Electronic Supporting Informations

For

7-Metalla-1,4-diphosphanorbornadienes: cycloaddition of monovalent group 13 NacNac complexes to a stable 1,4-diphosphinine

Abhishek Koner,[a] Bulat M. Gabidullin,[b] Zsolt Kelemen,[c] László Nyulászi,[c]* Georgii I. Nikonov,[d]* and Rainer Streubel[a]*

[a] *Institut für Anorganische Chemie, der Rheinischen Friedrich-Wilhelms-Universität Bonn, Gerhard-Domagk-Strasse 1, 53121 Bonn, Germany. E-Mail: r.streubel@uni-bonn.de*

[b] *X-Ray Core Facility, Faculty of Science, University of Ottawa, 150 Louis Pasteur, Ottawa, K1N 6N5, Ontario, Canada.*

[c] *Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics and MTA-BME Computation Driven Chemistry Research Group, Szt Gellert ter 4, 1111 Budapest, Hungary.*

[d] *Department of Chemistry, Brock University, 1812 Sir Isaac Brock Way, St. Catharines, L2S 3A1, Ontario, Canada. E-mail: gnikonov@brocku.ca*

Experimental Section

Materials and Methods

All manipulations were performed using standard inert atmosphere (N_2 gas) MBraun glovebox. HPLC grade toluene and ether were dried using a Grubbs-type solvent purification system. Benzene-d_6 was pre-dried and distilled from K/Na alloy and stored in the glovebox in a glass ampoule equipped with a Teflon stopcock. NMR spectra were obtained from solutions in C_6D_6 by using Young-type NMR tubes with a Bruker AVANCE III HD 400 MHz spectrometer (^{1}H, 400 MHz; ^{13}C, 101 MHz) at room temperature. The ^{1}H spectra very referenced to the residual solvent proton peak. Elemental analyses were obtained by the Elemental Analysis Service at the Université de Montréal. Compounds **1** - **3** were prepared according to literature procedures.

Preparation of compound 5. Suspension of 0.0538 g (0.121 mmol) of diphosphinine **4** in 3 mL of ether to a suspension of 0.0583g (0.121 mmol) of NacNacAl in 2 mL of ether results in immediate change of colour from deep red to deep purple. The mixture was stirred overnight at room temperature to give a light-purple crystalline precipitate under a brownish-yellow solution. The Mother liquor was removed by a pipette and the residue was washed by a small portion of ether and dried to give 0.0494 g of the product. Cooling the ether fraction to -30 C produced light red crystals. Cold supernatant solution was removed by pipette and the crystals dried under vacuo to give 0.016 g. The combined yield is 0.0654g (0.071 mmol, 58%).
^{1}H NMR (C_6D_6): 7.38 (t, ^3J(H-H)=7.8 Hz, 2H, *p*-Ar), 6.99 (t, ^3J(H-H)=7.8 Hz, 4H, *m*-Ar), 4.87 (s, 1H, CH), 4.48 (ddd, ^3J(H-H)=5.3 Hz, ^3J(H-H)=10.7 Hz, ^3J(H-H)=13.0 Hz, 4H, $^{\alpha}CH_2N$), 3.66 (ddd, ^3J(H-H)=5.2 Hz, ^3J(H-H)=10.8 Hz, ^3J(H-H)=13.1 Hz, $^{\alpha}CH_2N$), 2.89 (sept, ^3J(H-H)=6.8 Hz, 4H, CH in Pr^i), 2.01 (m, 4, $^{\beta}CH_2$), 1.53 (m, 4, $^{\beta}CH_2$), 1.50 (d, ^3J(H-H)=6.7 Hz, 12H, Me in Ar), 1.45 (s, 6H, Me of NacNac), 1.31 (m, 8, $^{\gamma}CH_2$), 0.88 (d, ^3J(H-H)=6.7 Hz, 12H, Me in Ar), 0.81 (t, ^3J(H-H)=7.4 Hz, 12H, Me in Bu). **^{13}C NMR** (C_6D_6): 172.1 (s, C=N), 166.5 (C=S), 140.7 (s, PCN), 141.8 (s, *i*-Ar), 138.7 (s, *o*-Ar), 128.0 (s, *p*-Ar), 125.1 (s, *m*-Ar), 98.2 (s, CH), 48.0 ($^{\alpha}CH_2N$), 30.3 (s, $^{\beta}CH_2$), 28.8 (s, CH in Ar), 24.8 (s, Me in Ar), 24.1 (s, Me in Ar), 23.8 (Me in NacNac), 20.2 (s, $^{\gamma}CH_2$) 13.4 (Me in Bu). ^{31}P NMR (C_6D_6): -134.1 (s). **ESI-Pos-MS**: Calc. for $[M+H]^+$($C_{51}H_{78}AlN_6P_2S_2$) 927.5; found 927.6. **Elem. Anal.** Calcd for $C_{51}H_{77}AlN_6P_2S_2$: N 9.06, C 66.60, H 8.37, S 6.91; Found N 8.71; C 64.85, H 7.71, S 5.87.

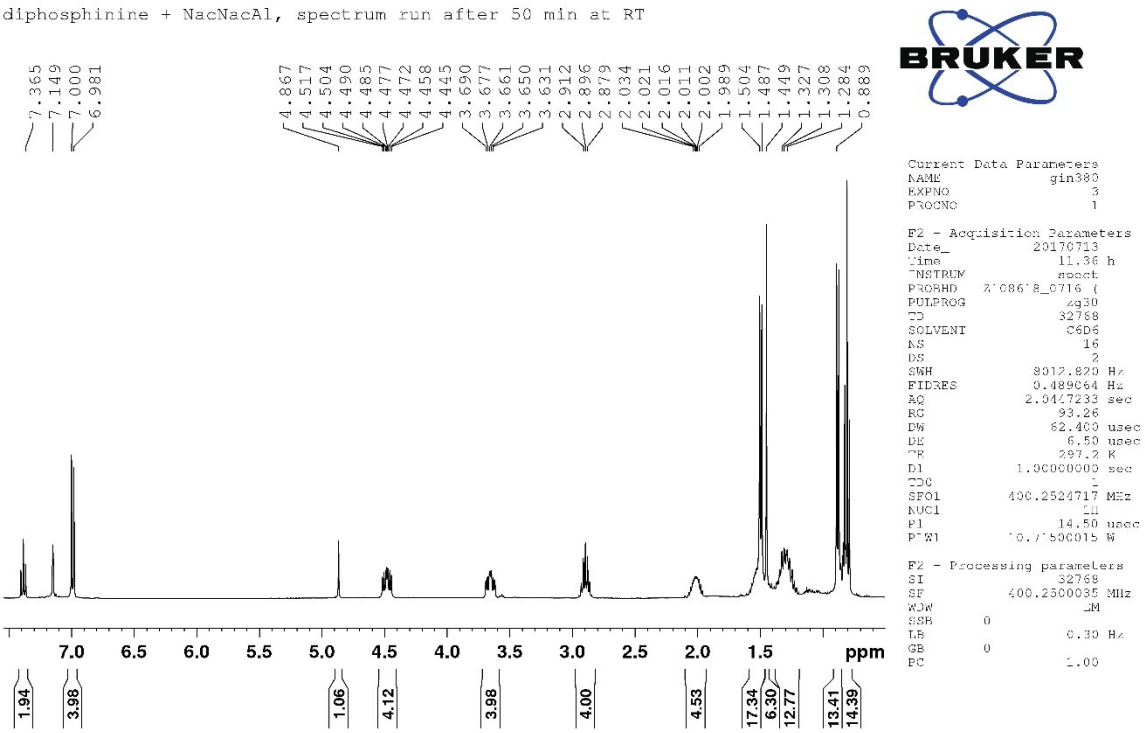


Figure 1. ^{1}H NMR spectrum of compound **5**.

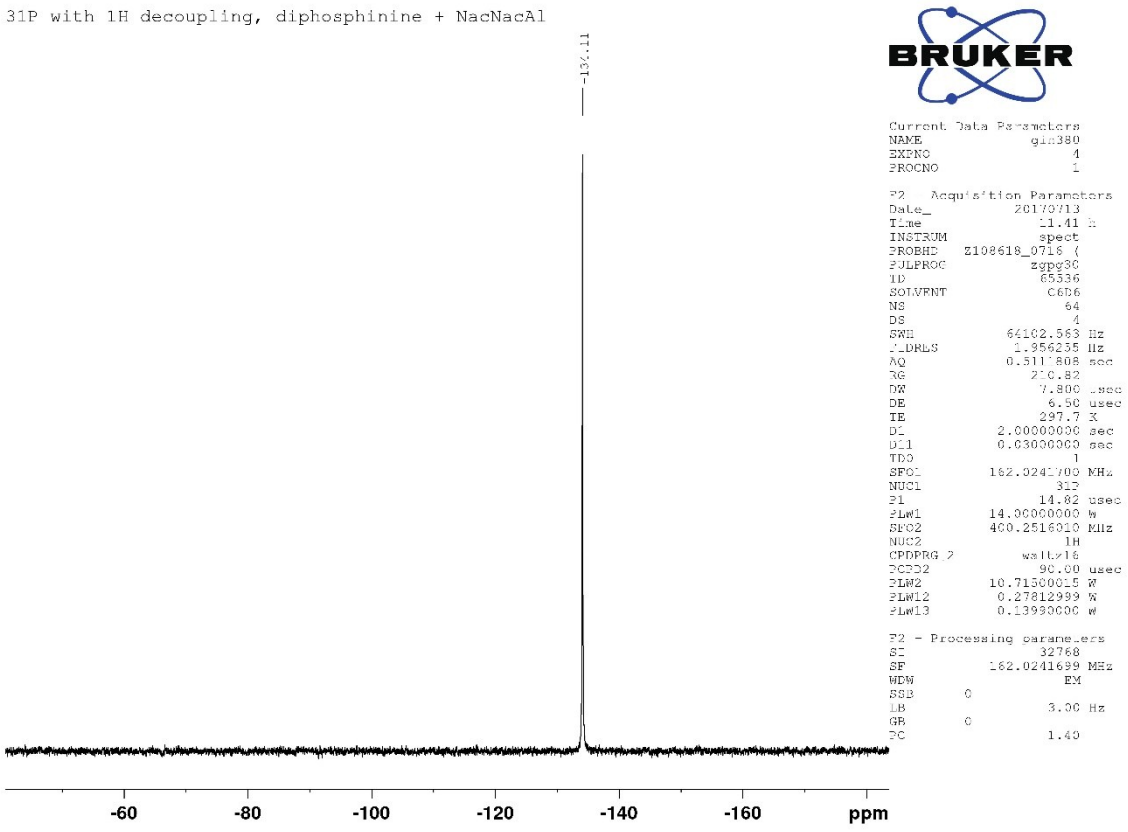
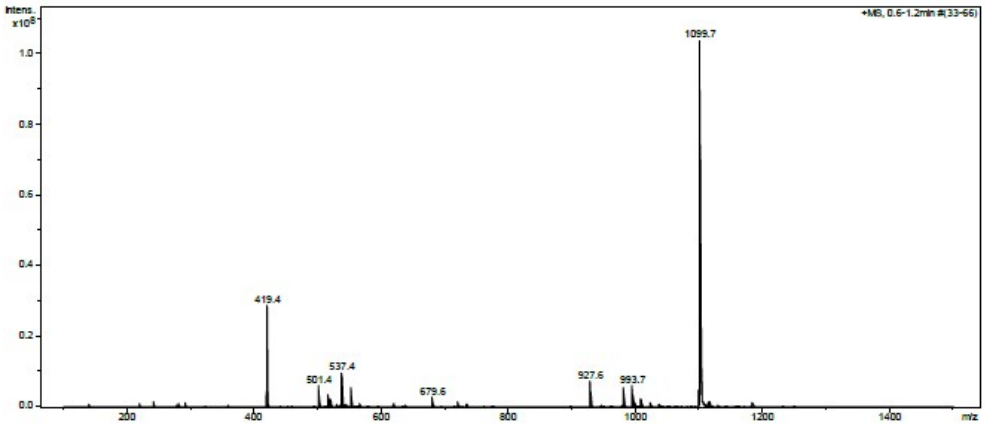
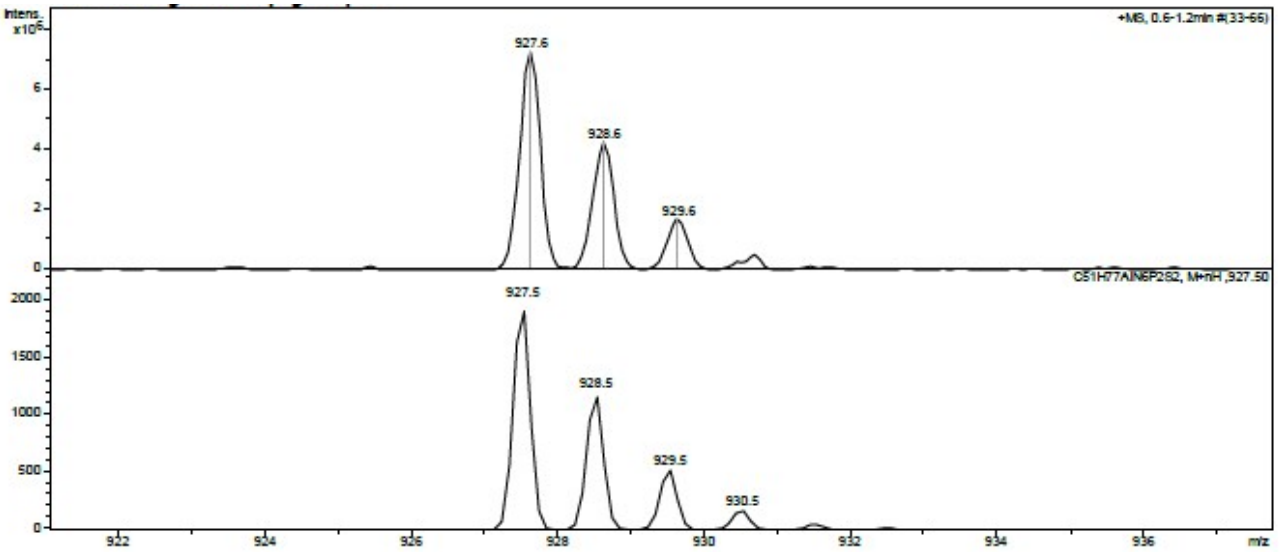


Figure 2. ^{31}P NMR spectrum of compound **5**.

ESI-Pos-MS Spectra for compound 5 (Solvent Acetonitrile)





Preparation of compound 6. Addition of 4 mL of a pale-yellow toluene solution of 0.100 g (0.206 mmol) of NacNacGa to 4 ml of bright-red toluene solution of diphosphinine **4** immediately led to a light-orange solution. NMR check showed quantitative formation of a single product. Volatiles were removed under reduced pressure and the residue was extracted by 7 mL of ether. The solubility in ether is low but cooling this ether fraction to -30 °C produces white crystalline material. The cold ether solution was transferred back to the main fraction and the procedure was repeated several times until extraction is complete. The volume of the ether fraction was slowly reduced to 1 mL. Then the cold ether solution was removed by a pipette and the residue was dried. Yield of white crystals 0.0926 g (0.096 mmol, 46%).

^{1}H NMR (C_6D_6): 7.38 (t, ^{3}J(H-H)=7.8 Hz, 2H, *p*-Ar), 7.00 (t, ^{3}J(H-H)=7.8 Hz, 4H, *m*-Ar), 4.77 (s, 1H, CH), 4.53 (ddd, ^{3}J(H-H)=5.3 Hz, ^{3}J(H-H)=10.6 Hz, ^{3}J(H-H)=13.3 Hz, 4H, CH_2N), 3.66 (ddd, ^{3}J(H-H)=5.3 Hz, ^{3}J(H-H)=11.0 Hz, ^{3}J(H-H)=13.1 Hz, $^{\alpha}CH_2N$), 2.92 (sept, ^{3}J(H-H)=6.8 Hz, 4H, CH in Pr^{i}), 1.99 (m, 4H, $^{\beta}CH_2$), 1.54 (m, 4H, $^{\beta}CH_2$), 1.48 (d, ^{3}J(H-H)=6.8 Hz, 12H, Me in Ar), 1.47 (s, 6H, Me of NacNac), 1.27 (m, 8, $^{\gamma}CH_2$), 0.91 (d, ^{3}J(H-H)=6.8 Hz, 12H, Me in Ar), 0.80 (t, ^{3}J(H-H)=7.4 Hz, 12H, Me in Bu). **^{13}C NMR** (C_6D_6): 169.6 (s, C=N), 166.3 (C=S), 142.1 (s, PCN), 141.2 (s, *i*-Ar), 140.4 (s, *o*-Ar), 127.8 (s, *p*-Ar), 124.9 (s, *m*-Ar), 96.3 (s, CH), 48.3 ($^{\alpha}CH_2N$), 30.3 (s, $^{\beta}CH_2$), 28.7 (s, CH in Ar), 24.8 (s, Me in Ar), 23.9 (s, Me in Ar), 23.9 (Me in NacNac), 20.1 (s, $^{\gamma}CH_2$) 13.5 (Me in Bu). ^{31}P NMR (C_6D_6): -110.1 (s). **ESI-Pos-MS**: Calc. for $[M+H]^{+}$($C_{51}H_{78}GaN_6P_2S_2$) 969.4; found 969.5. **Elem. Anal**. Calcd for $C_{51}H_{77}GaN_6P_2S_2$: N 8.66, C 63.15, H 8.00, S 6.61; Found N 8.44, C 62.87, H 7.25, S 5.81.

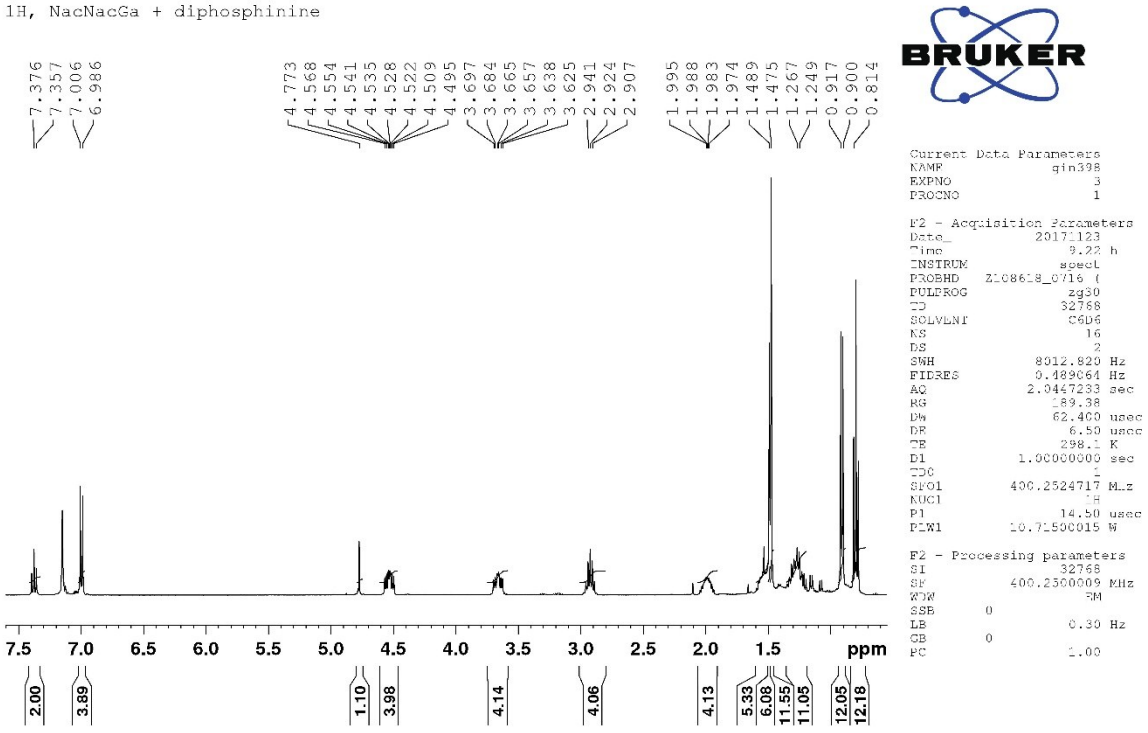


Figure 3. ^{1}H NMR spectrum of compound **6**.

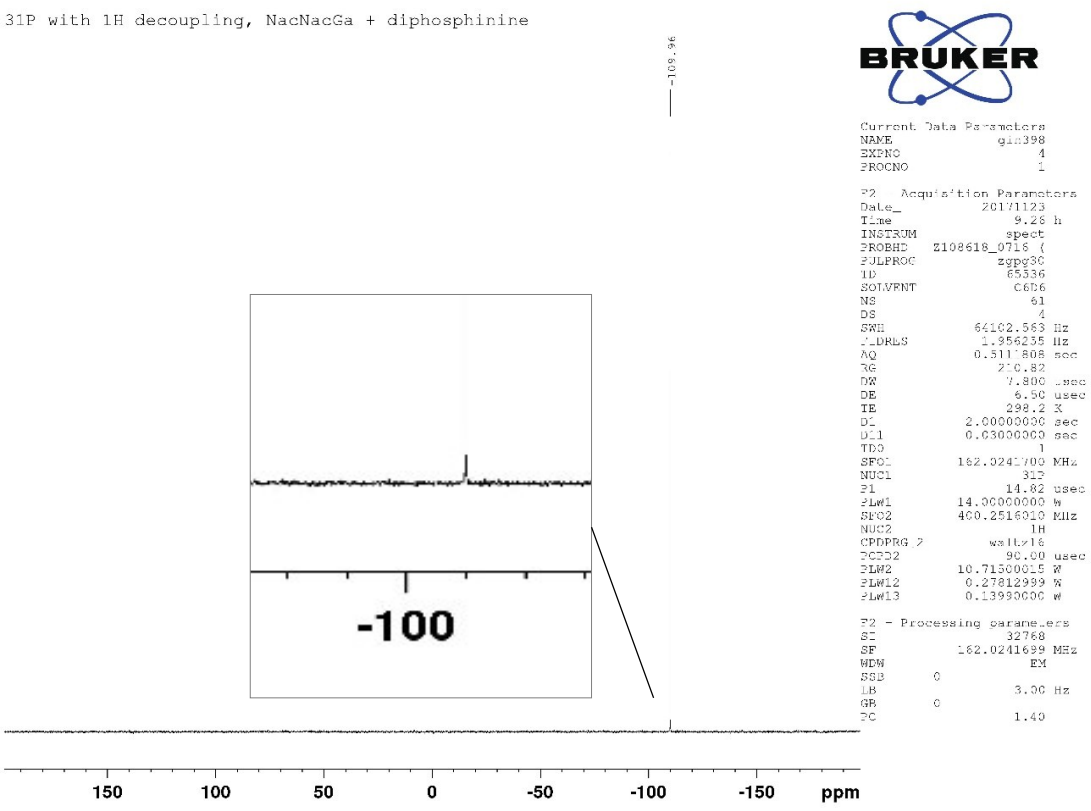
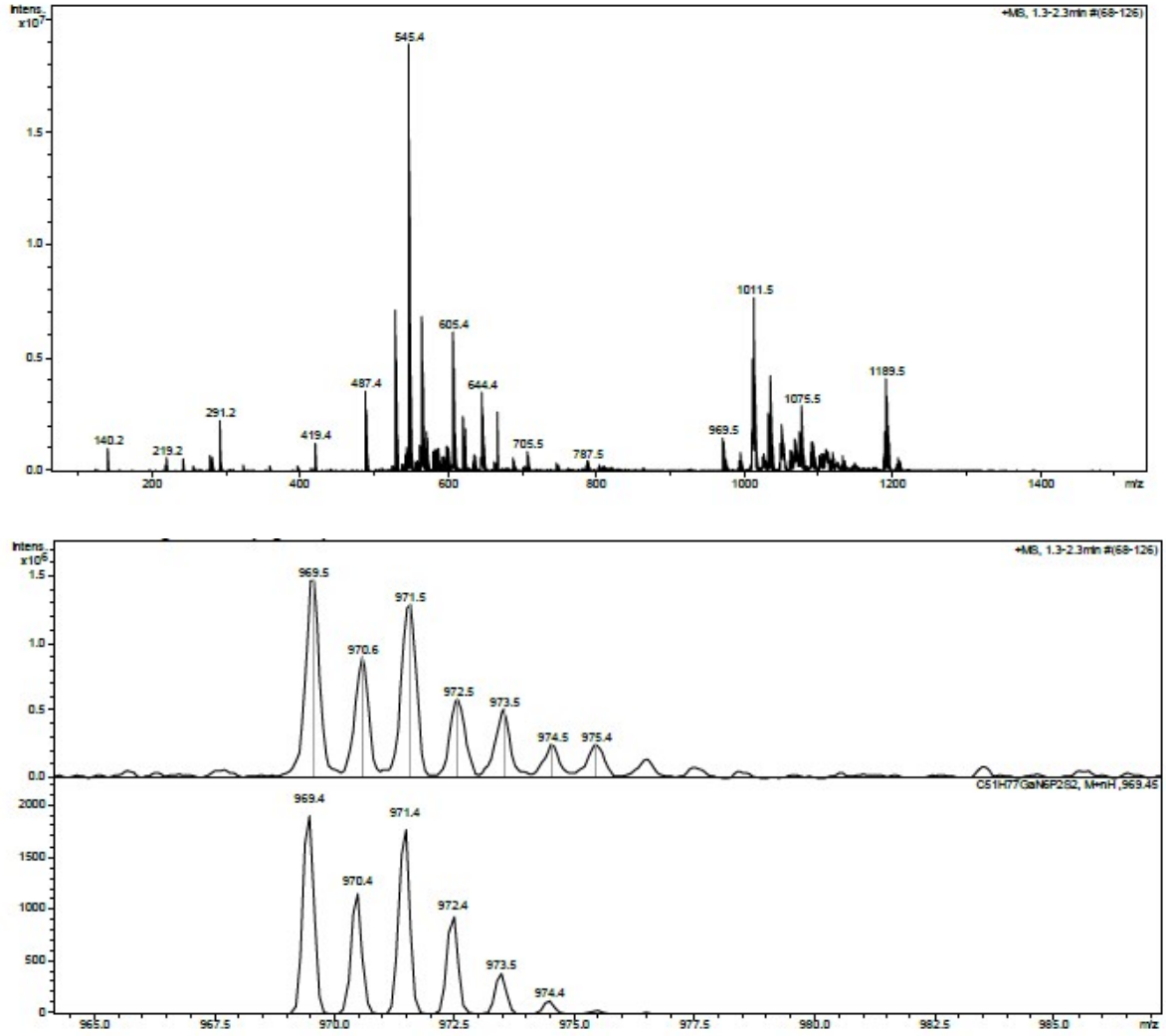


Figure 4. ^{31}P NMR spectrum of compound **6**.

ESI-Pos-MS Spectra for compound 6 (Solvent Acetonitrile)



X-ray diffraction study. Crystals of **5** and **6** were grown from ether solutions at -30 C. Data collection results for represent the best data sets obtained in several trials for each sample. The crystals were mounted on thin glass fiber using paraffin oil. Prior to data collection crystals were cooled to 200 K. Data were collected on a Bruker APEX II single crystal diffractometer equipped with a sealed Mo tube source (wavelength 0.71073 Å) and APEX II CCD detector. Raw data collection and processing were performed with APEX II software package from Bruker AXS. Semi-empirical absorption corrections based on equivalent reflections were applied. Systematic absences in the diffraction dataset and unit-cell parameters were consistent with monoclinic $P2_1/n$ (№14) for **5** and orthorhombic $Pna2_1$ (№33) for **6**. The structures were solved by direct methods, completed with difference Fourier synthesis, and refined with full-matrix least-squares procedures based on F^2. All hydrogen atom positions were calculated based on the geometry of related non-hydrogen atoms. For the refinement of **5** no additional restraints or constraints were required. In the structure of **6** the C(36)..C(39) butyl group is disordered over two positions with 0.586(14):0.414(14) occupancy ratio. The C(44)..C(47) butyl group is disordered over two positions with 0.721(14):0.279(14) occupancy ratio. These fragments were refined with bond distance and angle restraints (DFIX, SAME) as well as enhanced rigid-bond restraints (RIGU) applied to ADPs. A constraint (EADP) was applied to the ADPs of C(37) and C(37a). CCDC 1900182 (for **5**) and 1900183 (for **6**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

Z	**5**	**6**
Empirical formula	$C_{51}H_{77}AlN_6P_2S_2$	$C_{51}H_{77}GaN_6P_2S_2$
Formula weight	927.22	969.96
colour, habit	yellow, plate	colourless , plate

Wavelength, Å	V	0.71073
Crystal size, mm^3	0.737 x 0.583 x 0.104	0.350 x 0.340 x 0.210
Crystal system	Monoclinic	orthorhombic
Space group	$P2_1/n$	$Pna2_1$
Unit cell dimensions:		
a, Å	12.3978(5)	23.684(3)
b, Å	20.1923(9)	12.5765(17)
c, Å	21.8157(11)	17.783(3)
α, °	90	90
β, °	100.880(2)	90
γ, °	90	90
Volume, $Å^3$	5363.2(4)	5296.9(13)
Z	4	4
Density (calcd), g/cm^3	1.148	1.216
Absorption coefficient, mm^{-1}	0.214	0.697
F(000)	2000	2072
Temperature, K	200(2)	200(2) K
2θ range for data collection, °	1.386 to 30.088	1.720 to 31.276
Index ranges	-17≤h≤17, -26≤k≤26, -26≤l≤29	-34≤h≤34, -18≤k≤17, -24≤l≤25
Reflections collected	41871	54651
Independent reflections	14732 [R(int) = 0.0588]	16035 [R(int) = 0.0353]
Data / restraints / parameters	14732 / 0 / 563	16035 / 102 / 601
Goodness-of-fit on F^2	1.021	1.029
Final R indices [I>2σ(I)]	R_1 = 0.0607, wR_2 = 0.1368	R_1 = 0.0432, wR_2 = 0.0981
R indices (all data)	R_1 = 0.1190, wR_2 = 0.1638	R_1 = 0.0655, wR_2 = 0.1077
Absolute structure parameter	-	-0.005(4)
Largest diff. peak and hole, $e.Å^{-3}$	0.517 and -0.271	0.736 and -0.238

Computational details

All calculations were carried out with the Gaussian 09 program package.[12] Full geometry optimization calculations were performed, followed by calculation of the second derivatives at the optimized structures to establish the nature of the stationary points obtained. The Gibbs free energies were calculated based on the harmonic vibrational frequencies (atmospheric pressure, 298.15 K). The dispersion corrected M06-2X functional (ultrafine integration grid was applied for the M06-2X frequency calculations) was applied with the conjunction of the 6-31+G* (and for indium def2SVP) basis set. **4**, **5**, **6** and their derivatives were calculated with methyl substituents at the nitrogen atoms (instead of the *n*-butyl) to reduce the computational time and they were labeled by the special character ‘. For the visualization of the molecular structures and the molecular orbitals the MOLDEN program was used.[13]

4’

G(M06-2X/6-31+G*)= -2085.875965
E(M06-2X/6-31+G*)= -2086.0534474

N	-2.648334	1.090432	-0.002270
C	-1.317542	0.704662	-0.000816
C	-1.317538	-0.704637	0.000837
N	-2.648321	-1.090437	0.002285
C	-3.484772	-0.000007	0.000001
P	0.000014	1.852025	0.000002
C	1.317559	0.704650	0.000824
N	2.648347	1.090429	0.002283
C	3.484781	-0.000012	-0.000002
N	2.648320	-1.090435	-0.002282
C	1.317541	-0.704624	-0.000819
C	3.089781	2.471068	0.003765
P	-0.000034	-1.851967	-0.000005
C	3.089722	-2.471083	-0.003766
S	5.149954	-0.000032	-0.000005
C	-3.089734	-2.471081	0.003773
S	-5.149944	-0.000013	-0.000012
C	-3.089779	2.471066	-0.003765
H	-2.695839	2.984394	-0.886414
H	-4.179167	2.473956	-0.027832
H	-2.736047	2.975857	0.900658
H	-4.179124	-2.473977	0.027819
H	-2.735988	-2.975860	-0.900651
H	-2.695785	-2.984404	0.886421
H	2.736051	2.975846	-0.900666
H	4.179169	2.473947	0.027839
H	2.695817	2.984407	0.886395
H	4.179110	-2.473988	-0.027844
H	2.695742	-2.984413	-0.886395
H	2.735999	-2.975847	0.900674

NacNacAl

G(M06-2X/6-31+G*)= -1480.640204
E(M06-2X/6-31+G*)= -1481.214800

C	-3.479522	-1.139649	-0.497362
C	-2.690707	-0.048743	-0.092079
C	-3.109872	1.279598	-0.303147
C	-4.357486	1.495329	-0.891158
C	-5.162291	0.427603	-1.277102
C	-4.720844	-0.876522	-1.082941
N	-1.383119	-0.273401	0.445502
C	-1.221336	-0.294156	1.763915
C	-2.439122	-0.227060	2.654999
C	-2.219320	2.460832	0.056752
C	-2.950689	3.513797	0.897179
C	-3.007707	-2.573682	-0.320979
C	-4.013841	-3.418063	0.470891

Al	-0.000984	-0.461775	-1.031661
N	1.408349	-0.224831	0.419253
C	1.277643	-0.223066	1.741733
C	0.034820	-0.332110	2.385926
C	2.708791	0.004927	-0.125305
C	3.085988	1.325105	-0.442952
C	4.400157	1.540276	-0.865922
C	5.284936	0.478268	-1.027138
C	4.844178	-0.827923	-0.841226
C	3.540341	-1.093186	-0.414407
C	2.071296	2.465271	-0.397835
C	2.419304	3.595115	-1.371711
C	3.012757	-2.520134	-0.313217
C	3.107864	-3.118729	1.097724
C	2.495493	-0.041496	2.624081
C	3.688553	-3.460839	-1.315938
C	1.837362	3.048571	1.002735
C	-1.637993	3.099989	-1.213216
C	-2.717460	-3.221672	-1.682077
H	0.044590	-0.357198	3.468301
H	5.520720	-1.651204	-1.050533
H	6.305202	0.666498	-1.348754
H	4.735220	2.546796	-1.096951
H	-5.348120	-1.706191	-1.400439
H	-6.129127	0.612637	-1.736183
H	-4.702055	2.512602	-1.060888
H	1.112063	2.044980	-0.732332
H	1.948519	-2.475207	-0.577989
H	3.144468	-4.409905	-1.353887
H	3.702036	-3.032716	-2.323079
H	4.720183	-3.689621	-1.024195
H	1.177494	3.921792	0.934209
H	1.359531	2.331576	1.675438
H	2.783979	3.375212	1.450804
H	-1.376926	2.088270	0.651028
H	-0.933450	3.898705	-0.951432
H	-1.112275	2.362898	-1.831178
H	-2.436344	3.536030	-1.825451
H	-2.251378	4.295539	1.213215
H	-3.750305	3.998216	0.326017
H	-3.399395	3.073314	1.793693
H	-2.070444	-2.552346	0.245833
H	-2.307417	-4.228741	-1.546190
H	-3.636300	-3.304856	-2.274635
H	-1.997091	-2.629992	-2.255807
H	-3.612731	-4.422818	0.641879
H	-4.240677	-2.970061	1.444019
H	-4.957644	-3.526652	-0.075061
H	2.845350	0.995128	2.570450
H	2.253151	-0.271547	3.663445
H	3.329904	-0.667239	2.300798
H	-2.168379	-0.383436	3.700345
H	-2.923025	0.751675	2.558956
H	-3.179825	-0.974636	2.354743
H	1.572270	4.284054	-1.452601
H	3.279805	4.178512	-1.023774
H	2.643910	3.211164	-2.371657
H	2.837793	-4.180202	1.070753
H	4.131974	-3.039986	1.482976
H	2.433176	-2.626247	1.803096

NacNacGa

G(M06-2X/6-31+G*)= -3161.194756
E(M06-2X/6-31+G*)= -3161.702315

C	3.170306	1.303609	-0.466133
C	2.720038	0.013414	-0.145776
C	3.496037	-1.128951	-0.417253
C	4.776970	-0.946982	-0.941022
C	5.263716	0.330071	-1.213721
C	4.459213	1.440627	-0.992506
N	1.404849	-0.151015	0.407845
C	1.293608	-0.267861	1.731426
C	2.533421	-0.261534	2.597703
C	2.909119	-2.505098	-0.173320
C	3.843643	-3.677190	-0.458391
C	2.298621	2.527852	-0.284074
C	2.158274	3.015690	1.162806
Ga	0.001746	-0.252993	-1.007482
N	-1.363480	-0.184160	0.449213
C	-1.202752	-0.281526	1.767636
C	0.055138	-0.369557	2.380477
C	-2.696020	0.007680	-0.057885
C	-3.185354	1.320372	-0.204313
C	-4.454165	1.497504	-0.761806
C	-5.221462	0.409730	-1.163357
C	-4.721587	-0.878235	-1.012302
C	-3.456920	-1.104876	-0.461818
C	-2.364151	2.536744	0.197776
C	-1.844381	3.270136	-1.046778
C	-2.939329	-2.529500	-0.340090
C	-2.675634	-3.127879	-1.729072
C	-2.416531	-0.273193	2.666396
C	-3.900276	-3.424937	0.452892
C	-3.153106	3.499528	1.094868
H	0.070963	-0.464345	3.458793
H	5.402643	-1.808912	-1.150921
H	6.262065	0.453794	-1.623444
H	4.824283	2.434294	-1.242314
H	-5.321454	-1.725207	-1.336683
H	-6.205229	0.566967	-1.596292
H	-4.846487	2.503933	-0.886819
H	1.298107	2.329729	-0.691830
C	2.859934	3.595112	-1.089297
C	2.431151	-2.597573	1.192511
H	2.007439	-2.602804	-0.795447
H	3.334897	-4.621590	-0.244828
H	4.154043	-3.697456	-1.508011
H	4.745444	-3.634975	0.162252
H	1.642578	3.981388	1.188475
H	1.575448	2.315838	1.769477
H	3.140464	3.144732	1.631362
H	-1.493483	2.191410	0.766780
H	-1.214659	4.119535	-0.756871
H	-1.255480	2.602170	-1.685092
H	-2.679683	3.651966	-1.645430
H	-2.503081	4.309109	1.443991
H	-3.987113	3.957713	0.552351
H	-3.565606	2.990423	1.972386
H	-1.986173	-2.500958	0.199812

H	-2.246933	-4.132451	-1.640093
H	-3.609953	-3.207586	-2.297239
H	-1.982804	-2.503816	-2.302403
H	-3.463107	-4.419784	0.590817
H	-4.122261	-3.008795	1.441201
H	-4.851358	-3.551773	-0.076159
H	3.106503	0.657963	2.442878
H	2.267036	-0.340859	3.652903
H	3.199472	-1.090447	2.337795
H	-2.131303	-0.427912	3.708033
H	-2.942987	0.683966	2.581910
H	-3.126936	-1.050038	2.367047
H	2.252033	4.491797	-0.978243
H	3.876697	3.802669	-0.759091
H	2.872639	3.292419	-2.135307
H	2.010427	-3.587335	1.363637
H	3.259979	-2.431774	1.879152
H	1.664076	-1.843062	1.360530

NacNacIn

G(M06-2X/6-31+G*)= -1428.302933
E(M06-2X/6-31+G*)= -1428.877922

C	3.752300	-0.907415	-0.089875
C	2.788761	0.109388	0.067735
C	3.058824	1.435301	-0.343329
C	4.328195	1.728961	-0.847065
C	5.302001	0.741780	-0.968709
C	5.005870	-0.565929	-0.604989
N	1.483924	-0.193242	0.554206
C	1.290055	-0.325289	1.858533
C	2.477964	-0.254930	2.800374
C	1.991544	2.518181	-0.231514
C	1.852377	3.044615	1.203899
C	3.439325	-2.362422	0.223614
C	3.180993	-3.137145	-1.077186
In	-0.000908	-0.502276	-1.233001
N	-1.466494	-0.307096	0.571686
C	-1.244738	-0.412087	1.874754
C	0.029848	-0.507649	2.462694
C	-2.776813	0.018884	0.111301
C	-3.681210	-0.996396	-0.260579
C	-4.914152	-0.627374	-0.805009
C	-5.255696	0.709499	-0.978207
C	-4.355892	1.701953	-0.603575
C	-3.111061	1.380128	-0.057865
C	-3.339199	-2.468588	-0.097654
C	-3.117817	-3.132036	-1.464318
C	-2.146172	2.493412	0.325837
C	-1.654338	3.246176	-0.917570
C	-2.426948	-0.387799	2.822684
C	-2.771609	3.474688	1.325652
C	-4.415804	-3.228190	0.688642
C	2.213581	3.683837	-1.197977
C	4.546487	-3.048349	1.033655
H	0.040634	-0.621586	3.539423
H	5.760709	-1.338160	-0.730150
H	6.282590	0.990355	-1.363739
H	4.562143	2.741102	-1.161329
H	-5.619726	-1.400379	-1.100429
H	-6.217993	0.976768	-1.404712
H	-4.625017	2.746723	-0.741720
H	1.027161	2.059178	-0.491855

H	2.518626	-2.396502	0.815164
H	2.917115	-4.178791	-0.862274
H	2.366453	-2.687287	-1.655535
H	4.076467	-3.133886	-1.709604
H	1.101612	3.843520	1.242492
H	1.537319	2.258974	1.896391
H	2.806975	3.456076	1.553779
H	-1.272669	2.040026	0.808598
H	-0.935655	4.023896	-0.634074
H	-1.166982	2.571926	-1.632322
H	-2.489197	3.730007	-1.437908
H	-2.029773	4.215370	1.644223
H	-3.613047	4.016669	0.879389
H	-3.141749	2.957592	2.216652
H	-2.402133	-2.535062	0.466284
H	-2.829829	-4.182233	-1.342510
H	-4.036467	-3.098633	-2.061715
H	-2.333686	-2.623598	-2.035671
H	-4.092602	-4.257940	0.875311
H	-4.623138	-2.753649	1.653251
H	-5.357878	-3.273999	0.131076
H	2.150534	-0.208288	3.840114
H	3.115751	-1.136990	2.676891
H	3.100884	0.618132	2.581614
H	-2.110521	-0.555753	3.853204
H	-2.941013	0.578041	2.765303
H	-3.160566	-1.151524	2.544332
H	1.339736	4.342818	-1.192077
H	3.077575	4.291428	-0.905446
H	2.370409	3.334252	-2.223712
H	4.220261	-4.045144	1.348835
H	5.457380	-3.176232	0.438683
H	4.811758	-2.474564	1.927871

5’

G(M06-2X/6-31+G*)= -3566.574315
E(M06-2X/6-31+G*)= -3567.362872

C	3.162009	1.044113	-1.465065
C	2.718017	1.405996	-0.173579
C	3.459123	1.088991	0.980466
C	4.611745	0.310303	0.826657
C	5.043354	-0.098153	-0.429924
C	4.339813	0.299032	-1.564951
N	1.415531	2.010513	-0.054982
C	1.256550	3.332089	0.008991
C	2.458779	4.230495	0.147835
C	3.095711	1.629013	2.356469
C	2.877999	0.530589	3.397119
C	2.416323	1.498496	-2.715167
C	2.573471	0.546176	-3.899346
C	0.000001	3.957957	0.000216
C	-1.256540	3.332073	-0.008649
C	-2.458789	4.230460	-0.147456
N	-1.415504	2.010489	0.055151
Al	0.000002	0.738305	0.000066
P	-0.039889	-1.020204	1.681821
C	1.337789	-1.770803	0.719183
N	2.471265	-2.446907	1.148527
C	3.211878	-2.851579	0.072484
N	2.505829	-2.465033	-1.032845
C	1.362462	-1.778130	-0.651088
C	2.848672	-2.784139	2.501709

S	4.678108	-3.659250	0.106129
C	2.916666	-2.819716	-2.370826
P	0.039923	-1.020063	-1.681819
C	-1.337780	-1.770706	-0.719253
C	-1.362471	-1.778148	0.651016
N	-2.505853	-2.465058	1.032712
C	-3.211961	-2.851405	-0.072645
N	-2.471306	-2.446723	-1.148657
C	-2.916648	-2.819963	2.370649
S	-4.678201	-3.659051	-0.106337
C	-2.848749	-2.783841	-2.501857
C	-2.717988	1.405939	0.173635
C	-3.459055	1.089069	-0.980470
C	-4.611729	0.310437	-0.826780
C	-5.043412	-0.098111	0.429744
C	-4.339892	0.298925	1.564836
C	-3.162050	1.043950	1.465086
C	-3.095517	1.629184	-2.356401
C	-2.877741	0.530830	-3.397113
C	-2.416400	1.498152	2.715270
C	-2.573909	0.545816	3.899390
C	-2.848900	2.912257	3.125022
C	-4.185661	2.594458	-2.844094
C	4.185914	2.594213	2.844174
C	2.849050	2.912535	-3.124916
H	-2.152276	2.189866	-2.266823
H	2.152485	2.189736	2.267008
H	-5.920748	-0.738262	0.522953
H	-4.408108	3.373360	-2.101903
H	-3.598150	0.562796	4.301853
H	-3.025525	-3.865824	-2.567956
H	-2.039893	-2.482969	-3.178009
H	-3.785573	-2.276424	-2.771082
H	3.771170	-2.205913	-2.690743
H	3.235203	-3.870179	-2.376069
H	2.066877	-2.669534	-3.047955
H	3.025334	-3.866147	2.567749
H	3.785549	-2.276844	2.770979
H	2.039848	-2.483219	3.177877
H	-3.234897	-3.870516	2.375813
H	-2.066930	-2.669600	3.047825
H	-3.771335	-2.206416	2.690562
H	-0.000006	5.045966	0.000261
H	-4.708952	0.005793	2.548517
H	-5.185603	0.017704	-1.709292
H	4.708823	0.005978	-2.548674
H	5.920644	-0.738355	-0.523224
H	5.185636	0.017452	1.709118
H	-3.880409	3.081060	-3.782374
H	-5.121160	2.048308	-3.038076
H	1.343249	1.540564	-2.471978
H	-2.287753	5.184019	0.366817
H	-2.600673	4.449281	-1.217651
H	-3.377557	3.765547	0.227965
H	2.600646	4.449291	1.218036
H	3.377560	3.765609	-0.227587
H	2.287706	5.184065	-0.366407
H	-1.343286	1.539998	2.472213
H	-1.897779	0.847682	4.711861
H	-2.325833	-0.486381	3.620605

H	-2.339417	3.213991	4.052051
H	-2.610870	3.657351	2.354951
H	-3.934648	2.942702	3.304377
H	3.880705	3.080760	3.782497
H	5.121394	2.048011	3.038101
H	4.408373	3.373140	2.102015
H	1.897323	0.848240	-4.711728
H	3.597671	0.562928	-4.301923
H	2.325179	-0.485975	-3.620579
H	2.339534	3.214394	-4.051887
H	2.611232	3.657649	-2.354798
H	3.934785	2.942783	-3.304373
H	-2.611257	0.974257	-4.367923
H	-2.066697	-0.148636	-3.104796
H	-3.792046	-0.063563	-3.541563
H	2.611658	0.973953	4.367997
H	2.066897	-0.148827	3.104853
H	3.792287	-0.063867	3.541410

6’

G(M06-2X/6-31+G*)= -5247.131913
E(M06-2X/6-31+G*)= -5247.9196441

C	3.443854	1.040410	0.950435
C	2.732084	1.406728	-0.204097
C	3.170320	1.062546	-1.498502
C	4.337888	0.304329	-1.605254
C	5.023084	-0.130360	-0.473513
C	4.581379	0.244106	0.790269
N	1.437472	2.016240	-0.075396
C	1.260569	3.330712	-0.006694
C	2.455105	4.246757	0.104897
C	2.422802	1.537216	-2.739418
C	2.568846	0.592202	-3.934954
C	3.056467	1.556700	2.328377
C	2.861686	0.441106	3.357176
C	0.000008	3.947644	-0.000090
C	-1.260559	3.330724	0.006567
C	-2.455090	4.246769	-0.105090
N	-1.437469	2.016257	0.075340
Ga	-0.000005	0.702163	-0.000016
P	-0.099832	-1.050739	1.681805
C	1.309450	-1.794477	0.764641
N	2.406572	-2.507243	1.232577
C	3.182076	-2.917194	0.183598
N	2.535002	-2.495830	-0.943806
C	1.390507	-1.787618	-0.601457
C	2.699745	-2.890959	2.599672
S	4.628625	-3.770647	0.266177
C	2.991780	-2.835165	-2.275423
P	0.099798	-1.050764	-1.681801
C	-1.309488	-1.794480	-0.764626
C	-1.390545	-1.787607	0.601473
N	-2.535010	-2.495869	0.943827
C	-3.182121	-2.917182	-0.183573
N	-2.406598	-2.507272	-1.232553
C	-2.991737	-2.835292	2.275438
S	-4.628644	-3.770678	-0.266141
C	-2.699747	-2.891043	-2.599637
C	-2.732076	1.406753	0.204091
C	-3.170261	1.062610	1.498520
C	-4.337773	0.304310	1.605327
C	-5.022972	-0.130457	0.473617

C	-4.581340	0.244017	-0.790189
C	-3.443866	1.040383	-0.950409
C	-2.422750	1.537429	2.739391
C	-2.568550	0.592436	3.934971
C	-3.056555	1.556688	-2.328368
C	-2.861832	0.441106	-3.357191
C	-4.122325	2.540671	-2.836765
C	-2.874234	2.946933	3.151185
C	2.874104	2.946778	-3.151218
C	4.122222	2.540666	2.836842
H	-2.103252	2.091328	-2.239405
H	2.103172	2.091345	2.239371
H	-5.892793	-0.772371	0.573572
H	-4.329478	3.332421	-2.110922
H	-3.579275	0.628476	4.357309
H	-2.797781	-3.978103	-2.654291
H	-1.882968	-2.551850	-3.238180
H	-3.644126	-2.443964	-2.920695
H	3.884102	-2.256681	-2.531958
H	3.246047	-3.897085	-2.303056
H	2.186880	-2.619435	-2.979977
H	2.797795	-3.978015	2.654363
H	3.644120	-2.443854	2.920704
H	1.882968	-2.551754	3.238211
H	-3.245970	-3.897222	2.303022
H	-2.186823	-2.619578	2.979979
H	-3.884072	-2.256851	2.532026
H	0.000012	5.031523	-0.000129
H	-4.711072	0.030159	2.587870
H	-5.134961	-0.089596	-1.665072
H	4.711224	0.030163	-2.587780
H	5.892945	-0.772226	-0.573425
H	5.134984	-0.089466	1.665179
H	-3.800521	3.004365	-3.775804
H	-5.064592	2.014219	-3.026648
H	1.355492	1.593928	-2.492389
H	-2.300729	5.148186	0.493028
H	-2.557540	4.556070	-1.152223
H	-3.384288	3.763311	0.199667
H	2.557561	4.556123	1.152010
H	3.384299	3.763273	-0.199831
H	2.300748	5.148137	-0.493278
H	-1.355463	1.594303	2.492297
H	-1.872366	0.889547	4.725811
H	-2.344537	-0.442705	3.663649
H	-2.364307	3.253517	4.071164
H	-2.653733	3.692314	2.383508
H	-3.954480	2.960896	3.338007
H	3.800368	3.004360	3.775864
H	5.064470	2.014198	3.026780
H	4.329432	3.332416	2.111015
H	1.872664	0.889159	-4.725852
H	3.579593	0.628398	-4.357224
H	2.344997	-0.442970	-3.663606
H	2.364164	3.253277	-4.071218
H	2.653478	3.692140	-2.383558
H	3.954353	2.960886	-3.338006
H	-2.559215	0.863681	-4.321494
H	-2.087406	-0.259634	-3.038706
H	-3.788860	-0.120730	-3.514619
H	2.559026	0.863673	4.321469
H	2.087268	-0.259624	3.038648
H	3.788702	-0.120740	3.514644

In analouge of **6'**

G(M06-2X/6-31+G*)= -3514.166196
E(M06-2X/6-31+G*)= -3514.950966

C	3.106896	1.124498	-1.725603
C	2.768720	1.527889	-0.413210
C	3.567978	1.184905	0.692120
C	4.699411	0.392497	0.471076
C	5.046058	-0.020437	-0.808194
C	4.264196	0.362009	-1.895968
N	1.482909	2.127951	-0.207153
In	-0.000057	0.540308	-0.001086
P	-0.237970	-1.467403	1.707162
C	1.236747	-2.148445	0.862938
C	1.431083	-2.139387	-0.494728
N	2.716993	-2.615051	-0.722963
C	3.324517	-2.920363	0.462795
N	2.407826	-2.629709	1.436321
P	0.237955	-1.469745	-1.706641
C	-1.236742	-2.149683	-0.861481
N	-2.407861	-2.631611	-1.434225
C	-3.324669	-2.920668	-0.460332
N	-2.717141	-2.613732	0.725019
C	-1.431121	-2.138674	0.496157
C	-2.627454	-2.957924	-2.830602
S	-4.864291	-3.559157	-0.674940
C	-3.319491	-2.919591	2.007865
C	3.319477	-2.922601	-2.005337
S	4.864039	-3.558825	0.678139
C	2.627596	-2.953896	2.833162
C	3.240672	1.652428	2.101257
H	2.342377	2.278970	2.058681
C	2.249762	1.532304	-2.917694
C	2.548438	2.977430	-3.345286
C	1.273449	3.432783	-0.101497
C	2.463720	4.365885	-0.043630
C	-0.000211	4.029680	-0.003321
C	-1.273741	3.432793	0.096206
C	-2.464185	4.365629	0.037601
N	-1.483024	2.128070	0.203872
C	-2.768585	1.528280	0.412226
C	-3.105278	1.126874	1.725637
C	-4.262282	0.364489	1.898447
C	-5.045404	-0.019538	0.812127
C	-4.700301	0.391585	-0.468130
C	-3.569113	1.183662	-0.691651
C	-2.246977	1.536819	2.916173
C	-2.545461	2.982642	3.341565
C	-3.243428	1.648968	-2.101896
C	-4.386782	2.499460	-2.672910
H	-2.345265	2.275743	-2.061326
C	-2.394835	0.608933	4.124287
C	4.383238	2.504134	2.672056
C	2.398984	0.602295	-4.124015
H	5.914721	-0.656336	-0.951287
H	4.638133	3.332651	2.003122
H	3.379628	0.713803	-4.600523
H	2.645678	-4.040094	2.963521
H	1.820776	-2.518546	3.424296
H	3.591363	-2.552843	3.151589
H	-4.313137	-2.471703	2.060252
H	-3.418405	-4.003430	2.120714
H	-2.681044	-2.516521	2.795029
H	-2.645052	-4.044318	-2.959398
H	-3.591376	-2.557755	-3.149650

H	-1.820806	-2.523077	-3.422342
H	3.422114	-4.006417	-2.114881
H	2.678940	-2.524186	-2.793177
H	4.311540	-2.471431	-2.060003
H	-0.000267	5.113599	-0.004193
H	4.548793	0.036313	-2.892089
H	5.311122	0.076354	1.312594
H	-4.545686	0.040157	2.895357
H	-5.913895	-0.655248	0.957131
H	-5.312973	0.074177	-1.308470
C	2.940080	0.471549	3.030742
H	4.102136	2.918166	3.646438
H	5.287021	1.901232	2.812680
C	-2.943559	0.466553	-3.029672
H	-1.195119	1.500181	2.601921
H	2.229766	5.326591	-0.508022
H	2.709178	4.553422	1.009054
H	3.347283	3.936708	-0.520596
H	-2.710874	4.550772	-1.015222
H	-3.347167	3.937369	0.516474
H	-2.229877	5.327388	0.499613
H	1.197599	1.496037	-2.604433
H	1.641697	0.850226	-4.874560
H	2.265098	-0.447889	-3.847094
H	1.966447	3.237669	-4.236299
H	2.297610	3.697036	-2.561870
H	3.612083	3.089729	-3.586149
H	-4.106763	2.911987	-3.648242
H	-5.290562	1.896124	-2.811664
H	-4.641205	3.328998	-2.005057
H	-1.636938	0.858455	4.873694
H	-3.375070	0.721025	4.601497
H	-2.260850	-0.441707	3.849177
H	-1.962665	3.244494	4.231579
H	-2.295476	3.700944	2.556688
H	-3.608893	3.095201	3.583246
H	2.708244	0.823596	4.042016
H	2.085993	-0.110531	2.668067
H	3.801297	-0.203041	3.092094
H	-2.713332	0.816855	-4.041917
H	-2.088685	-0.114438	-2.667102
H	-3.804526	-0.208589	-3.088514

TS of the fomation of **5'**
G(M06-2X/6-31+G*)= -3566.510879
E(M06-2X/6-31+G*)= -3567.296469

N	-2.972489	-2.600545	-0.284939
C	-1.608014	-2.704438	-0.052491
C	-0.991311	-2.659533	-1.303899
N	-2.013696	-2.530627	-2.237080
C	-3.237027	-2.469440	-1.621210
P	-0.913749	-2.566922	1.549621
C	0.765325	-2.818939	1.117580
C	1.380557	-2.774879	-0.134233
N	2.748147	-2.746843	0.101696
C	3.017703	-2.756187	1.442443
N	1.792066	-2.826502	2.054397
C	3.740472	-2.729455	-0.954156
P	0.696902	-2.435987	-1.709498
C	1.581877	-2.822118	3.487794
S	4.519547	-2.675428	2.184298
C	-1.796586	-2.416044	-3.664844
S	-4.732419	-2.259707	-2.350767

C	-3.970482	-2.663567	0.763929
C	4.821653	0.454833	-0.337218
C	5.065131	0.360253	-1.702947
C	4.108038	0.809484	-2.604472
C	2.903657	1.365211	-2.161566
C	2.678948	1.460414	-0.772150
C	3.635066	1.005843	0.160921
N	1.433025	2.011090	-0.305668
C	1.306183	3.338445	-0.270839
C	2.447488	4.224711	-0.717118
C	1.891915	1.862555	-3.188330
C	1.126189	0.696205	-3.826974
C	3.545737	1.169728	1.678356
C	3.833075	2.616555	2.106749
Al	0.037348	0.628886	-0.002450
N	-1.277376	2.056190	0.430736
C	-1.077750	3.372531	0.503048
C	0.130741	3.983785	0.138716
C	-2.545554	1.534189	0.869432
C	-2.760304	1.338399	2.249736
C	-3.983614	0.802313	2.663550
C	-4.968105	0.467506	1.742151
C	-4.734687	0.660024	0.384938
C	-3.530608	1.198825	-0.083580
C	-1.717050	1.704588	3.299615
C	-1.015494	0.454817	3.847493
C	-3.451150	1.483686	-1.583475
C	-2.210243	0.988640	-2.333526
C	-2.165419	4.281007	1.030795
C	-3.674768	2.972817	-1.886065
C	-2.319717	2.516866	4.454573
C	2.548245	2.720139	-4.279355
C	2.271780	0.673859	2.369949
H	5.994912	-0.072657	-2.061744
H	3.002052	3.279576	1.839641
H	1.817003	0.001501	-4.320149
H	-1.923997	-0.020910	-2.021122
H	1.148177	-1.866224	3.804491
H	2.548983	-2.961956	3.970514
H	0.901922	-3.635263	3.756797
H	-3.760307	-1.898952	1.516758
H	-4.944961	-2.475755	0.313388
H	-3.953201	-3.655740	1.226490
H	-2.770129	-2.425133	-4.154809
H	-1.277323	-1.478413	-3.895127
H	-1.190402	-3.258880	-4.009057
H	4.723651	-2.645109	-0.491722
H	3.673300	-3.655459	-1.534308
H	3.567143	-1.869145	-1.607251
H	0.160133	5.065433	0.181859
H	4.299479	0.731263	-3.671684
H	5.562224	0.088212	0.369909
H	-4.167395	0.647407	3.723790
H	-5.912290	0.047219	2.077880
H	-5.497565	0.382664	-0.339040
H	4.357679	0.545562	2.070457
H	3.955271	2.665503	3.194591
H	4.748451	2.999532	1.643142
H	2.472057	0.544908	3.440508
H	1.447906	1.393109	2.277303

H	1.943141	-0.292738	1.973758
H	-4.296362	0.932336	-2.012888
H	-0.948442	2.324665	2.825298
H	2.457825	4.278120	-1.812385
H	2.318549	5.237377	-0.330393
H	3.418585	3.837050	-0.403747
H	-1.991730	5.310276	0.710959
H	-3.160160	3.964261	0.712386
H	-2.153043	4.260036	2.127176
H	1.154549	2.489297	-2.674848
H	0.415795	1.068516	-4.574768
H	0.570857	0.131680	-3.071657
H	1.778007	3.198594	-4.893184
H	3.187483	3.501826	-3.855461
H	3.166792	2.112308	-4.948474
H	-3.806977	3.118326	-2.964072
H	-4.565430	3.357590	-1.378017
H	-2.810163	3.571768	-1.577590
H	-2.429349	0.957746	-3.407719
H	-1.351583	1.658400	-2.196107
H	-0.277545	0.733073	4.609467
H	-1.741480	-0.230913	4.301162
H	-0.501604	-0.087771	3.048100
H	-1.521550	2.905545	5.095614
H	-2.915366	3.361742	4.093058
H	-2.969569	1.897760	5.082436

TS of the oxidative cleavage of the S=C bond in the presence of NacNacAl

G(M06-2X/6-31+G*)= -3566.482012
E(M06-2X/6-31+G*)= -3567.362479

C	-1.375092	3.662653	0.235493
C	-2.417278	2.726527	0.119772
C	-3.616681	3.036095	-0.555357
C	-3.764361	4.330259	-1.058389
C	-2.758135	5.282349	-0.922979
C	-1.568436	4.942446	-0.293703
N	-2.276759	1.409340	0.699247
C	-2.621531	1.256820	1.975781
C	-2.665294	0.007609	2.626596
C	-2.546144	-1.252039	2.018052
C	-2.757954	-2.469318	2.888239
C	-4.724800	2.006577	-0.733194
C	-5.485365	2.190641	-2.048179
C	-0.032839	3.314734	0.857952
C	1.052891	3.264420	-0.228733
N	-2.223747	-1.412872	0.735452
C	-2.497964	-2.700132	0.141195
C	-3.815987	-2.962424	-0.283228
C	-4.087700	-4.218252	-0.828427
C	-3.088976	-5.176632	-0.973718
C	-1.788677	-4.882223	-0.583129
C	-1.471845	-3.642212	-0.021630
C	-4.935567	-1.936457	-0.159600
C	-5.940759	-2.325220	0.934581
C	-0.033270	-3.317864	0.336064
C	0.606517	-4.357804	1.262284
Al	-1.710162	-0.013700	-0.502179
S	-2.385236	-0.140554	-2.474067
C	0.424392	0.056236	-0.369463

N	1.199628	-0.030739	0.742141
C	2.553496	-0.037119	0.436481
C	2.617181	0.065467	-0.958226
N	1.301339	0.117172	-1.398147
P	3.812412	-0.152447	1.651974
C	5.175732	-0.088449	0.573318
N	6.484107	-0.141940	1.015130
C	7.372873	-0.072261	-0.034546
N	6.588077	0.026308	-1.159927
C	5.241641	0.020488	-0.841244
S	9.030331	-0.100364	0.044280
C	6.860005	-0.256208	2.410597
P	3.991451	0.130174	-2.046609
C	7.095045	0.124792	-2.515204
C	0.720358	-0.105605	2.110876
C	0.982220	0.242388	-2.819737
C	-5.654593	-1.719892	-1.495534
C	0.798061	-3.145533	-0.944379
C	-5.694441	1.988059	0.456398
C	0.390540	4.286883	1.966752
C	-2.961983	2.469646	2.810715
H	-4.246223	1.025806	-0.803756
H	1.001726	-1.067175	2.554742
H	1.421487	1.170594	-3.198672
H	1.162929	0.706221	2.698002
H	1.408143	-0.612924	-3.353384
H	-2.911410	0.018799	3.680850
H	-4.678632	4.596693	-1.579362
H	-0.039039	-2.361850	0.869200
H	-2.896921	6.281916	-1.324941
H	-1.811281	-3.018769	2.967265
H	-3.482467	-3.161734	2.454395
H	-3.085624	-2.182025	3.888442
H	-3.322587	-6.145570	-1.405526
H	-5.098357	-4.447385	-1.156666
H	-0.772725	5.679574	-0.214897
H	-1.005107	-5.623742	-0.720790
H	-0.361602	-0.005009	2.125008
H	-3.658655	3.132795	2.291817
H	-2.053356	3.051589	3.000670
H	-3.391731	2.169949	3.767557
H	-0.119010	2.316690	1.300518
H	-4.489964	-0.976317	0.121370
H	0.022017	-4.494665	2.178333
H	1.619520	-4.044658	1.542229
H	0.688421	-5.333408	0.771034
H	-0.105557	0.248579	-2.941174
H	0.298181	-2.471623	-1.649109
H	0.927161	-4.111425	-1.446884
H	1.796103	-2.748935	-0.712490
H	-4.939910	-1.418274	-2.266988
H	-6.404260	-0.927273	-1.382831
H	-6.181593	-2.624519	-1.821156
H	0.727001	2.668077	-1.086176
H	1.985019	2.839293	0.166567
H	1.272251	4.274031	-0.595024
H	-0.366071	4.371962	2.752613
H	0.564237	5.291331	1.566173
H	1.327131	3.950991	2.427060
H	-6.137957	1.327664	-2.213639

H	-4.788177	2.246826	-2.889466
H	-6.119419	3.085630	-2.041181
H	-5.474122	-2.382584	1.923488
H	-6.395673	-3.299251	0.717796
H	-6.744228	-1.581999	0.987981
H	-6.509873	1.281481	0.260000
H	-6.136623	2.978927	0.621062
H	-5.204621	1.671249	1.383771
H	8.183278	0.107202	-2.468591
H	6.733164	-0.720820	-3.107920
H	6.756184	1.060691	-2.969692
H	6.450125	-1.180246	2.829831
H	7.947967	-0.274612	2.465021
H	6.473164	0.601546	2.969398

TS of the oxidative cleavage of the S=C bond in the presence of NacNacGa

G(M06-2X/6-31+G*)= -5247.037879
E(M06-2X/6-31+G*)=-5247.8233804

C	1.095010	3.781515	0.053329
C	2.152950	2.884834	0.275241
C	3.096004	3.131880	1.301553
C	3.016346	4.328778	2.013350
C	2.005013	5.250326	1.763101
C	1.040811	4.957660	0.808937
N	2.322447	1.702534	-0.514921
C	3.422304	1.640394	-1.301653
C	3.900537	2.909807	-1.966201
C	4.184282	2.129967	1.663291
C	5.574629	2.572734	1.186986
C	-0.018658	3.492628	-0.932316
C	-1.291838	3.144480	-0.148190
Ga	1.216353	0.099238	-0.398982
C	-0.598381	-0.471993	-1.527398
N	-1.606071	0.450726	-1.889495
C	-2.791868	0.160955	-1.250126
C	-2.578396	-1.043770	-0.528451
N	-1.325208	-1.497193	-0.885148
S	0.738073	-0.779680	-2.669447
C	-1.538382	1.346282	-3.025631
P	-4.233755	1.124727	-1.442420
C	-5.273536	0.252458	-0.327942
C	-5.018054	-0.857241	0.482868
N	-6.187426	-1.097527	1.193015
C	-7.165521	-0.197506	0.856906
N	-6.588843	0.622465	-0.078686
P	-3.584928	-1.860461	0.639683
C	-0.667519	-2.575227	-0.200085
C	-6.349278	-2.176999	2.145258
S	-8.724353	-0.116200	1.458539
C	-7.250911	1.740473	-0.718949
N	2.846565	-1.090683	-0.179727
C	3.979593	-0.735016	-0.743881
C	4.140427	0.472212	-1.487734
C	2.653971	-2.374439	0.430165
C	2.321420	-2.424175	1.799450
C	1.946724	-3.650409	2.354332
C	1.923036	-4.809550	1.590420
C	2.291850	-4.750754	0.252045
C	2.653637	-3.548095	-0.361662

C	2.396823	-1.208320	2.711696
C	1.030255	-0.843328	3.305735
C	3.028237	-3.596287	-1.839724
C	1.904112	-4.176934	-2.711168
C	5.233203	-1.560732	-0.588484
C	4.294096	-4.445810	-2.053399
C	3.419190	-1.454721	3.831014
C	4.216500	1.865455	3.173531
C	-0.260477	4.661926	-1.894650
H	3.943203	1.185054	1.167199
H	-2.108225	0.928273	-3.865073
H	-1.370528	-3.397543	-0.050242
H	-1.963356	2.318097	-2.760542
H	0.169136	-2.922926	-0.803850
H	5.040576	0.535506	-2.089725
H	3.752613	4.540604	2.784725
H	3.212222	-2.576629	-2.193687
H	1.956744	6.178339	2.325257
H	5.084974	-2.431574	0.049707
H	6.013892	-0.928428	-0.152877
H	5.589065	-1.892521	-1.569683
H	1.628915	-5.755061	2.036455
H	1.674902	-3.697486	3.405825
H	0.228007	5.659563	0.640927
H	2.288869	-5.662607	-0.339412
H	-0.498553	1.465442	-3.325811
H	4.067975	3.710976	-1.241224
H	3.121786	3.257726	-2.655718
H	4.821606	2.738936	-2.526823
H	0.275855	2.624281	-1.533407
H	2.750849	-0.354581	2.122782
H	5.113492	-4.163616	-1.387908
H	4.640946	-4.353218	-3.088472
H	4.076032	-5.504574	-1.872662
H	-0.285689	-2.234567	0.777364
H	0.993811	-3.577654	-2.655659
H	1.671370	-5.207677	-2.421209
H	2.223836	-4.191378	-3.759027
H	0.288273	-0.649270	2.524219
H	1.114802	0.059230	3.921482
H	0.649449	-1.649616	3.943437
H	-1.162537	2.220870	0.428285
H	-2.151784	3.011839	-0.811747
H	-1.540517	3.951492	0.550620
H	0.665370	4.959537	-2.397944
H	-0.656128	5.538052	-1.369870
H	-0.992553	4.385517	-2.660906
H	4.893207	1.032613	3.393270
H	3.220962	1.614205	3.555089
H	4.577980	2.738046	3.728449
H	4.417740	-1.641801	3.420448
H	3.137451	-2.323336	4.435616
H	3.475733	-0.589729	4.498777
H	6.328460	1.833906	1.482998
H	5.847705	3.533536	1.639676
H	5.623109	2.684189	0.100313
H	-6.215590	-3.140043	1.642580
H	-5.609263	-2.079213	2.945331
H	-7.355339	-2.110257	2.558707
H	-7.253072	1.598000	-1.803859

H	-8.274340	1.780932	-0.346832
H	-6.728730	2.671274	-0.475987

Product of the oxidative cleavage of the S=C bond in the presence of NacNacAl

G(M06-2X/6-31+G*)= -3566.578797
E(M06-2X/6-31+G*)= -3567.362479

C	-1.375092	3.662653	0.235493
C	-2.417278	2.726527	0.119772
C	-3.616681	3.036095	-0.555357
C	-3.764361	4.330259	-1.058389
C	-2.758135	5.282349	-0.922979
C	-1.568436	4.942446	-0.293703
N	-2.276759	1.409340	0.699247
C	-2.621531	1.256820	1.975781
C	-2.665294	0.007609	2.626596
C	-2.546144	-1.252039	2.018052
C	-2.757954	-2.469318	2.888239
C	-4.724800	2.006577	-0.733194
C	-5.485365	2.190641	-2.048179
C	-0.032839	3.314734	0.857952
C	1.052891	3.264420	-0.228733
N	-2.223747	-1.412872	0.735452
C	-2.497964	-2.700132	0.141195
C	-3.815987	-2.962424	-0.283228
C	-4.087700	-4.218252	-0.828427
C	-3.088976	-5.176632	-0.973718
C	-1.788677	-4.882223	-0.583129
C	-1.471845	-3.642212	-0.021630
C	-4.935567	-1.936457	-0.159600
C	-5.940759	-2.325220	0.934581
C	-0.033270	-3.317864	0.336064
C	0.606517	-4.357804	1.262284
Al	-1.710162	-0.013700	-0.502179
S	-2.385236	-0.140554	-2.474067
C	0.424392	0.056236	-0.369463
N	1.199628	-0.030739	0.742141
C	2.553496	-0.037119	0.436481
C	2.617181	0.065467	-0.958226
N	1.301339	0.117172	-1.398147
P	3.812412	-0.152447	1.651974
C	5.175732	-0.088449	0.573318
N	6.484107	-0.141940	1.015130
C	7.372873	-0.072261	-0.034546
N	6.588077	0.026308	-1.159927
C	5.241641	0.020488	-0.841244
S	9.030331	-0.100364	0.044280
C	6.860005	-0.256208	2.410597
P	3.991451	0.130174	-2.046609
C	7.095045	0.124792	-2.515204
C	0.720358	-0.105605	2.110876
C	0.982220	0.242388	-2.819737
C	-5.654593	-1.719892	-1.495534
C	0.798061	-3.145533	-0.944379
C	-5.694441	1.988059	0.456398
C	0.390540	4.286883	1.966752
C	-2.961983	2.469646	2.810715
H	-4.246223	1.025806	-0.803756
H	1.001726	-1.067175	2.554742
H	1.421487	1.170594	-3.198672

H	1.162929	0.706221	2.698002
H	1.408143	-0.612924	-3.353384
H	-2.911410	0.018799	3.680850
H	-4.678632	4.596693	-1.579362
H	-0.039039	-2.361850	0.869200
H	-2.896921	6.281916	-1.324941
H	-1.811281	-3.018769	2.967265
H	-3.482467	-3.161734	2.454395
H	-3.085624	-2.182025	3.888442
H	-3.322587	-6.145570	-1.405526
H	-5.098357	-4.447385	-1.156666
H	-0.772725	5.679574	-0.214897
H	-1.005107	-5.623742	-0.720790
H	-0.361602	-0.005009	2.125008
H	-3.658655	3.132795	2.291817
H	-2.053356	3.051589	3.000670
H	-3.391731	2.169949	3.767557
H	-0.119010	2.316690	1.300518
H	-4.489964	-0.976317	0.121370
H	0.022017	-4.494665	2.178333
H	1.619520	-4.044658	1.542229
H	0.688421	-5.333408	0.771034
H	-0.105557	0.248579	-2.941174
H	0.298181	-2.471623	-1.649109
H	0.927161	-4.111425	-1.446884
H	1.796103	-2.748935	-0.712490
H	-4.939910	-1.418274	-2.266988
H	-6.404260	-0.927273	-1.382831
H	-6.181593	-2.624519	-1.821156
H	0.727001	2.668077	-1.086176
H	1.985019	2.839293	0.166567
H	1.272251	4.274031	-0.595024
H	-0.366071	4.371962	2.752613
H	0.564237	5.291331	1.566173
H	1.327131	3.950991	2.427060
H	-6.137957	1.327664	-2.213639
H	-4.788177	2.246826	-2.889466
H	-6.119419	3.085630	-2.041181
H	-5.474122	-2.382584	1.923488
H	-6.395673	-3.299251	0.717796
H	-6.744228	-1.581999	0.987981
H	-6.509873	1.281481	0.260000
H	-6.136623	2.978927	0.621062
H	-5.204621	1.671249	1.383771
H	8.183278	0.107202	-2.468591
H	6.733164	-0.720820	-3.107920
H	6.756184	1.060691	-2.969692
H	6.450125	-1.180246	2.829831
H	7.947967	-0.274612	2.465021
H	6.473164	0.601546	2.969398

Product of the oxidative cleavage of the S=C bond in the presence of NacNacGa

G(M06-2X/6-31+G*)= -5247.118822
E(M06-2X/6-31+G*)= -5247.903700

N	6.594704	-0.116765	1.083824
C	5.288963	-0.084692	0.632330
C	5.363751	-0.014237	-0.784398
N	6.711960	-0.007086	-1.094280
C	7.490016	-0.069558	0.038551

P	3.919701	-0.129087	1.703944
C	2.668848	-0.056200	0.477553
N	1.312556	-0.047731	0.774355
C	0.549605	0.010633	-0.343219
N	1.427913	0.044021	-1.368395
C	2.741342	0.007136	-0.919061
Ga	-1.598088	-0.004451	-0.496540
S	-2.286764	-0.057842	-2.499936
C	0.819213	-0.109447	2.139061
P	4.121460	0.050514	-2.000856
C	1.116302	0.123612	-2.794707
C	7.227368	0.057842	-2.448397
S	9.146894	-0.084407	0.128559
C	6.962152	-0.189345	2.484364
N	-2.157362	-1.415651	0.784641
C	-2.461100	-1.227871	2.062782
C	-2.533841	0.036156	2.670765
C	-2.495496	1.284305	2.016732
N	-2.200961	1.437999	0.733604
C	-2.372613	2.741363	0.147152
C	-1.318754	3.667335	0.181902
C	-1.542267	4.949548	-0.326931
C	-2.774612	5.295852	-0.865382
C	-3.786274	4.342809	-0.946053
C	-3.606019	3.045712	-0.461521
C	0.066751	3.280665	0.668797
C	0.645564	4.245815	1.708382
C	-4.702237	1.997636	-0.600701
C	-5.611513	1.930123	0.633680
C	-2.477659	-2.686184	0.189474
C	-1.462799	-3.620778	-0.064703
C	-1.809536	-4.847596	-0.635183
C	-3.130572	-5.137850	-0.953063
C	-4.119279	-4.187268	-0.721655
C	-3.817808	-2.945367	-0.160048
C	-0.005667	-3.300699	0.211427
C	0.738812	-3.109598	-1.118798
C	-4.936086	-1.929708	0.038364
C	-5.532853	-1.513115	-1.312344
C	-2.738547	-2.432396	2.930029
C	-6.042959	-2.458696	0.961548
C	0.689752	-4.354199	1.080109
C	-2.792230	2.503298	2.859264
C	1.005677	3.169591	-0.542303
C	-5.532342	2.199429	-1.870460
H	-4.201051	1.030540	-0.714297
H	1.090266	-1.069792	2.591492
H	1.547569	1.045096	-3.198595
H	1.255931	0.706324	2.724444
H	1.556869	-0.742572	-3.298515
H	-2.748992	0.052852	3.731554
H	-4.729512	4.611788	-1.411086
H	0.023840	-2.354197	0.761083
H	-2.940207	6.298495	-1.249048
H	-1.913317	-3.148731	2.847598
H	-3.638678	-2.957408	2.600112
H	-2.863175	-2.140540	3.973975
H	-3.388203	-6.096351	-1.394247
H	-5.147648	-4.410351	-0.995199
H	-0.739585	5.682928	-0.305285

H	-1.034214	-5.582927	-0.837076
H	-0.262272	-0.006219	2.135543
H	-3.541753	3.143829	2.386800
H	-1.884170	3.108183	2.964423
H	-3.139673	2.213436	3.851936
H	-0.004637	2.290328	1.131298
H	-4.513809	-1.029144	0.500093
H	0.167738	-4.497121	2.032390
H	1.720602	-4.047862	1.294676
H	0.733409	-5.324834	0.574341
H	0.028812	0.119168	-2.928679
H	0.194401	-2.423108	-1.777336
H	0.828874	-4.068024	-1.643334
H	1.751620	-2.720121	-0.947074
H	-4.760734	-1.076726	-1.953874
H	-6.328534	-0.775471	-1.152435
H	-5.976497	-2.374116	-1.826373
H	0.552990	2.554914	-1.326526
H	1.970253	2.729399	-0.255163
H	1.196057	4.160855	-0.969444
H	-0.013029	4.353998	2.576177
H	0.800616	5.243123	1.283008
H	1.619327	3.884547	2.059702
H	-6.177183	1.330103	-2.029086
H	-4.880941	2.295962	-2.744276
H	-6.181106	3.081342	-1.804805
H	-5.663245	-2.758752	1.943532
H	-6.542671	-3.326929	0.516896
H	-6.801227	-1.683237	1.116641
H	-6.410717	1.197679	0.467276
H	-6.079076	2.903155	0.831424
H	-5.067719	1.621442	1.533008
H	8.315361	0.050468	-2.394099
H	6.876464	-0.806884	-3.019741
H	6.884176	0.977984	-2.930936
H	6.554629	-1.103464	2.926981
H	8.049820	-0.200115	2.546096
H	6.567166	0.681742	3.016180