.03515	−638.14679	0.157695	99.0	1
53	−638.17247	0.034611	−638.13786	0.166625	104.6	1

54	−638.17174	0.03582	−638.13592	0.168565	105.8	0
55	−638.1702	0.037148	−638.13305	0.171435	107.6	1
56	−638.16674	0.03514	−638.1316	0.172885	108.5	0
57	−638.15491	0.03109	−638.12382	0.180665	113.4	2
58	−638.16675	0.043054	−638.12369	0.180795	113.5	1
59	−638.15393	0.034623	−638.11931	0.185175	116.2	4
60	−638.09798	0.035609	−638.06237	0.242115	151.9	1
61	−638.04949	0.032952	−638.01653	0.287955	180.7	2
62	−637.99394	0.028693	−637.96524	0.339245	212.9	1

Table S2. Total energy (in a.u), zero-point vibrational energy (ZPVE; in a.u), ZPVE corrected total energy (E+ZPVE; in a.u), relative energy (ΔE + ZPVE; in a.u and kcal mol^{-1}), and the number of imaginary frequencies (NImag) of various $Al_2C_4H_2$ isomers calculated at B3LYP/6-311++G(2d,2p) level of theory.

B3LYP/6−311++G(2d,2p)						
Isomer	**Energy (a.u)**	**ZPVE (a.u)**	**E+ZPVE (a.u)**	**ΔE+ZPVE (a.u)**	**ΔE+ZPVE (kcal mol^{-1})**	**NImag**
1	−638.46707	0.0344	−638.43267	0.00053	0.3	0
2	−638.47392	0.040723	−638.4332	0	0.0	0
3	−638.47004	0.040297	−638.42974	0.00346	2.2	0
4	−638.44859	0.031694	−638.4169	0.0163	10	0
5	−638.44816	0.031502	−638.41666	0.01654	10	1
6	−638.46643	0.040538	−638.42589	0.00731	4.6	0
7	−638.46136	0.040567	−638.42079	0.01241	7.8	0
8	−638.4613733	0.040555	−638.420819	0.012381	7.8	0
9	−638.45689	0.032815	−638.42408	0.00912	5.7	0
10*	–	–	–	–	–	–
11	−638.45748	0.0392	−638.41828	0.01492	9.4	0
12	−638.44652	0.0386	−638.40792	0.02528	15.9	0
13	−638.44632	0.037859	−638.40846	0.02474	15.5	0
14	−638.44447	0.03905	−638.40542	0.02778	17.4	0
15	−638.43633	0.036413	−638.39992	0.03328	20.9	0
16	−638.44423	0.036521	−638.40771	0.02549	16.0	0
17	−638.43557	0.037451	−638.39812	0.03508	22.0	0
18	−638.43186	0.038165	−638.39369	0.03951	24.8	0
19	−638.43481	0.039372	−638.39544	0.03776	23.7	0
20	−638.42378	0.034366	−638.38942	0.04378	27.5	0
21	−638.42392	0.038278	−638.38564	0.04756	29.8	0
22	−638.42174	0.03635	−638.38539	0.04781	30.0	0
23	−638.43355	0.037795	−638.39575	0.03745	23.5	0

24	−638.42894	0.03949	−638.38945	0.04375	27.5	0
25*	–	–	–	–	–	–
26	−638.42785	0.036559	−638.39129	0.04191	26.3	0
27	−638.41742	0.035387	−638.38204	0.05116	32.1	0
28	−638.42584	0.039124	−638.38672	0.04648	29.2	0
29	−638.40242	0.030088	−638.37234	0.06086	38.2	1
30	−638.40606	0.032153	−638.3739	0.0593	37.2	0
31*	–	–	–	–	–	–
32	−638.40482	0.038319	−638.3665	0.0667	41.9	0
33*	–	–	–	–	–	–
34	−638.38982	0.032735	−638.35709	0.07611	47.8	0
35	−638.40038	0.03804	−638.36234	0.07086	44.5	0
36	−638.38901	0.03496	−638.35405	0.07915	49.7	0
37	−638.39095	0.033363	−638.35759	0.07561	47.4	0
38	−638.39066	0.038566	−638.35209	0.08111	50.9	0
39*	–	–	–	–	–	–
40	−638.3845	0.038687	−638.34581	0.08739	54.8	1
41	−638.38608	0.040395	−638.34568	0.08752	54.9	0
42	−638.37782	0.036071	−638.34175	0.09145	57.4	0
43	−638.37904	0.035622	−638.34342	0.08978	56.3	0
44	−638.36209	0.0369	−638.32519	0.10801	67.8	0
45	−638.36878	0.034359	−638.33442	0.09878	62.0	0
46	−638.34783	0.033576	−638.31425	0.11895	74.6	0
47	−638.37091	0.030329	−638.34058	0.09262	58.1	0
48	−638.33968	0.03068	−638.309	0.1242	77.9	0
49	−638.3162	0.033928	−638.28228	0.15092	94.7	0
50*	–	–	–	–	–	–
51*	–	–	–	–	–	–
52	−638.31415	0.034303	−638.27985	0.15335	96.2	1
53	−638.30983	0.033706	−638.27612	0.15708	98.6	1

54	−638.31897	0.035368	−638.28361	0.14959	93.9	0
55	−638.31708	0.036458	−638.28062	0.15258	95.7	1
56	−638.28788	0.034582	−638.2533	0.1799	112.9	0
57*	–	–	–	–	–	–
58*	–	–	–	–	–	–
59	−638.28315	0.037009	−638.24614	0.18706	117.4	3
60*	–	–	–	–	–	–
61*	–	–	–	–	–	–
62	−638.1255	0.028082	−638.09742	0.33578	210.7	1

The isomers marked with ***** are not converged at B3LYP/6-311++G(2d,2p) level of theory.

Table S3. Natural atomic charges of hydrogen in isomers **3**, **4**, **14**, **18**, **20**, **21**, **22**, **28**, **31**, **34**, and **40** from NBO analysis at the ωB97XD/6-311++G(2d,2p) level of theory

Isomers	**Atomic charge of H (when Al–H)** |***e***|	**Atomic charge of H (when C–H)** |***e***|
3	–	0.232 (H7, H8)
4	−0.365 (H7, H8)	–
14	–	0.231 (H7), 0.235 (H8)
18	–	0.214 (H2), 0.228 (H8)
20	−0.347 (H8)	0.227 (H3)
21	–	0.213 (H1), 0.215 (H7)
22	−0.373 (H8)	0.195 (H7)
28	−0.345 (H8)	0.205 (H7), 0.201 (H8)
31	–	0.234 (H3)
34	−0.378 (H7), −0.333 (H8)	–
40	–	0.257 (H7), 0.242 (H8)

Table S4. The hyper conjugative interaction between the donor → acceptor orbitals of lone pair of aluminum in the isomers **3**, **4**, **18**, **21**, **22**, **28**, and **31** as determined by NBO analysis at ωB97XD/6-311++G(2d,2p) level of theory.

Isomers	**Donor NBO (*i*)**	**Acceptor NBO (*j*)**	**$E^{(2)}$ (kcal/mol)**	**E*(j)*–E*(i)* (a.u)**	**F*(i.j)* (a.u)**
3	LPAl5	π*(C1–C4)	36.71	0.20	0.092
	LPAl6	π*(C1–C4)	36.71	0.20	0.092
4	LPAl4	LP2*Al5	9.11	0.50	0.062
	LPAl5	σ*(C1– Al4)	9.50	0.55	0.067
18	LPAl3	σ*(C4– C5)	15.29	1.03	0.112
21	LPAl5	σ*(C2– C8)	6.94	1.21	0.082
22	LPAl5	σ*(C1– C4)	3.43	0.93	0.051
28	LPAl2	σ*(C1– C5)	6.54	1.15	0.083
31	LPAl5	σ*(C2– C7)	35.04	0.40	0.108

Table S5. Occupancies of lone pairs for isomers **3**, **14**, **18**, **21**, **22**, **28**, **31**, and **40** from NBO analysis at ωB97XD/6-311++G(2d,2p) level of theory.

Isomers	Atom	Type of orbital	Occupancy	%s	%p	%d	NBO Hybrids
3	Al5	LP	1.75	83.96	15.97	0.07	$sp^{0.19}$
	Al6	LP	1.75	83.96	15.97	0.07	$sp^{0.19}$
14	Al4	LP	1.98	93.88	6.10	0.02	$sp^{0.06}$
	Al5	LP	1.81	86.50	13.41	0.08	$sp^{0.16}$
18	Al3	LP	1.97	91.22	8.77	0.01	$sp^{0.10}$
	C4	LP	1.78	47.64	51.74	0.62	$sp^{1.09}$
21	Al5	LP	1.97	90.12	9.84	0.04	$sp^{0.11}$
22	Al5	LP	1.99	92.48	7.50	0.02	$sp^{0.08}$
28	C1	LP	1.71	44.7	54.91	0.33	$sp^{1.23}$
	Al2	LP	1.72	81.25	18.70	0.05	$sp^{0.23}$
	C5	LP	1.78	56.16	43.48	0.36	$sp^{0.77}$
31	C1	LP	1.65	35.67	64.07	0.26	$sp^{1.80}$
	Al5	LP	1.68	93.11	6.87	0.02	$sp^{0.07}$
	C7	LP	1.90	59.90	39.90	0.20	$sp^{0.67}$
40	C3	LP	1.42	0.00	99.65	0.35	$sp^{1.00}$

Table S6. Optimized geometries of $Al_2C_4H_2$ isomers in Cartesian coordinates (in Angström units) obtained at ωB97XD/6-311++G(2d,2p) level of theory.

1

C	-3.520857	-1.225198	0.000000
H	-1.691932	2.482479	0.000000
H	-4.280181	-1.971133	0.000000
C	-2.656364	-0.383474	0.000000
C	0.519537	0.414710	0.000000
C	1.696329	0.083340	0.000000
Al	-1.307605	0.960963	0.000000
Al	3.585438	-0.494003	0.000000

2

C	0.788995	-0.675549	0.000000
C	-0.457850	-0.836448	0.000000
C	-1.665862	-0.149781	0.000000
C	-2.953913	-0.455652	0.000000
Al	2.716653	-0.248716	0.000000
Al	-0.198451	1.317679	0.000000
H	-3.302569	-1.481886	0.000000
H	-3.704952	0.322979	0.000000

3

C	-0.129653	0.713772	0.000000
C	1.284955	-1.318563	0.000000
C	-1.284955	1.318563	0.000000
C	0.129653	-0.713772	0.000000
Al	2.030791	0.541047	0.000000
Al	-2.030791	-0.541047	0.000000
H	1.497900	-2.372993	0.000000
H	-1.497900	2.372993	0.000000

4

C	-0.317990	1.357600	0.000000
C	1.537320	-1.160640	0.000000
C	-1.537320	1.160640	0.000000
C	0.317990	-1.357600	0.000000
Al	1.537320	0.747620	0.000000
Al	-1.537320	-0.747620	0.000000
H	2.759740	1.723170	0.000000
H	-2.759740	-1.723170	0.000000

5

C	-1.505283	0.612659	0.000000
C	-1.505283	-0.612659	0.000000
Al	0.000000	1.808016	0.000000
C	1.505283	0.612659	0.000000
C	1.505283	-0.612659	0.000000
Al	0.000000	-1.808016	0.000000
H	0.000000	-3.371889	0.000000
H	0.000000	3.371889	0.000000

6

C	-1.417980	0.041849	0.000000
C	-0.219983	0.285780	0.000000
C	1.188975	0.419431	0.000000
C	1.811170	1.607366	0.000000
Al	-3.347575	-0.233691	0.000000
Al	2.382389	-1.200057	0.000000
H	2.897185	1.672513	0.000000
H	1.283895	2.556438	0.000000

7

C	-2.229249	0.582887	0.000000
C	-1.155021	1.390865	0.000000
C	0.176182	0.862253	0.000000
C	1.297811	0.383395	0.000000
Al	-1.893530	-1.402756	0.000000
Al	3.115174	-0.357419	0.000000
H	-3.193081	1.089908	0.000000
H	-1.226629	2.475963	0.000000

8

C	-0.786055	0.425835	0.000000
C	0.628616	0.252494	0.000000
C	1.839562	0.117002	0.000000
Al	3.785123	-0.101752	0.000000
C	-1.692237	-0.569304	0.000000
Al	-3.591362	0.029077	0.000000
H	-1.284476	-1.578802	0.000000
H	-1.104971	1.470009	0.000000

9

C	0.000000	0.000000	-1.741228
C	0.000000	0.000000	-0.525991
C	0.000000	0.000000	0.842420
C	0.000000	0.000000	2.061850
Al	0.000000	0.000000	4.033474
Al	0.000000	0.000000	-3.650255
H	0.000000	1.383574	-4.402073
H	0.000000	-1.383574	-4.402073

10

C	2.355644	0.228058	0.000000
C	1.302557	0.980249	0.000000
C	-0.036991	0.914535	0.000000
C	-1.302837	1.251099	0.000000
Al	-2.166939	-0.571524	0.000000
H	-1.609869	2.291684	0.000000
Al	0.957244	-1.197745	0.000000
H	3.405740	0.460629	0.000000

11

C	0.000000	1.927103	0.910773
C	0.000000	0.649013	1.145972
C	0.000000	-0.649013	1.145972
C	0.000000	-1.927103	0.910773
Al	0.000000	1.637741	-1.077904
Al	0.000000	-1.637741	-1.077904
H	0.000000	-2.699200	1.667486
H	0.000000	2.699200	1.667486

12

H	0.000000	1.341644	-3.934316
H	0.000000	-1.341644	-3.934316
C	0.000000	0.684947	-3.069753
C	0.000000	-0.684947	-3.069753
Al	0.000000	0.000000	-1.355859
C	0.000000	0.000000	0.533290
Al	0.000000	0.000000	3.738827
C	0.000000	0.000000	1.754554

13

H	2.969085	1.760585	0.000000
C	-2.385535	-0.004871	0.000000
C	-3.591545	0.032295	0.000000
H	-4.655115	0.076920	0.000000
C	2.109447	1.113646	0.000000
C	0.837527	1.159896	0.000000
Al	2.025861	-0.973924	0.000000
Al	-0.499512	-0.222923	0.000000

14

C	0.649658	0.342177	0.000000
C	-0.110352	-0.776373	0.000000
C	0.299561	-2.119803	0.000000
Al	0.515788	2.445493	0.000000
Al	-1.502456	0.566695	0.000000
C	0.602209	-3.283429	0.000000
H	0.848719	-4.316767	0.000000
H	1.745422	0.240141	0.000000

15

H	-1.584837	2.176653	0.000000
H	-3.980265	-1.471882	0.000000
Al	-2.776079	-0.476960	0.000000
C	-1.864811	1.128603	0.000000
C	-0.992804	0.063863	0.000000
C	0.410457	0.031872	0.000000
Al	3.578780	-0.114218	0.000000
C	1.629872	-0.034750	0.000000

16

Al	0.000000	-1.546777	0.000000
H	-3.779689	0.000000	0.000000
C	1.494719	0.000000	0.000000
Al	0.000000	1.546777	0.000000
C	-2.713894	0.000000	0.000000
C	2.713894	0.000000	0.000000
C	-1.494719	0.000000	0.000000
H	3.779689	0.000000	0.000000

17

C	0.000000	2.689047	1.608824
H	0.000000	3.628058	2.109842
C	0.000000	1.613765	1.056533
C	0.000000	-1.613765	1.056533
C	0.000000	-2.689047	1.608824
Al	0.000000	0.000000	0.005653
H	0.000000	-3.628058	2.109842
Al	0.000000	0.000000	-2.758925

18

C	-0.784200	1.742701	0.003344
H	-1.197963	2.746151	0.005164
Al	-2.167835	-1.211163	-0.001608
C	-1.495098	0.593859	0.001335
Al	0.434536	0.338227	0.002387
C	2.216161	-0.258882	0.002222
C	3.349976	-0.667121	0.001891
H	4.352075	-1.026199	0.001628

19

H	-3.897751	-0.772962	0.000000
H	0.179646	-1.946888	0.000000
C	-1.636248	-0.873978	0.000000
C	0.605714	0.179495	0.000000
C	-2.836195	-0.822004	0.000000
C	-0.199409	-0.910724	0.000000
Al	2.414691	-0.650284	0.000000
Al	-0.249399	1.981711	0.000000

20

C	2.360644	-0.041733	0.000000
C	3.566127	0.000599	0.000000
H	4.629791	0.046050	0.000000
C	-2.127275	1.228853	0.000000
C	-0.872604	1.179835	0.000000
Al	-1.940235	-0.724272	0.000000
Al	0.475011	-0.221131	0.000000
H	-3.150333	-1.721443	0.000000

21

C	-0.641659	0.180390	0.000000
C	-0.116857	-1.081260	0.000000
C	1.680473	1.432419	0.000000
C	0.485298	1.094932	0.000000
Al	-2.633998	0.057312	0.000000
Al	1.801752	-0.551475	0.000000
H	-0.762985	-1.961112	0.000000
H	3.138645	-1.373654	0.000000

22

C	0.000000	-1.578124	0.652744
C	0.000000	-0.962094	-0.463496
H	0.000000	2.619385	0.922873
H	0.000000	-2.619385	0.922873
Al	0.000000	0.000000	1.919041
C	0.000000	1.578124	0.652744
C	0.000000	0.962094	-0.463496
Al	0.000000	0.000000	-2.235711

23

H	3.102346	-0.891848	-0.594409
H	0.557717	2.386896	0.708643
C	1.664681	0.751848	-0.206376
C	-0.649770	0.698848	0.022413
C	2.246373	-0.360715	-0.231568
C	0.471000	1.434719	0.191564
Al	-2.339748	-0.156323	-0.195461
Al	0.358016	-1.098674	0.293256

24

C	0.000000	0.685581	1.501577
C	0.000000	-0.685581	1.501577
H	0.000000	2.457944	-2.085703
C	0.000000	1.779900	0.935788
C	0.000000	-1.779900	0.935788
Al	0.000000	1.343948	-0.964499
Al	0.000000	-1.343948	-0.964499
H	0.000000	-2.457944	-2.085703

25

C	0.894727	0.109772	0.010032
C	-0.389035	0.173549	0.007343
C	-1.453061	1.076071	0.014263
H	-3.239721	2.464458	0.023865
Al	2.163806	-1.301413	-0.005077
Al	-0.406074	-1.910939	-0.020046
C	-2.404924	1.807955	0.020033
H	3.735098	-1.228481	-0.000366

26

Al	1.078123	0.861971	0.000000
C	2.828138	0.022861	0.000000
C	3.972929	-0.369394	0.000000
Al	-1.078123	-0.861971	0.000000
C	-2.828138	-0.022861	0.000000
C	-3.972929	0.369394	0.000000
H	-4.975852	0.726435	0.000000
H	4.975852	-0.726435	0.000000

27

Al	-0.949004	1.157641	0.000000
H	-1.760722	2.489812	0.000000
Al	-1.859246	-1.808679	0.000000
C	-0.308803	-0.673776	0.000000
C	0.687628	0.252103	0.000000
C	2.083638	0.080866	0.000000
C	3.281606	-0.010466	0.000000
H	4.339885	-0.100489	0.000000

28

C	1.518707	0.682544	0.000000
Al	-0.143990	1.829768	0.000000
C	-1.176426	-0.035850	0.000000
C	-2.485689	-0.227908	0.000000
C	2.281352	-0.318863	0.000000
Al	0.459866	-1.041123	0.000000
H	-3.173550	0.612472	0.000000
H	-2.936320	-1.214384	0.000000

29

C	0.000000	0.631648	-3.408267
C	0.000000	-0.631648	-3.408267
C	0.000000	0.000000	0.230510
C	0.000000	0.000000	1.447156
Al	0.000000	0.000000	-1.640103
Al	0.000000	0.000000	3.380267
H	0.000000	1.393129	4.105539
H	0.000000	-1.393129	4.105539

30

H	0.009499	1.597575	0.848412
C	-0.000621	-0.421965	-3.236954
Al	-0.005515	-0.027756	3.220763
C	0.007231	0.806437	-2.945846
C	0.001536	0.614413	1.318605
C	-0.005837	-0.483311	0.531643
Al	-0.001774	-0.221349	-1.363989
H	-0.013875	-1.475261	0.999972

31

C	0.318519	0.335128	0.000000
C	-1.187951	-0.113131	0.000000
H	2.303954	-0.423009	0.000000
C	1.248120	-0.638106	0.000000
Al	-0.796668	2.017858	0.000000
Al	-0.205295	-1.830644	0.000000
C	-2.309899	0.533332	0.000000
H	-0.692471	-3.318059	0.000000

32

C	0.222283	0.685324	0.000000
C	1.344472	1.426924	0.000000
C	-0.512903	-2.945290	0.000000
Al	0.236166	-1.213497	0.000000
Al	-1.182067	2.122935	0.000000
C	0.746525	-3.031133	0.000000
H	1.320790	2.528591	0.000000
H	2.363300	1.044129	0.000000

33

C	-0.021311	2.434485	0.002279
C	1.131790	-2.957194	-0.027816
C	-0.376267	1.265144	0.008699
C	0.461287	-1.884421	-0.011955
H	1.610621	-1.623979	-0.035133
Al	-0.928269	-0.554000	0.018705
Al	0.545407	4.336771	-0.004558
H	-2.423257	-1.016804	0.049780

34

C	0.534683	-0.683805	0.001732
C	0.494714	0.727905	-0.003029
C	-2.039387	-1.096101	-0.002102
C	-0.800267	-1.201623	0.001331
Al	-1.487846	0.822768	0.000326
Al	2.225173	0.061574	-0.000104
H	-2.506636	2.017507	0.009073
H	3.785600	0.012879	-0.006138

35

C	-1.587975	0.824603	0.000000
C	1.635842	0.366643	0.000000
C	-1.104028	-1.748351	0.000000
C	-1.510242	-0.436061	0.000000
Al	0.123855	1.383887	0.000000
Al	0.660437	-1.209069	0.000000
H	-1.742063	-2.612770	0.000000
H	2.698263	0.538339	0.000000

36

C	0.000000	0.000000	-3.759612
C	0.000000	-0.728309	1.025405
H	0.000000	0.000000	-4.824065
C	0.000000	0.000000	-2.554475
C	0.000000	0.728309	1.025405
H	0.000000	0.000000	4.293852
Al	0.000000	0.000000	-0.673048
Al	0.000000	0.000000	2.732340

37

C	3.276732	-1.150196	-0.018102
H	1.374682	2.569443	0.036314
H	4.014977	-1.917525	-0.029572
C	2.444513	-0.275863	-0.005080
Al	-1.344918	0.090243	0.003583
C	-3.238898	0.041400	0.000226
Al	1.066420	1.028296	0.014624
C	-2.785031	-1.136459	-0.006975

38

C	0.883565	-0.117687	0.348232
C	-0.298479	0.617860	0.013049
C	-1.523546	0.683133	-0.542459
Al	1.694450	-0.631434	-1.425965
Al	0.252559	-1.542899	1.629233
C	-1.033583	1.849302	0.035511
H	-2.342891	0.217686	-1.066794
H	1.616861	0.510812	0.881045

39

C	-0.508622	1.678973	0.000000
H	1.168154	-1.982703	-0.000000
C	-1.741759	1.838040	0.000000
C	0.360599	-1.235706	-0.000000
Al	1.065439	0.595454	0.000000
Al	-2.090047	-0.094317	-0.000000
H	2.574532	1.021107	0.000000
C	-0.828296	-1.820848	-0.000000

40

C	-0.189270	-0.192023	0.428319
C	-0.966814	0.767051	-0.124202
C	-1.190569	-1.356064	0.123153
C	-1.968693	-0.396909	-0.428493
Al	-0.473269	2.673855	-0.200089
H	-2.940464	-0.425064	-0.910358
Al	-1.685666	-3.262468	0.197554
H	0.782300	-0.164109	0.910586

41

C	-0.262646	0.957874	0.000000
C	-1.066609	-0.129930	0.000000
C	1.066609	0.129930	0.000000
C	0.262646	-0.957874	0.000000
Al	-3.035728	-0.041533	0.000000
H	0.467201	-2.022522	0.000000
Al	3.035728	0.041533	0.000000
H	-0.467201	2.022522	0.000000

42

Al	-1.072291	0.497226	2.909345
C	0.655586	0.582977	-0.076917
C	-0.437222	-0.251507	0.313322
C	0.111951	-0.409215	-0.991713
Al	1.507827	0.545862	-1.702453
C	-1.302261	-0.570588	1.280580
H	2.543162	0.968729	-2.775869
H	-2.006752	-1.363485	1.043705

43

C	1.142729	0.568823	0.006970
C	0.112104	1.280859	0.065224
C	-1.254302	1.717927	0.165624
Al	1.717103	-1.226312	0.047914
Al	-0.742021	-0.756367	0.251328
H	-1.505543	2.775527	0.131099
C	-2.148867	0.695510	0.302187
H	3.111040	-1.937936	-0.043871

44

C	-0.428549	-0.000000	1.575778
Al	0.502669	-0.000000	-0.172344
C	-1.398238	0.000000	0.389596
Al	1.161970	0.000000	-3.268152
C	1.754420	-0.000000	-1.457444
C	-1.773035	-0.000000	1.685347
H	2.790887	-0.000000	-1.115490
H	-2.610124	-0.000000	2.362709

45

Al	-0.186375	-0.004374	2.153626
C	0.401436	-0.004277	0.259391
C	-0.781807	0.010171	-0.301248
Al	0.307000	0.000174	-2.329506
C	1.572783	-0.015740	-0.523700
H	-1.810086	0.021169	0.027942
C	2.279388	-0.020415	-1.550480
H	-1.782338	0.013291	2.263975

46

C	-0.953741	0.000000	2.376723
C	0.767334	-0.000000	0.035734
C	-0.513282	0.000000	0.176640
Al	-0.638128	0.000000	-1.899313
Al	1.953421	-0.000000	-1.428061
C	-1.541141	0.000000	1.214605
H	3.525334	-0.000000	-1.476553
H	-2.599796	0.000000	1.000225

47

C	1.891210	0.506013	0.010683
Al	3.525784	-0.356863	0.005672
C	0.640335	0.466456	0.005734
C	-0.675919	0.449186	0.000730
C	-1.927506	0.458754	-0.004793
Al	-3.536217	-0.446822	-0.024185
H	4.985174	0.249972	0.019573
H	-5.018315	0.100575	-0.024143

48

Al	0.138253	-0.007466	-0.205994
H	-0.611266	-0.005893	1.157188
C	2.035263	0.002431	-0.771805
C	1.288879	-0.006461	-1.785556
C	-0.105538	-0.016364	-2.185372
C	-0.725716	-0.025073	-3.332049
Al	-2.286622	-0.037625	-4.288867
H	-2.541718	-0.043845	-5.844897

49

C	0.671456	0.023223	0.020544
H	0.503333	0.027578	1.084361
C	1.564637	0.024127	-1.049687
C	0.128810	0.012385	-1.197625
Al	-1.328501	-0.005621	-2.468650
C	-2.925197	-0.017698	-3.274340
Al	-2.422606	-0.028522	-4.998649
H	-2.373275	-0.038031	-6.571432

50

C	0.000000	-1.286238	1.176695
C	0.000000	0.000000	-1.104801
C	0.000000	1.286238	1.176695
C	0.000000	0.000000	0.645519
Al	0.000000	-1.724052	-0.607268
Al	0.000000	1.724052	-0.607268
H	0.000000	-1.569987	2.211937
H	0.000000	1.569987	2.211937

51

C	0.011166	0.721478	0.000000
C	-1.076896	-0.088814	0.000000
C	1.821513	-1.143024	0.000000
C	1.234003	-0.052121	0.000000
Al	-0.037276	-1.729250	0.000000
H	-2.084381	0.298861	0.000000
Al	-0.557925	-4.063518	0.000000
H	-0.002682	1.804698	0.000000

52

Al	0.020914	1.194076	-0.000000
C	1.323984	-0.345632	-0.000000
C	-1.915494	1.091939	-0.000000
C	0.158222	-0.934591	-0.000000
C	1.928770	0.838400	-0.000000
Al	-1.743573	-0.863561	-0.000000
H	2.973758	1.091519	-0.000000
H	-2.746581	-2.072149	-0.000000

53

Al	-0.283919	0.000000	-1.087279
H	-1.414618	0.000000	0.000743
C	1.731165	0.000000	-0.946820
Al	1.411272	0.000000	-2.842864
C	-0.439020	0.000000	-3.044100
C	-1.460624	0.000000	-3.968078
C	-2.368185	0.000000	-4.768856
H	-3.169410	0.000000	-5.465926

54

Al	-3.751353	-0.085522	2.292877
H	1.320275	0.109613	1.473004
C	0.533836	0.048776	0.726239
Al	0.950180	0.009811	-1.057288
C	1.968935	-0.000655	-2.586881
C	-0.768455	0.005001	1.201721
H	1.682279	-0.051358	-3.636462
C	-1.935696	-0.035665	1.586789

55

C	-1.616240	-3.181202	0.000000
H	-2.955405	-0.234369	0.000000
H	-1.482255	-4.234788	0.000000
C	-1.784141	-1.983689	0.000000
Al	-0.504555	0.562339	0.000000
C	0.825597	1.805029	0.000000
C	-1.932595	-0.599332	0.000000
Al	2.738245	2.237569	0.000000

56

C	-1.298743	-0.197145	-0.031398
C	1.581403	-0.748102	-0.007114
C	2.033819	0.409332	-0.071283
Al	0.178641	0.829425	-0.064891
Al	-0.175794	-1.726852	0.044350
H	-2.371623	-0.099625	-0.020626
C	-0.206108	-3.633542	0.443569
H	-0.308505	-4.380726	-0.353830

57

C	0.000000	0.000000	-1.513107
C	0.000000	0.000000	0.207889
H	0.000000	2.887463	1.795508
H	0.000000	-2.887463	1.795508
Al	0.000000	-1.828744	0.659155
Al	0.000000	1.828744	0.659155
C	0.000000	-1.230963	-1.074837
C	0.000000	1.230963	-1.074837

58

C	0.000000	1.903112	0.864028
C	0.000000	-1.903112	0.864028
H	0.000000	2.933258	1.231592
H	0.000000	-2.933258	1.231592
C	0.000000	-1.480168	-0.429924
C	0.000000	1.480168	-0.429924
Al	0.000000	0.000000	-1.518029
Al	0.000000	0.000000	0.927855

59

C	0.000000	0.000000	-0.295117
C	0.000000	1.273928	-1.004316
C	0.000000	-1.273928	-1.004316
Al	0.000000	0.000000	-2.327972
C	0.000000	0.000000	1.036946
Al	0.000000	0.000000	3.008403
H	0.000000	-2.269495	-0.612657
H	0.000000	2.269495	-0.612657

60

C	1.749553	0.486653	0.000000
C	0.502315	0.474701	0.000000
Al	-1.420382	-0.223317	0.000000
C	-3.101205	0.385664	0.000000
Al	1.664518	-1.368183	0.000000
C	-0.118830	-1.716346	0.000000
H	-3.305133	1.450230	0.000000
H	-3.979448	-0.246818	0.000000

61

C	0.277169	-2.610273	0.000000
H	-2.734351	0.259423	0.000000
C	0.841552	-3.719379	0.000000
C	-0.316293	-1.458135	0.000000
C	-0.048192	1.714256	0.000000
Al	-1.159796	0.220686	0.000000
Al	0.949056	3.103028	0.000000
H	1.322260	-4.665931	0.000000

62

H	-2.632241	1.788568	0.000000
C	1.334820	-0.128611	0.000000
C	-3.112164	0.794273	0.000000
C	0.139867	-0.374593	0.000000
Al	3.192594	0.224415	0.000000
Al	-1.760017	-0.700512	0.000000
C	5.070458	0.593539	0.000000
H	-2.233318	-2.197079	0.000000

Table S7. Optimized geometries of isomers of $Al_2C_4H_2$ in Cartesian coordinates (in Angström units) obtained at B3LYP/6-311++G(2d,2p) level of theory.

1

C	-1.218942	-3.544513	0.000000
H	-2.989348	0.184085	0.000000
H	-1.115963	-4.602474	0.000000
C	-1.332441	-2.340315	0.000000
C	0.000000	0.659970	0.000000
C	0.982334	1.395048	0.000000
Al	-1.553809	-0.446983	0.000000
Al	2.593779	2.554463	0.000000

2

C	-0.698362	-0.550140	0.000000
C	0.000000	0.683774	0.000000
C	0.588915	1.757265	0.000000
Al	1.538168	3.479313	0.000000
C	-0.132557	-1.779082	0.000000
Al	-1.362742	-3.358400	0.000000
H	0.956702	-1.794007	0.000000
H	-1.785211	-0.448760	0.000000

3

C	-0.310776	0.657391	0.000000
C	-0.310776	-1.813040	0.000000
C	0.310776	1.813040	0.000000
C	0.310776	-0.657391	0.000000
Al	-1.994488	-0.709642	0.000000
Al	1.994488	0.709642	0.000000
H	0.109162	-2.803593	0.000000
H	-0.109162	2.803593	0.000000

4

C	-0.352255	1.406262	0.000000
C	1.524623	-1.022362	0.000000
C	-1.524623	1.022362	0.000000
C	0.352255	-1.406262	0.000000
Al	1.524623	0.889953	0.000000
Al	-1.524623	-0.889953	0.000000
H	2.733261	1.881317	0.000000
H	-2.733261	-1.881317	0.000000

5

C	0.000000	1.507462	0.614218
C	0.000000	1.507462	-0.614218
Al	0.000000	0.000000	1.812755
C	0.000000	-1.507462	0.614218
C	0.000000	-1.507462	-0.614218
Al	0.000000	0.000000	-1.812755
H	0.000000	0.000000	-3.375701
H	0.000000	0.000000	3.375701

6

C	1.163376	0.780751	0.000000
C	0.000000	0.382718	0.000000
C	-1.260306	-0.239798	0.000000
C	-2.437646	0.413282	0.000000
Al	2.964125	1.546293	0.000000
Al	-1.340526	-2.268487	0.000000
H	-3.379330	-0.128867	0.000000
H	-2.519991	1.495674	0.000000

7

C	-2.295245	0.009785	0.000000
C	-1.411291	1.031610	0.000000
C	0.000000	0.839352	0.000000
C	1.215767	0.690245	0.000000
Al	-1.639452	-1.901532	0.000000
Al	3.179233	0.531604	0.000000
H	-3.342914	0.310341	0.000000
H	-1.729629	2.072787	0.000000

8

C	0.595213	-0.579535	0.299545
C	-0.658195	0.057430	0.116528
C	-1.747970	0.593054	-0.040642
Al	-3.496261	1.456731	-0.293770
C	1.799022	0.037264	0.328430
Al	3.415023	-1.111420	0.605321
H	1.775452	1.118377	0.196707
H	0.532603	-1.662160	0.424130

9

C	0.000000	0.000000	-1.745151
C	0.000000	0.000000	-0.522660
C	0.000000	0.000000	0.834463
C	0.000000	0.000000	2.061496
Al	0.000000	0.000000	4.041891
Al	0.000000	0.000000	-3.653492
H	0.000000	1.380765	-4.409030
H	0.000000	-1.380765	-4.409030

11

C	0.000000	1.925802	0.913791
C	0.000000	0.648878	1.171343
C	0.000000	-0.648878	1.171343
C	0.000000	-1.925802	0.913791
Al	0.000000	1.630958	-1.089260
Al	0.000000	-1.630958	-1.089260
H	0.000000	-2.718667	1.649575
H	0.000000	2.718667	1.649575

12

H	0.000000	1.347452	-3.942097
H	0.000000	-1.347452	-3.942097
C	0.000000	0.685468	-3.080902
C	0.000000	-0.685468	-3.080902
Al	0.000000	0.000000	-1.357089
C	0.000000	0.000000	0.531690
Al	0.000000	0.000000	3.750909
C	0.000000	0.000000	1.757536

13

H	-0.315726	-3.425736	0.000000
C	-1.061870	2.145807	0.000000
C	-1.624923	3.216925	0.000000
H	-2.132986	4.150716	0.000000
C	-0.094828	-2.372728	0.000000
C	-0.692544	-1.246184	0.000000
Al	1.791823	-1.424430	0.000000
Al	0.000000	0.563823	0.000000

14

C	0.004592	-0.771866	0.000000
C	-0.675566	0.402562	0.000000
C	-2.051108	0.643947	0.000000
Al	1.958747	-1.586645	0.000000
Al	1.157461	1.083898	0.000000
C	-3.225849	0.923585	0.000000
H	-4.259715	1.160997	0.000000
H	-0.564775	-1.714816	0.000000

15

H	2.360427	-1.363454	0.000000
H	-1.028975	-4.116858	0.000000
Al	-0.166575	-2.813759	0.000000
C	1.343029	-1.740511	0.000000
C	0.195787	-0.970175	0.000000
C	0.000000	0.409976	0.000000
Al	-0.542903	3.550826	0.000000
C	-0.223521	1.617118	0.000000

16

Al	0.000000	-1.546777	0.000000
H	-3.779689	0.000000	0.000000
C	1.494719	0.000000	0.000000
Al	0.000000	1.546777	0.000000
C	-2.713894	0.000000	0.000000
C	2.713894	0.000000	0.000000
C	-1.494719	0.000000	0.000000
H	3.779689	0.000000	0.000000

17

C	0.000000	2.701169	-1.600439
H	0.000000	3.643712	-2.091703
C	0.000000	1.615165	-1.061762
C	0.000000	-1.615165	-1.061762
C	0.000000	-2.701169	-1.600439
Al	0.000000	0.000000	-0.005125
H	0.000000	-3.643712	-2.091703
Al	0.000000	0.000000	2.784342

18

C	-0.807790	1.741011	0.000031
H	-1.220721	2.746144	0.000071
Al	-2.250639	-1.210134	-0.000001
C	-1.514502	0.589504	-0.000045
Al	0.426604	0.336315	-0.000087
C	2.226933	-0.202442	-0.000131
C	3.373856	-0.583267	-0.000159
H	4.383873	-0.914884	-0.000224

19

H	0.455860	-4.004351	0.000000
H	-1.873088	-0.485802	0.000000
C	-0.290108	-1.864456	0.000000
C	0.000000	0.606492	0.000000
C	0.100857	-3.004249	0.000000
C	-0.766387	-0.517207	0.000000
Al	-1.447372	1.998563	0.000000
Al	1.997454	0.552719	0.000000

20

C	-0.996203	2.148061	0.000000
C	-1.557053	3.219557	0.000000
H	-2.060768	4.155854	0.000000
C	-0.178562	-2.447905	0.000000
C	-0.682830	-1.295074	0.000000
Al	1.508727	-1.440633	0.000000
Al	0.000000	0.532226	0.000000
H	2.935198	-2.094401	0.000000

21

C	0.000000	0.663949	0.000000
C	-1.074046	-0.188739	0.000000
C	1.845602	-1.214141	0.000000
C	1.189801	-0.155663	0.000000
Al	-0.679193	2.559500	0.000000
Al	-0.030629	-1.898599	0.000000
H	-2.097092	0.189734	0.000000
H	-0.443369	-3.413888	0.000000

22

C	0.000000	1.585846	-0.644869
C	0.000000	0.998866	0.488317
H	0.000000	-2.622478	-0.934610
H	0.000000	2.622478	-0.934610
Al	0.000000	0.000000	-1.950161
C	0.000000	-1.585846	-0.644869
C	0.000000	-0.998866	0.488317
Al	0.000000	0.000000	2.238457

23

H	-3.919630	1.030593	0.114592
H	0.380503	0.459792	-0.293094
C	-1.751280	0.609095	0.159248
C	-0.626771	-1.437890	0.100476
C	-2.991789	0.525177	-0.059629
C	-0.505698	-0.097337	0.002144
Al	-0.438887	-3.336333	0.285677
Al	-2.646888	-1.497930	-0.522280

24

C	0.000085	0.680775	1.522886
C	-0.000085	-0.680775	1.522886
H	0.000250	2.476563	-2.092900
C	0.000189	1.769608	0.933014
C	-0.000189	-1.769608	0.933014
Al	0.000171	1.357663	-0.975837
Al	-0.000171	-1.357663	-0.975837
H	-0.000250	-2.476563	-2.092900

26

Al	1.086254	0.852647	0.000000
C	2.837079	0.001308	0.000000
C	3.991868	-0.372146	0.000000
Al	-1.086254	-0.852647	0.000000
C	-2.837079	-0.001308	0.000000
C	-3.991868	0.372146	0.000000
H	-4.998981	0.713308	0.000000
H	4.998981	-0.713308	0.000000

27

Al	1.510559	0.601456	0.000000
H	2.860855	1.381991	0.000000
Al	0.744912	-2.419124	0.000000
C	-0.001222	-0.631523	0.000000
C	-0.377790	0.678658	0.000000
C	-1.641345	1.278192	0.000000
C	-2.700403	1.855958	0.000000
H	-3.636456	2.355069	0.000000

28

C	0.179106	1.597464	0.000000
Al	1.592799	0.212967	0.000000
C	0.043773	-1.172716	0.000000
C	0.084807	-2.498423	0.000000
C	-0.939747	2.175434	0.000000
Al	-1.361394	0.214656	0.000000
H	1.026726	-3.038435	0.000000
H	-0.808439	-3.114116	0.000000

29

C	0.000000	0.632216	-3.417621
C	0.000000	-0.632216	-3.417621
C	0.000000	0.000000	0.231248
C	0.000000	0.000000	1.451921
Al	0.000000	0.000000	-1.642626
Al	0.000000	0.000000	3.385229
H	0.000000	1.391979	4.110922
H	0.000000	-1.391979	4.110922

30

H	1.546298	0.177655	0.000000
C	-0.664160	-2.846231	0.000000
Al	0.019736	2.854250	0.000000
C	0.603859	-2.864392	0.000000
C	0.691160	0.887319	0.000000
C	-0.675336	0.895191	0.000000
Al	0.000000	-1.069755	0.000000
H	-1.535994	0.192580	0.000000

32

C	-0.030605	-0.857486	0.000000
C	-0.954143	-1.838756	0.000000
C	-0.012271	2.851474	0.000000
Al	-0.443257	1.003558	0.000000
Al	1.694182	-1.925235	0.000000
C	-1.269276	2.715650	0.000000
H	-0.676653	-2.903959	0.000000
H	-2.033441	-1.702115	0.000000

34

C	-0.532085	0.688799	-0.000026
C	-0.496374	-0.728590	-0.000249
C	2.035136	1.096717	-0.000247
C	0.793076	1.209991	-0.000098
Al	1.500159	-0.836197	0.001615
Al	-2.235880	-0.059541	0.000026
H	2.527874	-2.025048	0.004842
H	-3.796460	-0.004268	-0.000151

35

C	-0.707264	1.599130	0.000000
C	1.694205	-0.561938	0.000000
C	-1.785263	-0.774821	0.000000
C	-1.390071	0.533979	0.000000
Al	1.045823	1.152774	0.000000
Al	-0.006230	-1.325855	0.000000
H	-2.784495	-1.168211	0.000000
H	2.666898	-1.020974	0.000000

36

C	0.000000	0.000000	-3.783548
C	0.000000	0.726496	1.016984
H	0.000000	0.000000	-4.846614
C	0.000000	0.000000	-2.575022
C	0.000000	-0.726496	1.016984
H	0.000000	0.000000	4.294134
Al	0.000000	0.000000	-0.694172
Al	0.000000	0.000000	2.734710

37

C	-3.299404	-1.149547	-0.000074
H	-1.382086	2.556297	0.000076
H	-4.045573	-1.907385	-0.000185
C	-2.455352	-0.282174	0.000057
Al	1.356192	0.088998	0.000082
C	3.261461	0.050485	-0.000348
Al	-1.067785	1.015630	0.000257
C	2.816354	-1.132637	0.000246

38

C	-0.439725	-0.000145	0.540633
C	0.947301	-0.000269	0.202037
C	1.943569	0.000050	-0.710466
Al	-1.190911	-1.767738	-0.132615
Al	-1.189833	1.767930	-0.132589
C	2.325584	-0.000870	0.625829
H	2.274891	0.000538	-1.737507
H	-0.598311	-0.000390	1.633812

40

C	0.000000	0.944092	0.000000
C	0.000000	0.000000	1.101852
C	0.000000	0.000000	-1.101852
C	0.000000	-0.944092	0.000000
Al	0.000000	0.000000	3.062624
H	0.000000	-2.035593	0.000000
Al	0.000000	0.000000	-3.062624
H	0.000000	2.035593	0.000000

41

C	-0.255204	0.962016	0.000000
C	-1.072275	-0.121511	0.000000
C	1.072275	0.121511	0.000000
C	0.255204	-0.962016	0.000000
Al	-3.061091	-0.060717	0.000000
H	0.449259	-2.029391	0.000000
Al	3.061091	0.060717	0.000000
H	-0.449259	2.029391	0.000000

42

Al	-2.855104	-0.577561	0.000106
C	0.725823	-0.515347	-0.000251
C	-0.228236	0.545614	-0.000295
C	1.156930	0.886315	-0.000499
Al	2.559780	-0.310441	-0.000318
C	-1.526405	0.885036	0.000025
H	4.038195	-0.772460	-0.000683
H	-1.730792	1.954304	-0.000032

43

C	-0.593206	1.103279	0.000193
C	0.662587	1.068060	0.000201
C	2.033496	0.657221	0.000214
Al	-2.112453	-0.019297	0.000217
Al	0.191489	-1.177768	0.000088
H	2.843146	1.384624	0.000294
C	2.207080	-0.695549	0.000146
H	-3.657475	0.270955	0.000300

44

C	1.794645	1.398917	0.000000
Al	0.010841	0.522417	0.000000
C	1.875657	-0.140895	0.000000
Al	-2.416771	-1.632691	0.000000
C	-1.764460	0.175816	0.000000
C	2.944708	0.687852	0.000000
H	-2.404453	1.060631	0.000000
H	4.019929	0.745169	0.000000

45

Al	2.477146	0.292886	0.000078
C	0.473080	0.192147	0.000379
C	0.255185	-1.115050	0.000989
Al	-1.926167	-0.736355	0.000893
C	-0.644656	1.051899	0.000138
H	0.918392	-1.967922	0.001224
C	-1.850930	1.377660	-0.000147
H	3.073159	-1.200166	0.000598

46

C	-2.846452	0.654153	0.000000
C	0.004987	0.814262	0.000000
C	-0.830792	-0.166860	0.000000
Al	0.857461	-1.481610	0.000000
Al	1.890148	1.004404	0.000000
C	-2.249784	-0.505719	0.000000
H	2.722317	2.341947	0.000000
H	-2.635346	-1.513305	0.000000

47

C	-1.906298	0.269358	-0.000116
Al	-3.661177	-0.386714	0.000005
C	-0.663149	0.205565	-0.000114
C	0.664351	0.204142	-0.000153
C	1.907575	0.266365	-0.000091
Al	3.661620	-0.391959	0.000392
H	-4.947166	0.542404	-0.001435
H	4.948723	0.535630	0.000888

48

Al	-1.811911	-0.849927	-0.000173
H	-2.373851	-2.299380	-0.000339
C	-2.531431	0.989047	-0.000023
C	-1.267595	1.032416	0.000017
C	-0.084820	0.216851	-0.000028
C	1.202699	0.393619	0.000112
Al	2.931313	-0.305923	-0.000041
H	4.214915	0.623221	-0.000023

49

C	-3.144191	0.313902	-0.001010
H	-3.854826	1.123866	-0.001801
C	-2.895946	-1.058374	0.000069
C	-1.857123	-0.048997	-0.000348
Al	0.054107	0.271277	-0.000148
C	1.688317	1.021088	-0.000050
Al	2.780310	-0.415255	-0.000185
H	4.026992	-1.377135	-0.000082

50

Al	-0.019295	-1.127842	0.000000
C	1.664523	0.083779	0.000000
C	-1.862463	-0.498992	0.000000
C	0.669667	0.930230	0.000000
C	1.947818	-1.219148	0.000000
Al	-1.206628	1.345593	0.000000
H	2.893461	-1.732176	0.000000
H	-1.840075	2.782099	0.000000

52

Al	-0.019295	-1.127842	0.000000
C	1.664523	0.083779	0.000000
C	-1.862463	-0.498992	0.000000
C	0.669667	0.930230	0.000000
C	1.947818	-1.219148	0.000000
Al	-1.206628	1.345593	0.000000
H	2.893461	-1.732176	0.000000
H	-1.840075	2.782099	0.000000

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Al	0.990477	-1.108065	0.000000
H	2.545674	-1.321975	0.000000
C	-0.576038	-2.379594	0.000000
Al	-1.433020	-0.637098	0.000000
C	-0.004199	0.606083	0.000000
C	0.311491	1.932105	0.000000
C	0.608024	3.114379	0.000000
H	0.873343	4.141419	0.000000

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Al	-3.740466	-0.273035	0.000519
H	0.899406	1.959211	-0.000815
C	0.684343	0.892725	-0.000278
Al	2.143371	-0.277299	-0.001152
C	3.960854	-0.528223	0.002131
C	-0.638252	0.536547	0.000631
H	4.542101	-1.449067	0.004155
C	-1.827484	0.186410	0.001647

55

C	-3.598810	-1.025306	0.000000
H	-2.191716	1.884406	0.000000
H	-4.323059	-1.800648	0.000000
C	-2.776936	-0.128324	0.000000
Al	0.031430	0.564586	0.000000
C	1.850079	0.456892	0.000000
C	-1.819735	0.863274	0.000000
Al	3.475356	-0.636315	0.000000

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C	-0.090693	-1.516648	-0.089897
C	-0.554248	1.366245	-0.121066
C	-1.782824	1.404558	0.085218
Al	-1.570312	-0.490079	0.206120
Al	0.973862	0.077186	-0.224838
H	0.188811	-2.556688	-0.050590
C	2.830378	0.469985	0.153081
H	3.638521	0.073882	-0.474057

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C	0.000000	0.000000	0.294786
C	0.000000	-1.274179	0.998501
C	0.000000	1.274179	0.998501
Al	0.000000	0.000000	2.355151
C	0.000000	0.000000	-1.041886
Al	0.000000	0.000000	-3.025421
H	0.000000	2.277405	0.625077
H	0.000000	-2.277405	0.625077

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H	-3.335224	-1.719163	0.000000
C	0.460943	0.503499	0.000000
C	-2.786103	-2.676995	0.000000
C	0.009642	-0.636899	0.000000
Al	1.198096	2.238648	0.000000
Al	-0.789435	-2.392545	0.000000
C	1.943198	4.022272	0.000000
H	0.189737	-3.619158	0.000000