Electronic supplementary information

Reactions of α-Diimine-Aluminum Complexes with sodium alkynides: Versatile Structures of Aluminum σ-alkynide Complexes

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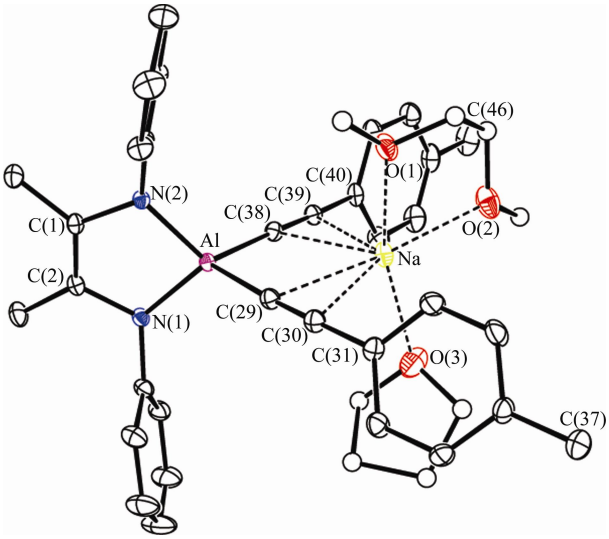

Figure S1. Molecular structure of **6b.** Thermal ellipsoids are set at the 30% probability level; hydrogen atoms and isopropyl groups of L are omitted for clarity. Selected bond lengths (Å) and bond angles (°): Al−N(1) 1.834(2), Al−N(2) 1.8346(19), Al–C(29) 1.972(3), Al–C(38) 1.987(2), C(29)−C(30) 1.214(3), C(38)−C(39) 1.207(3), Na–O(1) 2.332(2), Na–O(2) 2.334(2), Na–O(3) 2.325(2), N(1)–C(1) 1.433(3), N(2)–C(2) 1.427(3), C(1)–C(2) 1.347(3); N(1)–Al–N(2) 90.03(9), C(29)–Al–C(38) 100.74(10), C(31)–C(30)–C(29) 175.4(3), C(40)–C(39)–C(38) 176.8(3), Al–C(29)–C(30) 175.5(2), Al–C(38)–C(39) 178.6(2).

Table S1. Crystallographic data and refinement details for compounds **1** and **3–10**.

compound	**1**	**2**	**4**	2·**5**
empirical formula	$C_{28}H_{40}AlCl_2N_2$	$C_{32}H_{48}AlClN_2O$	$C_{69}H_{97}Al_2N_4NaO$	$2(C_{41}H_{55}AlN_2O)\cdot(THF)$
Fw	502.50	539.15	1075.46	1309.80
crystal system	Orthorhombic	Orthorhombic	Monoclinic	Monoclinic
space group	*Pnma*	*Pbcn*	*P2(1)/c*	*C2/c*
a /Å	12.542(2)	26.279(3)	14.510(2)	39.766(10)
b /Å	21.514(4)	15.6114(17)	19.288(3)	16.373(4)
c /Å	10.581(2)	15.8183(17)	24.629(4)	12.360(3)
α /°	90	90	90	90
β /°	90	90	101.942(2)	95.498(3)
γ /°	90	90	90	90
V /Å^3	2855.0(9)	6489.4(12)	6743.6(18)	8011(4)
Z	4	8	4	4
D_{calc} /g cm^{-3}	1.169	1.104	1.059	1.086
F (000)	1076	2336	2336	2848
μ /mm^{-1}	0.28	0.17	0.09	0.09
θ range	1.89–25.16	1.52–25.11	1.78–25.09	1.35–25.10
reflns collected	18172	41355	44436	25831
independent reflns	2630	5787	11886	7050
observed reflns	1558	3830	4597	4142
R(int)	0.100	0.069	0.091	0.078

R_1; wR_2 [$I > 2\sigma(I)$]	0.0491, 0.1127	0.0478, 0.1147	0.0811, 0.1177	0.0877, 0.1734
R_1; wR_2 (all data)	0.1070, 0.1430	0.0837, 0.1359	0.1969, 0.1386	0.1478, 0.1993
GOF (F^2)	1.02	1.00	1.00	1.08

compound	**6a**	**6b**	**2·6c**	**7**
empirical formula	$C_{52}H_{66}AlN_2NaO_2$	$C_{54}H_{72}AlN_2NaO_3 \cdot C_7H_8$	$2(C_{46}H_{76}AlN_2NaO_3Si_2) \cdot (C_7H_8)$	$C_{48}H_{58}AlN_2NaO \cdot 0.5(C_7H_8)$
Fw	801.04	939.24	1714.61	775.00
crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic
space group	*P2(1)/c*	*P2(1)/c*	*P−1*	*P2(1)/n*
a /Å	15.589 (8)	17.619(4)	12.6090(17)	15.289(7)
b /Å	15.119 (8)	15.448(3)	19.913(3)	15.214(7)
c /Å	23.000 (12)	21.942(5)	21.881(3)	22.131(10)
α /°	90	90	79.478(2)	90
β /°	107.223 (7)	110.058	86.486(2)	107.956(6)
γ /°	90	90	89.329(2)	90
V /Å^3	5178 (4)	5610(2)	5391.4(13)	4897(4)
Z	4	4	2	4
D_{calc} /g cm^{-3}	1.028	1.112	1.056	1.061
F (000)	1728	2032	1868	1684
μ /mm^{-1}	0.08	0.09	0.13	0.09
θ range	1.37−25.03	1.23–25.09	1.27−25.05	1.44−25.38
reflns collected	25343	34447	35871	31852
independent reflns	9091	9860	18471	8832
observed reflns	3810	6700	10463	4303
R(int)	0.065	0.068	0.1056	0.105
R_1; wR_2 [$I > 2\sigma(I)$]	0.0849, 0.1607	0.0541, 0.1082	0.0650, 0.1402	0.1320, 0.3015
R_1; wR_2 (all data)	0.1772, 0.1811	0.0901, 0.1239	0.1292, 0.1736	0.2110, 0.3269
GOF (F^2)	1.001	1.00	1.01	1.14

compound	**8**	**9**	**10**
empirical formula	$C_{83}H_{124}Al_2N_4Na_2Si_4$	$C_{44}H_{50}AlN_2Na$	$C_{100}H_{156}Al_2N_4Na_2O_2 \cdot 2C_7H_8$
Fw	1390.17	656.83	1730.50
crystal system	Monoclinic	Triclinic	Orthorhombic
space group	*P*2(1)/*n*	*P−1*	*Pbca*
a /Å	12.8201(15)	8.841(4)	19.7833 (17)
b /Å	32.219(4)	12.395(6)	19.3362 (17)
c /Å	23.498(3)	18.281(9)	28.545 (3)
α /°	90	84.253(6)	90
β /°	95.188(2)	87.165(6)	90
γ /°	90	76.832(7)	90
V /Å^3	9666(2)	1940.0(16)	10919.6 (16)
Z	4	2	4

D_{calc} /g cm^{-3}	0.955	1.124	1.053
F (000)	3016	704	3792
μ /mm^{-1}	0.13	0.10	0.08
θ range	1.53–24.96	1.94–25.07	1.43−25.32
reflns collected	47526	12559	71292
independent reflns	16811	6682	9957
observed reflns	7899	3625	6778
R(int)	0.081	0.060	0.072
R_1; wR_2 [$I > 2\sigma(I)$]	0.0927, 0.1733	0.0612, 0.1332	0.0689, 0.1309
R_1; wR_2 (all data)	0.1616, 0.1905	0.1201, 0.1597	0.1067, 0.1505
GOF (F^2)	1.08	1.00	1.001

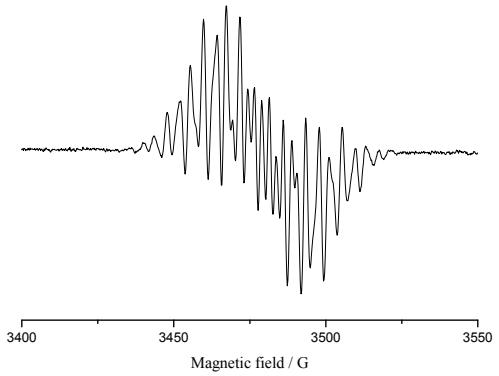

Figure S2. Room-temperature EPR spectrum of **1** recorded in THF solution.

DFT computations

The model compounds [L'AlCl$_2$] (**1H**) and [L'AlCl(THF)] (**2H**) [Na(H$_2$O)][L'Al−Al(C ≡ C(C$_6$H$_4$−Me))L'] (**4H**; L′ = [PhNCMe]$_2$), [L'Al(C ≡ C(C$_6$H$_4$−Me))] (**5H**), [Na(THF)(DME)][L'Al(C ≡ C(C$_6$H$_4$−Me))$_2$] (**6bH**) and [Na(H$_2$O)$_3$][L'Al(C ≡ CSi(Me)$_3$)$_2$] (**6cH**), [Na][(μ-Na)][LAl(C≡CSi(Me)$_3$)$_2$]$_2$ (**8H**) and[Na(H$_2$O)]$_2$[L′Al((CH=C(C$_4$H$_9$)(C≡C(C$_4$H$_9$))$_2$]$_2$ (**10H**), wherein the 2,6-diisopropylphenyl groups on the nitrogen atoms were replaced by phenyl groups and the THF and DME molecules by H$_2$O (except **6b)**, were used for the products **1**, **2**, **4**, **5**, **6b**, **6c 8** and **10**, respectively. The structure optimization and NBO bonding analysis for the model compounds were carried out at the DFT (B3LYP) level with the 6-31G* basis sets using the Gaussian 09 program.[1] The B3LYP method is a hybrid of the HF and DFT methods, incorporating Becke's three-parameter exchange functional (B3)[2] with the Lee, Yang, and Parr (LYP) correlation functional. Geometry optimizations gave bond distances that were in good agreement with the X-ray structures. All reported structural parameters refer to singlet ground state structures. Bonding analyses were performed by means of natural bond orbital (NBO) analysis and natural population analysis (NPA). Wiberg bond indices (WBI) were evaluated with Weinhold's natural bond orbital method.[3]

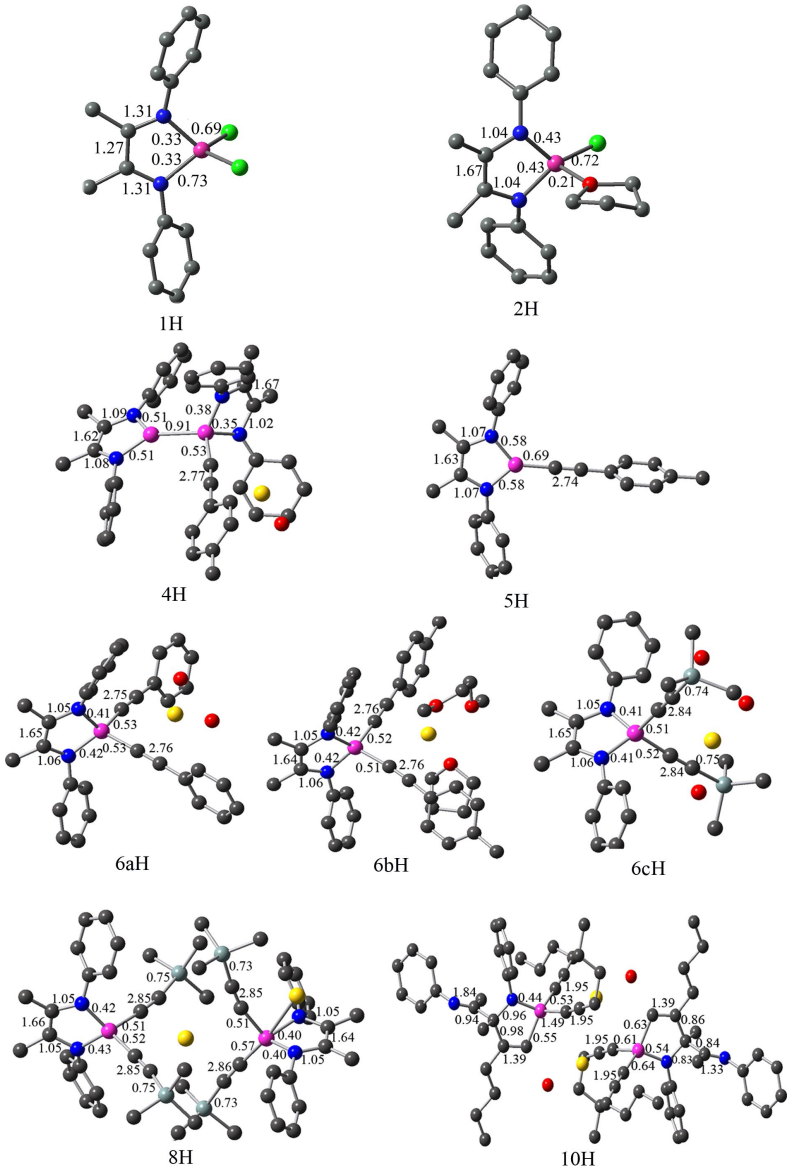

Figure S3. Optimized structures of **1H**, **2H**, **3H**−**6H**, **8H** and **10H** and their selected bond orders.

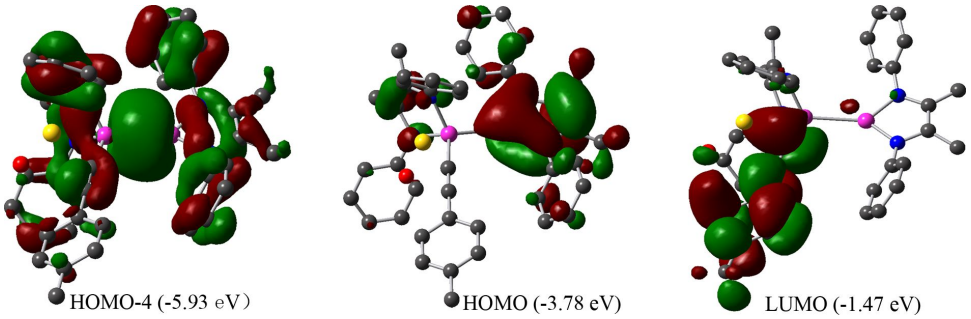

Figure S4. Al–Al bonding orbital (HOMO−4) of **4** (−5.93 eV) and selected Kohn-Sham orbital representations for the model species [Na(Et_2O)][LAl−Al(C≡C(C_6H_4−Me))L] (**4**).

Table S2. Natural charges of the model compounds **3H**−**6H**, **8H** and **10H** at B3LYP/6-31G* level.

	1H	**2H**	**3H**	**4H**	**5H**
Al	1.67	1.86	1.13	1.17, 1.22	1.73
L	−0.57	−1.42	−1.79	−1.25, −1.40	−1.18
alkynyl				−0.60	−0.55

	6aH	**6bH**	**6cH**	**8H**	**10H**
Al	1.76	1.74	1.75	1.74, 1.73	1.63
L	−1.46	−1.39	−1.38	−1.38, −1.36	−0.68
alkynyl	−0.50, −0.63	−0.61, −0.61,	−0.61, −0.61,	−0.60, −0.60, −0.55, −0.58	−0.56, −0.58(av.)

Table S3. Cartesian coordinates of the optimized geometry for **1H**.

Al	-0.93661300	0.02488400	0.00000000	C	2.87266400	-0.80139400	-1.49638200
Cl	-2.39299400	-1.54995700	0.00000000	H	2.63053500	-1.03894200	-2.53334400
Cl	-1.78636000	1.98077300	0.00000000	H	3.58697700	0.03267800	-1.50421300
N	0.43882500	-0.21009300	1.30577600	H	3.39201200	-1.66133000	-1.06169200
C	2.87266400	-0.80139400	1.49638200	C	1.62973200	-0.47346200	-0.71287800
H	2.63053500	-1.03894200	2.53334400	C	0.27755200	-0.02401200	-2.70643400
H	3.58697700	0.03267800	1.50421300	C	1.04493400	0.91469900	-3.41406000
H	3.39201200	-1.66133000	1.06169200	C	0.82938100	1.11107500	-4.77703200
C	1.62973200	-0.47346200	0.71287800	H	1.42641400	1.84469700	-5.31196600
C	0.27755200	-0.02401200	2.70643400	C	-0.15707100	0.38534400	-5.44787200
C	1.04493400	0.91469900	3.41406000	H	-0.32607000	0.54456500	-6.50898300
C	0.82938100	1.11107500	4.77703200	C	-0.93199800	-0.53725500	-4.74278200
H	1.42641400	1.84469700	5.31196600	H	-1.70608800	-1.10333500	-5.25335300
C	-0.15707100	0.38534400	5.44787200	C	-0.72065800	-0.74361400	-3.38008800
H	-0.32607000	0.54456500	6.50898300	H	1.78745000	1.50600600	2.88658700
C	-0.93199800	-0.53725500	4.74278200	H	-1.31773300	-1.46564800	2.83134900
H	-1.70608800	-1.10333500	5.25335300	H	1.78745000	1.50600600	-2.88658700
C	-0.72065800	-0.74361400	3.38008800	H	-1.31773300	-1.46564800	-2.83134900
N	0.43882500	-0.21009300	-1.30577600				

Table S4. Cartesian coordinates of the optimized geometry for **2H**.

Al	0.00734800	0.36654700	-0.48563900	O	0.01034700	2.18829200	0.17362400
Cl	-0.00412300	0.75497100	-2.58416400	N	1.33006100	-0.52883400	0.41264900

N	-1.30835500	-0.53833100	0.41721700	H	-5.41426800	0.66657300	-1.22048300
C	0.69921000	-1.29376200	1.44517500	C	-5.14761700	-1.47132200	-1.11528600
C	-0.66668900	-1.30160100	1.44639500	H	-6.13049100	-1.70224200	-1.51636400
C	1.57238800	-1.78552900	2.57213200	C	-4.26714900	-2.49681900	-0.76238900
H	1.00201200	-2.32755700	3.32765500	H	-4.55954200	-3.53517300	-0.90019600
H	2.07236300	-0.94042300	3.06857200	C	-3.00198800	-2.20625800	-0.25571400
H	2.36948400	-2.44946800	2.22337100	C	-0.06865900	3.45979400	-0.56345600
C	-1.53378700	-1.80737900	2.57215200	H	-1.06073400	3.51387000	-1.01918600
H	-0.96131200	-2.36820400	3.31230900	H	0.68802800	3.43188500	-1.34701100
H	-2.33706400	-2.45992400	2.21613200	C	0.15232400	4.52376200	0.50726700
H	-2.02604400	-0.97024900	3.08995200	H	1.22258800	4.71805200	0.63806800
C	2.62639600	-0.82795000	-0.05340400	H	-0.33551000	5.46692500	0.24602200
C	3.07802500	-2.14954800	-0.23566600	C	-0.43525300	3.87187300	1.77028000
C	4.35739800	-2.40478500	-0.72548400	H	-1.52803500	3.95030200	1.77139300
H	4.68076100	-3.43461800	-0.85794700	H	-0.05993500	4.31773600	2.69546100
C	5.21304000	-1.35530300	-1.06880200	C	-0.00690600	2.41603200	1.62897400
H	6.20708100	-1.55893800	-1.45694100	H	1.00518200	2.22634900	1.99553100
C	4.76904900	-0.04109900	-0.91188000	H	-0.69806300	1.68796300	2.05491800
H	5.42010400	0.78921100	-1.17509800	H	-2.30630400	-3.00892200	-0.02870700
C	3.49859800	0.21963600	-0.40084900	H	-3.19056600	1.18501600	-0.26421400
C	-2.59005400	-0.87269900	-0.06643400	H	2.40234300	-2.97147900	-0.01752100
C	-3.48723100	0.15032100	-0.42283500	H	3.17044600	1.24566600	-0.24843000
C	-4.74320600	-0.14538600	-0.95038200				

Table S5. Cartesian coordinates of the optimized geometry for **4H**.

Al	1.85827500	1.33709000	0.44469600	H	3.24921400	-3.88580800	1.64741600
Al	0.44383600	-0.81619600	0.22672400	C	0.21825400	-2.01536200	-2.42091800
Na	-2.39287400	-1.63038500	-2.00600400	C	-0.32517900	-3.20963400	-2.98232800
O	-4.64058200	-1.80490200	-2.15881900	C	-1.10048800	-3.17711800	-4.14394200
N	0.89693600	-1.97174200	-1.23045800	H	-1.49591900	-4.11085800	-4.53848400
N	0.72882300	-2.27781700	1.38264500	C	-1.38764800	-1.97000600	-4.79540200
N	3.67640600	1.64998600	0.32418600	H	-1.97961400	-1.95515900	-5.70550300
N	1.60564800	3.17308900	0.43446300	C	-0.85283400	-0.78431700	-4.26461700
C	1.51309700	-3.14440000	-0.67986400	H	-1.03834700	0.16493200	-4.76247900
C	1.41969800	-3.29110400	0.67161800	C	-0.06823500	-0.80131900	-3.11326200
C	2.49658900	-3.88766500	-1.55133800	C	0.00328800	-2.54807900	2.54722300
H	3.44114400	-3.32906300	-1.63090400	C	-0.16709400	-1.53226500	3.51160900
H	2.12458000	-4.02522800	-2.57209000	C	-0.92055900	-1.74825900	4.66196300
H	2.73140900	-4.87780500	-1.15112900	H	-1.02853600	-0.94336100	5.38555300
C	2.24445600	-4.28851500	1.45428400	C	-1.51817200	-2.98901700	4.90172600
H	2.36654100	-5.23521400	0.91994900	H	-2.09558200	-3.15967600	5.80614800
H	1.79433700	-4.50855600	2.42458300	C	-1.35867300	-4.00478600	3.95705100

H	-1.82415600	-4.97496600	4.11874200	H	-2.70499600	4.01476700	1.74321800
C	-0.62095400	-3.79072700	2.79315400	C	-0.67114800	3.60752900	1.18504100
C	3.95326400	3.03704200	0.32872300	C	-1.49343500	-0.36865100	0.11535800
C	2.85119500	3.84982700	0.38479000	C	-2.67069500	-0.01829600	0.18749900
C	5.38303800	3.50259400	0.42977700	C	-4.04084700	0.39208900	0.25928000
H	5.44515900	4.52623500	0.80517800	C	-4.44093900	1.66488300	-0.19509900
H	5.91795200	3.47931200	-0.52834000	H	-3.68964000	2.35529000	-0.56585000
H	5.94706700	2.86139500	1.11784800	C	-5.78088500	2.04041000	-0.15103100
C	2.88145300	5.34571000	0.56011200	H	-6.06526500	3.02865500	-0.50533200
H	2.18534000	5.65618200	1.34957500	C	-6.77085800	1.17617900	0.33970600
H	2.59315300	5.89751400	-0.34388300	C	-6.37003900	-0.08884800	0.79483000
H	3.87729600	5.69433800	0.84114900	H	-7.11434100	-0.77489700	1.19297600
C	4.65810100	0.67180100	0.05001900	C	-5.03104200	-0.47848200	0.76544100
C	4.76175400	-0.45691000	0.88309000	H	-4.73456000	-1.45051400	1.15105900
C	5.66379100	-1.48100900	0.59333700	C	-8.21603400	1.60788300	0.41198100
H	5.72355400	-2.34185100	1.25496100	H	-8.89633400	0.75338600	0.33324800
C	6.49937200	-1.39488900	-0.52158900	H	-8.46418500	2.31629900	-0.38535600
H	7.20980100	-2.18730600	-0.74067100	H	-8.43054200	2.10621600	1.36670300
C	6.40976200	-0.27486400	-1.35246700	H	-5.07309100	-1.34335900	-1.41589800
H	7.04429000	-0.19857300	-2.23241700	H	-5.17748900	-1.60708600	-2.94035200
C	5.49630400	0.74107800	-1.07926500	H	4.13268900	-0.51423000	1.76741000
C	0.37524900	3.84449000	0.27512800	H	5.40208100	1.58455000	-1.75634200
C	0.12405600	4.70922000	-0.80926200	H	-0.48537500	2.95714000	2.03540300
C	-1.11714400	5.32304700	-0.96168100	H	0.90706000	4.87483200	-1.54296400
H	-1.28301500	5.98824700	-1.80606600	H	0.35381200	0.12363400	-2.72937100
C	-2.14877800	5.07999000	-0.04985400	H	-0.15162500	-4.15165900	-2.47240600
H	-3.11328900	5.56731700	-0.16695700	H	-0.53843100	-4.57894500	2.04994200
C	-1.91769600	4.21156000	1.01950900	H	0.32190600	-0.57376200	3.35204500

Table S6. Cartesian coordinates of the optimized geometry for **5H**.

Al	-0.81570800	0.00051900	-0.00046900	H	-4.82220600	-2.10598100	-0.73561800
N	-2.07091500	1.30077100	-0.09714400	H	-5.46486000	-0.93348500	0.41902100
N	-2.07530500	-1.29543000	0.09698500	C	-1.88835200	2.70714000	-0.05472900
C	-3.35607400	0.68738400	-0.04299200	C	-1.15310000	3.34108100	-1.06884000
C	-3.35838000	-0.67768300	0.04350300	C	-0.90562400	4.71333100	-1.01946500
C	-4.58337200	1.54952800	-0.17193400	H	-0.33136400	5.18241500	-1.81431500
H	-5.46197300	0.95023000	-0.41684100	C	-1.40312200	5.48219700	0.03326700
H	-4.45294700	2.28294100	-0.97704600	H	-1.21735400	6.55211300	0.06779600
H	-4.81419600	2.12140000	0.73627800	C	-2.13813200	4.86090900	1.04600100
C	-4.58857300	-1.53565400	0.17285300	H	-2.51955700	5.44616400	1.87903300
H	-4.45999600	-2.27015000	0.97726000	C	-2.37100800	3.48727800	1.01054400

C	-1.89750900	-2.70241200	0.05468000	H	6.36076200	-0.07270500	-2.14649000
C	-1.16375600	-3.33864900	1.06843700	C	6.54366000	-0.01430000	0.00026900
C	-0.92090100	-4.71172400	1.01912300	C	5.82188600	0.01342600	1.20222600
H	-0.34770300	-5.18260600	1.81367600	H	6.35948000	0.02991500	2.14753500
C	-1.42162200	-5.47907600	-0.03318600	C	4.43130900	0.01844400	1.20981500
H	-1.23944200	-6.54960900	-0.06766900	H	3.88788100	0.03855000	2.14942100
C	-2.15518100	-4.85549100	-1.04556000	C	8.05340700	0.01321200	0.00075000
H	-2.53908400	-5.43959700	-1.87826100	H	8.43024800	1.04495800	0.00113800
C	-2.38345100	-3.48108400	-1.01016600	H	8.46417400	-0.48191500	-0.88536000
C	1.06135500	-0.00292300	-0.00075800	H	8.46346000	-0.48147000	0.88761700
C	2.28637600	-0.00512600	-0.00087800	H	-2.90818800	3.00286700	1.82036200
C	3.71227300	-0.00697200	-0.00065000	H	-0.79011900	2.74530700	-1.90220900
C	4.43184900	-0.03900400	-1.21042400	H	-0.79824000	-2.74395400	1.90146800
H	3.88899200	-0.06465100	-2.15022400	H	-2.91954000	-2.99499600	-1.81970200
C	5.82262800	-0.04381200	-1.20183200				

Table S7. Cartesian coordinates of the optimized geometry for **6aH**.

C	0.30291600	3.35443300	1.63396700	C	2.44309000	0.23283500	-2.62800600
C	0.41394100	3.48911600	3.03273300	C	1.38410800	-2.37166600	1.85243700
H	0.63865200	2.61060900	3.63084900	C	2.88909200	-2.39615900	-0.11755100
C	0.25779500	4.73440600	3.63697400	C	3.68082100	0.90564700	-2.72286500
H	0.35008400	4.82361700	4.71611100	C	1.40212200	0.66579000	-3.47930100
C	-0.00752400	5.86590900	2.86160700	C	0.44886600	2.07487600	1.00690900
H	-0.12589200	6.83631100	3.33570600	C	-0.25600000	-3.07333000	3.54162800
C	-0.11131100	5.74605600	1.47339200	H	-1.25769900	-3.43141200	3.77445900
H	-0.30604100	6.62487500	0.86445500	C	2.33007100	-2.25226600	2.89777600
C	0.04152100	4.50434500	0.86119200	C	1.58898200	1.71621300	-4.37469400
H	-0.02244000	4.40918800	-0.21886300	H	0.76642200	2.01927300	-5.01945600
Al	0.79124000	-0.75396200	-0.47833000	C	0.58606800	0.98096700	0.46214900
N	2.18087800	-0.78594500	-1.70638400	C	1.99020100	-2.54423500	4.21679600
C	4.27367900	-2.09646600	-2.23208200	H	2.74487900	-2.43650400	4.99294900
H	4.56317300	-3.14610700	-2.13105200	C	3.86510600	1.94204600	-3.63578100
H	5.18464200	-1.50020700	-2.08962500	H	4.83116300	2.44041300	-3.68249700
H	3.95433300	-1.94171400	-3.26840400	C	0.69790200	-2.95492000	4.55817600
C	3.67405500	-3.57455200	0.39785700	H	0.44420600	-3.19325500	5.58716100
H	2.99497000	-4.38220100	0.70166400	C	2.82520400	2.36037200	-4.46962600
H	4.29555000	-3.34433900	1.27326700	H	2.97519100	3.17120200	-5.17730700
H	4.34510800	-3.97347000	-0.36611900	Na	-1.91607200	0.60925200	0.88888900
N	1.65439500	-2.07107700	0.52229600	C	-1.09538700	-1.10438600	-0.98382700
C	3.15317600	-1.73663300	-1.28521100	C	-2.29188100	-1.21151300	-1.24654000
C	0.07600200	-2.78437400	2.21425100	C	-3.68863500	-1.28982400	-1.54955900

C	-6.44965000	-1.37543000	-2.09962100	O	-3.74241600	1.71895600	0.08291400
H	-7.51450600	-1.41028500	-2.31106400	O	-1.99474400	-0.37617600	2.92699500
C	-5.88403800	-2.27519800	-1.19233200	H	-1.82895000	0.13850100	3.73135600
H	-6.50991000	-3.01204500	-0.69656100	H	-1.33760300	-1.10394100	2.96222100
C	-4.51925900	-2.23623300	-0.91604000	H	-3.67415800	2.60132900	-0.31207600
H	-4.07919100	-2.93674300	-0.21301500	H	-4.19451300	1.17163100	-0.58505200
C	-5.63766000	-0.43613400	-2.74034700	H	4.48662900	0.62959700	-2.05122600
H	-6.06794900	0.25543100	-3.45985000	H	0.45071200	0.13953200	-3.44297500
C	-4.26922100	-0.39024900	-2.47217600	H	3.32803500	-1.89737700	2.66327800
H	-3.62777900	0.31653900	-2.99211000	H	-0.65099600	-2.93842900	1.41992600

Table S8. Cartesian coordinates of the optimized geometry for **6bH**.

Al	-0.53414600	1.79673100	-0.36099000	H	2.11761100	3.20295500	4.21335000
Na	0.93962300	-1.16847300	0.42008700	C	0.07356000	3.49808000	4.84109500
O	1.31815700	-0.86985500	2.76337000	H	0.31147500	3.55458600	5.90013000
O	2.69096000	-2.63585300	1.16658100	C	-1.24647100	3.63320200	4.40086100
O	0.60077700	-2.73024300	-1.30744200	H	-2.04714100	3.77551300	5.12376000
N	-1.57866400	2.56657900	-1.69463800	C	-1.55730300	3.57286900	3.04359400
N	-0.80848300	3.30071300	0.69915100	C	-1.35185200	0.13122400	0.35381600
C	-2.08547200	3.81597800	-1.22885500	C	-1.95403900	-0.87143200	0.73467300
C	-1.68475700	4.19781800	0.02102800	C	-2.71967300	-2.01508900	1.12730500
C	-2.79460900	4.70109100	-2.22189800	C	-3.93360000	-2.31412400	0.47520400
H	-2.89734700	5.72426800	-1.85626300	H	-4.27965900	-1.65843200	-0.31804400
H	-3.80089000	4.35055200	-2.48185500	C	-4.67839200	-3.43056500	0.84177900
H	-2.22923000	4.73783200	-3.16358500	H	-5.61148100	-3.63955500	0.32297100
C	-1.89881400	5.56299000	0.62154900	C	-4.25396400	-4.28894300	1.86711600
H	-0.93661300	6.00268800	0.91953300	C	-3.04594200	-3.99148600	2.51176200
H	-2.52186000	5.54773500	1.52411200	H	-2.69226500	-4.64176300	3.30904900
H	-2.37451400	6.24696100	-0.08308800	C	-2.29036800	-2.87713700	2.15503800
C	-2.15926400	1.86822900	-2.75790700	H	-1.35797900	-2.66421200	2.67056900
C	-3.55536500	1.72944200	-2.92857900	C	-5.08884400	-5.47757900	2.28086600
C	-4.08074900	0.99848700	-3.99217400	H	-5.87019400	-5.18461900	2.99505100
H	-5.16060700	0.91298400	-4.09599300	H	-4.47927200	-6.24825400	2.76425500
C	-3.24081800	0.36408700	-4.91196700	H	-5.59294600	-5.93327300	1.42155300
H	-3.65599200	-0.19980200	-5.74309300	C	1.32799600	1.23108400	-0.72147300
C	-1.85750300	0.47478200	-4.74603800	C	2.50009300	0.90559200	-0.90328800
H	-1.18520300	0.00230100	-5.45995500	C	3.87536500	0.56509000	-1.10505200
C	-1.32453900	1.21592700	-3.69230100	C	4.30416100	-0.06956800	-2.28718900
C	-0.54772500	3.39127500	2.07129600	H	3.57634500	-0.29201600	-3.06190900
C	0.77894000	3.24569800	2.53354400	C	5.64361400	-0.40270300	-2.46842000
C	1.08133200	3.29681700	3.89350000	H	5.94989800	-0.89080500	-3.39109300

C	6.60629000	-0.11598000	-1.48990900	H	3.04672000	-3.43512000	-0.66020900
C	6.17717600	0.51618600	-0.31386700	H	4.16959600	-3.99907700	0.61954500
H	6.90393100	0.75368200	0.46007100	C	-0.14323500	-3.94690700	-1.04666600
C	4.84088000	0.85497200	-0.11971800	H	-0.56709300	-3.86365200	-0.04167900
H	4.52990400	1.35634000	0.79230500	H	0.54758200	-4.79903400	-1.06550900
C	8.06381400	-0.44484100	-1.71024300	C	-1.23136400	-4.04940100	-2.13642100
H	8.59059200	0.39148000	-2.18917900	H	-2.20572400	-4.30969800	-1.71427900
H	8.18537000	-1.31803600	-2.36010300	H	-0.96650500	-4.81795800	-2.87124200
H	8.57720200	-0.65074900	-0.76486600	C	-1.22175300	-2.65317000	-2.78566500
C	0.40082600	-0.31158200	3.70777300	H	-1.54153600	-2.65985700	-3.83090600
H	-0.27980600	0.33217300	3.15209900	H	-1.86449600	-1.95763900	-2.23806200
H	0.93391800	0.28729200	4.45526200	C	0.23504500	-2.23881100	-2.61601500
C	2.23645500	-1.77799000	3.34981500	H	0.88190700	-2.70539500	-3.37499700
H	1.71123300	-2.69185300	3.67109800	H	0.39897900	-1.15929600	-2.62125600
H	2.71204200	-1.32910100	4.23543400	H	-0.24868200	1.34002400	-3.59367200
C	3.31194700	-2.11799500	2.33690600	H	-4.22024000	2.18012200	-2.19830700
H	3.89925000	-1.22323900	2.08128100	H	1.56895800	3.12434100	1.79711300
H	3.99278000	-2.86523800	2.77367500	H	-2.59152400	3.63845300	2.71983200
C	3.62775200	-3.13372200	0.21229000	H	-0.16763200	-1.10693600	4.21135100
H	4.34707300	-2.35678900	-0.07698100				

Table S9. Cartesian coordinates of the optimized geometry for **6cH**.

Si	2.92741200	-1.15243900	3.24520300	C	-2.45403500	1.87612500	1.40302100
Si	-2.25591900	-3.05883800	-2.58289400	C	-2.23027100	1.11774500	2.57993600
Al	-0.23191100	0.90172400	-0.15991200	C	-3.28672400	0.72376800	3.40409700
Na	-0.00381400	-2.34641600	0.74335000	H	-3.07499500	0.16780500	4.31611300
O	-2.13539300	-2.05231400	1.59685700	C	-4.60281600	1.07983300	3.09326500
O	1.61464500	-3.54463200	-0.25758600	H	-5.42432000	0.78211400	3.73836000
O	3.22253100	-1.44799700	-0.75172500	C	-4.83771300	1.83707200	1.94255000
N	-1.36449800	2.17206900	0.58432800	H	-5.85506600	2.11775800	1.67914900
N	0.47395100	2.18854500	-1.29770100	C	-3.79140100	2.22399900	1.10682100
C	-1.18064800	3.40286900	-0.10894800	C	1.67571600	2.06103100	-1.99051100
C	-0.19618300	3.42423100	-1.05549500	C	1.89015300	0.89432700	-2.76703700
C	-1.96218300	4.62231000	0.30985000	C	3.09656200	0.67647300	-3.43545200
H	-1.41935100	5.53848000	0.06534400	H	3.21186700	-0.21522200	-4.04991300
H	-2.12044400	4.61652500	1.39462600	C	4.13139200	1.61505000	-3.36460600
H	-2.95695200	4.69971400	-0.15163800	H	5.06580500	1.45145800	-3.89351600
C	0.09656700	4.62091900	-1.92701500	C	3.93229300	2.77251200	-2.60771500
H	-0.78317300	5.26307000	-2.01823200	H	4.72749500	3.51067300	-2.53028400
H	0.36802700	4.29535600	-2.93749600	C	2.73680500	2.99354800	-1.92666100
H	0.92242600	5.25110000	-1.56701600	C	1.04300600	0.06062700	1.12132500

C	1.77739700	-0.45340700	1.97048500	C	-1.75733900	-4.66219100	-1.70887700
C	2.67108900	-0.23127700	4.87239000	H	-0.66941600	-4.71456400	-1.58137800
H	2.86970300	0.83958800	4.75365800	H	-2.07235100	-5.53868800	-2.28842400
H	3.34547200	-0.61506600	5.64786200	H	-2.22293400	-4.73811800	-0.71805200
H	1.64348700	-0.34154000	5.23691900	C	-1.50786900	-2.99242700	-4.31583600
C	2.50145400	-2.98743500	3.45333500	H	-1.75046300	-2.04768400	-4.81480200
H	1.48164200	-3.11989600	3.83652900	H	-1.88938200	-3.81084800	-4.93882600
H	3.18426400	-3.47314900	4.16096700	H	-0.41604500	-3.07975800	-4.27780800
H	2.57817200	-3.51886100	2.49707300	H	2.15759400	-4.30367200	-0.00265800
C	4.69629700	-0.95148000	2.61643200	H	2.25248300	-2.84839200	-0.57851300
H	4.81835700	-1.38699700	1.61833500	H	3.20957400	-0.89678800	-1.55706800
H	5.41048700	-1.43827700	3.29197300	H	2.84724800	-0.86127600	-0.06597500
H	4.96768200	0.10835100	2.55026700	H	-2.34555900	-1.30838300	2.19382900
C	-1.10022000	-0.66317300	-1.01996600	H	-2.44391900	-1.72657300	0.72946300
C	-1.57684600	-1.63998900	-1.60445500	H	2.62730000	3.87869700	-1.31025500
C	-4.13733800	-2.90319900	-2.65362800	H	1.07042500	0.18800500	-2.87532800
H	-4.57901100	-2.93951900	-1.65099900	H	-1.20301200	0.89458500	2.85787900
H	-4.57417000	-3.72093700	-3.24016000	H	-4.00621500	2.77282700	0.19643500
H	-4.44013400	-1.95778100	-3.11734400				

Table S10. Cartesian coordinates of the optimized geometry for **8H**.

Si	1.26839900	0.71438900	3.83864000	H	7.91395000	-1.62363100	0.03597500
Si	0.46826400	-0.90311900	-4.34739600	H	8.42576000	-0.37113000	-1.09037800
Si	-0.24504000	-4.27192500	0.68357400	C	4.45562800	2.84390300	-0.58976400
Si	-1.54790900	4.37282200	-0.72904400	C	5.11681100	3.62899600	0.38176400
Al	3.64919300	0.05115300	-0.54771900	C	4.75807400	4.95691100	0.60078200
Al	-3.23225700	-0.26022500	0.19060000	H	5.28783300	5.53342400	1.35641800
Na	0.31355300	-0.31615000	-0.14868200	C	3.72052800	5.54769800	-0.12551800
Na	-4.70795000	2.11247700	-0.04618700	H	3.44963100	6.58687400	0.04149100
N	4.77737100	1.50550600	-0.83468700	C	3.04373400	4.77824700	-1.07646900
N	5.13488000	-1.05478400	-0.37352500	H	2.24841100	5.22651100	-1.66888400
N	-4.46934400	0.17015900	1.55708000	C	3.40277600	3.45085100	-1.30761700
N	-4.71816400	-0.24446000	-0.98156600	C	5.17551200	-2.28181100	0.30119200
C	6.12984500	1.04677800	-0.83891700	C	4.38185400	-3.35433300	-0.15545600
C	6.31428500	-0.28478600	-0.60113600	C	4.37983700	-4.58288300	0.50403700
C	7.17811700	1.98423500	-1.38348400	H	3.77011100	-5.39557200	0.11449500
H	8.16515600	1.52073200	-1.41967600	C	5.17418000	-4.78641500	1.63496800
H	7.27306700	2.90426000	-0.79662200	H	5.18317900	-5.74888800	2.13965000
H	6.91452300	2.29678800	-2.40494400	C	5.96064500	-3.73043100	2.10403100
C	7.60033900	-1.03698800	-0.83421700	H	6.57462400	-3.86436000	2.99228200
H	7.47633800	-1.75346000	-1.65964200	C	5.95740900	-2.49630600	1.45766900

C	-5.81603100	-0.03490900	1.10374800	H	0.76651400	-1.65026200	4.44825000
C	-5.94836700	-0.25326000	-0.24065300	C	2.27202800	-0.36907900	-1.92003500
C	-6.94916600	0.10410400	2.08845300	C	1.44407300	-0.59740700	-2.80696300
H	-6.80545900	0.97724700	2.73853400	C	-0.72902900	-2.33685100	-4.06784400
H	-7.03220700	-0.76101800	2.75698600	H	-0.18124000	-3.26129000	-3.85172100
H	-7.91066500	0.21472900	1.58297600	H	-1.34723600	-2.50997600	-4.95664400
C	-7.25257600	-0.38637100	-0.98568700	H	-1.40752400	-2.14452200	-3.22923000
H	-8.10077400	-0.07994500	-0.36996500	C	-0.46914900	0.68327200	-4.78015700
H	-7.44722300	-1.41370200	-1.31586400	H	-1.17697400	0.95411300	-3.98861000
H	-7.25437700	0.22950900	-1.89474800	H	-1.03633700	0.56022600	-5.71115600
C	-4.17596300	0.09568800	2.94921900	H	0.22468100	1.52071300	-4.91619800
C	-3.53007100	1.16600400	3.58861800	C	1.68702100	-1.32950600	-5.72813300
C	-3.22623900	1.11045200	4.95020100	H	2.40502700	-0.51704600	-5.88540100
H	-2.72970400	1.95399100	5.42217900	H	1.16225400	-1.50624200	-6.67554900
C	-3.56457800	-0.01494600	5.70243700	H	2.25690900	-2.23312800	-5.48471000
H	-3.33629900	-0.05508400	6.76374500	C	-1.98100300	-1.73629800	0.32973200
C	-4.19115300	-1.09386900	5.07399100	C	-1.22481700	-2.70187100	0.45115200
H	-4.44294200	-1.98433400	5.64440600	C	0.63148600	-4.65992200	-0.94145500
C	-4.48428000	-1.04556000	3.71213000	H	1.31901900	-3.85686700	-1.22856100
C	-4.69050500	-0.75418800	-2.31056100	H	-0.09049000	-4.79464200	-1.75474800
C	-4.17991400	0.03574200	-3.35382700	H	1.21592500	-5.58378100	-0.85228600
C	-4.13905800	-0.44510100	-4.66394800	C	0.96896400	-4.01421500	2.10027000
H	-3.74469300	0.18859700	-5.45372500	H	0.43918700	-3.77996700	3.03061500
C	-4.61018400	-1.72457300	-4.96073900	H	1.67150100	-3.19997600	1.89258800
H	-4.58886100	-2.09487600	-5.98180600	H	1.56552700	-4.91888800	2.26658800
C	-5.10113200	-2.52775400	-3.92847400	C	-1.49421600	-5.62856600	1.10226100
H	-5.45221500	-3.53411600	-4.14221600	H	-0.98418000	-6.58920900	1.24619700
C	-5.13122100	-2.05474300	-2.61768700	H	-2.22911900	-5.75523300	0.29946300
C	2.52718900	0.21466900	1.08541900	H	-2.03856400	-5.39648700	2.02442300
C	1.89409400	0.37218000	2.13305200	C	-2.21265000	1.40636600	-0.18559900
C	0.28652700	2.33236700	3.80173500	C	-1.87878400	2.57476000	-0.40747400
H	0.91367900	3.15552400	3.44109500	C	-3.26832800	5.18889000	-0.64004500
H	-0.07413800	2.59471100	4.80415900	H	-3.94863500	4.78175800	-1.40189300
H	-0.58306700	2.25391300	3.13939200	H	-3.20527700	6.26902700	-0.81952300
C	2.76979300	0.89559900	4.97282900	H	-3.72176100	5.05940700	0.35287700
H	3.36771200	-0.02250900	4.97963900	C	-0.82883200	4.57704100	-2.45819600
H	2.46241800	1.10750000	6.00481300	H	0.13749000	4.06759500	-2.53835500
H	3.41892700	1.71206300	4.63769900	H	-0.66908800	5.63692900	-2.69089200
C	0.18568400	-0.72137900	4.41688800	H	-1.49172100	4.15946100	-3.22449900
H	-0.67018900	-0.88098600	3.75157600	C	-0.42549500	5.08164800	0.60299400
H	-0.21006100	-0.53573800	5.42254400	H	-0.79563300	4.84968100	1.60787500

H	-0.36331300	6.17314800	0.50995700	H	6.54185100	-1.67100200	1.85387900
H	0.59210300	4.68529000	0.51637400	H	2.90264900	2.86842600	-2.07822800
H	-5.48934500	-2.69340200	-1.81518500	H	5.89789000	3.16951900	0.98026900
H	-3.81606600	1.03521900	-3.12683500	H	-4.94860100	-1.89727600	3.22282100
H	3.79934000	-3.21418100	-1.06285000	H	-3.26836600	2.04640100	3.00636900

Table S11. Cartesian coordinates of the optimized geometry for 10H.

Al	-0.05682400	-2.37760300	-1.80232300	C	-1.87056400	-2.12177800	-5.62156800
Na	-0.11104700	-1.30973400	1.32748300	H	-2.17757500	-3.10653300	-6.00351000
O	0.21174600	-1.08870800	3.54893500	H	-1.20368600	-1.72452600	-6.40067400
N	0.71373200	-3.45102000	-3.08346200	C	-3.10713900	-1.22152600	-5.52870000
N	-0.00436600	-5.31803600	-5.82662500	H	-3.78612500	-1.60163700	-4.75316400
C	0.09600200	-3.33252100	-4.42549500	H	-2.81056800	-0.21263800	-5.20263900
C	-0.49657000	-4.71155800	-4.81566000	C	-3.86360200	-1.11158700	-6.85919500
C	1.12107400	-2.86344400	-5.47915600	H	-4.17099900	-2.11591300	-7.18272300
H	1.48514100	-1.86601500	-5.20781300	H	-3.18134900	-0.73913700	-7.63651500
H	0.69267400	-2.82966900	-6.48367200	C	-5.09423300	-0.20262900	-6.77978500
H	1.96861400	-3.55025000	-5.51759900	H	-5.80917500	-0.56750700	-6.03214400
C	-1.61099100	-5.26079700	-3.94507400	H	-5.61601300	-0.15110500	-7.74200700
H	-2.58731000	-5.01215400	-4.38106700	H	-4.81575300	0.82075300	-6.49823600
H	-1.57284300	-4.83690900	-2.94073400	C	-0.85087200	-3.23427200	-0.19958900
H	-1.55522300	-6.35116200	-3.88340200	C	-1.33533000	-3.81733800	0.76694700
C	1.84891300	-4.28936800	-2.91013100	C	-1.90600600	-4.58511100	1.88193700
C	3.15475500	-3.77683200	-3.02422700	H	-2.78516700	-5.13803300	1.52050300
C	4.27207300	-4.58429000	-2.80283600	H	-2.27846400	-3.89757900	2.65426600
H	5.26917100	-4.16139600	-2.90234600	C	-0.91138900	-5.57934600	2.52506200
C	4.11391800	-5.92749900	-2.45674600	H	-0.04677400	-5.02042200	2.91007300
H	4.98320700	-6.55688900	-2.28469500	H	-1.40428200	-6.03306600	3.39589200
C	2.82644800	-6.45184100	-2.32817800	C	-0.42960000	-6.67946900	1.57329700
H	2.68823800	-7.49347100	-2.04734800	H	-1.30069800	-7.23564500	1.19816800
C	1.71028300	-5.64298800	-2.54996900	H	0.04297900	-6.21764100	0.69739400
C	-0.43798700	-6.59673100	-6.22875100	C	0.55173500	-7.65113200	2.23631500
C	0.28151400	-7.73711400	-5.83392500	H	1.44953200	-7.12825800	2.58870400
C	-0.09361900	-8.99816400	-6.29490400	H	0.87562900	-8.42794400	1.53485200
H	0.46932300	-9.87174700	-5.97487600	H	0.09805700	-8.15118900	3.10121300
C	-1.17689900	-9.14531800	-7.16455800	C	1.22855000	-1.08066200	-0.95757700
H	-1.46171000	-10.12942400	-7.52629300	C	2.18304600	-0.47273700	-0.47313600
C	-1.88428200	-8.01195300	-7.57020200	C	3.36841000	0.20002100	0.07824700
H	-2.72647600	-8.11048000	-8.25099900	H	3.99324500	0.55679500	-0.75339100
C	-1.52059800	-6.74661100	-7.11001700	H	3.05727000	1.09527900	0.63108800
C	-1.31583000	-1.69320400	-3.16049100	C	4.21784700	-0.70901100	0.99635000
H	-2.18188500	-1.02886500	-3.12400000	H	5.00232900	-0.08795800	1.44915800
C	-1.07134400	-2.31425400	-4.33939000	H	3.58884000	-1.06724400	1.82396500

C	4.85368500	-1.90262500	0.27532200	H	2.17757500	3.10653300	6.00351000
H	5.50966300	-1.52745900	-0.52330400	H	1.20368600	1.72452600	6.40067400
H	4.07284200	-2.49037600	-0.22252900	C	3.10713900	1.22152600	5.52870000
C	5.65779100	-2.80703800	1.21409200	H	3.78612500	1.60163700	4.75316400
H	6.47214700	-2.25729900	1.70252700	H	2.81056800	0.21263800	5.20263900
H	6.10023600	-3.64740800	0.66842400	C	3.86360200	1.11158700	6.85919500
H	5.02026600	-3.22510200	2.00360000	H	4.17099900	2.11591300	7.18272300
Al	0.05682400	2.37760300	1.80232300	H	3.18134900	0.73913700	7.63651500
Na	0.11104700	1.30973400	-1.32748300	C	5.09423300	0.20262900	6.77978500
O	-0.21174600	1.08870800	-3.54893500	H	5.80917500	0.56750700	6.03214400
N	-0.71373200	3.45102000	3.08346200	H	5.61601300	0.15110500	7.74200700
N	0.00436600	5.31803600	5.82662500	H	4.81575300	-0.82075300	6.49823600
C	-0.09600200	3.33252100	4.42549500	C	0.85087200	3.23427200	0.19958900
C	0.49657000	4.71155800	4.81566000	C	1.33533000	3.81733800	-0.76694700
C	-1.12107400	2.86344400	5.47915600	C	1.90600600	4.58511100	-1.88193700
H	-1.48514100	1.86601500	5.20781300	H	2.78516700	5.13803300	-1.52050300
H	-0.69267400	2.82966900	6.48367200	H	2.27846400	3.89757900	-2.65426600
H	-1.96861400	3.55025000	5.51759900	C	0.91138900	5.57934600	-2.52506200
C	1.61099100	5.26079700	3.94507400	H	0.04677400	5.02042200	-2.91007300
H	2.58731000	5.01215400	4.38106700	H	1.40428200	6.03306600	-3.39589200
H	1.57284300	4.83690900	2.94073400	C	0.42960000	6.67946900	-1.57329700
H	1.55522300	6.35116200	3.88340200	H	1.30069800	7.23564500	-1.19816800
C	-1.84891300	4.28936800	2.91013100	H	-0.04297900	6.21764100	-0.69739400
C	-3.15475500	3.77683200	3.02422700	C	-0.55173500	7.65113200	-2.23631500
C	-4.27207300	4.58429000	2.80283600	H	-1.44953200	7.12825800	-2.58870400
H	-5.26917100	4.16139600	2.90234600	H	-0.87562900	8.42794400	-1.53485200
C	-4.11391800	5.92749900	2.45674600	H	-0.09805700	8.15118900	-3.10121300
H	-4.98320700	6.55688900	2.28469500	C	-1.22855000	1.08066200	0.95757700
C	-2.82644800	6.45184100	2.32817800	C	-2.18304600	0.47273700	0.47313600
H	-2.68823800	7.49347100	2.04734800	C	-3.36841000	-0.20002100	-0.07824700
C	-1.71028300	5.64298800	2.54996900	H	-3.99324500	-0.55679500	0.75339100
C	0.43798700	6.59673100	6.22875100	H	-3.05727000	-1.09527900	-0.63108800
C	-0.28151400	7.73711400	5.83392500	C	-4.21784700	0.70901100	-0.99635000
C	0.09361900	8.99816400	6.29490400	H	-5.00232900	0.08795800	-1.44915800
H	-0.46932300	9.87174700	5.97487600	H	-3.58884000	1.06724400	-1.82396500
C	1.17689900	9.14531800	7.16455800	C	-4.85368500	1.90262500	-0.27532200
H	1.46171000	10.12942400	7.52629300	H	-5.50966300	1.52745900	0.52330400
C	1.88428200	8.01195300	7.57020200	H	-4.07284200	2.49037600	0.22252900
H	2.72647600	8.11048000	8.25099900	C	-5.65779100	2.80703800	-1.21409200
C	1.52059800	6.74661100	7.11001700	H	-6.47214700	2.25729900	-1.70252700
C	1.31583000	1.69320400	3.16049100	H	-6.10023600	3.64740800	-0.66842400
H	2.18188500	1.02886500	3.12400000	H	-5.02026600	3.22510200	-2.00360000
C	1.07134400	2.31425400	4.33939000	H	-2.06344100	-5.86353500	-7.43656000
C	1.87056400	2.12177800	5.62156800	H	1.13154800	-7.61607200	-5.16852400

H	3.27763600	-2.72985400	-3.28520600	H	-3.27763600	2.72985400	3.28520600
H	0.71136800	-6.05223100	-2.43250600	H	0.89622000	-1.50573500	4.09320500
H	-1.13154800	7.61607200	5.16852400	H	0.33548600	-0.12076400	3.68595000
H	2.06344100	5.86353500	7.43656000	H	-0.33548600	0.12076400	-3.68595000
H	-0.71136800	6.05223100	2.43250600	H	-0.89622000	1.50573500	-4.09320500

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