

The Divergent Reactivity of β -diketiminato Aluminium Hydrides with Organophosphoryl Compounds

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NMR Spectra

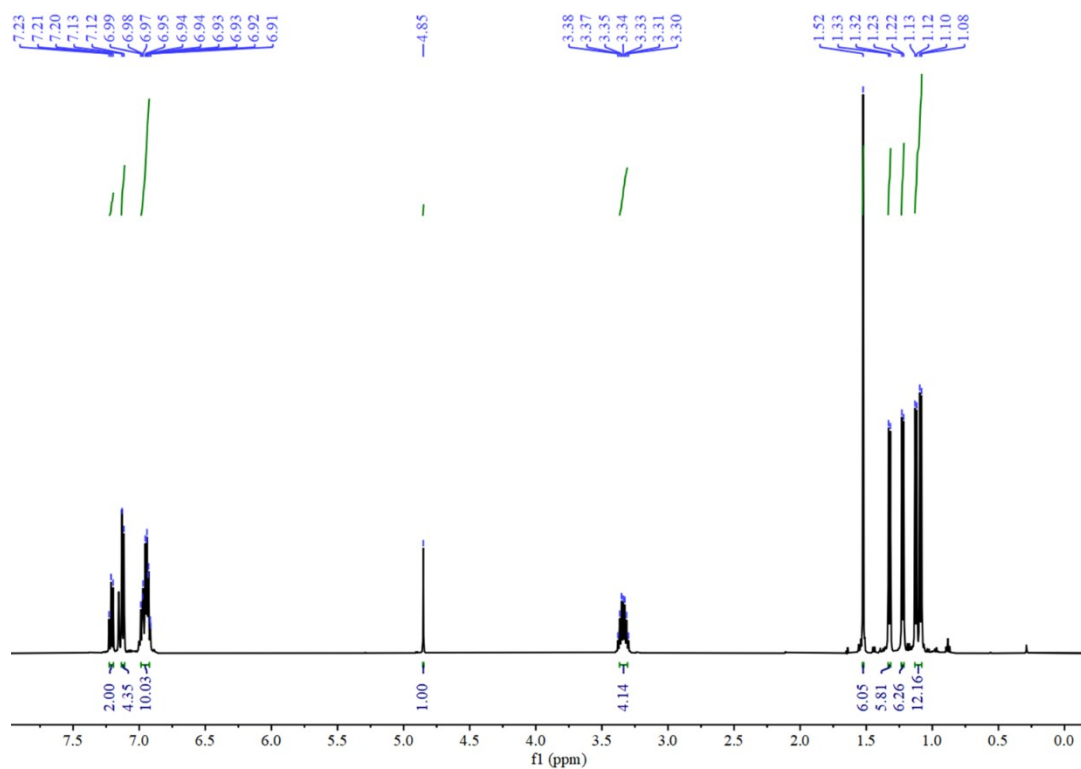


Figure S1.1 ¹H NMR of compound 2.

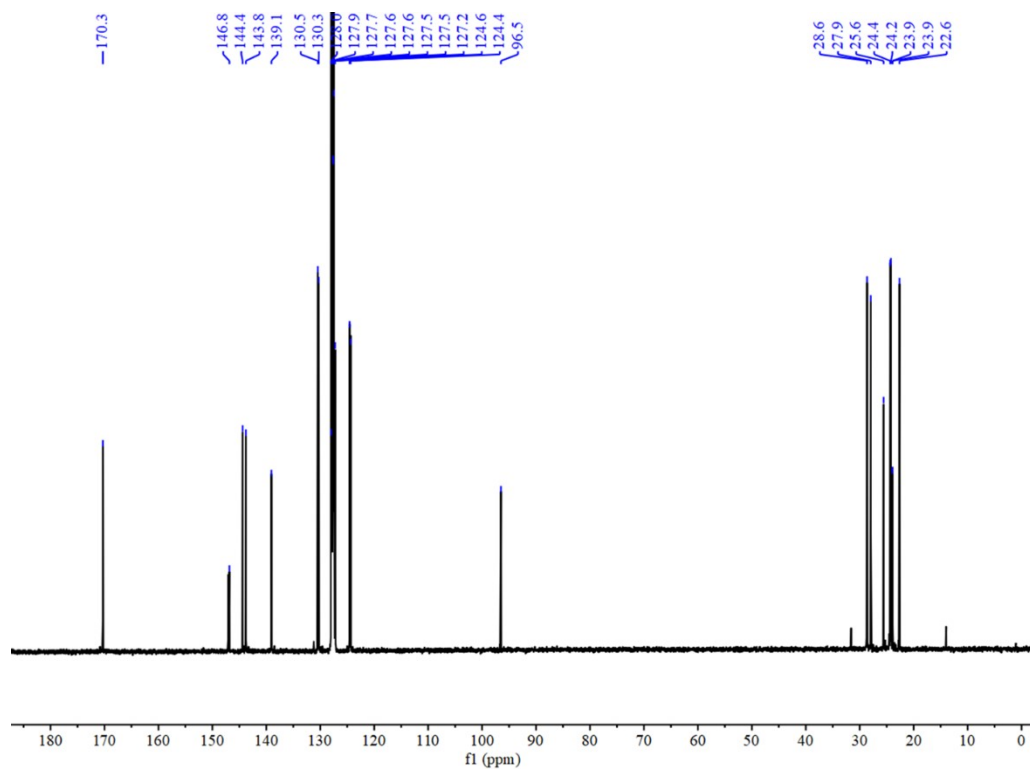


Figure S1.2 ¹³C NMR of compound 2.

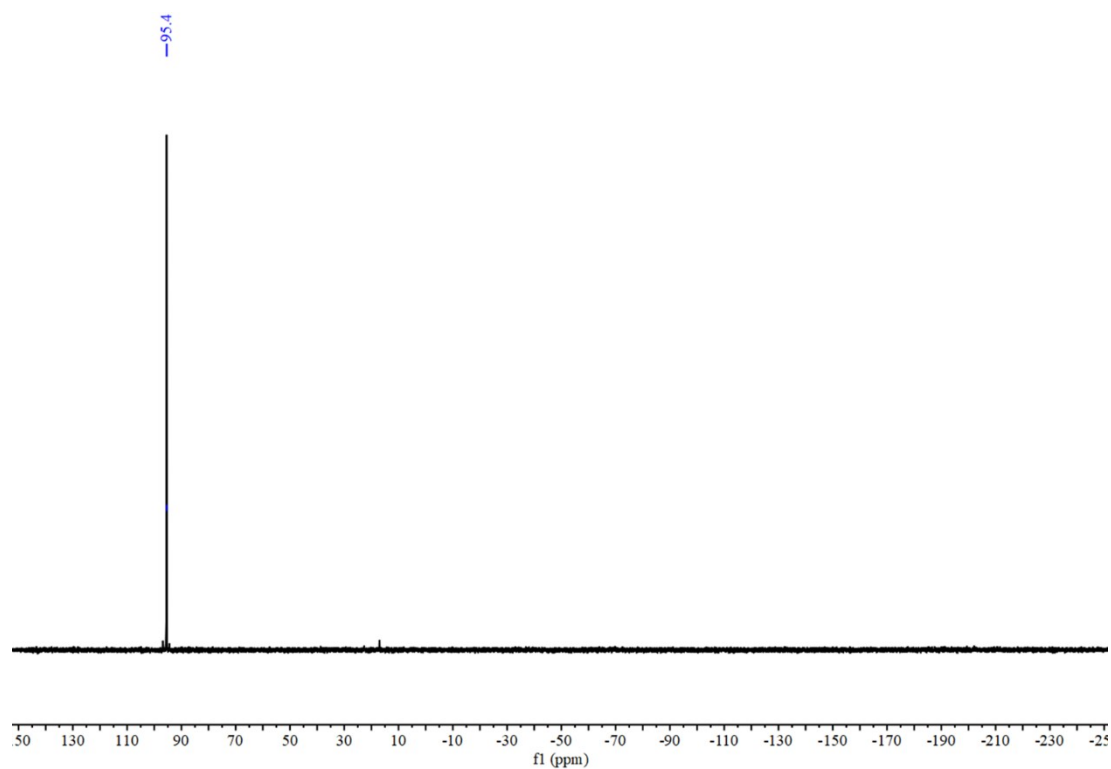


Figure S1.3 ^{31}P NMR of compound **2**.

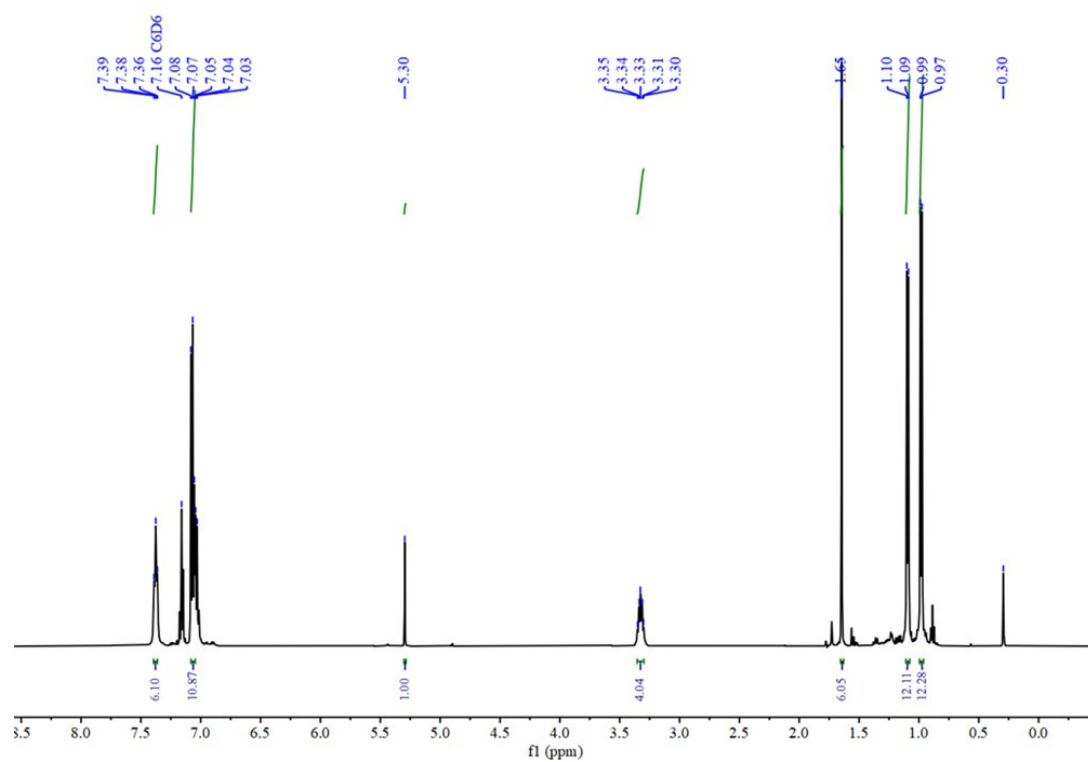


Figure S2.1 ^1H NMR of compound **3**.

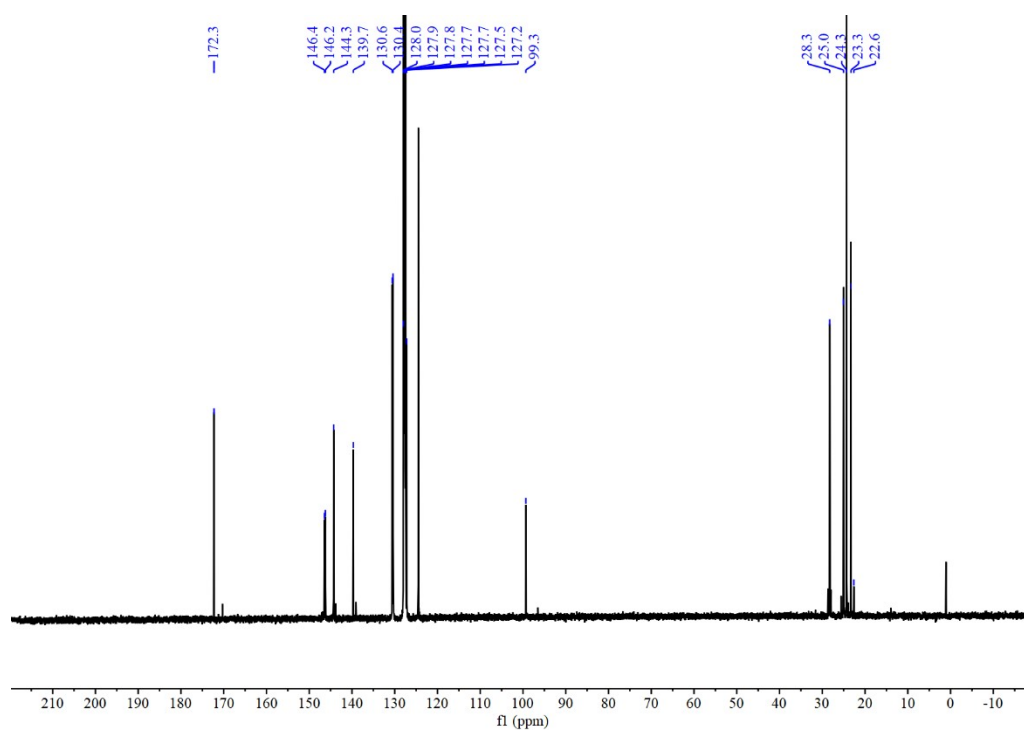


Figure S2.2 ^{13}C NMR of compound **3**.

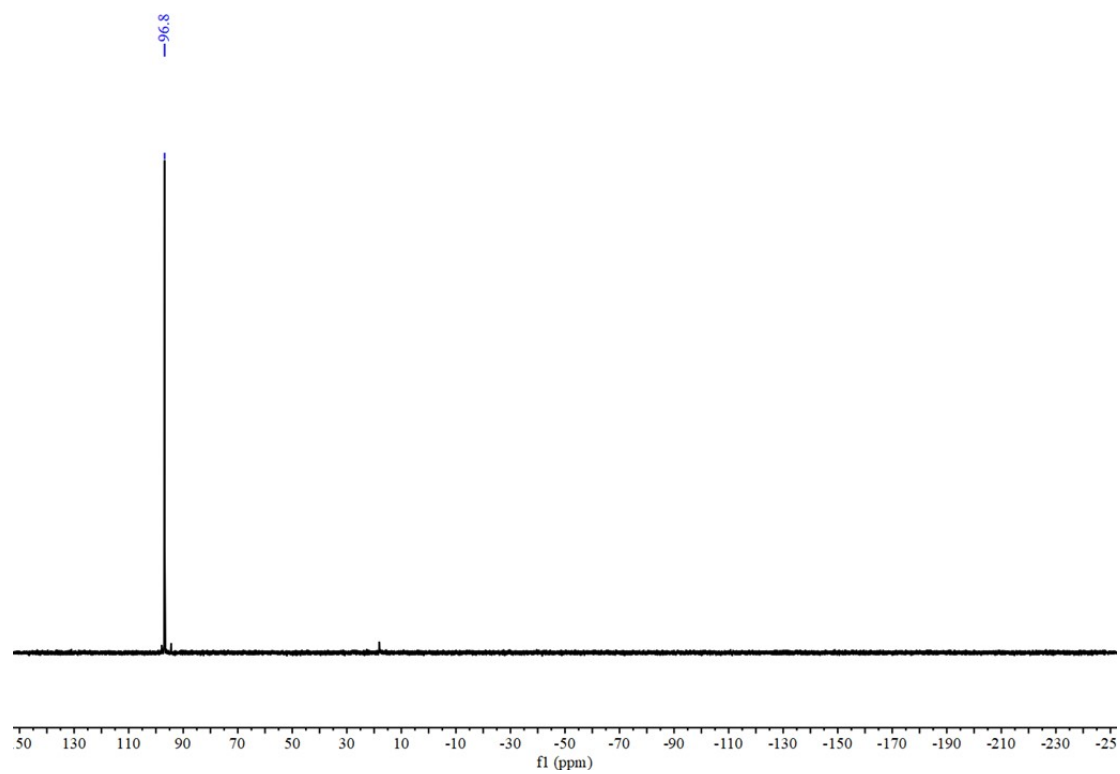


Figure S2.3 ^{31}P NMR of compound **3**.

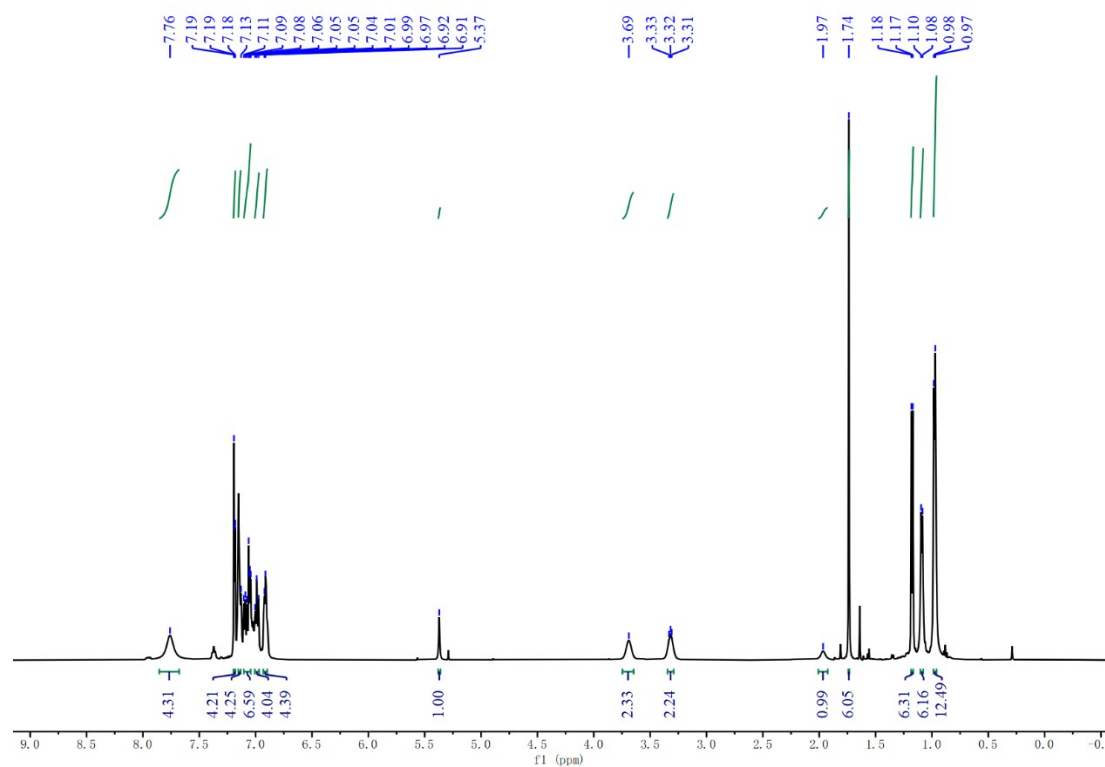


Figure S3.1 ¹H NMR of compound 4 and 4a.

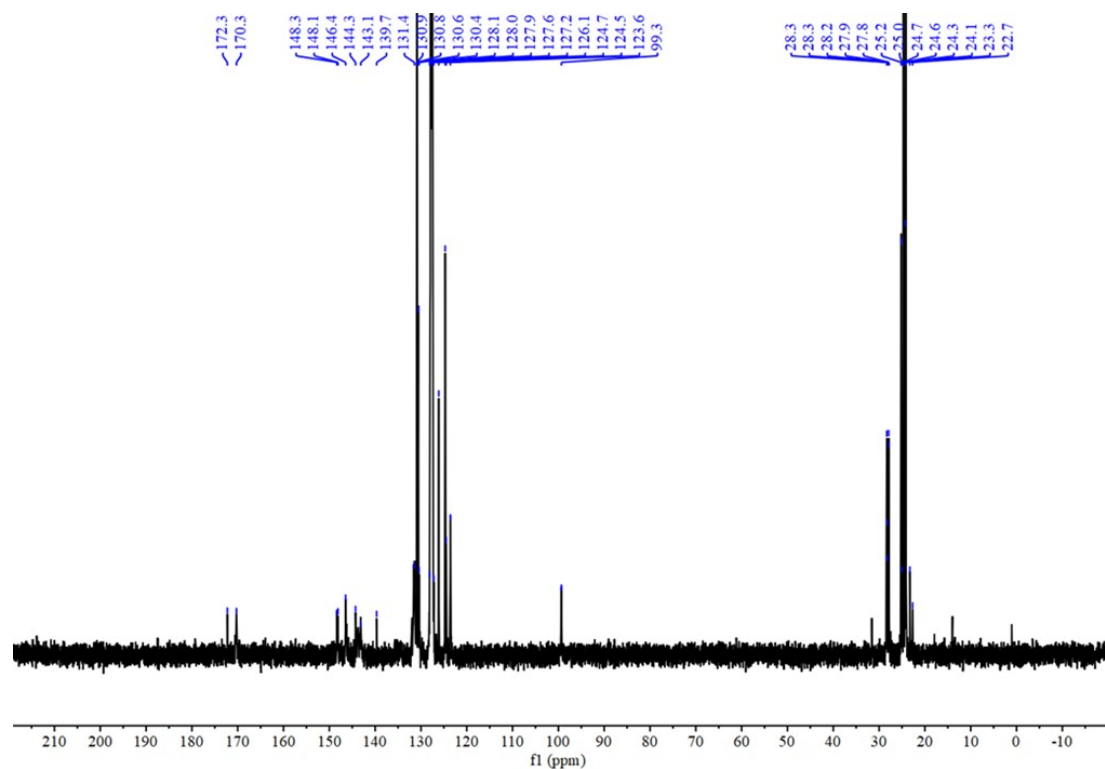


Figure S3.2 ¹³C NMR of compound 4 and 4a.

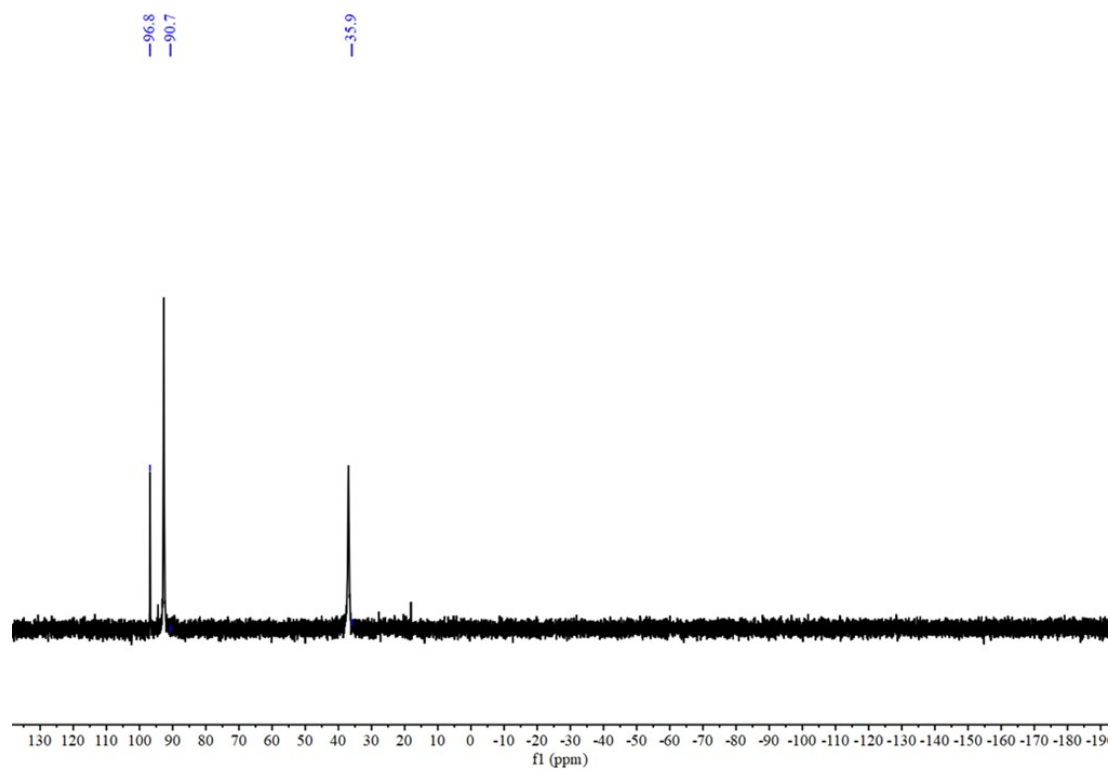


Figure S3.3 ³¹P NMR of compound **4** and **4a**.

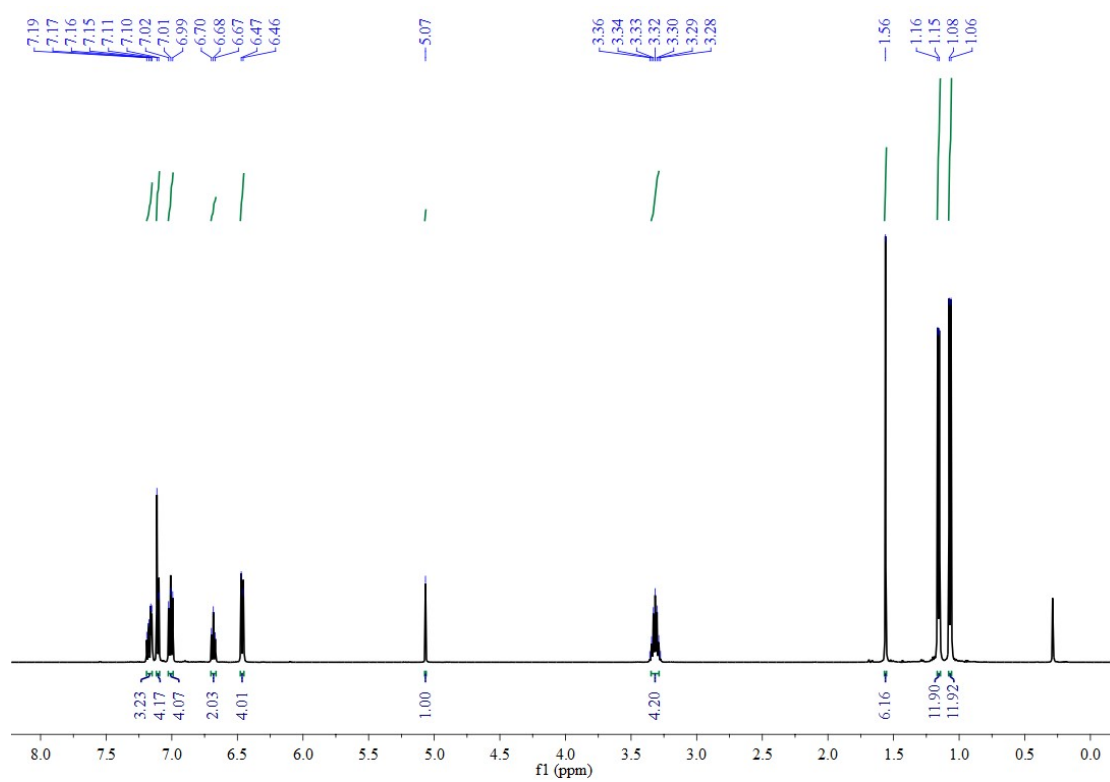


Figure S4.1 ¹H NMR of compound **5**.

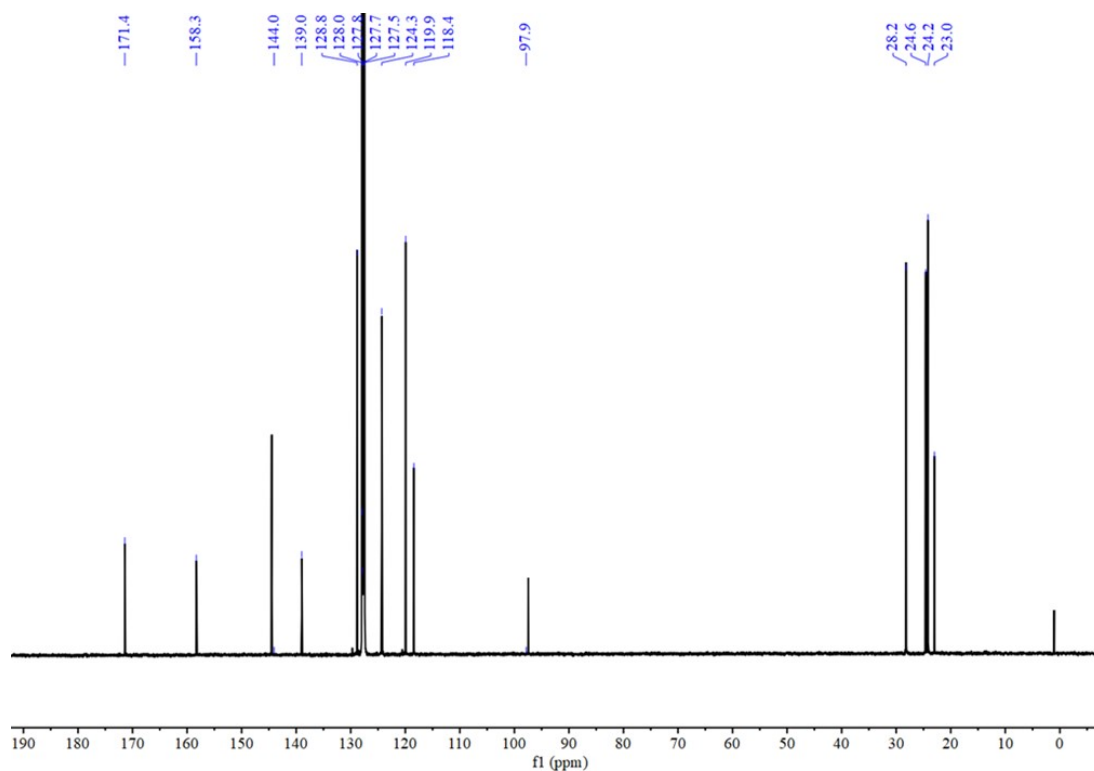


Figure S4.2 ^{13}C NMR of compound **5**.

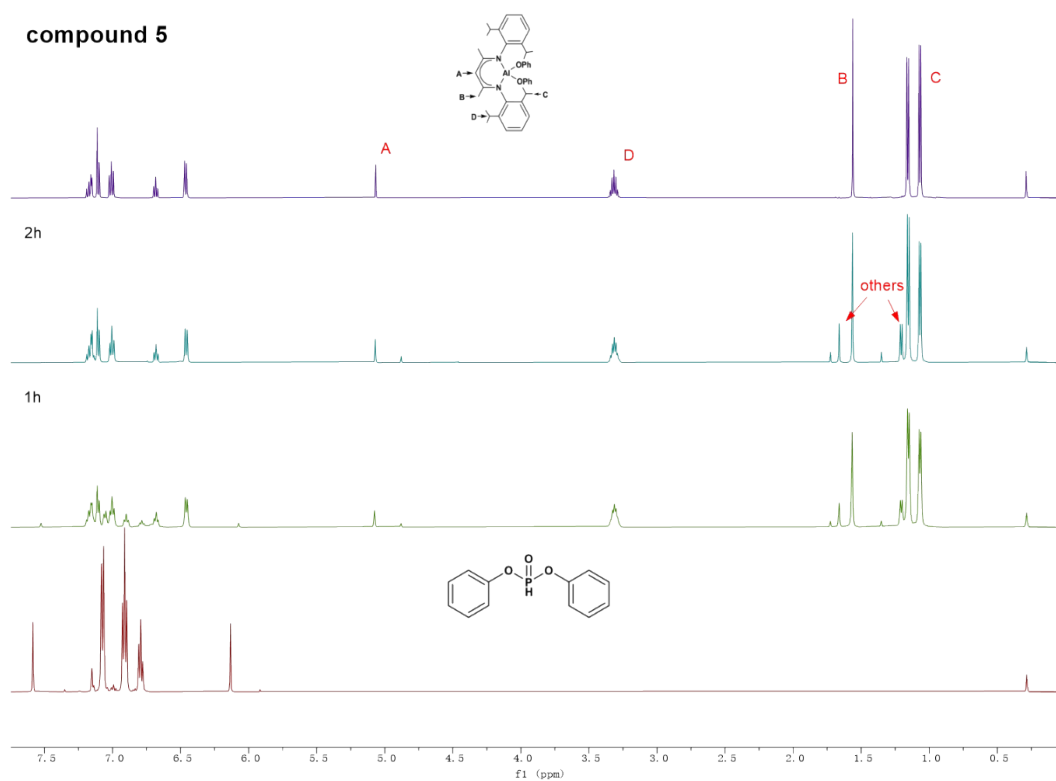


Figure S5.1 ^1H NMR of the reaction of compound **1** with $(\text{PhO})_2\text{P}(\text{O})\text{H}$.

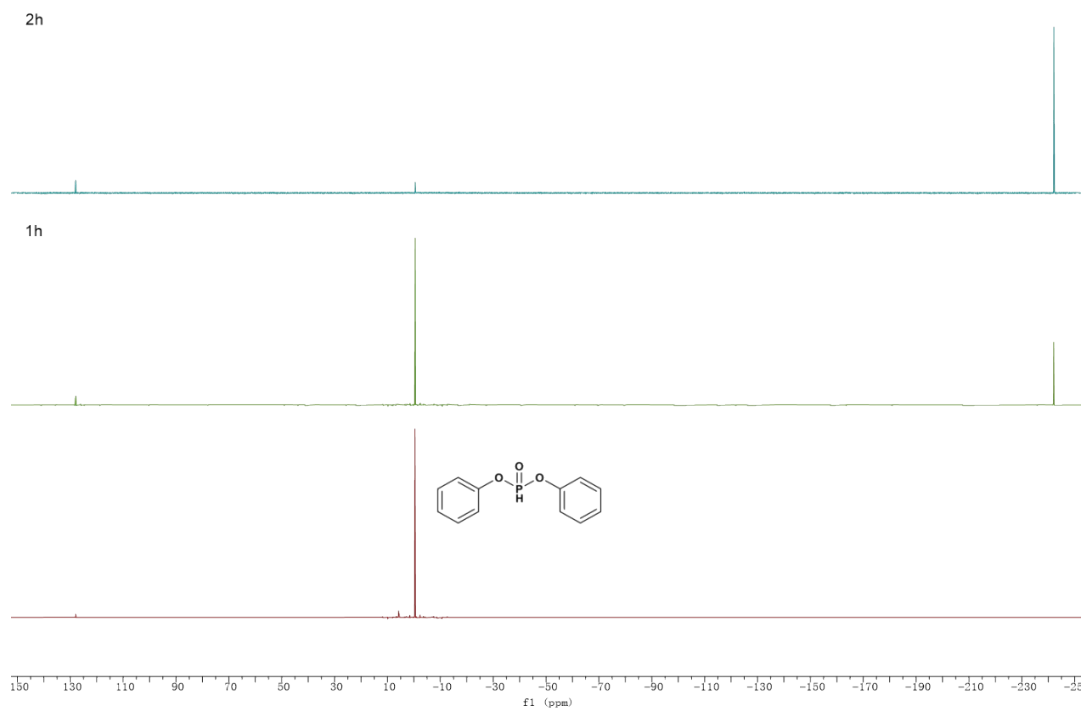


Figure S5.2 ^{31}P NMR of the reaction of compound **1** with $(\text{PhO})_2\text{P}(\text{O})\text{H}$.

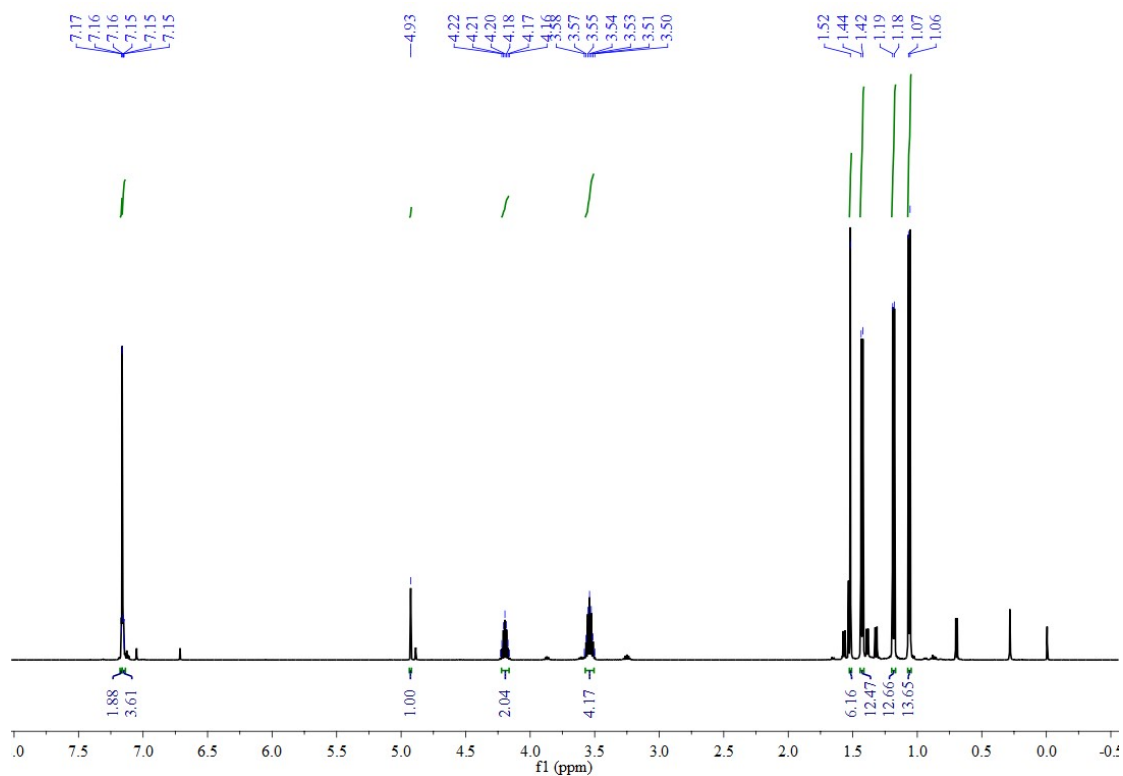


Figure S6.1 ^1H NMR of compound **6**.

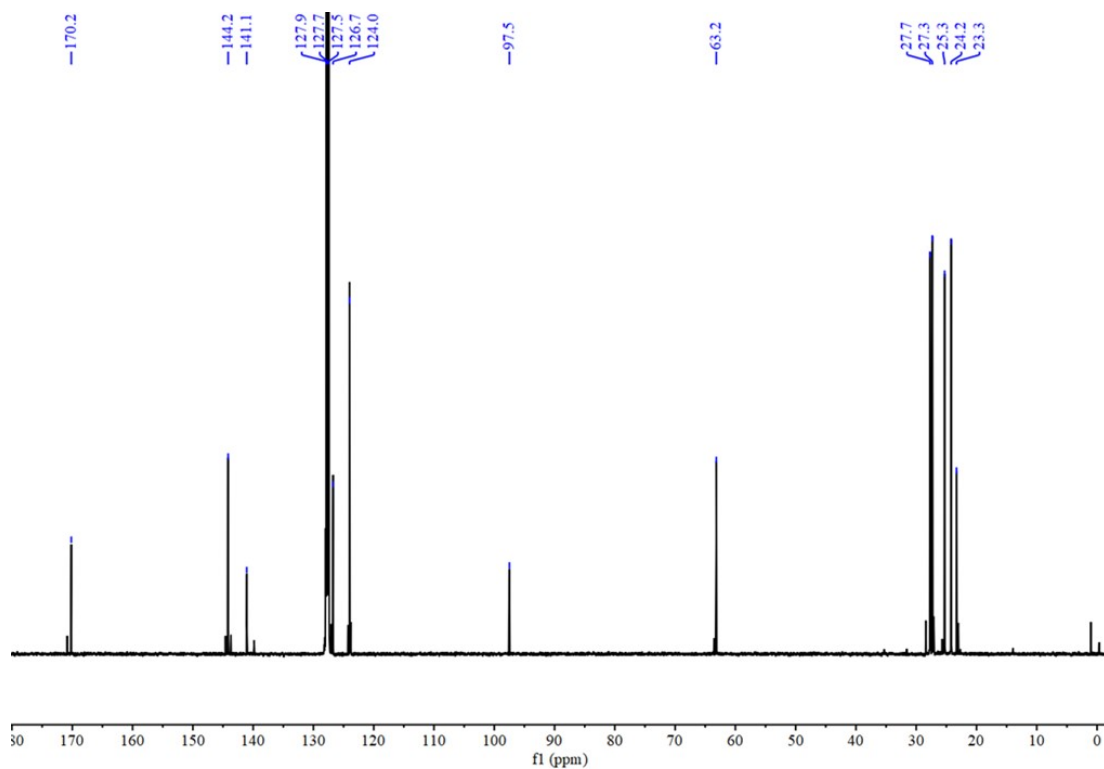


Figure S6.2 ¹³C NMR of compound 6.

IR Spectra

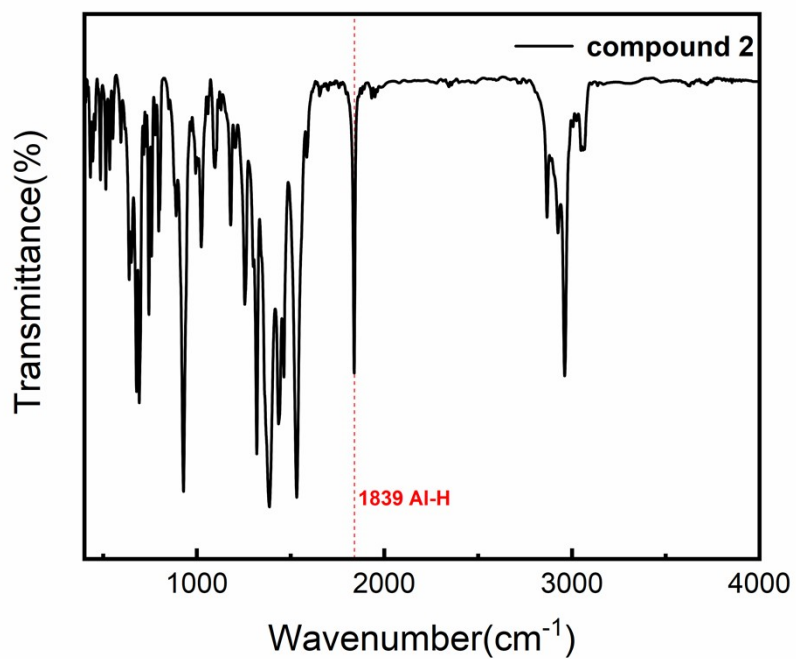


Figure S7 IR spectrum of compound 2.

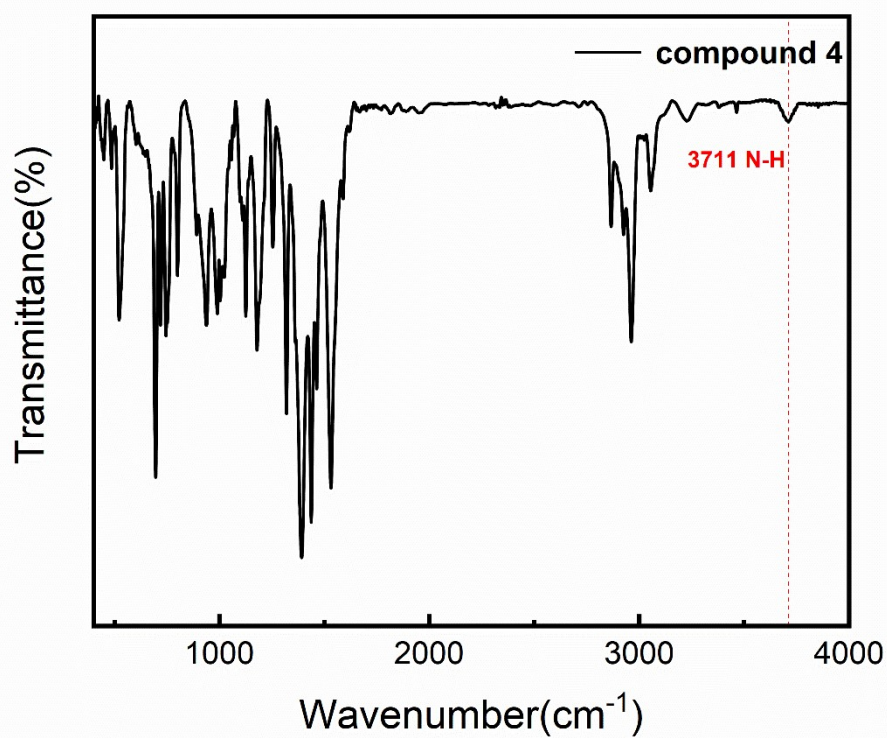


Figure S8 IR spectrum of compounds **4** and **4a**.

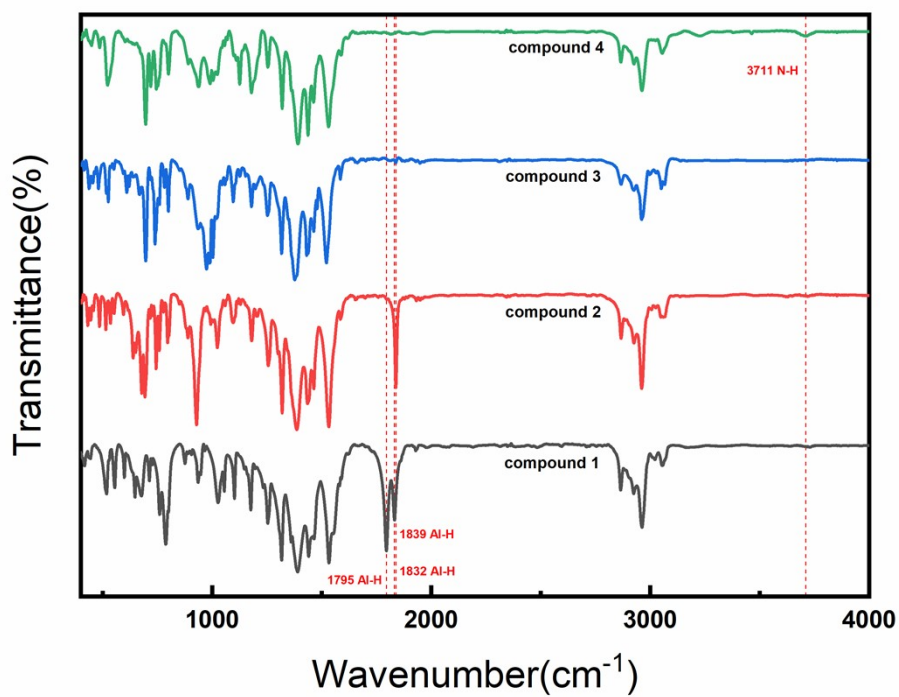


Figure S9 IR spectra of compounds **1-4**.

X-Ray Diffraction

Crystallographic analysis: All crystals were selected under cooling. The diffraction data were collected using an Incoatec Mo Microsource¹ and a Bruker D8 VENTURE. The data were integrated with SAINT.² A multi-scan absorption correction was applied using SADABS.³ The structures were solved by SHELXT⁴ and refined on F² using SHELXL⁵ in the graphical user interface ShelXle.⁶ An overview of the crystallographic data can be found in Table S1, while selected bond lengths and angles are listed in Table S2. In compound 5, the C-C bond length of the benzene was fixed to 1.4 Å and solvent (hexane) was squeezed by PLATON program due to heavily disorder.

Table S1. Crystal data and structure refinement for compounds 2-6.

Compound	2	3	4	5	6
CCDC	2415387	2415388	2415389	2415831	2415390
Empirical formula	C ₄₁ H ₅₂ AlN ₂ OP	C ₄₁ H ₅₂ AlN ₂ O ₃ P	C ₄₁ H ₅₂ AlN ₃ O ₂ P	C ₄₁ H ₅₁ AlN ₂ O ₂	C ₃₅ H ₅₅ AlN ₂ O ₂
Formula weight	646.79	678.83	676.82	630.81	562.79
Temperature (K)	150.0	150.0	150.0	150.00	150.0
Crystal system	monoclinic	monoclinic	monoclinic	orthorhombic	orthorhombic
Space group	P2 ₁ /n	P2 ₁ /n	P2 ₁ /n	Cmce	P2 ₁ 2 ₁ 2 ₁
<i>a</i> (Å)	11.8077(12)	11.868(3)	11.8186(4)	21.5775(7)	9.6913(4)
<i>b</i> (Å)	19.836(2)	19.828(5)	19.8525(6)	24.3473(7)	17.2251(6)
<i>c</i> (Å)	17.0505(18)	17.151(5)	17.2381(4)	16.4561(5)	20.4705(7)
α (deg)	90	90	90	90	90
β (deg)	107.820(4)	107.416(9)	107.2790(10)	90	90
γ (deg)	90	90	90	90	90
<i>V</i> (Å ³)	3802.0(7)	3851.2(19)	3862.0(2)	8645.3(5)	3417.2(2)
<i>Z</i>	4	2	2	8	4
μ /mm ⁻¹	0.128	0.131	0.128	0.638	0.744
Θ max (deg)	26.430	25.020	26.735	74.805	74.640
Reflections collected	66184	38418	42248	57923	27994
Independent reflections (<i>R</i> _{int})	7801 (0.1019)	6753 (0.0863)	8188 (0.0612)	4530(0.1382)	6910(0.1516)
Data/restraints/parameters	7801/0/426	6753/7/443	8188/0/449	4530/81/252	6910/8/404
<i>R</i> 1 ^a (<i>I</i> > 2 σ (<i>I</i>))	0.0517	0.0506	0.0462	0.1165	0.0452
<i>wR</i> 2 ^b (all data)	0.1410	0.1332	0.1146	0.2671	0.1269
$\Delta\rho_{\max}/\Delta\rho_{\min}$ (e Å ⁻³)	0.46/-0.28	0.31/-0.36	0.43/-0.90	0.68/-0.55	0.88/-0.31

$$^a R1 = \sum ||F_o| - |F_c|| / \sum |F_o|, ^b wR2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$$

Table S2. Selected Bond Lengths and Bond Angles for Compounds 1–6

selected bond lengths (Å)							
	1	2	3	4	4a	5	6
Al-NacNac (Å)	0	0.591	0.832	0.764	0.780	0.408	0.504
Al-N	1.8989	Al1-N1 1.886(2)	Al1-N1 1.8833(17)	Al1-N1 1.883(4)	Al4-N6 1.909(4)	1.865(4)	Al1-N2 1.901(2)
		Al1-N2 1.885(2)	Al1-N2 1.8787(17)	Al1-N4 1.884(3)	Al4-N8 1.957(3)		Al1-N3 1.907(2)

Al-O	–	1.7378(17)	Al1-O1	1.718(3)	Al4-O4	Al1-O2	Al1-O3
			1.7238(15)		1.747(3)	1.703(5)	1.712(2)
			Al1-O2		Al4-O6	Al1-O3	Al1-O4
			1.7095(15)		2.059(3)	1.720(5)	1.700(2)
P-O	–	1.6121(16)	P1-O2	P1-O2	P3-O4	–	–
			1.6143(15)	1.439(4)	1.591(3)		
			P2-O1	P2-O1	P5-O6		
			1.6078(15)	1.600(3)	1.513(3)		
selected bond angles (°)							
	1	2	3	4	4a	5	6
Al-O-P	–	127.94(10)	Al1-O1-P2	150.5(2)	Al4-O4-P3	–	–
			142.22		145.21(18)		
			Al1-O2-P1		Al4-O6-P5		
			141.43		92.89(15)		
O-Al-O	–	–	–	–	–	109.3(2)	114.24(12)
N-Al-N	96.41(5)	96.81(8)	98.86(7)	98.61(15)	94.06(15)	97.9(2)	98.06(9)

Theoretical Calculations

All calculations were performed with the Gaussian 16 software package.⁷ The geometry optimizations and frequency calculations were optimized in conjunction with the SMD⁸ continuum solvation model at the B3LYP⁹/def2-SVP¹⁰ level of theory, in which the solvent of *n*-hexane has been used according our experiments. The electronic energies were refined with the larger basis set def2-TZVP¹⁰ for all atoms. The same solvation model and dispersion corrections were included in all calculations.

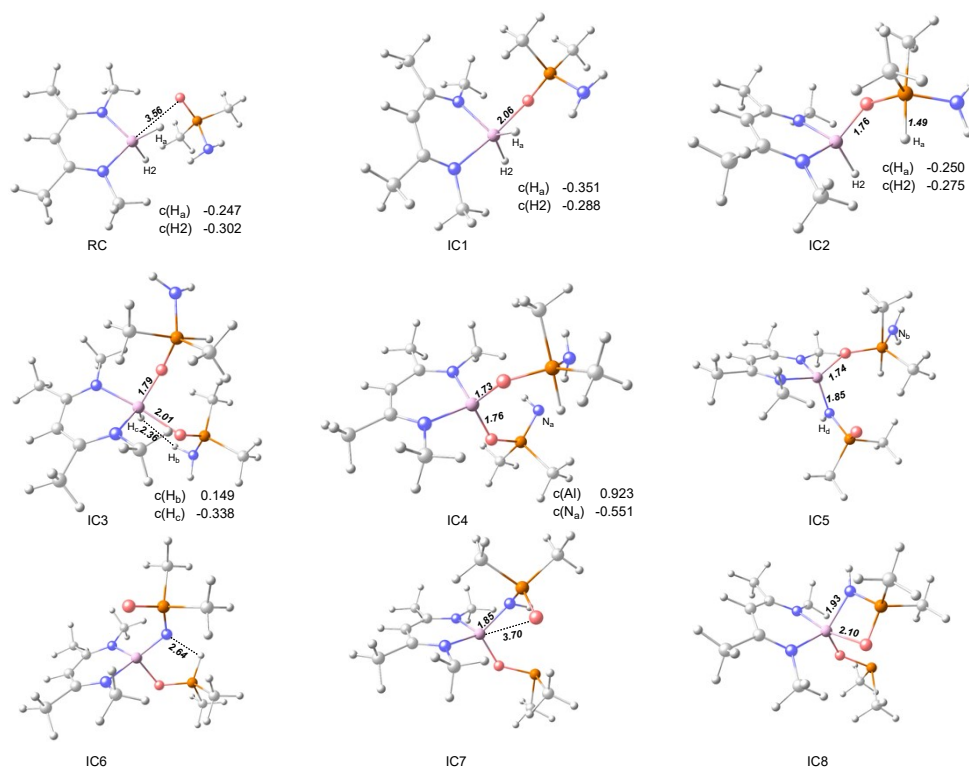


Figure S10. Optimized geometries of key species. The key distances are given in angstrom

Cartesian Coordinates

RC				Al	0.276252000	-0.861222000	0.723574000
H	-3.905034000	3.188901000	-0.270629000	N	0.556990000	1.075428000	0.735218000
H	-2.543646000	3.599000000	0.805884000	C	2.914267000	-0.319012000	-0.449921000
Al	-0.547581000	-0.531376000	0.325132000	C	2.446844000	0.984836000	-0.769743000
N	-1.169695000	1.273984000	0.176964000	H	3.048757000	1.562997000	-1.470775000
N	3.060594000	-1.734277000	0.121817000	C	1.415134000	1.669426000	-0.107356000
C	-3.398824000	-0.746721000	-0.104908000	C	1.313226000	3.162189000	-0.339390000
C	-3.493778000	0.659025000	-0.153816000	H	1.592661000	3.722231000	0.568828000
H	-4.490580000	1.068082000	-0.311816000	N	2.246740000	-1.128294000	0.351486000
C	-2.449672000	1.600522000	-0.021292000	C	4.241725000	-0.745869000	-1.038202000
C	-2.826616000	3.060600000	-0.113328000	H	4.147576000	-1.703074000	-1.577266000
H	-2.294503000	3.553659000	-0.943295000	H	4.990822000	-0.902231000	-0.243787000
P	3.505363000	-0.099254000	-0.017315000	H	4.638229000	0.006332000	-1.733174000
O	2.677658000	0.925683000	0.718761000	C	-0.280767000	1.912661000	1.585675000
N	-2.248061000	-1.393390000	0.084721000	H	-0.809764000	1.284707000	2.312181000
H	2.134761000	-1.880301000	-0.290823000	H	0.311764000	2.655062000	2.148078000
C	-4.671739000	-1.541770000	-0.275197000	H	-1.053527000	2.468493000	1.020473000
H	-4.865317000	-2.168836000	0.610894000	C	2.816183000	-2.413774000	0.717288000
H	-4.598604000	-2.225170000	-1.137260000	H	2.882084000	-3.104021000	-0.145134000
H	-5.539081000	-0.887214000	-0.428415000	H	3.829227000	-2.326332000	1.149081000
C	-0.159074000	2.328301000	0.296353000	H	2.173665000	-2.888353000	1.473229000
H	0.836413000	1.881771000	0.438320000	H	-0.098486000	-1.571905000	-0.719994000
H	-0.118284000	2.959910000	-0.608547000	N	-2.891266000	-1.910703000	-0.973421000
H	-0.356544000	2.988625000	1.158912000	P	-2.721837000	-0.400573000	-0.263681000
C	-2.221085000	-2.850158000	0.123407000	O	-1.732642000	-0.464853000	0.898850000
H	-2.838949000	-3.262654000	0.940170000	C	-2.230373000	0.837122000	-1.500404000
H	-2.562157000	-3.303827000	-0.823832000	H	-1.237128000	0.563865000	-1.886433000
H	-1.188607000	-3.192816000	0.294343000	H	-2.953032000	0.861060000	-2.331203000
C	5.240347000	-0.110279000	0.532221000	H	-2.177366000	1.833443000	-1.035833000
H	5.267491000	-0.348886000	1.607443000	C	-4.380999000	0.044860000	0.292169000
H	5.834167000	-0.851799000	-0.022093000	H	-5.092982000	0.034111000	-0.548193000
H	5.667414000	0.894907000	0.394568000	H	-4.698879000	-0.684708000	1.051566000
C	3.518130000	0.144991000	-1.819621000	H	-4.359299000	1.050466000	0.738681000
H	4.159583000	-0.593050000	-2.323384000	H	-1.973870000	-2.330229000	-1.148228000
H	2.485144000	0.046824000	-2.188357000	H	-3.500518000	-1.974201000	-1.787496000
H	3.872305000	1.164065000	-2.037504000	H	0.254765000	-1.634194000	2.132322000
H	0.031725000	-0.934542000	1.761270000	TS1			
H	0.391604000	-0.969266000	-0.909792000	H	-3.840439000	-2.024900000	-1.646014000
H	3.011557000	-2.027434000	1.099427000	H	-2.460785000	-3.114145000	-1.337542000
IC1				Al	0.020501000	-0.082319000	1.057634000
H	1.980093000	3.485974000	-1.149422000	N	-1.359427000	-1.412847000	0.548947000
H	0.283940000	3.464149000	-0.593210000	C	-2.151338000	1.316807000	-0.303521000

C	-2.657214000	0.101812000	-0.793791000	N	0.929742000	1.393136000	-0.690486000
H	-3.452296000	0.166731000	-1.535773000	C	2.226229000	2.949443000	0.697675000
C	-2.319679000	-1.195537000	-0.336704000	H	1.332109000	3.462025000	1.088535000
C	-3.120723000	-2.355414000	-0.885715000	H	2.604118000	3.562714000	-0.137135000
H	-3.682113000	-2.861043000	-0.082325000	H	2.990991000	2.935749000	1.484466000
N	-1.146980000	1.398294000	0.581023000	C	1.737832000	-2.771146000	-0.856614000
C	-2.808118000	2.587396000	-0.797678000	H	1.023036000	-2.947232000	-1.674550000
H	-2.064542000	3.297606000	-1.194577000	H	2.731445000	-3.086408000	-1.217637000
H	-3.333450000	3.104732000	0.022397000	H	1.452496000	-3.431358000	-0.018811000
H	-3.541576000	2.376896000	-1.586951000	C	0.277277000	2.556777000	-1.284127000
C	-1.087404000	-2.768730000	1.000982000	H	-0.322965000	3.122223000	-0.550053000
H	-0.373409000	-2.730224000	1.836855000	H	1.000520000	3.252078000	-1.743106000
H	-1.990836000	-3.288861000	1.363687000	H	-0.409115000	2.223219000	-2.075757000
H	-0.635112000	-3.387698000	0.204592000	H	-2.344780000	0.999849000	-0.867941000
C	-0.812975000	2.701688000	1.146801000	N	-4.081495000	-0.293862000	-0.680790000
H	-0.385216000	3.396067000	0.400122000	P	-2.604990000	-0.073248000	0.139052000
H	-1.689130000	3.194473000	1.601797000	O	-1.149201000	-0.750677000	-0.192837000
H	-0.055269000	2.572910000	1.931256000	C	-2.538716000	1.236764000	1.462266000
H	1.381259000	1.052221000	1.063164000	H	-3.344789000	1.958462000	1.255284000
N	3.579700000	0.058041000	1.028107000	H	-2.643927000	0.855927000	2.489773000
P	2.501851000	-0.023488000	-0.260823000	H	-1.573898000	1.759719000	1.365826000
O	1.183678000	-0.882909000	-0.190293000	C	-3.010173000	-1.507711000	1.323487000
C	2.377158000	1.561936000	-1.162354000	H	-3.968830000	-1.344896000	1.846780000
H	2.747992000	2.375445000	-0.526167000	H	-3.058899000	-2.463583000	0.776305000
H	2.962389000	1.523515000	-2.095506000	H	-2.209705000	-1.591729000	2.073913000
H	1.319998000	1.746071000	-1.399191000	H	-4.210733000	0.151125000	-1.583694000
C	3.516719000	-1.044566000	-1.399100000	H	-4.679459000	-1.097025000	-0.509438000
H	4.503442000	-0.589310000	-1.575664000	H	0.066212000	-0.500431000	-2.731529000
H	3.645721000	-2.054184000	-0.979239000	IC3			
H	2.983218000	-1.140647000	-2.356558000	H	5.152085000	1.133281000	-1.563129000
H	3.186975000	0.390020000	1.904536000	H	4.725658000	-0.581921000	-1.771625000
H	4.183146000	-0.753948000	1.145963000	Al	0.220723000	0.449724000	-0.473719000
H	0.194734000	-0.502773000	2.606539000	N	2.011356000	-0.038636000	-1.237726000
IC2				C	2.295051000	1.672496000	1.148402000
H	4.168031000	-1.300949000	1.812622000	C	3.218883000	1.542715000	0.101146000
H	3.030080000	-2.652659000	1.563371000	H	4.157418000	2.087110000	0.202229000
Al	0.255529000	-0.327039000	-1.160497000	C	3.116706000	0.638930000	-0.988439000
N	1.702435000	-1.361024000	-0.482719000	C	4.343493000	0.449528000	-1.853655000
C	1.886682000	1.555036000	0.229139000	H	4.110666000	0.617930000	-2.917912000
C	2.618137000	0.483514000	0.782790000	N	1.080354000	1.098847000	1.145972000
H	3.354530000	0.746891000	1.540765000	C	2.734623000	2.472833000	2.356036000
C	2.565239000	-0.878461000	0.414875000	H	2.899627000	1.815785000	3.226474000
C	3.551069000	-1.817807000	1.066770000	H	1.971774000	3.209983000	2.653969000
H	4.223898000	-2.264274000	0.315791000	H	3.674338000	3.004944000	2.157846000

C	1.988581000	-1.004122000	-2.326252000
H	1.045040000	-1.563456000	-2.285514000
H	2.056532000	-0.517040000	-3.317090000
H	2.811064000	-1.737769000	-2.259507000
C	0.319134000	1.089812000	2.392955000
H	0.931408000	0.759156000	3.248492000
H	-0.106757000	2.079702000	2.639225000
H	-0.524817000	0.398335000	2.302242000
H	-2.007017000	-2.716066000	-0.155051000
N	-0.386743000	-4.159791000	-0.195363000
P	-0.629955000	-2.579749000	0.407418000
O	-0.433588000	-1.210352000	-0.424834000
C	-1.421775000	-2.386574000	2.089339000
H	-1.902534000	-3.347961000	2.332795000
H	-0.727182000	-2.114814000	2.898947000
H	-2.208810000	-1.620635000	2.005509000
C	1.160093000	-2.567352000	1.091733000
H	1.326750000	-3.402139000	1.795604000
H	1.897210000	-2.638256000	0.275204000
H	1.354206000	-1.622564000	1.620643000
H	-1.061449000	-4.535140000	-0.854290000
H	0.535345000	-4.584037000	-0.240624000
H	-0.139948000	1.288557000	-1.839581000
O	-1.504104000	1.142961000	0.292916000
P	-2.787057000	1.337510000	-0.529896000
C	-3.170448000	-0.060784000	-1.601976000
H	-3.095400000	-0.991838000	-1.021519000
H	-4.172774000	0.063700000	-2.037202000
H	-2.416878000	-0.105575000	-2.401479000
C	-4.170773000	1.612066000	0.598570000
H	-3.938577000	2.471154000	1.247032000
H	-5.098478000	1.806287000	0.041090000
H	-4.293730000	0.720923000	1.232228000
N	-2.814152000	2.673170000	-1.557922000
H	-2.051947000	2.616458000	-2.238457000
H	-2.732626000	3.559780000	-1.057565000
TS2			
H	4.497890000	-1.829688000	-2.074291000
H	3.187329000	-3.000272000	-2.341744000
Al	0.256299000	-0.093161000	-0.032467000
N	1.298677000	-1.200426000	-1.207195000
C	2.796049000	-0.544359000	1.287294000
C	3.351553000	-0.918394000	0.038634000
H	4.435042000	-1.024489000	-0.003777000

C	2.632629000	-1.312353000	-1.100876000
C	3.416730000	-1.926430000	-2.238880000
H	3.165860000	-1.453723000	-3.202089000
N	1.498106000	-0.340392000	1.454553000
C	3.739923000	-0.409470000	2.460208000
H	3.512713000	-1.162056000	3.233670000
H	3.640231000	0.578068000	2.939668000
H	4.785598000	-0.543465000	2.154080000
C	0.622022000	-1.860831000	-2.321621000
H	-0.463576000	-1.828410000	-2.160843000
H	0.818203000	-1.369787000	-3.291833000
H	0.917453000	-2.919746000	-2.408601000
C	0.975050000	-0.027941000	2.778271000
H	1.285619000	-0.765624000	3.537892000
H	1.297698000	0.970951000	3.124908000
H	-0.121542000	-0.040639000	2.735835000
H	-2.991239000	0.104392000	-0.209057000
N	-3.155852000	-1.730659000	-1.365577000
P	-2.657997000	-1.279971000	0.208721000
O	-1.179556000	-0.787107000	0.710515000
C	-3.957038000	-1.134481000	1.532177000
H	-4.923861000	-0.977988000	1.027623000
H	-4.032075000	-2.003453000	2.203794000
H	-3.728075000	-0.233174000	2.123135000
C	-2.212269000	-3.095346000	0.607940000
H	-3.075457000	-3.771076000	0.470003000
H	-1.379635000	-3.447254000	-0.024105000
H	-1.881595000	-3.159379000	1.655805000
H	-3.235369000	-0.999975000	-2.066079000
H	-2.980793000	-2.658652000	-1.740319000
H	-0.746336000	0.260456000	-1.644788000
O	0.427789000	1.728596000	0.142675000
P	-0.407560000	2.906447000	-0.497411000
C	-1.859633000	3.144251000	0.549031000
H	-1.557414000	3.276134000	1.598734000
H	-2.441273000	4.012505000	0.205505000
H	-2.479445000	2.237293000	0.460237000
C	0.624047000	4.391223000	-0.395040000
H	1.534032000	4.232747000	-0.994261000
H	0.076159000	5.263359000	-0.782316000
H	0.915830000	4.567272000	0.651803000
N	-0.928824000	2.572158000	-2.001238000
H	-0.895315000	1.225680000	-1.886090000
H	-0.230178000	2.802054000	-2.712229000

IC4			
H	-4.313552000	-0.064410000	2.893124000
H	-2.894190000	-0.934520000	3.528096000
Al	-0.474415000	-0.175224000	-0.318944000
N	-1.305759000	-0.161626000	1.379007000
C	-3.231333000	-0.449943000	-0.921161000
C	-3.534643000	-0.256284000	0.443117000
H	-4.593106000	-0.226242000	0.697757000
C	-2.633552000	-0.162947000	1.526033000
C	-3.216625000	-0.076485000	2.915309000
H	-2.869127000	0.831691000	3.434606000
N	-1.983084000	-0.499591000	-1.395411000
C	-4.384899000	-0.625757000	-1.877874000
H	-4.354955000	-1.623486000	-2.346614000
H	-4.336325000	0.111421000	-2.695884000
H	-5.350747000	-0.516439000	-1.368953000
C	-0.430033000	-0.129684000	2.548803000
H	0.618748000	-0.145621000	2.222653000
H	-0.574099000	0.783791000	3.151675000
H	-0.589307000	-1.000122000	3.207722000
C	-1.732172000	-0.765294000	-2.809177000
H	-2.204938000	-1.702112000	-3.148503000
H	-2.089852000	0.054012000	-3.457081000
H	-0.649497000	-0.873810000	-2.968900000
H	2.563872000	-0.428919000	-0.877033000
N	3.069529000	-0.862223000	1.205126000
P	2.272943000	-1.639630000	-0.082061000
O	0.667249000	-1.469857000	-0.473957000
C	3.294823000	-2.596563000	-1.309015000
H	4.279142000	-2.106317000	-1.370762000
H	3.426742000	-3.664313000	-1.075649000
H	2.799812000	-2.496138000	-2.288844000
C	1.841457000	-3.165952000	0.983708000
H	2.750151000	-3.619278000	1.418802000
H	1.150778000	-2.899548000	1.800902000
H	1.341672000	-3.920763000	0.356381000
H	2.997022000	0.166947000	1.197087000
H	2.993940000	-1.259024000	2.138822000
O	0.137254000	1.433766000	-0.699442000
P	1.285370000	2.420521000	-0.149374000
C	2.461766000	2.568421000	-1.517862000
H	1.931366000	2.777040000	-2.458681000
H	3.183942000	3.370260000	-1.304062000
H	3.000213000	1.613057000	-1.606965000

C	0.391376000	4.012439000	-0.055180000
H	-0.374393000	3.938821000	0.733646000
H	1.090156000	4.823268000	0.200524000
H	-0.110100000	4.236759000	-1.009243000
N	2.081861000	2.003522000	1.158384000
H	1.538474000	2.155012000	2.010406000
TS _{IC4toIC5}			
H	4.606212000	-2.146438000	-1.742382000
H	3.363972000	-3.407608000	-1.558846000
Al	0.343603000	-0.142180000	-0.037329000
N	1.405244000	-1.481829000	-0.931087000
C	2.925899000	0.078548000	1.106886000
C	3.453295000	-0.627225000	0.004584000
H	4.539279000	-0.651788000	-0.079072000
C	2.734371000	-1.449101000	-0.894368000
C	3.529297000	-2.347167000	-1.813422000
H	3.217875000	-2.221276000	-2.863187000
N	1.616525000	0.236745000	1.322549000
C	3.909805000	0.641960000	2.105966000
H	3.834493000	0.110949000	3.069685000
H	3.705277000	1.704728000	2.312960000
H	4.943307000	0.546772000	1.748487000
C	0.709592000	-2.442994000	-1.777869000
H	-0.364280000	-2.418626000	-1.545462000
H	0.832083000	-2.218783000	-2.853895000
H	1.054627000	-3.477877000	-1.611214000
C	1.146356000	0.799945000	2.586044000
H	1.587520000	0.281764000	3.453946000
H	1.371369000	1.876975000	2.669463000
H	0.056566000	0.698473000	2.638339000
H	-2.486202000	-0.381338000	-0.948201000
N	-3.331993000	-2.363288000	-0.718664000
P	-2.623978000	-1.186078000	0.296935000
O	-1.018857000	-1.053236000	0.572120000
C	-3.660818000	0.181644000	1.014745000
H	-4.487936000	0.389806000	0.316831000
H	-4.070045000	-0.030444000	2.014579000
H	-3.001992000	1.063342000	1.062986000
C	-2.780034000	-2.350909000	1.795471000
H	-3.830586000	-2.630813000	1.992224000
H	-2.186676000	-3.266769000	1.641040000
H	-2.382787000	-1.838856000	2.685051000
H	-3.548484000	-2.126530000	-1.681622000
H	-3.769711000	-3.209077000	-0.365014000

O	-0.798765000	1.958879000	0.697575000
P	-0.596485000	2.397399000	-0.752448000
C	-2.150165000	2.778056000	-1.618333000
H	-2.669827000	3.609643000	-1.116846000
H	-1.956037000	3.051367000	-2.668036000
H	-2.784609000	1.880096000	-1.588427000
C	0.411975000	3.906360000	-0.907081000
H	1.367529000	3.733923000	-0.388832000
H	0.612361000	4.139887000	-1.965234000
H	-0.102814000	4.760651000	-0.439545000
N	0.176515000	1.110563000	-1.423683000
H	0.489129000	1.081189000	-2.388910000
ICS			
H	5.014154000	-1.401834000	-1.737531000
H	3.819607000	-2.718701000	-1.822406000
Al	0.477743000	-0.020678000	-0.087316000
N	1.723123000	-0.966907000	-1.158935000
C	3.003560000	0.563393000	1.094147000
C	3.645654000	-0.133347000	0.044047000
H	4.734497000	-0.138397000	0.069487000
C	3.046463000	-0.878812000	-0.990726000
C	3.958341000	-1.629928000	-1.931466000
H	3.735750000	-1.385158000	-2.982717000
N	1.680064000	0.689744000	1.193779000
C	3.882543000	1.184969000	2.153152000
H	3.627002000	0.795183000	3.151931000
H	3.738749000	2.277389000	2.193988000
H	4.944825000	0.984141000	1.965236000
C	1.159748000	-1.843269000	-2.182342000
H	0.077097000	-1.948292000	-2.018040000
H	1.314608000	-1.449675000	-3.203371000
H	1.582963000	-2.860592000	-2.143292000
C	1.080596000	1.393090000	2.329753000
H	1.202588000	0.824981000	3.268651000
H	1.521113000	2.393569000	2.476016000
H	0.006063000	1.535279000	2.143523000
H	-2.214505000	-1.021860000	-0.831030000
N	-2.362648000	-3.172043000	-0.616385000
P	-2.069991000	-1.831805000	0.407079000
O	-0.597980000	-1.154104000	0.677314000
C	-3.491402000	-0.897960000	1.151564000
H	-4.352825000	-0.985345000	0.469518000
H	-3.784171000	-1.241762000	2.155556000
H	-3.178073000	0.158211000	1.196350000

C	-1.790598000	-2.993343000	1.888299000
H	-2.683039000	-3.608943000	2.100488000
H	-0.930795000	-3.658189000	1.705134000
H	-1.565288000	-2.385966000	2.777783000
H	-2.716618000	-3.001708000	-1.552872000
H	-2.529499000	-4.107521000	-0.255531000
O	-1.809584000	2.039275000	0.861087000
P	-1.522803000	2.268815000	-0.607773000
C	-2.991117000	1.992995000	-1.654592000
H	-3.806017000	2.666092000	-1.344988000
H	-2.760071000	2.163377000	-2.718400000
H	-3.312548000	0.949483000	-1.520172000
C	-1.019402000	3.987068000	-0.972610000
H	-0.122940000	4.217843000	-0.376594000
H	-0.786659000	4.122363000	-2.041237000
H	-1.825230000	4.681798000	-0.687863000
N	-0.295719000	1.280992000	-1.147000000
H	0.070959000	1.484901000	-2.074880000
TS3			
H	-3.935504000	0.232102000	2.653229000
H	-2.498369000	0.046842000	3.696832000
Al	-0.023942000	-0.589920000	-0.140582000
N	-0.828413000	-0.470532000	1.562785000
N	0.322417000	1.021618000	-0.837868000
C	-2.549086000	-1.726331000	-0.544845000
C	-2.972391000	-1.025757000	0.599376000
H	-4.048001000	-0.969891000	0.762021000
C	-2.160593000	-0.426765000	1.596709000
C	-2.844093000	0.341642000	2.694384000
H	-2.578790000	1.403064000	2.540369000
P	-0.426350000	2.425221000	-0.483785000
O	-1.034524000	2.597135000	0.903572000
N	-1.266205000	-1.771420000	-0.935446000
C	-3.592260000	-2.445724000	-1.364459000
H	-3.399360000	-3.531561000	-1.376203000
H	-3.576418000	-2.107950000	-2.413742000
H	-4.600593000	-2.284726000	-0.962343000
C	-0.043410000	0.160217000	2.619902000
H	1.018040000	-0.088072000	2.468855000
H	-0.154251000	1.256129000	2.573041000
H	-0.322279000	-0.205803000	3.621720000
C	-0.869265000	-2.556222000	-2.096788000
H	-1.168724000	-3.614925000	-2.010754000
H	-1.291114000	-2.161397000	-3.038781000

H	0.226716000	-2.535539000	-2.183304000
C	0.798497000	3.757027000	-0.817637000
H	1.609709000	3.676852000	-0.076034000
H	1.227100000	3.666418000	-1.828790000
H	0.326986000	4.746182000	-0.706306000
C	-1.728321000	2.722768000	-1.749510000
H	-1.322650000	2.639312000	-2.770316000
H	-2.506879000	1.954875000	-1.612544000
H	-2.189255000	3.714099000	-1.610852000
H	4.042730000	-1.471450000	-0.965547000
H	1.536981000	0.825401000	-1.360674000
N	2.635216000	0.282890000	-1.660601000
P	3.068790000	-0.996592000	-0.049892000
O	1.549880000	-1.464196000	-0.143496000
C	3.559890000	-2.229174000	1.262233000
H	3.395519000	-3.249464000	0.879336000
H	4.630217000	-2.113599000	1.508583000
H	2.963963000	-2.105892000	2.180616000
C	3.489960000	0.550706000	0.841189000
H	4.387964000	1.001128000	0.390786000
H	2.648406000	1.248819000	0.724998000
H	3.679116000	0.360778000	1.906671000
H	2.487669000	-0.270807000	-2.509276000
H	3.388200000	0.942874000	-1.874886000
IC6			
H	2.304223000	2.532654000	4.214582000
H	1.328621000	1.105252000	4.646495000
Al	-0.043757000	0.507071000	0.268738000
N	0.785647000	0.526357000	1.973562000
N	0.079552000	-0.827133000	-0.868579000
C	0.753550000	3.219808000	0.636586000
C	1.181833000	2.909364000	1.940257000
H	1.567533000	3.740734000	2.528737000
C	1.269378000	1.629317000	2.539341000
C	1.979054000	1.542391000	3.871222000
H	2.868962000	0.896537000	3.791757000
P	1.471894000	-1.599897000	-1.125105000
O	2.654402000	-1.325870000	-0.195641000
N	0.267573000	2.306776000	-0.213034000
C	0.885410000	4.651441000	0.175210000
H	-0.077033000	5.039706000	-0.196192000
H	1.602963000	4.728040000	-0.658795000
H	1.234447000	5.305368000	0.984542000
C	1.034346000	-0.801408000	2.536156000

H	0.198121000	-1.467031000	2.269961000
H	1.938262000	-1.230414000	2.070309000
H	1.121379000	-0.800866000	3.632052000
C	-0.062308000	2.668762000	-1.587526000
H	-0.930721000	3.349766000	-1.646064000
H	0.781672000	3.149476000	-2.110819000
H	-0.303965000	1.749574000	-2.142001000
C	1.123259000	-3.417250000	-1.135687000
H	0.869194000	-3.724664000	-0.107665000
H	0.281926000	-3.666938000	-1.802693000
H	2.016402000	-3.982884000	-1.446933000
C	1.995399000	-1.305457000	-2.872286000
H	1.183701000	-1.544735000	-3.578398000
H	2.244745000	-0.236469000	-2.973373000
H	2.891149000	-1.897070000	-3.122732000
H	-2.482042000	-0.780234000	-1.485278000
P	-2.694450000	-0.712907000	-0.097559000
O	-1.884326000	0.422028000	0.599832000
C	-4.448101000	-0.332958000	0.143997000
H	-4.660199000	0.665177000	-0.268209000
H	-5.077800000	-1.080451000	-0.363310000
H	-4.675171000	-0.328767000	1.221011000
C	-2.397561000	-2.359374000	0.576091000
H	-3.095595000	-3.079913000	0.121141000
H	-1.360105000	-2.624716000	0.335532000
H	-2.550950000	-2.333045000	1.666078000
TS4			
H	-4.384289000	-1.760608000	-2.182330000
H	-2.928270000	-1.590983000	-3.199919000
Al	-0.390073000	0.180106000	0.136558000
N	-1.308966000	-0.982393000	-1.044553000
N	1.066587000	-0.244198000	1.088894000
C	-3.137630000	0.544070000	0.806737000
C	-3.498347000	-0.269715000	-0.286073000
H	-4.565801000	-0.373355000	-0.475491000
C	-2.642825000	-1.004149000	-1.135866000
C	-3.291795000	-1.861999000	-2.195453000
H	-3.043116000	-2.925675000	-2.046155000
P	2.070829000	-1.485362000	0.791228000
O	2.555640000	-1.673973000	-0.651318000
N	-1.868915000	0.777524000	1.152897000
C	-4.248187000	1.159755000	1.622749000
H	-4.135506000	2.254592000	1.681383000
H	-4.228040000	0.782376000	2.658813000

H	-5.234170000	0.934547000	1.196946000
C	-0.497260000	-1.783965000	-1.966128000
H	-0.588605000	-1.422280000	-3.005520000
H	0.563526000	-1.733350000	-1.673984000
H	-0.787712000	-2.847736000	-1.951809000
C	-1.554760000	1.581936000	2.330246000
H	-1.824668000	2.644419000	2.192482000
H	-2.066171000	1.216083000	3.236219000
H	-0.473884000	1.518732000	2.522846000
C	3.519272000	-1.287675000	1.901532000
H	4.065932000	-0.379867000	1.598411000
H	3.203478000	-1.176861000	2.950520000
H	4.199630000	-2.148485000	1.805261000
C	1.291296000	-3.045677000	1.376085000
H	1.020186000	-2.980418000	2.441420000
H	0.373630000	-3.216199000	0.790240000
H	1.971570000	-3.897406000	1.215321000
H	1.915949000	1.080148000	0.596620000
P	1.741411000	1.957630000	-0.641690000
O	0.203451000	1.592884000	-0.871392000
C	1.867776000	3.772728000	-0.706369000
H	1.253699000	4.209084000	0.096059000
H	2.915372000	4.084279000	-0.571221000
H	1.499187000	4.137148000	-1.679140000
C	2.715537000	1.285270000	-2.012854000
H	3.733838000	1.706319000	-1.999184000
H	2.769019000	0.192894000	-1.847856000
H	2.230429000	1.515918000	-2.974858000
IC7			
H	3.990643000	-0.831026000	2.886979000
H	2.513624000	-0.212040000	3.672048000
Al	0.261730000	0.353582000	-0.242227000
N	1.036538000	-0.342278000	1.337201000
N	-0.914812000	-0.784620000	-1.114103000
C	3.063866000	0.386730000	-0.778372000
C	3.307911000	-0.083904000	0.528391000
H	4.354094000	-0.201469000	0.806727000
C	2.361506000	-0.408721000	1.522184000
C	2.894027000	-0.855698000	2.862428000
H	2.567397000	-1.882941000	3.093932000
P	-1.667645000	-2.129950000	-0.458327000
O	-2.456896000	-1.919816000	0.817354000
N	1.836226000	0.599835000	-1.257753000
C	4.256268000	0.657465000	-1.662543000

H	4.263486000	1.705332000	-2.004562000
H	4.225189000	0.028290000	-2.567565000
H	5.199776000	0.458580000	-1.138956000
C	0.125542000	-0.639361000	2.448246000
H	0.135653000	0.166898000	3.202387000
H	-0.899327000	-0.756712000	2.069971000
H	0.379080000	-1.584816000	2.953136000
C	1.648447000	1.085917000	-2.621375000
H	2.082693000	2.089609000	-2.769528000
H	2.087783000	0.406484000	-3.371351000
H	0.572952000	1.158592000	-2.840227000
C	-2.708331000	-2.794306000	-1.802064000
H	-3.516419000	-2.073578000	-2.006125000
H	-2.125849000	-2.960624000	-2.720725000
H	-3.168038000	-3.739221000	-1.473924000
C	-0.316319000	-3.335056000	-0.231380000
H	0.177823000	-3.567402000	-1.186615000
H	0.426795000	-2.906688000	0.458328000
H	-0.722387000	-4.254392000	0.217134000
H	-1.594985000	-0.249035000	-1.660718000
P	-2.108864000	2.343003000	-0.208742000
O	-0.537295000	1.876783000	0.047882000
C	-2.008654000	4.079916000	0.428752000
H	-1.401752000	4.691300000	-0.258462000
H	-3.019395000	4.518678000	0.480541000
H	-1.546170000	4.106559000	1.430134000
C	-2.965323000	1.562367000	1.240593000
H	-3.999488000	1.942457000	1.307327000
H	-3.005891000	0.468439000	1.102840000
H	-2.437928000	1.787963000	2.183791000
IC8			
H	-4.476690000	1.169159000	2.114550000
H	-3.399939000	0.394947000	3.298643000
Al	-0.155907000	-0.120765000	-0.094851000
N	-1.301316000	0.305354000	1.385545000
N	0.123296000	1.079998000	-1.579463000
C	-2.845401000	-0.904589000	-0.865062000
C	-3.353817000	-0.081731000	0.168152000
H	-4.430412000	0.085700000	0.175535000
C	-2.631165000	0.403493000	1.273710000
C	-3.425048000	1.030996000	2.397841000
H	-3.008926000	2.009055000	2.688212000
P	1.203688000	2.042887000	-0.830022000
O	1.190372000	1.349027000	0.556217000

N	-1.550379000	-1.151574000	-1.008618000
C	-3.843644000	-1.540400000	-1.806185000
H	-3.836500000	-2.638056000	-1.698723000
H	-3.596429000	-1.324210000	-2.858495000
H	-4.864590000	-1.187868000	-1.609720000
C	-0.661931000	0.658969000	2.650459000
H	-1.167112000	0.193407000	3.512724000
H	0.376546000	0.308563000	2.642450000
H	-0.631228000	1.750754000	2.814598000
C	-1.096579000	-2.082723000	-2.032815000
H	-1.595769000	-3.064705000	-1.961923000
H	-1.264517000	-1.697098000	-3.056032000
H	-0.020367000	-2.252748000	-1.900817000
C	2.855165000	2.047496000	-1.577729000
H	3.213539000	1.006541000	-1.597512000
H	2.817062000	2.450697000	-2.602447000
H	3.545197000	2.656859000	-0.972868000
C	0.688944000	3.781828000	-0.733205000
H	0.639681000	4.227596000	-1.739721000
H	-0.308582000	3.820388000	-0.270513000
H	1.398727000	4.357147000	-0.118174000
H	-0.204631000	1.173081000	-2.534350000
P	2.623113000	-1.526979000	0.194082000
O	0.982597000	-1.442668000	0.184713000
C	2.826108000	-3.362883000	0.387812000
H	2.522663000	-3.868604000	-0.543465000
H	3.883337000	-3.609965000	0.584339000
H	2.200897000	-3.743067000	1.213999000
C	3.024884000	-1.034345000	1.940294000
H	4.088388000	-1.232836000	2.158511000
H	2.837071000	0.045290000	2.039843000
H	2.397306000	-1.582702000	2.664208000
4a			
H	1.236889000	6.017458000	1.786567000
C	2.719694000	3.639508000	2.164215000
H	3.597321000	3.930346000	1.567593000
H	2.836063000	2.578542000	2.435499000
H	2.751574000	4.235549000	3.090272000
H	4.892501000	2.457121000	0.623872000
C	4.100151000	-1.156816000	2.458915000
H	3.618547000	-0.774165000	3.363788000
C	5.479327000	-1.367689000	2.443602000
H	6.075614000	-1.141637000	3.331032000
C	6.096795000	-1.872740000	1.291465000

H	7.176832000	-2.041452000	1.282701000
H	-1.261321000	3.769542000	5.207004000
C	0.003015000	3.824947000	3.453454000
H	0.777764000	4.413015000	3.950416000
P	-2.414980000	-1.064686000	-1.611749000
Al	0.082008000	0.419434000	-0.209364000
P	1.544869000	-1.165386000	1.299952000
O	-1.519870000	-0.273678000	-0.509603000
N	-0.623271000	2.252329000	0.129545000
N	0.955471000	0.916101000	-1.863583000
C	0.176774000	3.445667000	2.114994000
C	3.335874000	-1.438746000	1.313829000
C	-3.160015000	-5.193287000	0.427493000
H	-3.312413000	-6.172956000	0.888855000
C	-2.336988000	-4.245016000	1.042384000
H	-1.835529000	-4.474834000	1.985644000
C	-2.143107000	-2.992930000	0.450628000
H	-1.486124000	-2.262588000	0.919180000
C	-2.770405000	-2.667976000	-0.760728000
C	-0.846182000	2.694928000	1.478288000
C	1.432174000	3.875944000	1.363279000
H	1.494656000	3.262731000	0.455664000
C	1.328575000	5.344605000	0.917346000
H	0.452925000	5.510256000	0.272002000
H	2.223733000	5.645958000	0.348833000
C	-1.031054000	2.991035000	-0.896898000
C	-1.978968000	4.146025000	-0.676837000
H	-1.994638000	4.829293000	-1.536045000
H	-1.732955000	4.714526000	0.230659000
H	-2.996310000	3.744784000	-0.536110000
C	-0.616830000	2.733448000	-2.224172000
H	-1.025104000	3.394571000	-2.987359000
C	0.394876000	1.853037000	-2.650541000
C	2.112744000	0.207048000	-2.361260000
C	1.969489000	-0.917935000	-3.210427000
C	0.615790000	-1.501403000	-3.595867000
H	-0.167689000	-0.831575000	-3.218369000
C	0.425555000	-1.617675000	-5.117942000
H	0.639296000	-0.672997000	-5.642524000
H	-0.615007000	-1.900964000	-5.345305000
H	1.079409000	-2.390258000	-5.555255000
C	0.390948000	-2.870363000	-2.930497000
H	1.138141000	-3.604952000	-3.277545000
H	-0.607202000	-3.259807000	-3.186140000

H	0.462488000	-2.792659000	-1.838139000
C	3.129313000	-1.535814000	-3.703688000
H	3.029895000	-2.404769000	-4.358408000
C	4.398097000	-1.061488000	-3.383080000
H	5.288588000	-1.546964000	-3.791682000
C	4.525983000	0.023148000	-2.517465000
H	5.524133000	0.365446000	-2.243384000
C	3.400697000	0.660003000	-1.975001000
C	3.577673000	1.804854000	-0.978558000
H	2.762992000	1.713765000	-0.244429000
C	3.448122000	3.183971000	-1.648253000
H	4.184736000	3.293099000	-2.461767000
H	3.634806000	3.988155000	-0.918556000
H	2.447153000	3.350661000	-2.068484000
C	4.893105000	1.719947000	-0.191982000
H	5.037678000	0.725629000	0.254149000
H	5.769104000	1.942317000	-0.823037000
C	-4.057913000	-0.187444000	-1.473045000
C	-4.099934000	1.109249000	-2.021759000
H	-3.187986000	1.542005000	-2.445140000
C	-5.282318000	1.851895000	-2.027397000
H	-5.289883000	2.860185000	-2.451063000
C	-6.458553000	1.301277000	-1.504070000
H	-7.388843000	1.875450000	-1.517041000
C	-6.433394000	0.013459000	-0.962245000
H	-7.345178000	-0.422422000	-0.544042000
C	-5.241462000	-0.721690000	-0.939621000
H	-5.239686000	-1.720514000	-0.498142000
C	-3.779358000	-4.885879000	-0.790517000
H	-4.417174000	-5.625589000	-1.282691000
C	-3.576843000	-3.637489000	-1.385066000
H	-4.054975000	-3.414031000	-2.344306000
C	5.336535000	-2.155953000	0.154091000
H	5.817484000	-2.536464000	-0.749915000
C	3.955852000	-1.934111000	0.157964000
H	3.359039000	-2.125558000	-0.735605000
C	0.867454000	-2.288887000	2.558439000
C	1.276318000	-3.632726000	2.606577000
H	2.036072000	-4.000568000	1.911201000
C	0.708303000	-4.501863000	3.539495000
H	1.022825000	-5.548349000	3.569233000
C	-0.263768000	-4.034179000	4.432793000
H	-0.705748000	-4.716247000	5.163560000
C	-0.672499000	-2.697559000	4.388456000

H	-1.433670000	-2.331349000	5.082118000
C	-0.111218000	-1.825149000	3.451767000
H	-0.438677000	-0.784077000	3.407459000
C	0.876998000	2.012866000	-4.073623000
H	0.414268000	2.883379000	-4.555463000
H	0.636900000	1.118451000	-4.665047000
H	1.970025000	2.127784000	-4.109871000
C	-2.021295000	2.340371000	2.183596000
C	-2.141791000	2.735273000	3.525804000
H	-3.043110000	2.461481000	4.079589000
C	-1.144219000	3.469206000	4.162259000
C	-3.154351000	1.551218000	1.542601000
H	-2.908152000	1.407120000	0.485693000
C	-4.496500000	2.295470000	1.618092000
H	-4.855320000	2.394118000	2.656380000
H	-5.263087000	1.747231000	1.050157000
H	-4.425314000	3.310247000	1.195381000
C	-3.270905000	0.149291000	2.158013000
H	-2.333993000	-0.408124000	2.035329000
H	-4.061240000	-0.427825000	1.654242000
H	-3.514680000	0.196618000	3.233163000
O	0.979434000	-1.395314000	-0.129516000
N	1.016620000	0.363907000	1.479929000
H	1.100709000	0.941587000	2.308237000
4			
H	-0.447955000	-3.659748000	4.164131000
H	-0.392712000	-1.929202000	4.600207000
C	-0.180324000	0.880830000	3.975427000
H	0.503413000	0.199661000	3.451164000
C	0.079005000	0.714759000	5.481604000
H	-0.485894000	1.450806000	6.077473000
H	1.149656000	0.868693000	5.697079000
H	-0.198838000	-0.287227000	5.848515000
Al	-0.021348000	-0.558800000	0.332320000
N	-0.873963000	-1.177730000	1.922410000
N	-1.118289000	0.231306000	-0.898986000
C	0.808037000	-3.216622000	0.439550000
C	0.495103000	-3.178131000	1.814963000
H	0.883368000	-4.001206000	2.413936000
C	-0.388976000	-2.295560000	2.482631000
C	-0.802581000	-2.659203000	3.886375000
H	-1.896389000	-2.623626000	3.995970000
C	-1.921780000	-0.422320000	2.578523000
C	-1.607258000	0.531327000	3.575201000

C	-4.277915000	0.086430000	2.821445000
H	-5.317404000	-0.059253000	2.528028000
C	-3.265848000	-0.633208000	2.171205000
C	-3.625029000	-1.608919000	1.052102000
H	-2.828765000	-1.527865000	0.297770000
C	-3.660981000	-3.066859000	1.543210000
H	-2.679184000	-3.416235000	1.890493000
H	-3.978912000	-3.741181000	0.731931000
H	-4.377752000	-3.181371000	2.373453000
C	-4.940335000	-1.254493000	0.345841000
H	-5.816703000	-1.431235000	0.990581000
H	-5.071346000	-1.880829000	-0.547676000
H	-4.957772000	-0.203636000	0.025265000
C	-1.851887000	-3.561666000	-1.658399000
H	-1.806794000	-3.093265000	-0.666399000
C	-1.749722000	-5.084986000	-1.442819000
H	-2.597011000	-5.447475000	-0.839224000
H	-0.817074000	-5.350036000	-0.923093000
C	-3.203992000	-3.184894000	-2.278360000
H	-3.303151000	-2.095833000	-2.408929000
H	-4.025902000	-3.522818000	-1.630568000
H	-3.356953000	-3.657447000	-3.261359000
C	0.166208000	2.310112000	3.520152000
H	-0.015641000	2.441753000	2.443782000
H	1.222385000	2.536658000	3.736297000
H	-0.452830000	3.050494000	4.055656000
H	-2.430020000	1.965807000	4.959805000
P	-1.502858000	1.844854000	-0.838886000
O	-1.076190000	2.482971000	0.459860000
C	-6.091988000	2.138366000	-1.350906000
H	-7.179222000	2.197523000	-1.449185000
C	-5.325806000	1.592774000	-2.387249000
H	-5.813188000	1.226473000	-3.294577000
C	-3.936654000	1.518725000	-2.263843000
C	-3.307309000	1.981432000	-1.098297000
C	-2.660817000	1.225532000	4.190702000
C	-3.984921000	1.001375000	3.831561000
H	-4.791112000	1.552057000	4.323665000
C	-4.077097000	2.525686000	-0.061665000
H	-3.573702000	2.869993000	0.844520000
C	-5.467107000	2.605857000	-0.191476000
H	-6.064757000	3.028485000	0.620330000
P	2.638118000	0.697620000	1.743913000
C	4.077952000	-0.372992000	1.229652000

C	3.973530000	-1.735373000	1.571254000
H	3.057538000	-2.102558000	2.044406000
C	5.018654000	-2.625298000	1.315044000
H	4.912470000	-3.680414000	1.582205000
C	6.207155000	-2.162672000	0.737343000
H	7.032750000	-2.853683000	0.548252000
C	6.328699000	-0.811531000	0.402843000
H	7.249886000	-0.442489000	-0.056596000
C	5.269322000	0.074026000	0.636181000
H	5.378616000	1.122185000	0.350904000
O	1.467170000	0.255123000	0.692372000
N	0.422618000	-2.256034000	-0.409770000
H	-1.512928000	-0.316921000	-1.661029000
C	1.643035000	-4.358074000	-0.071038000
H	2.690132000	-4.010763000	-0.141489000
H	1.348646000	-4.678275000	-1.075699000
H	1.618017000	-5.221952000	0.609075000
C	0.456630000	-2.442251000	-1.837698000
C	-0.670055000	-3.036763000	-2.466140000
C	-0.669305000	-3.153622000	-3.863672000
H	-1.521354000	-3.616818000	-4.365069000
C	0.399951000	-2.688261000	-4.628709000
H	0.378220000	-2.783512000	-5.717560000
C	1.495194000	-2.104800000	-3.997309000
H	2.331762000	-1.740693000	-4.597887000
C	1.551753000	-1.976320000	-2.600652000
C	2.778139000	-1.341173000	-1.962716000
H	2.671970000	-1.415229000	-0.874198000
C	4.069441000	-2.077529000	-2.351240000
H	4.014969000	-3.150277000	-2.104428000
H	4.924589000	-1.650116000	-1.808312000
H	4.281269000	-1.993453000	-3.430429000
C	2.864940000	0.155553000	-2.299534000
H	3.000380000	0.318507000	-3.382897000
H	3.713953000	0.619252000	-1.774722000
H	1.955405000	0.686224000	-1.986597000
H	-1.767068000	-5.617161000	-2.408830000
C	3.125255000	2.346393000	1.074521000
C	2.405871000	2.956177000	0.034626000
C	2.750385000	4.237388000	-0.407886000
H	2.181088000	4.691991000	-1.223591000
C	3.808289000	4.929834000	0.189083000
H	4.076025000	5.931604000	-0.158579000
C	4.514391000	4.340233000	1.245980000

H	5.333055000	4.881291000	1.729347000	C	-0.725937000	2.656328000	-2.282824000
C	4.167841000	3.062156000	1.691984000	H	-3.342566000	1.103600000	-3.083745000
H	4.717650000	2.615209000	2.527488000	C	0.333277000	2.595005000	-4.467023000
C	0.514897000	3.980683000	-4.420974000	H	0.683065000	2.023323000	-5.330581000
H	1.002897000	4.496627000	-5.252040000	C	-0.282141000	1.932824000	-3.400178000
C	0.082519000	4.705797000	-3.304479000	H	-0.391313000	0.846286000	-3.431879000
H	0.235304000	5.787632000	-3.260914000	H	1.558892000	2.434700000	-0.410121000
C	-0.533001000	4.046974000	-2.237616000				
H	-0.847164000	4.602394000	-1.350310000				

References

1. T. Schulz, K. Meindl, D. Leusser, D. Stern, J. Graf, C. Michaelson, M. Ruf, G. M. Sheldrick, D. Stalke, *J. Appl. Crystallogr.* **2009**, *42*, 885-891.
2. Bruker AXS Inc., in Bruker Apex CCD, SAINT v8.30C (Ed.: Bruker AXS Inst. Inc.), WI, USA, Madison, **2013**.
3. L. Krause, R. Herbst-Irmer, G. M. Sheldrick, D. Stalke, *J. Appl. Crystallogr.* **2015**, *48*, 3-10.
4. G. M. Sheldrick, *Acta Crystallogr. Sect. A* **2015**, *71*, 3-8.
5. G. M. Sheldrick, *Acta Crystallogr. Sect. C* **2015**, *71*, 3-8.
6. C. B. Hübschle, G. M. Sheldrick, B. Dittrich, *J. Appl. Crystallogr.* **2011**, *44*, 1281-1284.
7. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, Williams, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, Jr. Montgomery, J. A., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, *Gaussian 16 (Rev. A.03)*; Gaussian, Inc.: Wallingford, CT, **2016**.
8. (a) A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2009**, *113*, 6378-6396. (b) M. Garcia-Ratés, F. Neese, *J. Comput. Chem.* **2020**, *41*, 922-939.
9. (a) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785-789. (b) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648-5652. (c) A. D. Becke, *J. Chem. Phys.* **1992**, *97*, 9173-9177.
10. F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305.