Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Ligand Effects on the Electrochemical Behavior of $[Fe_2(CO)_5(L)\{\mu\text{-}(SCH_2)_2(Ph)P{=}O\}]$ (L = PPh_3, $P(OEt)_3$) Hydrogenase Model Complexes

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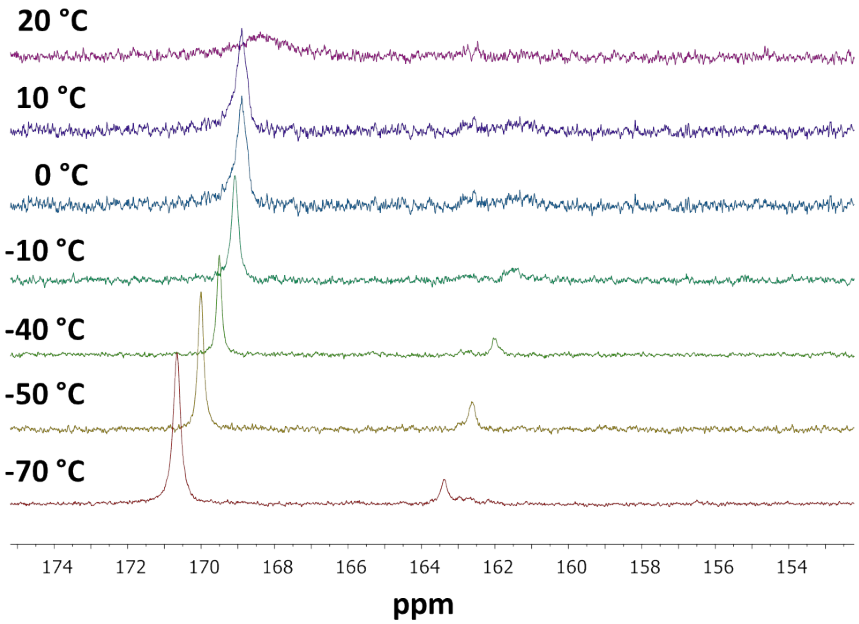


Figure S1. Variable temperature $^{31}P\{^{1}H\}$ NMR spectra at 400 MHz of complex **3** in MeOD. Only the resonance due to the $P(OEt)_3$ ligand is shown.

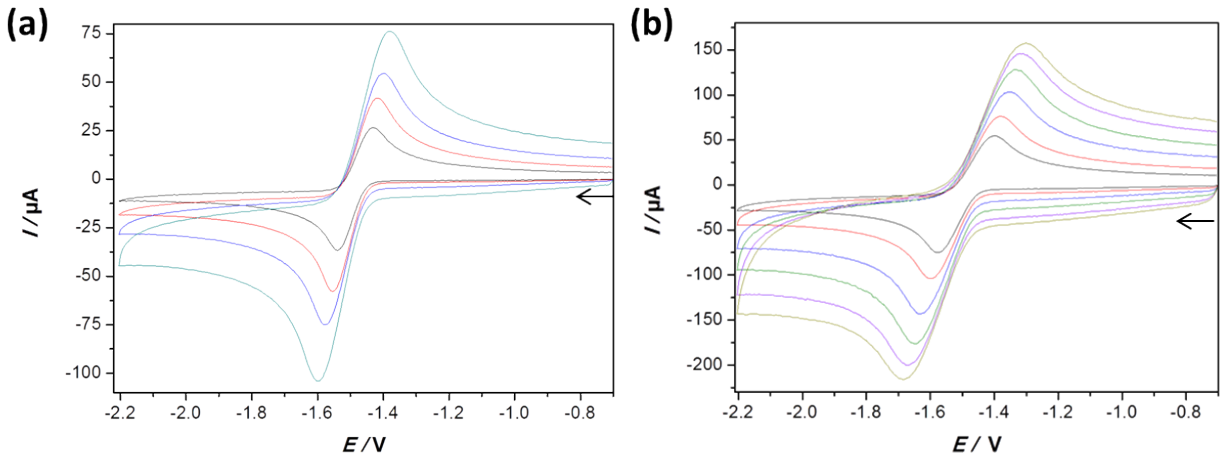


Figure S2. Cyclic voltammetry of 0.65 mM complex **1** (CH_2Cl_2/NBu_4PF_6 solution) at scan rates ($V \cdot s^{-1}$) = (a) 0.2 (black), 0.5 (red), 1 (blue), 2 (green), (b) 1 (black), 2 (red), 4 (blue), 6 (green), 8 (violet) and 10 (dark yellow). *E* is in V against the ferrocenium/ferrocene couple. The arrows indicate the scan direction.

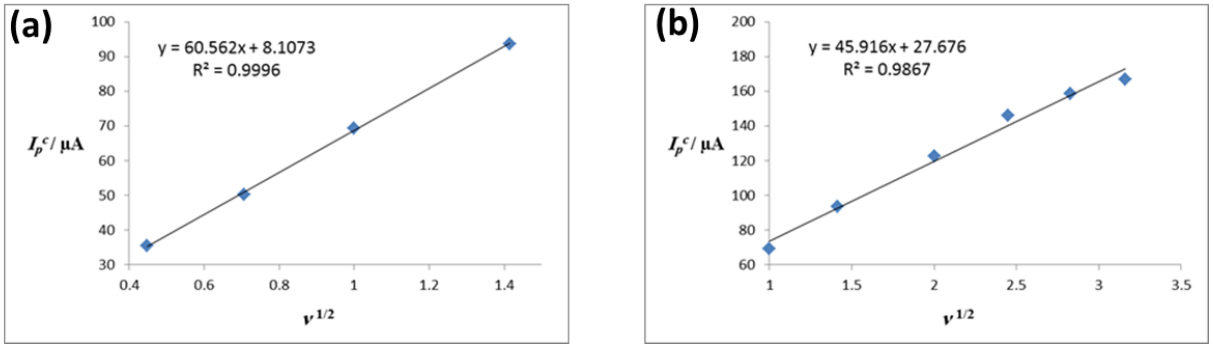


Figure S3. Plots of the cathodic current (I_p^c) versus square root of scan rate ($v^{1/2}$/ $(V \cdot s^{-1})^{1/2}$) obtained from the cyclic voltammetry of complex **1** in (a) Figures S2a and (b) Figure S2b.

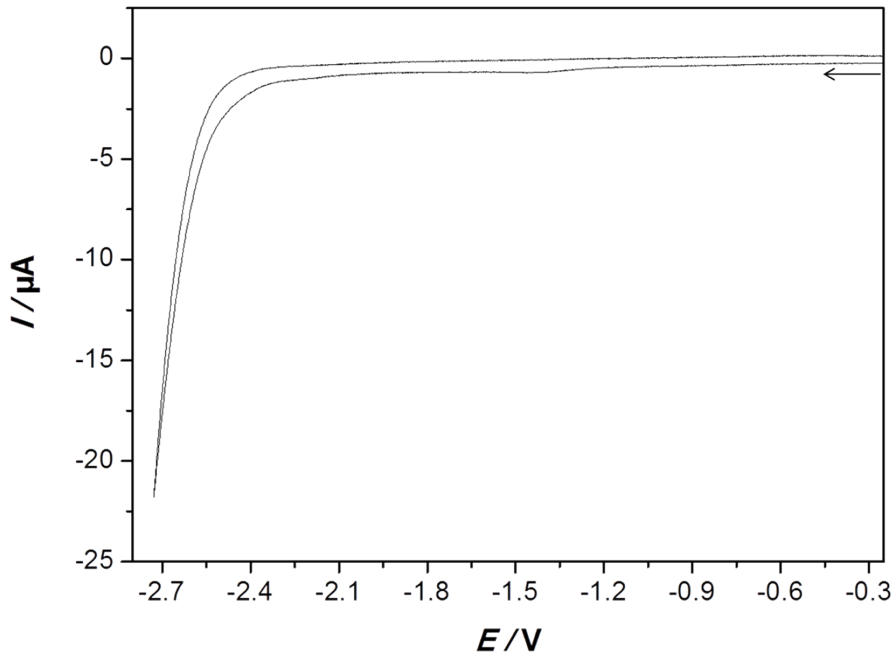


Figure S4. Cyclic voltammetry of 3.13 mM O=P(Ph)(CH_2Cl)$_2$ (CH_2Cl_2/NBu_4PF_6 solution) at 0.2 V·s^{-1}). *E* is in V against the ferrocenium/ferrocene couple. Glassy carbon disk (d = 1.6 mm). The arrows indicate the scan direction.

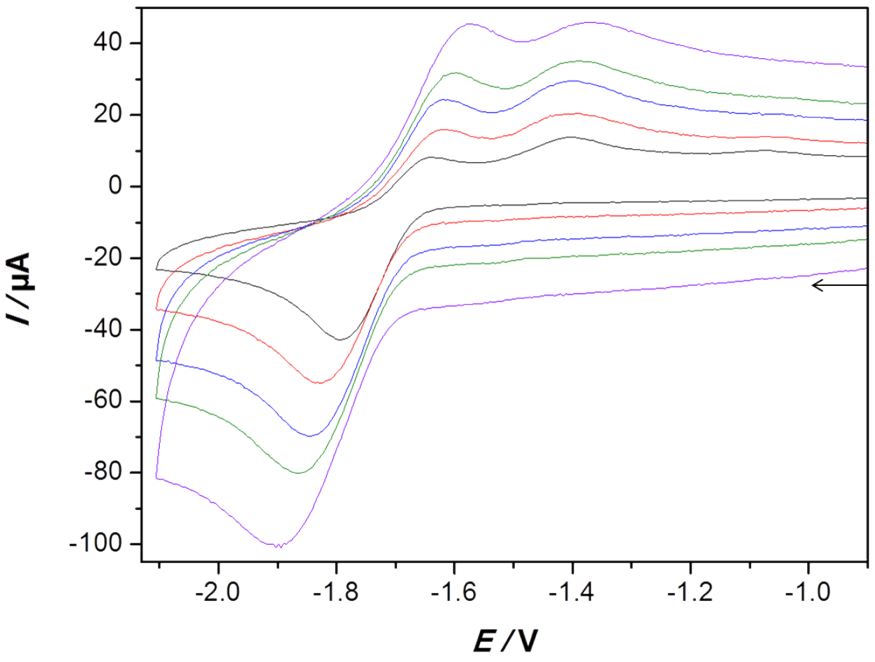


Figure S5. Cyclic voltammetry of 0.408 mM complex **2** (CH_2Cl_2/NBu_4PF_6 solution) at scan rates ($V \cdot s^{-1}$) equal to 1 (black), 2 (red), 3 (blue), 4 (green) and 6 (purple). *E* is in V against the ferrocenium/ferrocene couple. The arrow indicates the scan direction.

Table S1. Results of DFT calculations of **5** and **6** in the neutral, monoanionic and dianionic state as well as P1, P2 and the reduced species derived from them (See the paragraph discussing the structure of **P** and Figures S10 and S11).

	E_T [a.u.]	*NImag*	Stabilization [kJ·mol^{-1}]
5	-2799.196753	1*	0
5^{-}	-2799.260484	1*	-167.3
5^{2-}	-2799.206017	0	-24.3
5a^{2-}	-2799.225453	0	-75.4
5b^{2-}	-2799.212985	0	-42.6
6	-3024.944206	0	0
6^{-}	-3025.014420	0	-184.3
6^{2-}	-3024.951196	0	-18.4
6a^{2-}	-3024.963479	0	-50.6
6b^{2-}	-3024.956772	0	-33.0
P1	-3256.248118	0	
P2	-3256.238331	0	
P1^{-}	-3256.269607	0	
P1^{0}	-3256.190197	0	
P2^{0}	-3256.182587	0	

* One imaginary frequency corresponds to the rotation of the PMe_3 ligand with respect to the $[Fe_2S_2]$ cluster core and is of very low intensity.

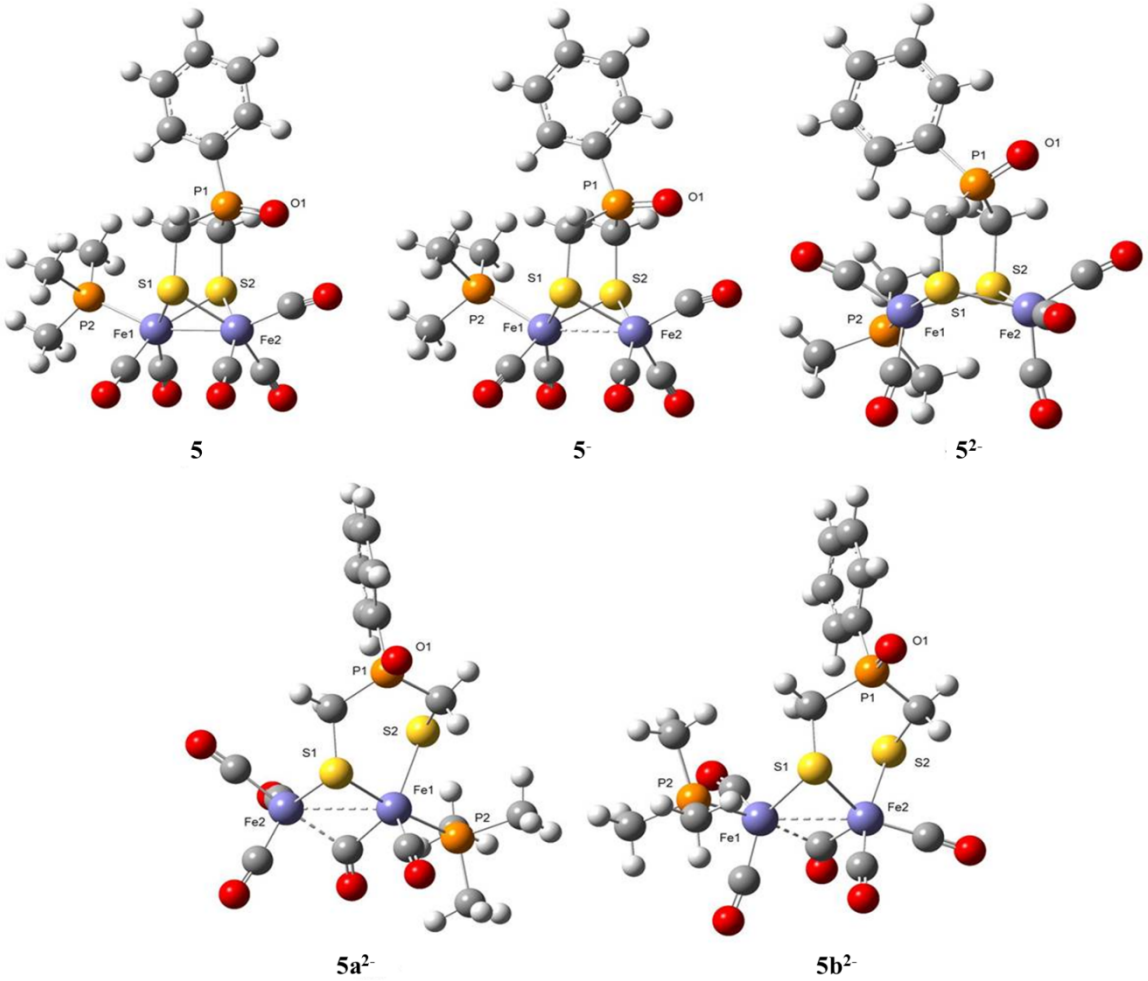


Figure S6. Calculated molecular structures and selected bond lengths [pm] of **5**: Fe1-Fe2 249.7, Fe1-S1 234.0, Fe1-S2 234.4, Fe2-S1 234.7, Fe2-S2 234.3, Fe1-P2 226.3, P1-O1 149.7; **5**$^{-}$: Fe1-Fe2 274.0, Fe1-S1 237.8, Fe1-S2 237.9, Fe2-S1 240.0, Fe2-S2 239.7, Fe1-P2 234.1, P1-O1 150.0; **5**$^{2-}$: Fe1-Fe2 350.7, Fe1-S1 236.9, Fe1-S2 244.7, Fe2-S1 242.2, Fe2-S2 239.9, Fe1-P2 220.0, P1-O1 151.2; **5a**$^{2-}$: Fe1-Fe2 265.2, Fe1-S1 231.1, Fe1-S2 254.3, Fe2-S1 237.9, Fe1-P2 224.0, P1-O1 151.5; **5b**$^{2-}$: Fe1-Fe2 271.8, Fe1-S1 244.0, Fe2-S1 234.7, Fe2-S2 245.1, Fe1-P2 220.2, P1-O1 151.6.

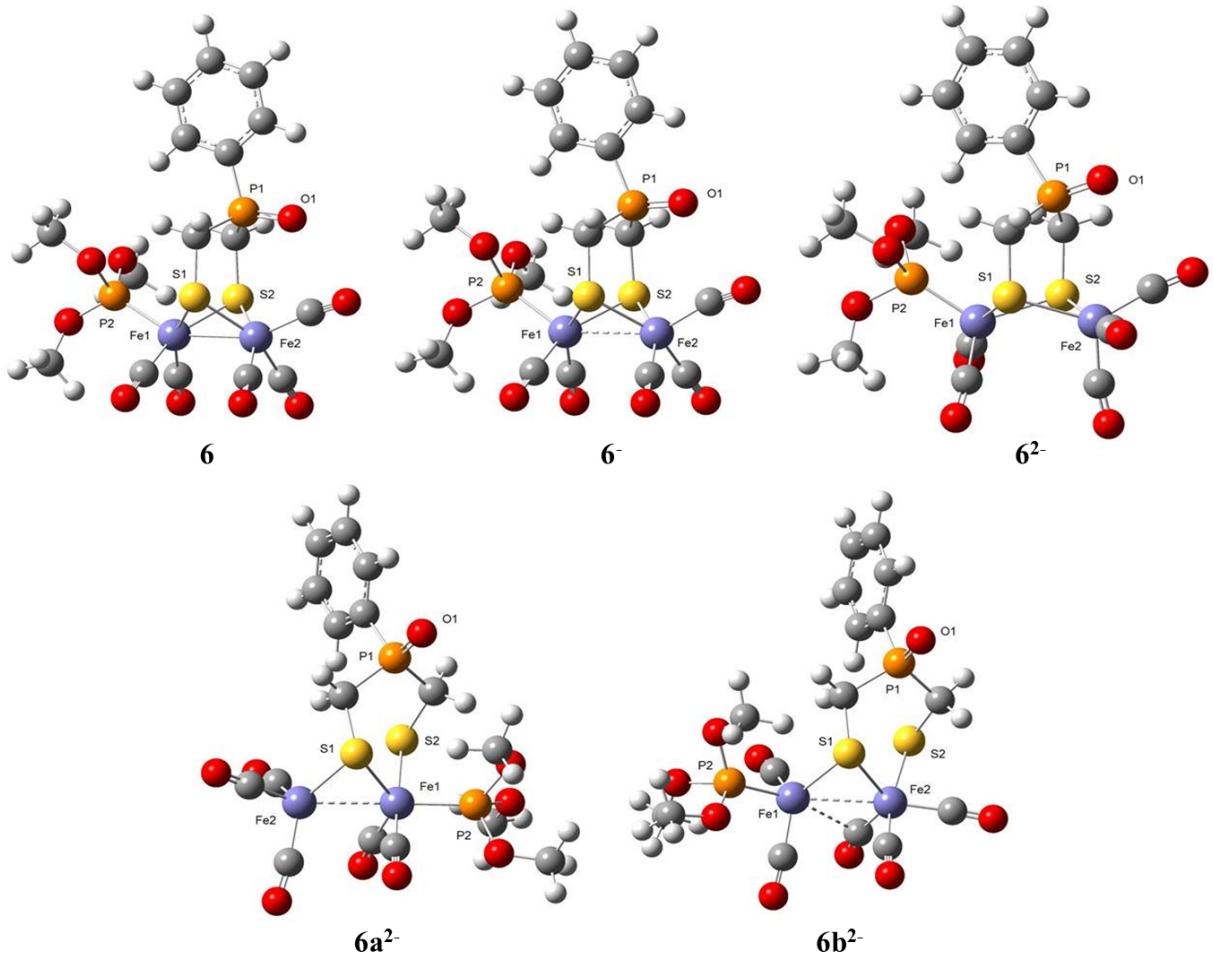


Figure S7. Calculated molecular structures and selected bond lengths [pm] of **6**: Fe1-Fe2 250.6, Fe1-S1 232.6, Fe1-S2 233.1, Fe2-S1 233.1, Fe2-S2 233.3, Fe1-P2 219.0, P1-O1 149.8; **6**$^{-}$: Fe1-Fe2 276.3, Fe1-S1 236.9, Fe1-S2 237.8, Fe2-S1 237.7, Fe2-S2 238.4, Fe1-P2 219.8, P1-O1 150.2; **6**$^{2-}$: Fe1-Fe2 344.7, Fe1-S1 240.7, Fe1-S2 240.4, Fe2-S1 244.0, Fe2-S2 239.7, Fe1-P2 210.0, P1-O1 150.8; **6a**$^{2-}$: Fe1-Fe2 272.5, Fe1-S1 236.7, Fe1-S2 245.7, Fe2-S1 232.9, Fe1-P2 214.7, P1-O1 151.6; **6b**$^{2-}$: Fe1-Fe2 273.9, Fe1-S1 234.7, Fe2-S1 235.9, Fe2-S2 244.6, Fe1-P2 211.1, P1-O1 151.6.

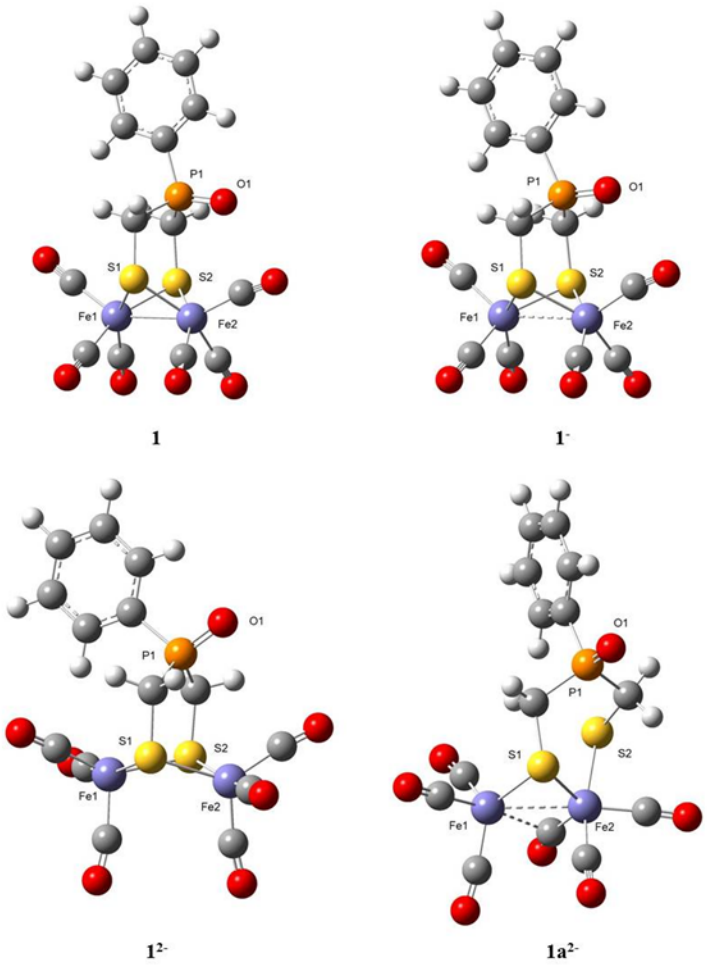


Figure S8. Calculated molecular structures and selected bond lengths [pm] of **1**: Calculated molecular structures and selected bond lengths [pm] of **1**: HF = -2451.489710 a.u., *NImag* = 0, Fe1-Fe2 251.2, Fe1-S1 231.9, Fe1-S2 231.9, Fe2-S1 232.7, Fe2-S2 232.7, P1-O1 149.7; $\mathbf{1}^{-}$: HF = -2451.571974 a.u. (-216.0 kJ·mol^{-1} relative to **1**), *NImag* = 0, Fe1-Fe2 281.0, Fe1-S1 237.3, Fe1-S2 237.3, Fe2-S1 236.9, Fe2-S2 236.9, P1-O1 150.1; $\mathbf{1}^{2-}$: HF = -2451.521008 a.u. (-82.2 kJ·mol^{-1} relative to **1**), *NImag* = 0, Fe1-Fe2 352.7, Fe1-S1 239.3, Fe1-S2 240.8, Fe2-S1 241.3, Fe2-S2 239.5, P1-O1 151.2; $\mathbf{1a}^{2-}$: HF = -2451.528961 a.u. (-13.1 kJ·mol^{-1} relative to **1**), *NImag* = 0, Fe1-Fe2 273.0, Fe1-S1 234.8, Fe2-S1 235.9, Fe2-S2 244.2, P1-O1 151.5.

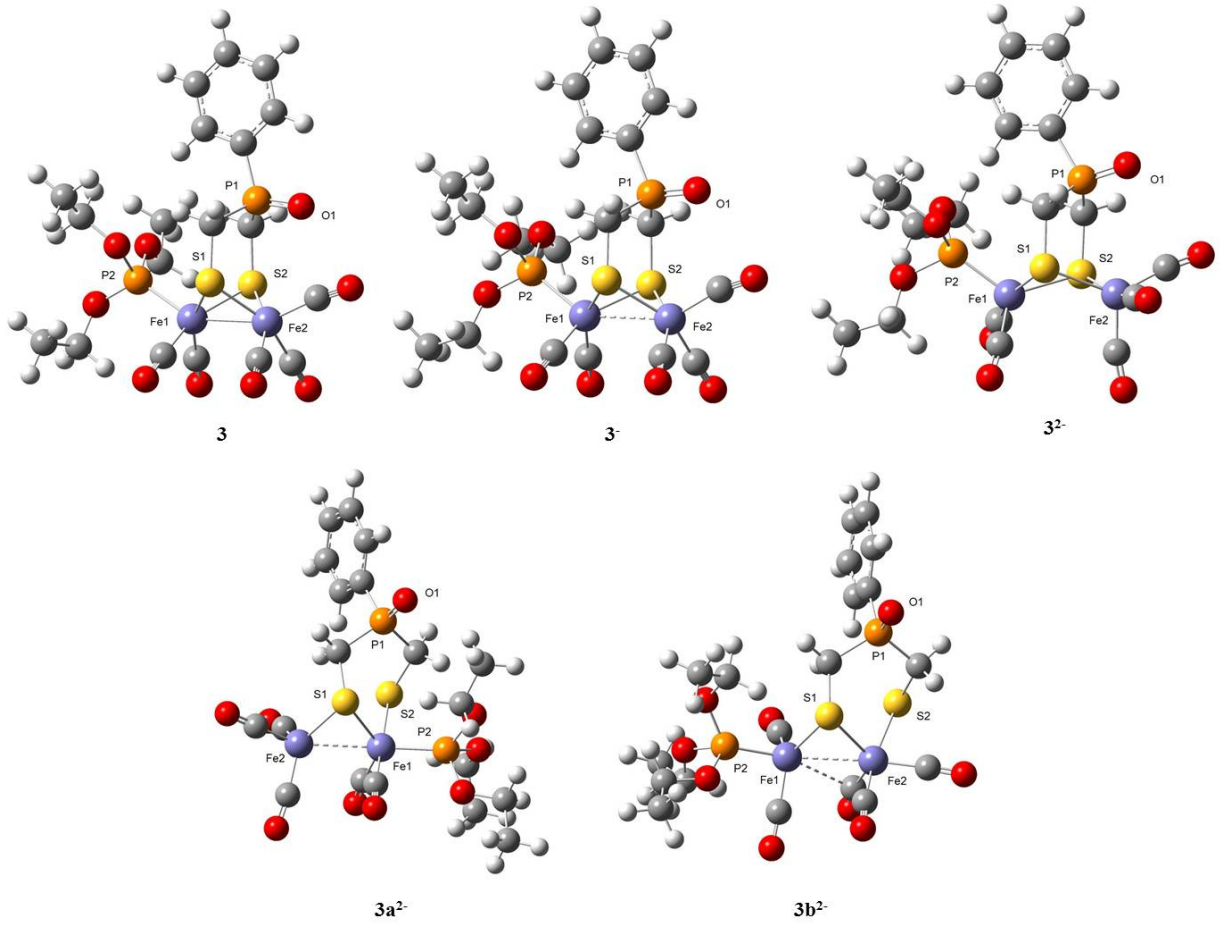


Figure S9. Calculated molecular structures and selected bond lengths [pm] of **3**: HF = -3142.854678 a.u., *NImag* = 0, Fe1-Fe2 251.7, Fe1-S1 232.6, Fe1-S2 232.9, Fe2-S1 233.0, Fe2-S2 232.9, Fe1-P2 220.8, P1-O1 150.0; $\mathbf{3}^{-}$: HF = -3142.922307 a.u. (-177.6 kJ·mol^{-1} relative to **3**), *NImag* = 0, Fe1-Fe2 278.5, Fe1-S1 236.3, Fe1-S2 237.1, Fe2-S1 237.9, Fe2-S2 237.6, Fe1-P2 221.9, P1-O1 150.3; $\mathbf{3}^{2-}$: HF = -3142.860589 a.u. (-15.5 kJ·mol^{-1} relative to **3**), *NImag* = 0, Fe1-Fe2 344.8, Fe1-S1 240.9, Fe1-S2 241.1, Fe2-S1 244.5, Fe2-S2 239.7, Fe1-P2 210.8, P1-O1 151.0; $\mathbf{3a}^{2-}$: HF = -3142.872079 a.u. (-45.7 kJ·mol^{-1} relative to **3**), *NImag* = 0, Fe1-Fe2 272.6, Fe1-S1 236.7, Fe1-S2 245.8, Fe2-S1 232.6, Fe1-P2 215.3, P1-O1 151.7; $\mathbf{3b}^{2-}$: HF = -3142.867376 a.u. (-33.3 kJ·mol^{-1} relative to **3**), *NImag* = 0, Fe1-Fe2 274.3, Fe1-S1 235.1, Fe2-S1 236.4, Fe2-S2 244.7, Fe1-P2 211.7, P1-O1 151.5.

Structure of P.

Another important question that arose during the electrochemical investigations was the molecular structure of compound **P**, which is formed by the reaction of the doubly reduced form of **3** with CO. We therefore calculated compounds with one additional CO ligand starting either from $\mathbf{3}^{2-}$ or $\mathbf{3a}^{2-}$. In the case of $\mathbf{3a}^{2-}$ as the substrate, we used a compound with two bridging CO ligands as the starting point for geometry optimization. Nevertheless, a convergence in the calculations was only reached after significant structural changes in the cluster core ending up with a situation in which a Lewis acid-Lewis base adduct, namely **P1**, consisting of a trigonal pyramidal $[Fe(CO)_4]$ and a square planar $\{Fe(CO)_2(P(OEt)_3)[(SCH_2)_2(Ph)P{=}O]\}$ fragment linked by an iron iron contact is observed (Figure S10). By forming this adduct, the coordination geometry of the first iron is completed to a distorted trigonal bipyramidal coordination environment and the second iron then shows a distorted octahedral geometry. The iron-iron interaction is quite weak with a bond length of 312.5 pm. Perhaps this long distance shows how the compound might decompose. If on the other hand the thermodynamically less stable dianion $\mathbf{3}^{2-}$ is used as the substrate for CO addition, one of the Fe-S bonds in the symmetrical $[Fe_2S_2]$ core is broken upon geometry optimization. The resulting structure **P2** still shows one bridging sulfur that coordinates a $[Fe(CO)_4]$ and a $\{Fe(CO)_2(P(OEt)_3)[(SCH_2)_2(Ph)P{=}O]\}$ fragment (Figure S10). Both iron atoms exhibit trigonal bipyramidal coordination environments. The overall reactions for the formation of **P1** and **P2** from the respective starting compounds are slightly exothermic with an enthalpy of -33.9 $kJ{\cdot}mol^{-1}$ (**P1**) and -38.4 $kJ{\cdot}mol^{-1}$ (**P2**). Nevertheless, **P1** is 25.7 $kJ{\cdot}mol^{-1}$more stable than **P2** if only those calculated compounds are compared. Table S1 above shows the DFT total energies E_T and the number of imaginary

frequencies for all stationary points calculated for **P1** and **P2** as well as selected calculated bond lengths.

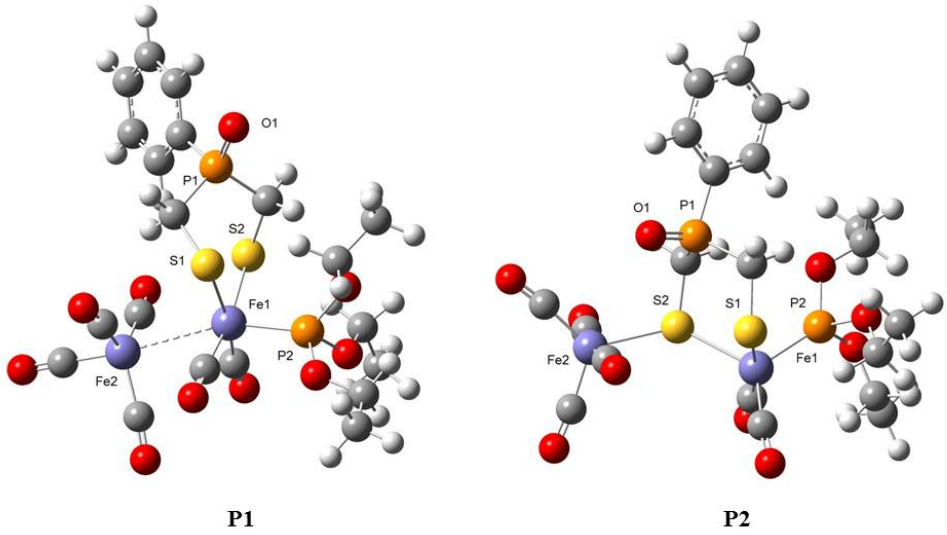
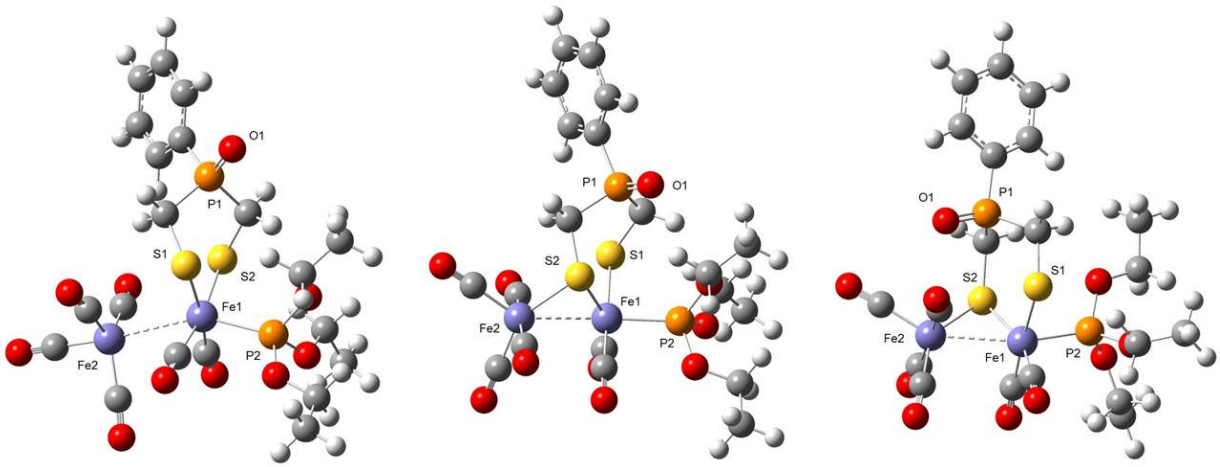


Figure S10. Calculated molecular structures and selected bond lengths [pm] of dianionic species **P1**: Fe1-Fe2 312.5, Fe1-S1 242.9, Fe1-S2 243.4, Fe1-P2 219.5, P1-O1 151.8; **P2**: Fe1-Fe2 451.3, Fe1-S1 241.2, Fe1-S2 248.5, Fe2-S2 243.9, Fe1-P2 212.1, P1-O1 150.7.

It has also been shown by cyclic voltammetry (Figure 6 and Scheme 3) that compound **P** undergoes a reversible oxidation process. We therefore calculated both monoanionic and neutral species with the calculated structures of **P1** and **P2** as the starting geometries. Whereas the geometry optimization of **P2** after one-electron oxidation did not converge, the corresponding monoanionic species from **P1** could be calculated. In both cases neutral compounds that would be obtained from the loss of two electrons from **P1** or **P2**, respectively, could be calculated. The corresponding structures are depicted in Figure S11. The monoanion derived from **P1** shows the

same connectivity pattern although it is obvious that upon loss of one electron the iron-iron bond length as well as the distances of Fe1 towards the coordinating sulfur atoms are shortened. If another electron is removed, electron demand in the cluster core is compensated by one of the sulfur atoms moving into a bridging position again. In addition, the iron-iron distance is further diminished. The same trend is observed if **P2** is oxidized. If two electrons are removed the iron atoms are again moved into close proximity to each other resulting in the same $[Fe_2S_2]$ cluster core for $\mathbf{P2^0}$ as in $\mathbf{P1^0}$. Both compounds are therefore isomers, which just differ in the dihedral angle of the $Fe(CO)_4$ group with respect to the rest of the molecule as well as in the conformation of the six-membered FeS_2C_2P ring. In summary, the addition of CO to the reduced species followed by oxidation of the resulting cluster compounds **P1** and **P2** results in the formation of compounds with the same connectivity as it has been observed for $\mathbf{3a^{2-}}$ and $\mathbf{3b^{2-}}$. As it is expected from the Wade-Mingos rules, the composition of a transition metal cluster compound is determined by the number of electrons in the cluster irrespective whether electrons are provided by additional ligands ($\mathbf{P1^0}$, $\mathbf{P2^0}$) or by reduction ($\mathbf{3a^{2-}}$, $\mathbf{3b^{2-}}$).



P1^{-} **P1**^{0} **P2**^{0}

Figure S11. Calculated molecular structures and selected bond lengths of **P1**$^{-}$: Fe1-Fe2 303.1, Fe1-S1 235.9, Fe1-S2 236.1, Fe1-P2 228.4, P1-O1 151.0; **P1**^{0}: Fe1-Fe2 283.6, Fe1-S1 240.3, Fe1-S2 230.1, Fe2-S2 235.8, Fe1-P1 223.1, P1-O1 150.6; **P2**^{0}: Fe1-Fe2 282.4, Fe1-S1 240.0, Fe1-S2 227.3, Fe2-S2 235.7, Fe1-P1 221.2, P1-O1 150.2.

Molecular coordinates of **1**

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Molecular coordinates of **1**$^{-}$

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   -3.7613   -1.6933   -2.0880 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.1572    2.5257    2.0905 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.1573    2.5256   -2.0905 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.6924    3.6814   -0.0001 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.2766   -0.0680    1.4827 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.6510    0.9534    1.5798 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.6528   -0.6514    2.3279 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.2766   -0.0681   -1.4826 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.6528   -0.6515   -2.3279 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.6511    0.9533   -1.5798 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.7619   -0.2306    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.1052    1.1279   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.3341    1.8915   -0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.4436    1.5158   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.6984    2.5702   -0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.4517    0.5512   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.4932    0.8553   -0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.1174   -0.8021    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.8987   -1.5550    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.7785   -1.1917    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.4976   -2.2393    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9546   -2.9440   -0.0001 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9703   -1.5126    1.2707 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9704   -1.5125   -1.2706 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4576    2.1243    1.2647 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4577    2.1242   -1.2647 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.0511    2.7925   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  1 30  1  0  0  0  0
  1 31  1  0  0  0  0
  1 32  1  0  0  0  0
  2 33  1  0  0  0  0
  2 34  1  0  0  0  0
  2 35  1  0  0  0  0
  3 13  1  0  0  0  0
  4 16  1  0  0  0  0
  5  6  2  0  0  0  0
```

5	13	1	0	0	0	0
5	16	1	0	0	0	0
5	19	1	0	0	0	0
7	30	3	0	0	0	0
8	31	3	0	0	0	0
9	32	3	0	0	0	0
10	33	3	0	0	0	0
11	34	3	0	0	0	0
12	35	2	0	0	0	0
13	14	1	0	0	0	0
13	15	1	0	0	0	0
16	17	1	0	0	0	0
16	18	1	0	0	0	0
19	20	4	0	0	0	0
19	28	4	0	0	0	0
20	21	1	0	0	0	0
20	22	4	0	0	0	0
22	23	1	0	0	0	0
22	24	4	0	0	0	0
24	25	1	0	0	0	0
24	26	4	0	0	0	0
26	27	1	0	0	0	0
26	28	4	0	0	0	0
28	29	1	0	0	0	0

Molecular coordinates of **1^{2-}**

```
12-, Fe2-Komplex, S2-Phosphanoxid-verbrueckt, Dianion

Created by GaussView 5.0.8
 35 33  0  0  0  0  0  0  0  0  0    0
    1.3877   -1.6309    0.0250 P   0  0  0  0  0  0  0  0  0  0  0  0
    0.6609   -0.9186    1.5791 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.6697   -0.9383   -1.5441 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.4193   -1.8154    2.1570 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8422    0.1481    1.5310 S   0  0  0  0  0  0  0  0  0  0  0  0
    1.4560   -0.3756    2.0969 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.1475   -1.0292    0.0117 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.4257   -3.1448    0.0432 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.4190   -1.8381   -2.1133 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8076    0.1639   -1.5224 S   0  0  0  0  0  0  0  0  0  0  0  0
    1.4734   -0.4129   -2.0658 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.5055    0.3234   -0.0368 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.1544   -2.0004    0.0470 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.8498    0.6944   -0.0470 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.7281    1.0824   -0.0630 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.4989   -1.6283    0.0362 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.8556   -3.0431    0.0805 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.8499   -0.2785   -0.0104 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.1126    1.7469   -0.0817 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.2721   -2.3912    0.0635 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.8961    0.0142   -0.0180 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.2483    1.9159    0.0293 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    0.8832    2.5092    1.2245 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.6325    2.7383   -1.2450 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.7414    2.8835    0.1496 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.5950    2.9314    2.0548 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.2113    3.2762   -2.1060 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5529    3.7105    0.2627 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3162   -0.9524   -0.0382 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -3.1213   -1.7779    1.2874 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1714   -2.4530   -0.9447 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.7093    0.0385   -0.5043 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.6409   -2.3165    2.1797 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2049   -3.4127   -1.6128 O   0  0  0  0  0  0  0  0  0  0  0  0
   -4.7115    0.5153   -0.8661 O   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1  3  1  0  0  0  0
  1  7  1  0  0  0  0
  1  8  2  0  0  0  0
  2  4  1  0  0  0  0
  2  5  1  0  0  0  0
  2  6  1  0  0  0  0
  3  9  1  0  0  0  0
  3 10  1  0  0  0  0
```

3	11	1	0	0	0	0
7	12	4	0	0	0	0
7	13	4	0	0	0	0
12	14	4	0	0	0	0
12	15	1	0	0	0	0
13	16	4	0	0	0	0
13	17	1	0	0	0	0
14	18	4	0	0	0	0
14	19	1	0	0	0	0
16	18	4	0	0	0	0
16	20	1	0	0	0	0
18	21	1	0	0	0	0
22	23	1	0	0	0	0
22	24	1	0	0	0	0
22	25	1	0	0	0	0
23	26	2	0	0	0	0
24	27	2	0	0	0	0
25	28	2	0	0	0	0
29	30	1	0	0	0	0
29	31	1	0	0	0	0
29	32	1	0	0	0	0
30	33	2	0	0	0	0
31	34	2	0	0	0	0
32	35	2	0	0	0	0

Molecular coordinates of **1a^{2-}**

```
1a2-, Fe2(CO)6-Komplex, Dianion umgelagert

Created by GaussView 5.0.8
 35 33  0  0  0  0  0  0  0  0  0    0
    2.4101    0.7150   -1.0873 P   0  0  0  0  0  0  0  0  0  0  0  0
    1.1403   -0.6082   -1.1465 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.7821    2.0106    0.0510 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.4648   -1.3127   -1.9176 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.1409   -1.1117   -0.1823 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.5975   -0.1000   -1.5321 S   0  0  0  0  0  0  0  0  0  0  0  0
    3.8152   -0.0890   -0.1769 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.9249    1.2256   -2.4178 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.6554    2.4987    0.4942 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.2655    2.7424   -0.5741 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.6632    1.3805    1.3702 S   0  0  0  0  0  0  0  0  0  0  0  0
    3.6948   -0.6341    1.1096 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.0547   -0.1401   -0.8245 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.8002   -1.2143    1.7317 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.7397   -0.5869    1.6226 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.1575   -0.7267   -0.2030 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.1284    0.2880   -1.8189 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.0323   -1.2650    1.0780 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.6949   -1.6318    2.7282 H   0  0  0  0  0  0  0  0  0  0  0  0
    7.1134   -0.7637   -0.7180 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.8888   -1.7235    1.5639 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9179   -1.3882   -0.0797 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -1.8219   -2.8084   -1.0780 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.6817   -1.4227   -0.0873 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0963   -2.1070    1.3101 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.7495   -3.7593   -1.7510 O   0  0  0  0  0  0  0  0  0  0  0  0
   -4.8415   -1.5714   -0.0276 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6775   -2.6993    2.2265 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4597    1.2922    0.1659 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -2.2690    0.5335    1.5708 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9271    1.5179   -0.7976 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3320    3.0256    0.3699 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.8040    0.4187    2.6022 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.8727    1.7628   -1.4173 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3011    4.1792    0.5372 O   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1  3  1  0  0  0  0
  1  7  1  0  0  0  0
  1  8  2  0  0  0  0
  2  4  1  0  0  0  0
  2  5  1  0  0  0  0
  2  6  1  0  0  0  0
  3  9  1  0  0  0  0
  3 10  1  0  0  0  0
```

3	11	1	0	0	0	0
7	12	4	0	0	0	0
7	13	4	0	0	0	0
12	14	4	0	0	0	0
12	15	1	0	0	0	0
13	16	4	0	0	0	0
13	17	1	0	0	0	0
14	18	4	0	0	0	0
14	19	1	0	0	0	0
16	18	4	0	0	0	0
16	20	1	0	0	0	0
18	21	1	0	0	0	0
22	23	1	0	0	0	0
22	24	1	0	0	0	0
22	25	1	0	0	0	0
23	26	2	0	0	0	0
24	27	2	0	0	0	0
25	28	2	0	0	0	0
29	30	1	0	0	0	0
29	31	1	0	0	0	0
29	32	1	0	0	0	0
30	33	2	0	0	0	0
31	34	3	0	0	0	0
32	35	2	0	0	0	0

Molecular coordinates of **2**

```
2, Fe2-Komplex, S2-Phosphanoxid-verbrueckt, PPh3

Created by GaussView 5.0.8
 67 68  0  0  0  0  0  0  0  0  0    0
    1.8811   -0.7444    0.0116 P   0  0  0  0  0  0  0  0  0  0  0  0
    1.1590   -2.0868   -1.0450 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.2033   -1.5860    1.6330 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.8836   -1.8019   -2.3919 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.8624   -3.3647   -0.5557 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.6192   -0.5923   -0.6362 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.7565    1.2782    0.0129 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    3.2067   -2.5611    1.7469 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.4567   -1.2514    2.7670 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.3508   -2.7772   -3.2303 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.0767   -0.8120   -2.7883 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.3166   -4.3370   -1.3957 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.0604   -3.6113    0.4796 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.4923    0.2714    0.0420 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.0965   -1.2869   -1.7522 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.7464    2.0040   -1.2884 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.7471    2.0480    1.2794 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.4409   -3.1963    2.9626 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.8140   -2.8183    0.8871 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.6932   -1.8896    3.9855 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.7016   -0.4777    2.7072 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.0651   -4.0495   -2.7345 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.1518   -2.5394   -4.2692 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.0957   -5.3220   -0.9993 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.8053    0.4358   -0.3868 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.1556    0.8142    0.9169 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.4126   -1.1150   -2.1850 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.4527   -1.9692   -2.2911 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.3621    2.4894   -2.1238 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.3682    2.5699    2.0914 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.6818   -2.8639    4.0854 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.2216   -3.9454    3.0351 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.1093   -1.6128    4.8560 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3549   -4.8069   -3.3864 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.2697   -0.2549   -1.5061 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.4642    1.1072    0.1521 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.7633   -1.6598   -3.0545 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.8697   -3.3550    5.0336 H   0  0  0  0  0  0  0  0  0  0  0  0
    7.2910   -0.1216   -1.8441 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2068    2.8523    0.0018 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -0.6889    3.9933   -1.2879 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.7231    4.0093    1.2930 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9822    3.3092   -0.0211 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3644    4.7236   -2.1055 O   0  0  0  0  0  0  0  0  0  0  0  0
```

-0.4209	4.7500	2.1096	O	0	0	0	0	0	0	0	0	0	0	0	0
-4.0227	3.7685	-0.0431	O	0	0	0	0	0	0	0	0	0	0	0	0
-2.0950	-0.2694	1.4634	C	0	0	0	0	0	0	0	0	0	0	0	0
-3.2400	-0.2685	0.0368	P	0	0	0	0	0	0	0	0	0	0	0	0
-2.7187	-0.2690	2.3602	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.4980	-1.1836	1.4654	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.9571	1.1762	1.6136	S	0	0	0	0	0	0	0	0	0	0	0	0
-2.1519	-0.2396	-1.4325	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.0124	-1.9305	0.0436	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.2748	0.8160	0.0744	O	0	0	0	0	0	0	0	0	0	0	0	0
-2.8101	-0.1806	-2.3025	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.5872	-1.1703	-1.4986	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.9601	1.1612	-1.5879	S	0	0	0	0	0	0	0	0	0	0	0	0
-3.2829	-3.1254	-0.0040	C	0	0	0	0	0	0	0	0	0	0	0	0
-5.4098	-1.9770	0.1078	C	0	0	0	0	0	0	0	0	0	0	0	0
-3.9452	-4.3505	0.0146	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.1997	-3.1123	-0.0607	H	0	0	0	0	0	0	0	0	0	0	0	0
-6.0685	-3.2051	0.1261	C	0	0	0	0	0	0	0	0	0	0	0	0
-5.9624	-1.0450	0.1424	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.3381	-4.3911	0.0805	C	0	0	0	0	0	0	0	0	0	0	0	0
-3.3758	-5.2725	-0.0228	H	0	0	0	0	0	0	0	0	0	0	0	0
-7.1512	-3.2347	0.1758	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.8516	-5.3460	0.0954	H	0	0	0	0	0	0	0	0	0	0	0	0

1	2	1	0	0	0	0
1	3	1	0	0	0	0
1	6	1	0	0	0	0
1	7	1	0	0	0	0
2	4	4	0	0	0	0
2	5	4	0	0	0	0
3	8	4	0	0	0	0
3	9	4	0	0	0	0
4	10	4	0	0	0	0
4	11	1	0	0	0	0
5	12	4	0	0	0	0
5	13	1	0	0	0	0
6	14	4	0	0	0	0
6	15	4	0	0	0	0
7	16	1	0	0	0	0
7	17	1	0	0	0	0
8	18	4	0	0	0	0
8	19	1	0	0	0	0
9	20	4	0	0	0	0
9	21	1	0	0	0	0
10	22	4	0	0	0	0
10	23	1	0	0	0	0
12	22	4	0	0	0	0
12	24	1	0	0	0	0
14	25	4	0	0	0	0
14	26	1	0	0	0	0
15	27	4	0	0	0	0
15	28	1	0	0	0	0
16	29	3	0	0	0	0

17	30	3	0	0	0	0
18	31	4	0	0	0	0
18	32	1	0	0	0	0
20	31	4	0	0	0	0
20	33	1	0	0	0	0
22	34	1	0	0	0	0
25	35	4	0	0	0	0
25	36	1	0	0	0	0
27	35	4	0	0	0	0
27	37	1	0	0	0	0
31	38	1	0	0	0	0
35	39	1	0	0	0	0
40	41	1	0	0	0	0
40	42	1	0	0	0	0
40	43	1	0	0	0	0
41	44	3	0	0	0	0
42	45	3	0	0	0	0
43	46	3	0	0	0	0
47	48	1	0	0	0	0
47	49	1	0	0	0	0
47	50	1	0	0	0	0
47	51	1	0	0	0	0
48	52	1	0	0	0	0
48	53	1	0	0	0	0
48	54	2	0	0	0	0
52	55	1	0	0	0	0
52	56	1	0	0	0	0
52	57	1	0	0	0	0
53	58	4	0	0	0	0
53	59	4	0	0	0	0
58	60	4	0	0	0	0
58	61	1	0	0	0	0
59	62	4	0	0	0	0
59	63	1	0	0	0	0
60	64	4	0	0	0	0
60	65	1	0	0	0	0
62	64	4	0	0	0	0
62	66	1	0	0	0	0
64	67	1	0	0	0	0

Molecular coordinates of **2**$^{-}$

2-, Fe2-Komplex, S2-Phosphanoxid-verbrueckt, PPh3

Created by GaussView 5.0.8

67	67	0	0	0	0	0	0	0	0	0	0				
-1.9698	0.3835	0.0055	P	0	0	0	0	0	0	0	0	0	0	0	0
-1.6609	1.8265	-1.1274	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.4160	1.2064	1.6188	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.7561	3.1728	-0.7500	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.2584	1.5305	-2.4410	C	0	0	0	0	0	0	0	0	0	0	0	0
-3.6802	-0.1383	-0.5309	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.5768	1.0115	2.7209	C	0	0	0	0	0	0	0	0	0	0	0	0
-3.5770	1.9777	1.7850	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.4778	4.1916	-1.6622	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.0484	3.4332	0.2595	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.9919	2.5487	-3.3531	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.1315	0.4971	-2.7435	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.3342	0.3556	-1.6648	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.3299	-1.1169	0.2381	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.8741	1.5963	3.9535	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.7052	0.3741	2.6203	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.8729	2.5613	3.0140	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.2587	2.1140	0.9531	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.1016	3.8850	-2.9680	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.5572	5.2273	-1.3479	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.6827	2.2948	-4.3613	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.6001	-0.1134	-2.0209	C	0	0	0	0	0	0	0	0	0	0	0	0
-3.8627	1.1117	-2.2792	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.5947	-1.5780	-0.1130	C	0	0	0	0	0	0	0	0	0	0	0	0
-3.8472	-1.5237	1.1184	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.0180	2.3753	4.1021	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.2137	1.4285	4.7975	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.7744	3.1551	3.1252	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.8834	4.6777	-3.6753	H	0	0	0	0	0	0	0	0	0	0	0	0
-6.2365	-1.0794	-1.2470	C	0	0	0	0	0	0	0	0	0	0	0	0
-6.0857	0.2818	-2.9072	H	0	0	0	0	0	0	0	0	0	0	0	0
-6.0749	-2.3358	0.4968	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.2518	2.8256	5.0611	H	0	0	0	0	0	0	0	0	0	0	0	0
-7.2188	-1.4455	-1.5254	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.4489	-1.4901	-0.0056	Fe	0	0	0	0	0	0	0	0	0	0	0	0
-1.2744	-2.4533	1.2340	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.2856	-2.3738	-1.3030	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.7826	-3.1136	2.0365	O	0	0	0	0	0	0	0	0	0	0	0	0
-1.7994	-2.9725	-2.1458	O	0	0	0	0	0	0	0	0	0	0	0	0
2.0487	-2.6372	-0.0076	Fe	0	0	0	0	0	0	0	0	0	0	0	0
1.7708	-3.8676	-1.2529	C	0	0	0	0	0	0	0	0	0	0	0	0
1.8656	-3.8688	1.2545	C	0	0	0	0	0	0	0	0	0	0	0	0
3.8721	-2.5163	-0.0499	C	0	0	0	0	0	0	0	0	0	0	0	0
1.6247	-4.6716	-2.0703	O	0	0	0	0	0	0	0	0	0	0	0	0

```
   1.7721   -4.6705    2.0810 O   0  0  0  0  0  0  0  0  0  0  0  0
   5.0022   -2.7244   -0.0954 O   0  0  0  0  0  0  0  0  0  0  0  0
   2.0009    0.6012    1.4993 C   0  0  0  0  0  0  0  0  0  0  0  0
   3.0658    0.9711    0.0561 P   0  0  0  0  0  0  0  0  0  0  0  0
   2.6489    0.7287    2.3711 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.2116    1.3554    1.5576 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.2338   -1.0769    1.6264 S   0  0  0  0  0  0  0  0  0  0  0  0
   2.0883    0.5945   -1.4469 C   0  0  0  0  0  0  0  0  0  0  0  0
   3.2009    2.8175    0.0625 C   0  0  0  0  0  0  0  0  0  0  0  0
   4.4447    0.3772    0.1038 O   0  0  0  0  0  0  0  0  0  0  0  0
   2.7987    0.6752   -2.2746 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.3327    1.3710   -1.5792 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.2577   -1.0509   -1.6046 S   0  0  0  0  0  0  0  0  0  0  0  0
   2.1052    3.6878    0.0161 C   0  0  0  0  0  0  0  0  0  0  0  0
   4.4928    3.3527    0.1225 C   0  0  0  0  0  0  0  0  0  0  0  0
   2.2984    5.0678    0.0319 C   0  0  0  0  0  0  0  0  0  0  0  0
   1.0941    3.2996   -0.0388 H   0  0  0  0  0  0  0  0  0  0  0  0
   4.6856    4.7335    0.1381 C   0  0  0  0  0  0  0  0  0  0  0  0
   5.3320    2.6666    0.1556 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.5891    5.5934    0.0940 C   0  0  0  0  0  0  0  0  0  0  0  0
   1.4411    5.7314   -0.0070 H   0  0  0  0  0  0  0  0  0  0  0  0
   5.6918    5.1371    0.1846 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.7380    6.6682    0.1059 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  3  1  0  0  0  0
 1  6  1  0  0  0  0
 2  4  4  0  0  0  0
 2  5  4  0  0  0  0
 3  7  4  0  0  0  0
 3  8  4  0  0  0  0
 4  9  4  0  0  0  0
 4 10  1  0  0  0  0
 5 11  4  0  0  0  0
 5 12  1  0  0  0  0
 6 13  4  0  0  0  0
 6 14  4  0  0  0  0
 7 15  4  0  0  0  0
 7 16  1  0  0  0  0
 8 17  4  0  0  0  0
 8 18  1  0  0  0  0
 9 19  4  0  0  0  0
 9 20  1  0  0  0  0
11 19  4  0  0  0  0
11 21  1  0  0  0  0
13 22  4  0  0  0  0
13 23  1  0  0  0  0
14 24  4  0  0  0  0
14 25  1  0  0  0  0
15 26  4  0  0  0  0
15 27  1  0  0  0  0
17 26  4  0  0  0  0
17 28  1  0  0  0  0
```

19	29	1	0	0	0	0
22	30	4	0	0	0	0
22	31	1	0	0	0	0
24	30	4	0	0	0	0
24	32	1	0	0	0	0
26	33	1	0	0	0	0
30	34	1	0	0	0	0
35	36	1	0	0	0	0
35	37	1	0	0	0	0
36	38	3	0	0	0	0
37	39	3	0	0	0	0
40	41	1	0	0	0	0
40	42	1	0	0	0	0
40	43	1	0	0	0	0
41	44	3	0	0	0	0
42	45	3	0	0	0	0
43	46	3	0	0	0	0
47	48	1	0	0	0	0
47	49	1	0	0	0	0
47	50	1	0	0	0	0
47	51	1	0	0	0	0
48	52	1	0	0	0	0
48	53	1	0	0	0	0
48	54	2	0	0	0	0
52	55	1	0	0	0	0
52	56	1	0	0	0	0
52	57	1	0	0	0	0
53	58	4	0	0	0	0
53	59	4	0	0	0	0
58	60	4	0	0	0	0
58	61	1	0	0	0	0
59	62	4	0	0	0	0
59	63	1	0	0	0	0
60	64	4	0	0	0	0
60	65	1	0	0	0	0
62	64	4	0	0	0	0
62	66	1	0	0	0	0
64	67	1	0	0	0	0

Molecular coordinates of **2^{2-}**

```
22-, Fe2-Komplex, S2-Phosphanoxid-verbrueckt, PPh3

Created by GaussView 5.0.8
 67 68  0  0  0  0  0  0  0  0  0    0
    2.1427    0.2151    0.0255 P   0  0  0  0  0  0  0  0  0  0  0  0
    2.0899    1.7531    1.0825 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.8180   -1.0270    1.2589 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.3570    1.7327    2.2813 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.6456    2.9700    0.6658 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.6847    0.5511   -0.9987 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.2829   -0.3142   -1.0692 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    3.5916   -0.6867    2.3776 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.5218   -2.3761    1.0383 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.2024    2.8888    3.0414 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.8917    0.8072    2.6038 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.4858    4.1287    1.4262 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.2029    3.0185   -0.2621 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.9793    0.5910   -0.4628 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.5278    0.7690   -2.3722 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.0735   -1.5482   -2.0311 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.1492    1.2223   -1.8805 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.0710   -1.6719    3.2406 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.8047    0.3539    2.5945 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.9989   -3.3625    1.9000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.8868   -2.6464    0.2030 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.7680    4.0938    2.6204 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.6263    2.8498    3.9606 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.9222    5.0608    1.0796 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.0838    0.8512   -1.2722 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.1337    0.4069    0.5930 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.6317    1.0353   -3.1838 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.5331    0.7160   -2.7974 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.6061   -2.2432   -2.8124 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.1523    2.1720   -2.5855 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.7784   -3.0148    3.0016 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.6614   -1.3875    4.1070 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.7310   -4.3971    1.7158 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.6385    4.9960    3.2100 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.9127    1.0788   -2.6382 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.0783    0.8709   -0.8361 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.4847    1.1994   -4.2465 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.1390   -3.7812    3.6812 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.7724    1.2783   -3.2711 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8183   -3.8521    0.0780 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1033   -2.6378    0.0189 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -0.0974   -4.7606    0.2292 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.2355   -3.5863   -0.9316 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.1790   -2.6847    1.4128 C   0  0  0  0  0  0  0  0  0  0  0  0
```

```
   -3.9832   -4.2042   -1.5753 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.8097   -2.8265    2.3859 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.0371    0.4521    1.3532 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.3904    0.8182    0.1358 P   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5951    0.2141    2.2643 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8134   -0.8943    1.0468 S   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4825    1.3781    1.5195 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9898    0.2631   -1.5842 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.3759    2.6774    0.0325 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.7668    0.4026    0.6025 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.9654   -0.0484   -1.9697 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.8047   -1.1240   -1.8483 S   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6474    1.1252   -2.1605 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2582    3.4300   -0.3487 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.5618    3.3428    0.3641 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3291    4.8219   -0.3977 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3327    2.9337   -0.6173 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.6321    4.7352    0.3164 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.4162    2.7422    0.6582 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.5146    5.4788   -0.0648 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4545    5.3897   -0.6983 H   0  0  0  0  0  0  0  0  0  0  0  0
   -5.5584    5.2397    0.5769 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.5663    6.5632   -0.1029 H   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1  3  1  0  0  0  0
  1  6  1  0  0  0  0
  1  7  1  0  0  0  0
  2  4  4  0  0  0  0
  2  5  4  0  0  0  0
  3  8  4  0  0  0  0
  3  9  4  0  0  0  0
  4 10  4  0  0  0  0
  4 11  1  0  0  0  0
  5 12  4  0  0  0  0
  5 13  1  0  0  0  0
  6 14  4  0  0  0  0
  6 15  4  0  0  0  0
  7 16  1  0  0  0  0
  7 17  1  0  0  0  0
  8 18  4  0  0  0  0
  8 19  1  0  0  0  0
  9 20  4  0  0  0  0
  9 21  1  0  0  0  0
 10 22  4  0  0  0  0
 10 23  1  0  0  0  0
 12 22  4  0  0  0  0
 12 24  1  0  0  0  0
 14 25  4  0  0  0  0
 14 26  1  0  0  0  0
 15 27  4  0  0  0  0
 15 28  1  0  0  0  0
 16 29  2  0  0  0  0
```

17	30	2	0	0	0	0
18	31	4	0	0	0	0
18	32	1	0	0	0	0
20	31	4	0	0	0	0
20	33	1	0	0	0	0
22	34	1	0	0	0	0
25	35	4	0	0	0	0
25	36	1	0	0	0	0
27	35	4	0	0	0	0
27	37	1	0	0	0	0
31	38	1	0	0	0	0
35	39	1	0	0	0	0
40	41	1	0	0	0	0
40	42	2	0	0	0	0
41	43	1	0	0	0	0
41	44	1	0	0	0	0
43	45	2	0	0	0	0
44	46	2	0	0	0	0
47	48	1	0	0	0	0
47	49	1	0	0	0	0
47	50	1	0	0	0	0
47	51	1	0	0	0	0
48	52	1	0	0	0	0
48	53	1	0	0	0	0
48	54	2	0	0	0	0
52	55	1	0	0	0	0
52	56	1	0	0	0	0
52	57	1	0	0	0	0
53	58	4	0	0	0	0
53	59	4	0	0	0	0
58	60	4	0	0	0	0
58	61	1	0	0	0	0
59	62	4	0	0	0	0
59	63	1	0	0	0	0
60	64	4	0	0	0	0
60	65	1	0	0	0	0
62	64	4	0	0	0	0
62	66	1	0	0	0	0
64	67	1	0	0	0	0

Molecular coordinates of **2a**$^{2-}$

2a2-, Fe2-Komplex, S2 mit Phosphanoxidbruecke und PPh3

Created by GaussView 5.0.8

67	68	0	0	0	0	0	0	0	0	0	0					
1.9166	-0.7163	0.0335	P	0	0	0	0	0	0	0	0	0	0	0	0	
3.5120	-0.1052	-0.7291	C	0	0	0	0	0	0	0	0	0	0	0	0	
1.5645	-2.1689	-1.1059	C	0	0	0	0	0	0	0	0	0	0	0	0	
4.2081	0.9147	-0.0624	C	0	0	0	0	0	0	0	0	0	0	0	0	
4.0353	-0.5811	-1.9372	C	0	0	0	0	0	0	0	0	0	0	0	0	
2.6417	-1.6431	1.5020	C	0	0	0	0	0	0	0	0	0	0	0	0	
0.3811	0.8505	0.4886	Fe	0	0	0	0	0	0	0	0	0	0	0	0	
0.8133	-1.9235	-2.2644	C	0	0	0	0	0	0	0	0	0	0	0	0	
1.9896	-3.4819	-0.8569	C	0	0	0	0	0	0	0	0	0	0	0	0	
5.4070	1.4105	-0.5667	C	0	0	0	0	0	0	0	0	0	0	0	0	
3.8064	1.3249	0.8550	H	0	0	0	0	0	0	0	0	0	0	0	0	
5.2283	-0.0721	-2.4538	C	0	0	0	0	0	0	0	0	0	0	0	0	
3.5144	-1.3583	-2.4820	H	0	0	0	0	0	0	0	0	0	0	0	0	
3.9893	-2.0200	1.5955	C	0	0	0	0	0	0	0	0	0	0	0	0	
1.7808	-1.9839	2.5540	C	0	0	0	0	0	0	0	0	0	0	0	0	
1.1920	2.3477	-0.2700	C	0	0	0	0	0	0	0	0	0	0	0	0	
1.0114	1.2922	2.0548	C	0	0	0	0	0	0	0	0	0	0	0	0	
0.5036	-2.9543	-3.1491	C	0	0	0	0	0	0	0	0	0	0	0	0	
0.4323	-0.9257	-2.4505	H	0	0	0	0	0	0	0	0	0	0	0	0	
1.6773	-4.5146	-1.7414	C	0	0	0	0	0	0	0	0	0	0	0	0	
2.5603	-3.7061	0.0354	H	0	0	0	0	0	0	0	0	0	0	0	0	
5.9240	0.9207	-1.7657	C	0	0	0	0	0	0	0	0	0	0	0	0	
5.9223	2.2029	-0.0333	H	0	0	0	0	0	0	0	0	0	0	0	0	
5.6118	-0.4563	-3.3946	H	0	0	0	0	0	0	0	0	0	0	0	0	
4.4626	-2.7225	2.7045	C	0	0	0	0	0	0	0	0	0	0	0	0	
4.6782	-1.7628	0.8003	H	0	0	0	0	0	0	0	0	0	0	0	0	
2.2535	-2.6924	3.6585	C	0	0	0	0	0	0	0	0	0	0	0	0	
0.7373	-1.6754	2.5066	H	0	0	0	0	0	0	0	0	0	0	0	0	
2.2133	2.8806	-0.5797	O	0	0	0	0	0	0	0	0	0	0	0	0	
1.4105	1.6102	3.1013	O	0	0	0	0	0	0	0	0	0	0	0	0	
0.9357	-4.2543	-2.8928	C	0	0	0	0	0	0	0	0	0	0	0	0	
-0.1133	-2.7421	-4.0147	H	0	0	0	0	0	0	0	0	0	0	0	0	
2.0076	-5.5260	-1.5218	H	0	0	0	0	0	0	0	0	0	0	0	0	
6.8509	1.3198	-2.1670	H	0	0	0	0	0	0	0	0	0	0	0	0	
3.5944	-3.0655	3.7405	C	0	0	0	0	0	0	0	0	0	0	0	0	
5.5117	-2.9996	2.7567	H	0	0	0	0	0	0	0	0	0	0	0	0	
1.5674	-2.9404	4.4627	H	0	0	0	0	0	0	0	0	0	0	0	0	
0.6757	-5.0610	-3.5713	H	0	0	0	0	0	0	0	0	0	0	0	0	
3.9622	-3.6099	4.6055	H	0	0	0	0	0	0	0	0	0	0	0	0	
-0.7533	3.0865	-0.2361	Fe	0	0	0	0	0	0	0	0	0	0	0	0	
-0.1031	4.2898	0.8611	C	0	0	0	0	0	0	0	0	0	0	0	0	
-0.7643	4.0978	-1.6800	C	0	0	0	0	0	0	0	0	0	0	0	0	
-2.3421	3.0883	0.5859	C	0	0	0	0	0	0	0	0	0	0	0	0	
0.3191	5.1063	1.5727	O	0	0	0	0	0	0	0	0	0	0	0	0	

-0.8126	4.8064	-2.6037	O	0	0	0	0	0	0	0	0	0	0	0	0
-3.3721	3.2055	1.1159	O	0	0	0	0	0	0	0	0	0	0	0	0
-2.7219	0.4202	-1.1029	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.9324	-1.3841	-0.8486	P	0	0	0	0	0	0	0	0	0	0	0	0
-3.3437	0.6806	-1.9641	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.1226	0.9082	-0.2190	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.0170	1.0576	-1.4188	S	0	0	0	0	0	0	0	0	0	0	0	0
-1.7660	-1.8900	0.4763	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.6162	-1.4930	-0.0770	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.9134	-2.2343	-2.1030	O	0	0	0	0	0	0	0	0	0	0	0	0
-2.2374	-2.7262	1.0022	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.8829	-2.2781	-0.0332	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.3358	-0.5452	1.6611	S	0	0	0	0	0	0	0	0	0	0	0	0
-4.9497	-0.8718	1.1351	C	0	0	0	0	0	0	0	0	0	0	0	0
-5.5842	-2.2491	-0.7465	C	0	0	0	0	0	0	0	0	0	0	0	0
-6.2338	-1.0102	1.6614	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.1957	-0.2986	1.6655	H	0	0	0	0	0	0	0	0	0	0	0	0
-6.8699	-2.3809	-0.2207	C	0	0	0	0	0	0	0	0	0	0	0	0
-5.3038	-2.7274	-1.6792	H	0	0	0	0	0	0	0	0	0	0	0	0
-7.1970	-1.7607	0.9852	C	0	0	0	0	0	0	0	0	0	0	0	0
-6.4822	-0.5254	2.6003	H	0	0	0	0	0	0	0	0	0	0	0	0
-7.6149	-2.9673	-0.7510	H	0	0	0	0	0	0	0	0	0	0	0	0
-8.1977	-1.8598	1.3961	H	0	0	0	0	0	0	0	0	0	0	0	0

1	2	1	0	0	0	0
1	3	1	0	0	0	0
1	6	1	0	0	0	0
1	7	1	0	0	0	0
2	4	4	0	0	0	0
2	5	4	0	0	0	0
3	8	4	0	0	0	0
3	9	4	0	0	0	0
4	10	4	0	0	0	0
4	11	1	0	0	0	0
5	12	4	0	0	0	0
5	13	1	0	0	0	0
6	14	4	0	0	0	0
6	15	4	0	0	0	0
7	16	1	0	0	0	0
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9	21	1	0	0	0	0
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12	24	1	0	0	0	0
14	25	4	0	0	0	0
14	26	1	0	0	0	0
15	27	4	0	0	0	0
15	28	1	0	0	0	0
16	29	2	0	0	0	0

17	30	2	0	0	0	0
18	31	4	0	0	0	0
18	32	1	0	0	0	0
20	31	4	0	0	0	0
20	33	1	0	0	0	0
22	34	1	0	0	0	0
25	35	4	0	0	0	0
25	36	1	0	0	0	0
27	35	4	0	0	0	0
27	37	1	0	0	0	0
31	38	1	0	0	0	0
35	39	1	0	0	0	0
40	41	1	0	0	0	0
40	42	1	0	0	0	0
40	43	1	0	0	0	0
41	44	2	0	0	0	0
42	45	2	0	0	0	0
43	46	2	0	0	0	0
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58	60	4	0	0	0	0
58	61	1	0	0	0	0
59	62	4	0	0	0	0
59	63	1	0	0	0	0
60	64	4	0	0	0	0
60	65	1	0	0	0	0
62	64	4	0	0	0	0
62	66	1	0	0	0	0
64	67	1	0	0	0	0

Molecular coordinates of **3**

```
3, Fe2-Komplex, S2-Phosphanoxid-verbrueckt, P(OEt)3

Created by GaussView 5.0.8
 58 56  0  0  0  0  0  0  0  0  0    0
    0.7755    2.1419    0.1464 P   0  0  0  0  0  0  0  0  0  0  0  0
    1.6001    0.0965    0.0372 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -0.2571    2.5191    1.3623 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.8319    0.3060   -1.2413 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.8174    0.2333    1.3393 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.7775    3.4289    0.3328 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1795    2.5428   -1.1041 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.1815    2.5780    2.7434 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.6206    0.4093   -2.0680 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.6053    0.3080    2.1700 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.1272    3.5352   -0.1748 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8461    3.8314   -1.2235 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9882    3.0383    3.5907 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.5237    1.5844    3.0484 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.0181    3.2776    2.8130 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.1669    4.1243   -1.5745 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.6408    4.1835    0.5373 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.6085    2.5558   -0.1433 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3806    3.9539   -2.6363 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6471    3.8724   -0.4819 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1273    4.6219   -0.9967 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6825    3.0930    4.6392 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3288    4.0282    3.2791 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.8264    2.3419    3.5164 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.6868    5.1054   -1.5961 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.6697    3.4734   -2.2972 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.2068    4.2456   -1.8910 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.8991    4.9101   -2.7514 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.0879    3.1524   -2.8603 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.5694    3.9113   -3.3660 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.2197   -2.3897   -0.0629 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    2.3768   -2.8704   -1.3573 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.3458   -2.9497    1.2273 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.1822   -3.8971   -0.1276 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.1121   -3.1773   -2.1763 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.0630   -3.3047    2.0432 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3224   -4.9155   -0.1652 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4745   -0.5654   -1.5090 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3726   -1.3236   -0.1084 P   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9280   -0.9629   -2.4200 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5939    0.5189   -1.5050 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.3302   -0.9126   -1.6295 S   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5396   -0.6830    1.3900 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.0218   -0.5252   -0.1075 C   0  0  0  0  0  0  0  0  0  0  0  0
```

```
  -2.4763   -2.8182   -0.1729 O   0  0  0  0  0  0  0  0  0  0  0  0
  -2.0344   -1.1520    2.2436 H   0  0  0  0  0  0  0  0  0  0  0  0
  -1.6725    0.3977    1.4610 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.2619   -1.0350    1.5715 S   0  0  0  0  0  0  0  0  0  0  0  0
  -4.2083    0.8601   -0.0102 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.1358   -1.3657   -0.2103 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.4938    1.3958   -0.0161 C   0  0  0  0  0  0  0  0  0  0  0  0
  -3.3564    1.5273    0.0736 H   0  0  0  0  0  0  0  0  0  0  0  0
  -6.4208   -0.8256   -0.2172 C   0  0  0  0  0  0  0  0  0  0  0  0
  -4.9783   -2.4359   -0.2822 H   0  0  0  0  0  0  0  0  0  0  0  0
  -6.6008    0.5528   -0.1202 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.6331    2.4683    0.0611 H   0  0  0  0  0  0  0  0  0  0  0  0
  -7.2802   -1.4818   -0.2974 H   0  0  0  0  0  0  0  0  0  0  0  0
  -7.6010    0.9715   -0.1249 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  3  1  0  0  0  0
 1  6  1  0  0  0  0
 1  7  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 3  8  1  0  0  0  0
 4  9  3  0  0  0  0
 5 10  3  0  0  0  0
 6 11  1  0  0  0  0
 7 12  1  0  0  0  0
 8 13  1  0  0  0  0
 8 14  1  0  0  0  0
 8 15  1  0  0  0  0
11 16  1  0  0  0  0
11 17  1  0  0  0  0
11 18  1  0  0  0  0
12 19  1  0  0  0  0
12 20  1  0  0  0  0
12 21  1  0  0  0  0
13 22  1  0  0  0  0
13 23  1  0  0  0  0
13 24  1  0  0  0  0
16 25  1  0  0  0  0
16 26  1  0  0  0  0
16 27  1  0  0  0  0
19 28  1  0  0  0  0
19 29  1  0  0  0  0
19 30  1  0  0  0  0
31 32  1  0  0  0  0
31 33  1  0  0  0  0
31 34  1  0  0  0  0
32 35  3  0  0  0  0
33 36  3  0  0  0  0
34 37  3  0  0  0  0
38 39  1  0  0  0  0
38 40  1  0  0  0  0
38 41  1  0  0  0  0
```

38	42	1	0	0	0	0
39	43	1	0	0	0	0
39	44	1	0	0	0	0
39	45	2	0	0	0	0
43	46	1	0	0	0	0
43	47	1	0	0	0	0
43	48	1	0	0	0	0
44	49	4	0	0	0	0
44	50	4	0	0	0	0
49	51	4	0	0	0	0
49	52	1	0	0	0	0
50	53	4	0	0	0	0
50	54	1	0	0	0	0
51	55	4	0	0	0	0
51	56	1	0	0	0	0
53	55	4	0	0	0	0
53	57	1	0	0	0	0
55	58	1	0	0	0	0

Molecular coordinates of **3**$^{-}$

```
3-, Fe2-Komplex, S2-Phosphanoxid-verbrueckt, P(OEt)3

Created by GaussView 5.0.8
 58 56  0  0  0  0  0  0  0  0  0    0
   -0.3711    2.1130   -0.0518 P   0  0  0  0  0  0  0  0  0  0  0  0
    1.3939    0.7684   -0.0671 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -1.5251    2.0566    1.1504 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.3751    1.4550   -1.3761 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.4191    1.5355    1.1586 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1284    3.7679    0.0667 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4265    2.0279   -1.3165 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1611    2.2906    2.5253 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.0219    1.8926   -2.2294 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.0934    2.0352    1.9562 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.9685    4.4211   -0.5929 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5757    2.8861   -1.4644 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.7895    3.5807    3.0290 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5221    1.4320    3.0987 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.0733    2.3166    2.6298 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.9138    5.8984   -0.2434 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.9125    3.9806   -0.2633 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.8910    4.2763   -1.6762 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.1413    2.6813   -2.8585 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2718    3.9248   -1.3071 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.3113    2.6315   -0.6959 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4180    4.4334    2.4580 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5437    3.7282    4.0861 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.8782    3.5435    2.9322 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.0030    6.0411    0.8364 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.7374    6.4288   -0.7311 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.0287    6.3435   -0.5733 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.0183    3.3204   -3.0047 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.4437    1.6420   -3.0068 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3977    2.9322   -3.6187 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.2453   -1.8831   -0.0163 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    3.5270   -1.8161    1.2158 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.4684   -1.9223   -1.3075 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.8212   -3.6762    0.0561 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.3576   -1.7937    2.0169 O   0  0  0  0  0  0  0  0  0  0  0  0
    4.2601   -1.9696   -2.1455 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.8137   -4.8236    0.1051 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.9559   -0.7331    0.1740 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.3448   -0.6180    0.2042 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.3536   -1.9936    0.0667 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.3469    0.1622    0.2438 H   0  0  0  0  0  0  0  0  0  0  0  0
   -6.1451   -1.7585    0.1265 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.8024    0.3619    0.2920 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5223   -2.2610    0.0221 P   0  0  0  0  0  0  0  0  0  0  0  0
```

```
  -4.1624   -3.1327   -0.0066 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.5517   -3.0155    0.0210 C   0  0  0  0  0  0  0  0  0  0  0  0
  -7.2260   -1.6662    0.1503 H   0  0  0  0  0  0  0  0  0  0  0  0
  -0.9783   -1.3481   -1.4686 C   0  0  0  0  0  0  0  0  0  0  0  0
  -0.9237   -1.3458    1.4941 C   0  0  0  0  0  0  0  0  0  0  0  0
  -1.2295   -3.7354    0.0123 O   0  0  0  0  0  0  0  0  0  0  0  0
  -3.6802   -4.1014   -0.0799 H   0  0  0  0  0  0  0  0  0  0  0  0
  -6.1699   -3.9055   -0.0368 H   0  0  0  0  0  0  0  0  0  0  0  0
  -1.2302   -2.0027   -2.3079 H   0  0  0  0  0  0  0  0  0  0  0  0
  -1.5542   -0.4257   -1.5640 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.8050   -0.8996   -1.6344 S   0  0  0  0  0  0  0  0  0  0  0  0
  -1.1198   -2.0114    2.3394 H   0  0  0  0  0  0  0  0  0  0  0  0
  -1.5339   -0.4490    1.6131 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.8481   -0.8334    1.5940 S   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  3  1  0  0  0  0
 1  6  1  0  0  0  0
 1  7  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 3  8  1  0  0  0  0
 4  9  3  0  0  0  0
 5 10  3  0  0  0  0
 6 11  1  0  0  0  0
 7 12  1  0  0  0  0
 8 13  1  0  0  0  0
 8 14  1  0  0  0  0
 8 15  1  0  0  0  0
11 16  1  0  0  0  0
11 17  1  0  0  0  0
11 18  1  0  0  0  0
12 19  1  0  0  0  0
12 20  1  0  0  0  0
12 21  1  0  0  0  0
13 22  1  0  0  0  0
13 23  1  0  0  0  0
13 24  1  0  0  0  0
16 25  1  0  0  0  0
16 26  1  0  0  0  0
16 27  1  0  0  0  0
19 28  1  0  0  0  0
19 29  1  0  0  0  0
19 30  1  0  0  0  0
31 32  1  0  0  0  0
31 33  1  0  0  0  0
31 34  1  0  0  0  0
32 35  3  0  0  0  0
33 36  3  0  0  0  0
34 37  3  0  0  0  0
38 39  4  0  0  0  0
38 40  4  0  0  0  0
38 41  1  0  0  0  0
```

39	42	4	0	0	0	0
39	43	1	0	0	0	0
40	44	1	0	0	0	0
40	45	4	0	0	0	0
42	46	4	0	0	0	0
42	47	1	0	0	0	0
44	48	1	0	0	0	0
44	49	1	0	0	0	0
44	50	2	0	0	0	0
45	46	4	0	0	0	0
45	51	1	0	0	0	0
46	52	1	0	0	0	0
48	53	1	0	0	0	0
48	54	1	0	0	0	0
48	55	1	0	0	0	0
49	56	1	0	0	0	0
49	57	1	0	0	0	0
49	58	1	0	0	0	0

Molecular coordinates of **3^{2-}**

```
32-, Fe2-Komplex, S2-Phosphanoxid-verbrueckt, P(OEt)3

Created by GaussView 5.0.8
 58 56  0  0  0  0  0  0  0  0  0    0
   -2.0839   -0.7841    0.1550 P   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1648   -1.5497   -0.2615 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -3.3948   -1.8803    0.0910 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.1630   -3.0659    0.5616 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6640   -2.3892   -1.7147 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9859    0.3776   -0.7366 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4115   -0.0651    1.6284 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.2561   -3.1890    0.6410 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.2843   -4.0888    1.1116 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9617   -2.9515   -2.6937 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9568    0.3455   -2.1604 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.7013    0.4129    2.0131 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.5606   -3.9395    0.4090 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4200   -3.7094    0.1682 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.0341   -3.1305    1.7146 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.2075   -0.3103   -2.7395 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.8856    1.3861   -2.5001 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.0557   -0.1750   -2.5057 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.7081    0.5944    3.5243 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.9033    1.3635    1.5069 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.4702   -0.3006    1.6990 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.7739   -4.0130   -0.6611 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.4918   -4.9534    0.8187 H   0  0  0  0  0  0  0  0  0  0  0  0
   -5.3994   -3.4263    0.8897 H   0  0  0  0  0  0  0  0  0  0  0  0
   -5.1071    0.2244   -2.4180 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.1669   -0.2983   -3.8353 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.2838   -1.3442   -2.3997 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9293    1.2973    3.8308 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.6783    0.9824    3.8572 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.5201   -0.3576    4.0279 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5447    3.3274   -0.2223 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4875    4.3524   -0.3128 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1830    3.6270   -0.0876 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.8874    2.2988   -0.2569 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.0856    5.6881   -0.2722 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.5390    4.1016   -0.4150 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.1808    2.3582    0.0518 P   0  0  0  0  0  0  0  0  0  0  0  0
    0.2114    4.9702   -0.0445 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.7311    5.9942   -0.1380 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.8225    6.4831   -0.3434 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.6820    1.3046    1.4794 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.0658    1.4184   -1.5417 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.4621    3.1317    0.2484 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.2697    5.1818    0.0666 H   0  0  0  0  0  0  0  0  0  0  0  0
```

```
  -0.4082    7.0310   -0.1042 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.1956    1.7722    2.3253 H   0  0  0  0  0  0  0  0  0  0  0  0
  -0.3947    1.3832    1.6397 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.1388   -0.4855    1.4618 S   0  0  0  0  0  0  0  0  0  0  0  0
   1.7738    1.9453   -2.1897 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.4720   -0.3873   -1.5971 S   0  0  0  0  0  0  0  0  0  0  0  0
   0.0619    1.5535   -1.9506 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.1526   -0.6756    0.0881 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   4.1474   -0.6229    1.5350 C   0  0  0  0  0  0  0  0  0  0  0  0
   4.2107    0.4722   -0.7244 C   0  0  0  0  0  0  0  0  0  0  0  0
   3.5017   -2.3619   -0.3357 C   0  0  0  0  0  0  0  0  0  0  0  0
   4.7914   -0.5890    2.5050 O   0  0  0  0  0  0  0  0  0  0  0  0
   4.9834    1.1084   -1.3275 O   0  0  0  0  0  0  0  0  0  0  0  0
   3.9311   -3.4002   -0.6532 O   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  3  1  0  0  0  0
 1  6  1  0  0  0  0
 1  7  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 3  8  1  0  0  0  0
 4  9  2  0  0  0  0
 5 10  2  0  0  0  0
 6 11  1  0  0  0  0
 7 12  1  0  0  0  0
 8 13  1  0  0  0  0
 8 14  1  0  0  0  0
 8 15  1  0  0  0  0
11 16  1  0  0  0  0
11 17  1  0  0  0  0
11 18  1  0  0  0  0
12 19  1  0  0  0  0
12 20  1  0  0  0  0
12 21  1  0  0  0  0
13 22  1  0  0  0  0
13 23  1  0  0  0  0
13 24  1  0  0  0  0
16 25  1  0  0  0  0
16 26  1  0  0  0  0
16 27  1  0  0  0  0
19 28  1  0  0  0  0
19 29  1  0  0  0  0
19 30  1  0  0  0  0
31 32  4  0  0  0  0
31 33  4  0  0  0  0
31 34  1  0  0  0  0
32 35  4  0  0  0  0
32 36  1  0  0  0  0
33 37  1  0  0  0  0
33 38  4  0  0  0  0
35 39  4  0  0  0  0
35 40  1  0  0  0  0
```

37	41	1	0	0	0	0
37	42	1	0	0	0	0
37	43	2	0	0	0	0
38	39	4	0	0	0	0
38	44	1	0	0	0	0
39	45	1	0	0	0	0
41	46	1	0	0	0	0
41	47	1	0	0	0	0
41	48	1	0	0	0	0
42	49	1	0	0	0	0
42	50	1	0	0	0	0
42	51	1	0	0	0	0
52	53	1	0	0	0	0
52	54	1	0	0	0	0
52	55	1	0	0	0	0
53	56	2	0	0	0	0
54	57	2	0	0	0	0
55	58	2	0	0	0	0

Molecular coordinates of **3a^{2-}**

```
3a2-, Fe2-Komplex, Dianion umgelagert, P(OEt)3

Created by GaussView 5.0.8
 58 56  0  0  0  0  0  0  0  0  0    0
    2.1355   -1.4273    0.1694 P   0  0  0  0  0  0  0  0  0  0  0  0
    1.0942    0.4570    0.1902 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    3.7357   -1.2934   -0.3174 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.3354    1.1718   -0.8551 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.5407    1.4372    1.5885 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.6786   -2.7391   -0.7769 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.3281   -2.4121    1.4945 O   0  0  0  0  0  0  0  0  0  0  0  0
    4.6039   -2.4179   -0.4322 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.1779    1.5674   -1.5416 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.9300    1.9644    2.5524 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.4414   -2.4984   -2.1770 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.3510   -1.8771    2.8261 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.9661   -1.9154   -0.8879 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.1938   -3.1370   -1.1513 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.6786   -2.9310    0.5333 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.6566   -3.6677   -2.7485 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.8886   -1.5627   -2.3056 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.4088   -2.3916   -2.6876 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.7553   -1.4682    3.2563 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.6514   -1.0442    2.8979 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.9723   -2.6827    3.4632 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.3791   -1.2115   -0.1606 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.6641   -2.7534   -1.0008 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.8817   -1.3969   -1.8464 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.5632   -3.5485   -3.8337 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.1673   -4.6148   -2.5445 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3523   -3.6963   -2.3324 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.7351   -1.1149    4.2935 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.4512   -2.3118    3.1912 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.1306   -0.6550    2.6311 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1098    2.8439   -0.3429 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -1.0714    3.8788   -1.3516 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.2855    3.9165   -0.4345 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0959    3.0241    1.1133 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.7254    4.5627   -2.0383 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.1254    4.7336   -0.4301 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.7115    3.3230    2.0613 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3354   -1.9560    0.5495 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4869   -1.4116   -0.7746 P   0  0  0  0  0  0  0  0  0  0  0  0
   -1.8941   -2.6432    1.1919 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.5467   -2.5312    0.0629 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6559   -0.5827    1.5683 S   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1608    0.3617   -1.1093 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.1525   -1.3638    0.0414 C   0  0  0  0  0  0  0  0  0  0  0  0
```

```
  -2.5500   -2.3347   -1.9773 O   0  0  0  0  0  0  0  0  0  0  0  0
  -2.8175    0.6410   -1.9385 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.4565    0.9166   -0.2214 H   0  0  0  0  0  0  0  0  0  0  0  0
  -0.4420    0.8889   -1.5576 S   0  0  0  0  0  0  0  0  0  0  0  0
  -4.4010   -0.6590    1.2281 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.1946   -2.0782   -0.5586 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.6731   -0.6747    1.7990 C   0  0  0  0  0  0  0  0  0  0  0  0
  -3.5948   -0.1100    1.7048 H   0  0  0  0  0  0  0  0  0  0  0  0
  -6.4683   -2.0877    0.0109 C   0  0  0  0  0  0  0  0  0  0  0  0
  -4.9809   -2.6224   -1.4728 H   0  0  0  0  0  0  0  0  0  0  0  0
  -6.7102   -1.3854    1.1918 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.8545   -0.1250    2.7172 H   0  0  0  0  0  0  0  0  0  0  0  0
  -7.2712   -2.6429   -0.4660 H   0  0  0  0  0  0  0  0  0  0  0  0
  -7.7011   -1.3893    1.6364 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  3  1  0  0  0  0
 1  6  1  0  0  0  0
 1  7  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 3  8  1  0  0  0  0
 4  9  3  0  0  0  0
 5 10  2  0  0  0  0
 6 11  1  0  0  0  0
 7 12  1  0  0  0  0
 8 13  1  0  0  0  0
 8 14  1  0  0  0  0
 8 15  1  0  0  0  0
11 16  1  0  0  0  0
11 17  1  0  0  0  0
11 18  1  0  0  0  0
12 19  1  0  0  0  0
12 20  1  0  0  0  0
12 21  1  0  0  0  0
13 22  1  0  0  0  0
13 23  1  0  0  0  0
13 24  1  0  0  0  0
16 25  1  0  0  0  0
16 26  1  0  0  0  0
16 27  1  0  0  0  0
19 28  1  0  0  0  0
19 29  1  0  0  0  0
19 30  1  0  0  0  0
31 32  1  0  0  0  0
31 33  1  0  0  0  0
31 34  1  0  0  0  0
32 35  2  0  0  0  0
33 36  2  0  0  0  0
34 37  2  0  0  0  0
38 39  1  0  0  0  0
38 40  1  0  0  0  0
38 41  1  0  0  0  0
```

38	42	1	0	0	0	0
39	43	1	0	0	0	0
39	44	1	0	0	0	0
39	45	2	0	0	0	0
43	46	1	0	0	0	0
43	47	1	0	0	0	0
43	48	1	0	0	0	0
44	49	4	0	0	0	0
44	50	4	0	0	0	0
49	51	4	0	0	0	0
49	52	1	0	0	0	0
50	53	4	0	0	0	0
50	54	1	0	0	0	0
51	55	4	0	0	0	0
51	56	1	0	0	0	0
53	55	4	0	0	0	0
53	57	1	0	0	0	0
55	58	1	0	0	0	0

Molecular coordinates of **3b^{2-}**

```
3b2-, Fe2-Komplex, Dianion umgelagert, P(OEt)3

Created by GaussView 5.0.8
 58 56  0  0  0  0  0  0  0  0  0    0
    0.5214    2.4319   -0.1582 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -1.3075    0.4662    0.4015 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    0.2551    0.4100   -1.3547 S   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5925   -1.1681    0.0027 P   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6577   -0.2205    1.8859 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.7049    1.5307    0.4586 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.5641    3.7793   -0.5715 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.2561    2.6660    1.4331 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.5703    1.6888    0.9539 S   0  0  0  0  0  0  0  0  0  0  0  0
   -0.7720    3.1492   -1.1356 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.5422   -0.8048   -0.8126 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.9064   -0.8474   -0.9913 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.3898   -1.9265    1.2625 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1399   -2.6567   -0.6139 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3753   -0.6453    2.9423 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.6501    2.2055    0.6314 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.2140    4.7183   -0.8052 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.5765    3.0978    2.4669 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.6217    1.2613   -0.4944 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5390    3.6966   -1.8054 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.2947   -0.4092   -1.1791 P   0  0  0  0  0  0  0  0  0  0  0  0
    1.4504   -0.9367    0.2629 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.3450   -1.7599   -1.3065 H   0  0  0  0  0  0  0  0  0  0  0  0
   -5.0120   -1.7386   -1.1189 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.8473   -1.1804    2.3956 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3417   -2.7508   -1.7995 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.4612    1.9671   -1.3124 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.6801    1.2958   -0.2190 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.2240   -1.5751   -0.0715 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.7583   -0.6236   -2.6058 O   0  0  0  0  0  0  0  0  0  0  0  0
   -5.8925   -1.2375   -2.2547 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.5764   -1.7651   -0.1789 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.6587   -2.7573   -1.3157 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.8012   -2.0852    3.6167 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.2176   -0.2989    2.5384 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.8730   -0.8354    2.2040 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1073   -3.4657   -2.9066 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0170   -1.7598   -2.1275 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.4472   -3.3249   -1.5358 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.0434   -1.6397    1.3180 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.1532   -2.4289   -0.6767 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.3412   -1.2354   -3.1990 H   0  0  0  0  0  0  0  0  0  0  0  0
   -6.7757   -1.8778   -2.3664 H   0  0  0  0  0  0  0  0  0  0  0  0
   -6.2225   -0.2148   -2.0559 H   0  0  0  0  0  0  0  0  0  0  0  0
```

-4.4055	-2.9850	3.4618	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.1862	-1.5523	4.4935	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.7706	-2.3850	3.8186	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.4544	-4.4475	-2.5692	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.4559	-3.6081	-3.7762	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.9747	-2.8805	-3.2224	H	0	0	0	0	0	0	0	0	0	0	0	0
4.7857	-2.5416	2.0804	C	0	0	0	0	0	0	0	0	0	0	0	0
3.3340	-0.9735	1.7975	H	0	0	0	0	0	0	0	0	0	0	0	0
5.8908	-3.3338	0.0872	C	0	0	0	0	0	0	0	0	0	0	0	0
5.2797	-2.3653	-1.7526	H	0	0	0	0	0	0	0	0	0	0	0	0
5.7080	-3.3920	1.4690	C	0	0	0	0	0	0	0	0	0	0	0	0
4.6370	-2.5819	3.1549	H	0	0	0	0	0	0	0	0	0	0	0	0
6.6064	-3.9934	-0.3955	H	0	0	0	0	0	0	0	0	0	0	0	0
6.2787	-4.0973	2.0664	H	0	0	0	0	0	0	0	0	0	0	0	0

1	7	1	0	0	0	0
1	8	1	0	0	0	0
1	10	1	0	0	0	0
2	4	1	0	0	0	0
2	5	1	0	0	0	0
2	6	1	0	0	0	0
3	11	1	0	0	0	0
4	12	1	0	0	0	0
4	13	1	0	0	0	0
4	14	1	0	0	0	0
5	15	2	0	0	0	0
6	16	2	0	0	0	0
7	17	2	0	0	0	0
8	18	2	0	0	0	0
9	19	1	0	0	0	0
10	20	3	0	0	0	0
11	21	1	0	0	0	0
11	22	1	0	0	0	0
11	23	1	0	0	0	0
12	24	1	0	0	0	0
13	25	1	0	0	0	0
14	26	1	0	0	0	0
19	21	1	0	0	0	0
19	27	1	0	0	0	0
19	28	1	0	0	0	0
21	29	1	0	0	0	0
21	30	2	0	0	0	0
24	31	1	0	0	0	0
24	32	1	0	0	0	0
24	33	1	0	0	0	0
25	34	1	0	0	0	0
25	35	1	0	0	0	0
25	36	1	0	0	0	0
26	37	1	0	0	0	0
26	38	1	0	0	0	0
26	39	1	0	0	0	0
29	40	4	0	0	0	0
29	41	4	0	0	0	0

31	42	1	0	0	0	0
31	43	1	0	0	0	0
31	44	1	0	0	0	0
34	45	1	0	0	0	0
34	46	1	0	0	0	0
34	47	1	0	0	0	0
37	48	1	0	0	0	0
37	49	1	0	0	0	0
37	50	1	0	0	0	0
40	51	4	0	0	0	0
40	52	1	0	0	0	0
41	53	4	0	0	0	0
41	54	1	0	0	0	0
51	55	4	0	0	0	0
51	56	1	0	0	0	0
53	55	4	0	0	0	0
53	57	1	0	0	0	0
55	58	1	0	0	0	0

Molecular coordinates of **5**

```
5, Fe2-Komplex, S2-Phosphanoxid-verbrueckt, PMe3

Created by GaussView 5.0.8
 46 44  0  0  0  0  0  0  0  0  0    0
    2.3215   -0.8030    0.0086 P   0  0  0  0  0  0  0  0  0  0  0  0
    1.4997   -0.0978   -1.4675 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.4850   -0.0113    1.4317 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.9527   -0.5864   -2.3333 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.7105    0.9702   -1.5411 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3227   -0.3496   -1.6213 S   0  0  0  0  0  0  0  0  0  0  0  0
    4.0128   -0.0976   -0.0019 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.3462   -2.2992    0.0532 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.9495   -0.4234    2.3304 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.6755    1.0637    1.4229 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3309   -0.2979    1.6037 S   0  0  0  0  0  0  0  0  0  0  0  0
    4.2824    1.2768   -0.0264 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.0768   -1.0062    0.0164 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.5963    1.7353   -0.0332 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.4727    1.9995   -0.0380 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.3910   -0.5440    0.0092 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.8562   -2.0672    0.0368 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.6518    0.8240   -0.0157 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.7977    2.8004   -0.0520 H   0  0  0  0  0  0  0  0  0  0  0  0
    7.2108   -1.2531    0.0234 H   0  0  0  0  0  0  0  0  0  0  0  0
    7.6751    1.1819   -0.0212 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6609    0.7271   -0.0256 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -1.0562    2.9074    0.0178 P   0  0  0  0  0  0  0  0  0  0  0  0
   -2.8661    0.9025   -1.3314 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9084    0.8989    1.2372 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3810    3.5511    1.6119 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4627    4.0695   -0.2696 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.1766    3.5297   -1.2104 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.6393    1.0148   -2.1711 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.7126    1.0129    2.0477 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0944    3.3476    2.4123 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1990    4.6278    1.5581 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.5519    3.0444    1.8612 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.2441    3.8883    0.4709 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1381    5.1106   -0.1972 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.8875    3.8973   -1.2602 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1518    3.2717   -2.2186 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.2924    4.6143   -1.1360 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.1471    3.0621   -1.0382 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2737   -1.7391    0.0085 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -2.4362   -2.2329   -1.2714 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4223   -2.2157    1.3083 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.2803   -3.2804    0.0188 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.1775   -2.5446   -2.0837 O   0  0  0  0  0  0  0  0  0  0  0  0
```

```
  -3.1531   -2.5180    2.1336 O   0  0  0  0  0  0  0  0  0  0  0  0
   0.1748   -4.3228    0.0220 O   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  3  1  0  0  0  0
 1  7  1  0  0  0  0
 1  8  2  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 2  6  1  0  0  0  0
 3  9  1  0  0  0  0
 3 10  1  0  0  0  0
 3 11  1  0  0  0  0
 7 12  4  0  0  0  0
 7 13  4  0  0  0  0
12 14  4  0  0  0  0
12 15  1  0  0  0  0
13 16  4  0  0  0  0
13 17  1  0  0  0  0
14 18  4  0  0  0  0
14 19  1  0  0  0  0
16 18  4  0  0  0  0
16 20  1  0  0  0  0
18 21  1  0  0  0  0
22 23  1  0  0  0  0
22 24  1  0  0  0  0
22 25  1  0  0  0  0
23 26  1  0  0  0  0
23 27  1  0  0  0  0
23 28  1  0  0  0  0
24 29  3  0  0  0  0
25 30  3  0  0  0  0
26 31  1  0  0  0  0
26 32  1  0  0  0  0
26 33  1  0  0  0  0
27 34  1  0  0  0  0
27 35  1  0  0  0  0
27 36  1  0  0  0  0
28 37  1  0  0  0  0
28 38  1  0  0  0  0
28 39  1  0  0  0  0
40 41  1  0  0  0  0
40 42  1  0  0  0  0
40 43  1  0  0  0  0
41 44  3  0  0  0  0
42 45  3  0  0  0  0
43 46  3  0  0  0  0
```

Molecular coordinates of **5**$^{-}$

```
5-, Fe2-Komplex, S2-Phosphanoxid-verbrueckt, PMe3

Created by GaussView 5.0.8
 46 44  0  0  0  0  0  0  0  0  0    0
    2.1479   -1.1496    0.0035 P   0  0  0  0  0  0  0  0  0  0  0  0
    1.3703   -0.3953    1.4827 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.3709   -0.4074   -1.4827 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.7642   -0.9684    2.3269 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.7314    0.6304    1.5857 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.4718   -0.3894    1.6312 S   0  0  0  0  0  0  0  0  0  0  0  0
    3.8613   -0.4396    0.0002 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.2388   -2.6470    0.0097 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.7616   -0.9906   -2.3214 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.7361    0.6158   -1.5966 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.4712   -0.3927   -1.6309 S   0  0  0  0  0  0  0  0  0  0  0  0
    4.1503    0.9304   -0.0041 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.9201   -1.3536    0.0025 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.4693    1.3780   -0.0062 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.3468    1.6596   -0.0060 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.2403   -0.9068    0.0004 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.6820   -2.4116    0.0060 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.5176    0.4585   -0.0040 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.6787    2.4426   -0.0096 H   0  0  0  0  0  0  0  0  0  0  0  0
    7.0530   -1.6258    0.0021 H   0  0  0  0  0  0  0  0  0  0  0  0
    7.5452    0.8066   -0.0057 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5476    0.9654   -0.0010 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -0.4000    3.0055    0.0079 P   0  0  0  0  0  0  0  0  0  0  0  0
   -2.7158    1.3875    1.2645 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.7016    1.4047   -1.2734 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5879    4.4342    0.0102 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.6746    3.5172    1.4404 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.6770    3.5230   -1.4209 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.4783    1.6629    2.0899 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.4532    1.6946   -2.1039 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2267    4.3673    0.8932 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0723    5.4002    0.0105 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2287    4.3689   -0.8713 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.1223    3.3503    2.3676 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.9731    4.5692    1.3821 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.5732    2.8981    1.4758 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.1241    3.3645   -2.3492 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.9801    4.5733   -1.3557 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.5728    2.8999   -1.4603 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5565   -1.7749   -0.0012 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -2.7552   -2.0915    1.2666 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.8007   -2.0267   -1.2400 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6794   -3.3794   -0.0352 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.5251   -2.3128    2.0986 O   0  0  0  0  0  0  0  0  0  0  0  0
```

```
  -3.6004   -2.2106   -2.0533 O   0  0  0  0  0  0  0  0  0  0  0  0
  -0.3828   -4.4903   -0.0658 O   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  3  1  0  0  0  0
 1  7  1  0  0  0  0
 1  8  2  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 2  6  1  0  0  0  0
 3  9  1  0  0  0  0
 3 10  1  0  0  0  0
 3 11  1  0  0  0  0
 7 12  4  0  0  0  0
 7 13  4  0  0  0  0
12 14  4  0  0  0  0
12 15  1  0  0  0  0
13 16  4  0  0  0  0
13 17  1  0  0  0  0
14 18  4  0  0  0  0
14 19  1  0  0  0  0
16 18  4  0  0  0  0
16 20  1  0  0  0  0
18 21  1  0  0  0  0
22 23  1  0  0  0  0
22 24  1  0  0  0  0
22 25  1  0  0  0  0
23 26  1  0  0  0  0
23 27  1  0  0  0  0
23 28  1  0  0  0  0
24 29  3  0  0  0  0
25 30  3  0  0  0  0
26 31  1  0  0  0  0
26 32  1  0  0  0  0
26 33  1  0  0  0  0
27 34  1  0  0  0  0
27 35  1  0  0  0  0
27 36  1  0  0  0  0
28 37  1  0  0  0  0
28 38  1  0  0  0  0
28 39  1  0  0  0  0
40 41  1  0  0  0  0
40 42  1  0  0  0  0
40 43  1  0  0  0  0
41 44  3  0  0  0  0
42 45  3  0  0  0  0
43 46  3  0  0  0  0
```

Molecular coordinates of **5**$^{2-}$

52-, Fe2-Komplex, S2-Phosphanoxid-verbrueckt, PMe3

Created by GaussView 5.0.8

46	44	0	0	0	0	0	0	0	0	0	0					
-1.7580	-1.7121	0.0943	P	0	0	0	0	0	0	0	0	0	0	0	0
-0.9876	-1.3626	-1.5558	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.9365	-0.8406	1.5181	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.0029	-2.3474	-2.0322	H	0	0	0	0	0	0	0	0	0	0	0	0
0.7306	-0.6975	-1.6733	S	0	0	0	0	0	0	0	0	0	0	0	0
-1.6551	-0.6990	-2.1108	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.4342	-0.9002	0.0126	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.9938	-3.1834	0.3492	O	0	0	0	0	0	0	0	0	0	0	0	0
-0.8946	-1.6239	2.2808	H	0	0	0	0	0	0	0	0	0	0	0	0
0.7446	-0.1020	1.3419	S	0	0	0	0	0	0	0	0	0	0	0	0
-1.6225	-0.0612	1.8588	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.6396	0.4477	-0.3058	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.5428	-1.7061	0.2964	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.9303	0.9748	-0.3356	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.7951	1.0841	-0.5434	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.8323	-1.1763	0.2719	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.3627	-2.7501	0.5306	H	0	0	0	0	0	0	0	0	0	0	0	0
-6.0297	0.1676	-0.0438	C	0	0	0	0	0	0	0	0	0	0	0	0
-5.0718	2.0194	-0.5954	H	0	0	0	0	0	0	0	0	0	0	0	0
-6.6837	-1.8133	0.4967	H	0	0	0	0	0	0	0	0	0	0	0	0
-7.0339	0.5823	-0.0673	H	0	0	0	0	0	0	0	0	0	0	0	0
0.6485	1.4041	-0.5837	Fe	0	0	0	0	0	0	0	0	0	0	0	0
0.6365	3.1139	0.8005	P	0	0	0	0	0	0	0	0	0	0	0	0
2.1826	1.9079	-1.2661	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.7295	2.0150	-1.4485	C	0	0	0	0	0	0	0	0	0	0	0	0
2.0952	3.2942	1.9368	C	0	0	0	0	0	0	0	0	0	0	0	0
0.5809	4.8185	0.0554	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.7460	3.2562	2.0390	C	0	0	0	0	0	0	0	0	0	0	0	0
3.0987	2.3878	-1.8240	O	0	0	0	0	0	0	0	0	0	0	0	0
-1.5473	2.5502	-2.1207	O	0	0	0	0	0	0	0	0	0	0	0	0
2.9971	3.3914	1.3296	H	0	0	0	0	0	0	0	0	0	0	0	0
2.0044	4.1561	2.6086	H	0	0	0	0	0	0	0	0	0	0	0	0
2.1804	2.3756	2.5201	H	0	0	0	0	0	0	0	0	0	0	0	0
1.4524	4.9403	-0.5914	H	0	0	0	0	0	0	0	0	0	0	0	0
0.5718	5.6119	0.8117	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.3112	4.8950	-0.5698	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.6948	3.3213	1.5029	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.6335	4.1273	2.6957	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.7527	2.3455	2.6408	H	0	0	0	0	0	0	0	0	0	0	0	0
1.9538	-1.7742	0.1182	Fe	0	0	0	0	0	0	0	0	0	0	0	0
2.5191	-3.0060	-1.0001	C	0	0	0	0	0	0	0	0	0	0	0	0
1.5208	-2.9857	1.3202	C	0	0	0	0	0	0	0	0	0	0	0	0
3.5257	-0.9988	0.3852	C	0	0	0	0	0	0	0	0	0	0	0	0
2.8817	-3.8135	-1.7562	O	0	0	0	0	0	0	0	0	0	0	0	0

```
   1.3557   -3.7529    2.1867 O   0  0  0  0  0  0  0  0  0  0  0  0
   4.6017   -0.6387    0.6568 O   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  3  1  0  0  0  0
 1  7  1  0  0  0  0
 1  8  2  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 2  6  1  0  0  0  0
 3  9  1  0  0  0  0
 3 10  1  0  0  0  0
 3 11  1  0  0  0  0
 7 12  4  0  0  0  0
 7 13  4  0  0  0  0
12 14  4  0  0  0  0
12 15  1  0  0  0  0
13 16  4  0  0  0  0
13 17  1  0  0  0  0
14 18  4  0  0  0  0
14 19  1  0  0  0  0
16 18  4  0  0  0  0
16 20  1  0  0  0  0
18 21  1  0  0  0  0
22 23  1  0  0  0  0
22 24  1  0  0  0  0
22 25  1  0  0  0  0
23 26  1  0  0  0  0
23 27  1  0  0  0  0
23 28  1  0  0  0  0
24 29  2  0  0  0  0
25 30  2  0  0  0  0
26 31  1  0  0  0  0
26 32  1  0  0  0  0
26 33  1  0  0  0  0
27 34  1  0  0  0  0
27 35  1  0  0  0  0
27 36  1  0  0  0  0
28 37  1  0  0  0  0
28 38  1  0  0  0  0
28 39  1  0  0  0  0
40 41  1  0  0  0  0
40 42  1  0  0  0  0
40 43  1  0  0  0  0
41 44  2  0  0  0  0
42 45  2  0  0  0  0
43 46  2  0  0  0  0
```

Molecular coordinates of **5a**$^{2-}$

```
5a2-, PME3 an Fe mit zwei S-Koordinationen

Created by GaussView 5.0.8
 46 44  0  0  0  0  0  0  0  0  0    0
   -1.2092    0.6971   -0.5264 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -2.3699    2.0193    0.8593 P   0  0  0  0  0  0  0  0  0  0  0  0
   -0.0327   -1.0559   -1.4655 S   0  0  0  0  0  0  0  0  0  0  0  0
   -4.2239    1.9493    0.8316 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1006    3.8447    0.6514 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.0527    1.8368    2.6780 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6818   -0.3556   -0.8852 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3088    1.7741   -1.8693 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.8300    1.6412    0.6646 S   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6016   -1.8386    0.1428 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    1.6753   -1.1373   -0.7632 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.5716    2.1000   -0.1921 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.5499    0.9578    1.1482 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.6581    2.7090    1.4912 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0299    4.0337    0.7474 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4169    4.1398   -0.3518 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6567    4.4259    1.3958 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6075    2.5830    3.2593 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3529    0.8345    2.9859 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9823    1.9522    2.8575 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.7783   -0.3574   -1.3641 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4599    2.4667   -2.8016 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.9667    1.7990   -0.7734 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2369   -3.2203   -0.7492 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.8159   -1.6106    1.3657 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3960   -2.4303    1.3064 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.8108    0.2317   -1.2183 P   0  0  0  0  0  0  0  0  0  0  0  0
    1.6167   -1.1595    0.3225 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.1461   -2.0587   -1.1176 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.4187    2.1096   -1.6663 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.7528    2.5363   -0.5809 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6892   -4.1768   -1.2412 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.6433   -1.4759    2.1856 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.3328   -2.8892    2.0954 O   0  0  0  0  0  0  0  0  0  0  0  0
    4.1989    0.0560    0.0058 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.3994    0.1835   -2.6136 O   0  0  0  0  0  0  0  0  0  0  0  0
    4.0271    0.1271    1.3958 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.4834   -0.1470   -0.5112 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.1262   -0.0008    2.2453 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.0348    0.3040    1.7981 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.5803   -0.2818    0.3407 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.5971   -0.1935   -1.5894 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.4035   -0.2085    1.7225 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.9816    0.0575    3.3198 H   0  0  0  0  0  0  0  0  0  0  0  0
```

```
   7.5716   -0.4435   -0.0736 H   0  0  0  0  0  0  0  0  0  0  0  0
   7.2551   -0.3145    2.3887 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  7  1  0  0  0  0
 1  8  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 2  6  1  0  0  0  0
 3 11  1  0  0  0  0
 4 12  1  0  0  0  0
 4 13  1  0  0  0  0
 4 14  1  0  0  0  0
 5 15  1  0  0  0  0
 5 16  1  0  0  0  0
 5 17  1  0  0  0  0
 6 18  1  0  0  0  0
 6 19  1  0  0  0  0
 6 20  1  0  0  0  0
 7 21  2  0  0  0  0
 8 22  2  0  0  0  0
 9 23  1  0  0  0  0
10 24  1  0  0  0  0
10 25  1  0  0  0  0
10 26  1  0  0  0  0
11 27  1  0  0  0  0
11 28  1  0  0  0  0
11 29  1  0  0  0  0
23 27  1  0  0  0  0
23 30  1  0  0  0  0
23 31  1  0  0  0  0
24 32  2  0  0  0  0
25 33  2  0  0  0  0
26 34  2  0  0  0  0
27 35  1  0  0  0  0
27 36  2  0  0  0  0
35 37  4  0  0  0  0
35 38  4  0  0  0  0
37 39  4  0  0  0  0
37 40  1  0  0  0  0
38 41  4  0  0  0  0
38 42  1  0  0  0  0
39 43  4  0  0  0  0
39 44  1  0  0  0  0
41 43  4  0  0  0  0
41 45  1  0  0  0  0
43 46  1  0  0  0  0
```

Molecular coordinates of **5b^{2-}**

```
5b2-, PMe3 an Fe mit nur einer S-Koordination

Created by GaussView 5.0.8
 46 44  0  0  0  0  0  0  0  0  0    0
   -0.8626    1.8921   -0.0988 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -1.8912   -0.5566    0.4761 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -0.3824   -0.0235   -1.3663 S   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3074   -2.4806   -0.5116 P   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1561   -1.3004    1.8792 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.6116   -0.2705    0.5411 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.7355    1.3229    1.4445 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6257    3.6061    0.0609 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.3181    1.8780    1.0206 S   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3043    2.1965   -1.0637 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.2618   -0.7249   -0.8875 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.5018   -3.6055    0.3670 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.0721   -2.4475   -2.2053 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9237   -3.6883   -0.8125 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8514   -1.8624    2.8679 O   0  0  0  0  0  0  0  0  0  0  0  0
   -4.7786   -0.1934    0.6961 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1064    1.7200    2.4910 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.4951    4.7642    0.1469 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.4071    1.9604   -0.4613 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.2229    2.4858   -1.7105 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.7346    0.3226   -1.2153 P   0  0  0  0  0  0  0  0  0  0  0  0
    1.2362   -0.9507    0.1765 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.4323   -1.6483   -1.4492 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.0917   -3.8485    1.3500 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.6873   -4.5305   -0.1913 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.4423   -3.0721    0.5182 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4183   -1.8664   -2.8582 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.2175   -3.4527   -2.6195 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.0333   -1.9332   -2.1411 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.4145   -3.8844    0.1334 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.2061   -3.2399   -1.5006 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2905   -4.6312   -1.2350 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.9447    2.5732   -1.2385 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.3771    2.4003   -0.2092 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.0490   -0.4538   -0.1556 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.2296    0.3483   -2.6484 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.9325   -0.6231    1.2319 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.2121   -0.8926   -0.7987 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.9666   -1.2175    1.9551 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.0393   -0.2715    1.7382 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.2428   -1.4921   -0.0742 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.2843   -0.7522   -1.8724 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.1219   -1.6561    1.3060 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.8654   -1.3413    3.0289 H   0  0  0  0  0  0  0  0  0  0  0  0
```

```
   7.1390   -1.8314   -0.5863 H   0  0  0  0  0  0  0  0  0  0  0  0
   6.9217   -2.1243    1.8728 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  7  1  0  0  0  0
 1  8  1  0  0  0  0
 1 10  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 2  6  1  0  0  0  0
 3 11  1  0  0  0  0
 4 12  1  0  0  0  0
 4 13  1  0  0  0  0
 4 14  1  0  0  0  0
 5 15  2  0  0  0  0
 6 16  2  0  0  0  0
 7 17  2  0  0  0  0
 8 18  2  0  0  0  0
 9 19  1  0  0  0  0
10 20  2  0  0  0  0
11 21  1  0  0  0  0
11 22  1  0  0  0  0
11 23  1  0  0  0  0
12 24  1  0  0  0  0
12 25  1  0  0  0  0
12 26  1  0  0  0  0
13 27  1  0  0  0  0
13 28  1  0  0  0  0
13 29  1  0  0  0  0
14 30  1  0  0  0  0
14 31  1  0  0  0  0
14 32  1  0  0  0  0
19 21  1  0  0  0  0
19 33  1  0  0  0  0
19 34  1  0  0  0  0
21 35  1  0  0  0  0
21 36  2  0  0  0  0
35 37  4  0  0  0  0
35 38  4  0  0  0  0
37 39  4  0  0  0  0
37 40  1  0  0  0  0
38 41  4  0  0  0  0
38 42  1  0  0  0  0
39 43  4  0  0  0  0
39 44  1  0  0  0  0
41 43  4  0  0  0  0
41 45  1  0  0  0  0
43 46  1  0  0  0  0
```

Molecular coordinates of **6**

```
6, Fe2S2 Phosphanoxid-verbrueckt, Laith, P(OMe)3

Created by GaussView 5.0.8
 49 47  0  0  0  0  0  0  0  0  0    0
    0.7300    2.4514   -0.0139 P   0  0  0  0  0  0  0  0  0  0  0  0
    1.5964    0.4401   -0.0328 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -0.2852    2.8832    1.1953 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.8015    0.6321   -1.3416 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.8371    0.6692    1.2349 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.7110    3.7658    0.0876 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.2423    2.7838   -1.2709 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.1792    3.0435    2.5486 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.5740    0.7320   -2.1826 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.6388    0.8053    2.0436 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.9672    3.8747   -0.6014 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8932    4.0622   -1.4415 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.9044    3.8569    2.6036 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.6234    2.1163    2.9193 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6981    3.2895    3.1448 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.6903    3.1535   -0.2158 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.8450    3.7333   -1.6778 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.3295    4.8835   -0.4090 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6084    4.2331   -0.6359 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1562    4.8666   -1.4534 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4064    4.0131   -2.4000 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.2869   -2.0463   -0.0067 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    2.4443   -2.5355   -1.2984 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.4535   -2.5056    1.2883 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.3010   -3.5908    0.0105 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.1810   -2.8413   -2.1157 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.1966   -2.7902    2.1078 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1668   -4.6267    0.0217 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4898   -0.3709   -1.4724 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3270   -1.0979   -0.0183 P   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9547   -0.8171   -2.3543 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6408    0.7087   -1.5104 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.3209   -0.6763   -1.6264 S   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4910   -0.3473    1.4265 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.0046   -0.3653   -0.0193 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3652   -2.5953   -0.0057 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9568   -0.7807    2.3143 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6547    0.7313    1.4413 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.3223   -0.6449    1.5893 S   0  0  0  0  0  0  0  0  0  0  0  0
   -4.2400    1.0158   -0.0095 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.0880   -1.2504   -0.0298 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.5438    1.5029   -0.0105 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.4117    1.7167    0.0012 H   0  0  0  0  0  0  0  0  0  0  0  0
   -6.3914   -0.7581   -0.0315 C   0  0  0  0  0  0  0  0  0  0  0  0
```

```
  -4.8920   -2.3164   -0.0356 H   0  0  0  0  0  0  0  0  0  0  0  0
  -6.6200    0.6159   -0.0219 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.7211    2.5724   -0.0018 H   0  0  0  0  0  0  0  0  0  0  0  0
  -7.2275   -1.4481   -0.0397 H   0  0  0  0  0  0  0  0  0  0  0  0
  -7.6350    0.9973   -0.0227 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  3  1  0  0  0  0
 1  6  1  0  0  0  0
 1  7  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 3  8  1  0  0  0  0
 4  9  3  0  0  0  0
 5 10  3  0  0  0  0
 6 11  1  0  0  0  0
 7 12  1  0  0  0  0
 8 13  1  0  0  0  0
 8 14  1  0  0  0  0
 8 15  1  0  0  0  0
11 16  1  0  0  0  0
11 17  1  0  0  0  0
11 18  1  0  0  0  0
12 19  1  0  0  0  0
12 20  1  0  0  0  0
12 21  1  0  0  0  0
22 23  1  0  0  0  0
22 24  1  0  0  0  0
22 25  1  0  0  0  0
23 26  3  0  0  0  0
24 27  3  0  0  0  0
25 28  3  0  0  0  0
29 30  1  0  0  0  0
29 31  1  0  0  0  0
29 32  1  0  0  0  0
29 33  1  0  0  0  0
30 34  1  0  0  0  0
30 35  1  0  0  0  0
30 36  2  0  0  0  0
34 37  1  0  0  0  0
34 38  1  0  0  0  0
34 39  1  0  0  0  0
35 40  4  0  0  0  0
35 41  4  0  0  0  0
40 42  4  0  0  0  0
40 43  1  0  0  0  0
41 44  4  0  0  0  0
41 45  1  0  0  0  0
42 46  4  0  0  0  0
42 47  1  0  0  0  0
44 46  4  0  0  0  0
44 48  1  0  0  0  0
46 49  1  0  0  0  0
```

Molecular coordinates of **6**$^{-}$

```
6-, Fe2-Komplex, S2-Phosphanoxid-verbrueckt, P(OMe)3

Created by GaussView 5.0.8
 49 47  0  0  0  0  0  0  0  0  0    0
    0.0708    2.5018   -0.0015 P   0  0  0  0  0  0  0  0  0  0  0  0
    1.4748    0.8116   -0.0715 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -0.8962    2.7627    1.3291 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.5847    1.2596   -1.3813 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.6657    1.2923    1.1509 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.6642    4.0660   -0.0414 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1520    2.6071   -1.1107 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.2960    2.9661    2.6122 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.3096    1.5354   -2.2388 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.4453    1.6034    1.9477 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.8374    4.4046   -0.7825 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.0564    3.7184   -1.1675 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.3536    2.1288    2.8801 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.2775    3.8973    2.6225 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1128    3.0343    3.3322 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.7095    3.8583   -0.4177 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.7145    4.2014   -1.8505 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.9944    5.4750   -0.6373 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5101    4.6547   -1.3034 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6485    3.7818   -0.2514 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.7100    3.5449   -2.0231 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.7375   -1.9375    0.0009 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    2.9535   -2.1651    1.2821 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.9833   -2.1842   -1.2492 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.9503   -3.6130    0.0207 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.7342   -2.3215    2.1158 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.7845   -2.3561   -2.0602 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.7028   -4.7330    0.0277 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2771   -0.7589   -1.5105 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.0066   -1.5313   -0.0201 P   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6528   -1.3464   -2.3527 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6428    0.2648   -1.6088 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.5630   -0.6981   -1.6533 S   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2851   -0.6928    1.4411 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.7618   -0.9491   -0.0315 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9693   -3.0320    0.0160 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6623   -1.2476    2.3046 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6672    0.3285    1.4969 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.5545   -0.6147    1.5935 S   0  0  0  0  0  0  0  0  0  0  0  0
   -4.1310    0.4016   -0.0581 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.7589   -1.9295   -0.0091 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.4765    0.7622   -0.0612 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.3707    1.1745   -0.0769 H   0  0  0  0  0  0  0  0  0  0  0  0
   -6.1046   -1.5667   -0.0132 C   0  0  0  0  0  0  0  0  0  0  0  0
```

```
  -4.4554   -2.9704    0.0118 H   0  0  0  0  0  0  0  0  0  0  0  0
  -6.4653   -0.2211   -0.0389 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.7532    1.8111   -0.0807 H   0  0  0  0  0  0  0  0  0  0  0  0
  -6.8711   -2.3346    0.0042 H   0  0  0  0  0  0  0  0  0  0  0  0
  -7.5128    0.0622   -0.0414 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  3  1  0  0  0  0
 1  6  1  0  0  0  0
 1  7  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 3  8  1  0  0  0  0
 4  9  3  0  0  0  0
 5 10  3  0  0  0  0
 6 11  1  0  0  0  0
 7 12  1  0  0  0  0
 8 13  1  0  0  0  0
 8 14  1  0  0  0  0
 8 15  1  0  0  0  0
11 16  1  0  0  0  0
11 17  1  0  0  0  0
11 18  1  0  0  0  0
12 19  1  0  0  0  0
12 20  1  0  0  0  0
12 21  1  0  0  0  0
22 23  1  0  0  0  0
22 24  1  0  0  0  0
22 25  1  0  0  0  0
23 26  3  0  0  0  0
24 27  3  0  0  0  0
25 28  3  0  0  0  0
29 30  1  0  0  0  0
29 31  1  0  0  0  0
29 32  1  0  0  0  0
29 33  1  0  0  0  0
30 34  1  0  0  0  0
30 35  1  0  0  0  0
30 36  2  0  0  0  0
34 37  1  0  0  0  0
34 38  1  0  0  0  0
34 39  1  0  0  0  0
35 40  4  0  0  0  0
35 41  4  0  0  0  0
40 42  4  0  0  0  0
40 43  1  0  0  0  0
41 44  4  0  0  0  0
41 45  1  0  0  0  0
42 46  4  0  0  0  0
42 47  1  0  0  0  0
44 46  4  0  0  0  0
44 48  1  0  0  0  0
46 49  1  0  0  0  0
```

Molecular coordinates of **6^{2-}**

62-, Fe2-Komplex, S2-Phosphanoxid-verbrueckt, P(OMe)3

Created by GaussView 5.0.8

49	47	0	0	0	0	0	0	0	0	0	0				
-1.3065	2.2071	-0.2784	P	0	0	0	0	0	0	0	0	0	0	0	0
0.6305	1.5781	0.2348	Fe	0	0	0	0	0	0	0	0	0	0	0	0
-1.6185	3.8830	-0.2804	O	0	0	0	0	0	0	0	0	0	0	0	0
1.8958	2.5349	-0.5259	C	0	0	0	0	0	0	0	0	0	0	0	0
0.6897	2.5424	1.6975	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.7725	1.9300	0.5789	O	0	0	0	0	0	0	0	0	0	0	0	0
-1.9761	1.8049	-1.7532	O	0	0	0	0	0	0	0	0	0	0	0	0
-0.6063	4.7842	-0.7108	C	0	0	0	0	0	0	0	0	0	0	0	0
2.6668	3.2439	-1.0384	O	0	0	0	0	0	0	0	0	0	0	0	0
0.7557	3.1608	2.6847	O	0	0	0	0	0	0	0	0	0	0	0	0
-2.7710	2.1508	1.9779	C	0	0	0	0	0	0	0	0	0	0	0	0
-3.2349	2.2960	-2.1949	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.2302	4.5359	-1.7091	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.0655	5.7785	-0.7368	H	0	0	0	0	0	0	0	0	0	0	0	0
0.2435	4.7953	-0.0241	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.8869	1.7103	2.4538	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.7918	3.2231	2.2086	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.6686	1.6786	2.3892	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.0531	1.8684	-1.6075	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.2823	3.3871	-2.1166	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.3422	1.9990	-3.2417	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.4782	-1.2876	0.1961	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.8600	-1.4643	0.2657	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.6310	-2.3916	0.0381	C	0	0	0	0	0	0	0	0	0	0	0	0
-3.0773	-0.2820	0.2646	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.4150	-2.7410	0.1787	C	0	0	0	0	0	0	0	0	0	0	0	0
-5.5010	-0.5961	0.3865	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.7697	-2.2948	-0.0737	P	0	0	0	0	0	0	0	0	0	0	0	0
-3.1962	-3.6693	-0.0495	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.5775	-3.8444	0.0207	C	0	0	0	0	0	0	0	0	0	0	0	0
-6.4920	-2.8739	0.2327	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.4609	-1.1768	-1.5067	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.2893	-1.4867	1.5240	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.2777	-3.7087	-0.2554	O	0	0	0	0	0	0	0	0	0	0	0	0
-2.5223	-4.5104	-0.1736	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.0004	-4.8430	-0.0486	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.3377	-1.8747	-2.3405	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.3426	-0.5623	-1.6957	H	0	0	0	0	0	0	0	0	0	0	0	0
1.0213	-0.0745	-1.4711	S	0	0	0	0	0	0	0	0	0	0	0	0
-0.0775	-2.3390	2.1774	H	0	0	0	0	0	0	0	0	0	0	0	0
1.1579	-0.3337	1.5935	S	0	0	0	0	0	0	0	0	0	0	0	0
-1.1610	-0.9596	1.9178	H	0	0	0	0	0	0	0	0	0	0	0	0
2.6723	-1.1836	-0.0583	Fe	0	0	0	0	0	0	0	0	0	0	0	0
3.4492	-1.8542	-1.4857	C	0	0	0	0	0	0	0	0	0	0	0	0

```
   2.7262   -2.7435    0.7582 C   0  0  0  0  0  0  0  0  0  0  0  0
   3.9927   -0.0920    0.3999 C   0  0  0  0  0  0  0  0  0  0  0  0
   3.9488   -2.2879   -2.4433 O   0  0  0  0  0  0  0  0  0  0  0  0
   2.8893   -3.7237    1.3707 O   0  0  0  0  0  0  0  0  0  0  0  0
   4.9585    0.4615    0.7490 O   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  3  1  0  0  0  0
 1  6  1  0  0  0  0
 1  7  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 3  8  1  0  0  0  0
 4  9  2  0  0  0  0
 5 10  2  0  0  0  0
 6 11  1  0  0  0  0
 7 12  1  0  0  0  0
 8 13  1  0  0  0  0
 8 14  1  0  0  0  0
 8 15  1  0  0  0  0
11 16  1  0  0  0  0
11 17  1  0  0  0  0
11 18  1  0  0  0  0
12 19  1  0  0  0  0
12 20  1  0  0  0  0
12 21  1  0  0  0  0
22 23  4  0  0  0  0
22 24  4  0  0  0  0
22 25  1  0  0  0  0
23 26  4  0  0  0  0
23 27  1  0  0  0  0
24 28  1  0  0  0  0
24 29  4  0  0  0  0
26 30  4  0  0  0  0
26 31  1  0  0  0  0
28 32  1  0  0  0  0
28 33  1  0  0  0  0
28 34  2  0  0  0  0
29 30  4  0  0  0  0
29 35  1  0  0  0  0
30 36  1  0  0  0  0
32 37  1  0  0  0  0
32 38  1  0  0  0  0
32 39  1  0  0  0  0
33 40  1  0  0  0  0
33 41  1  0  0  0  0
33 42  1  0  0  0  0
43 44  1  0  0  0  0
43 45  1  0  0  0  0
43 46  1  0  0  0  0
44 47  2  0  0  0  0
45 48  2  0  0  0  0
46 49  2  0  0  0  0
```

Molecular coordinates of **6a^{2-}**

6a2-, Fe2-Komplex, S2 mit Phosphanoxidbruecke, P(OMe)3

Created by GaussView 5.0.8

49	47	0	0	0	0	0	0	0	0	0	0						
1.3951	-0.0194	0.1946	Fe	0	0	0	0	0	0	0	0	0	0	0	0
0.6796	2.5837	-0.1779	Fe	0	0	0	0	0	0	0	0	0	0	0	0
0.0159	0.8148	-1.5392	S	0	0	0	0	0	0	0	0	0	0	0	0
-0.5489	-0.8399	1.4540	S	0	0	0	0	0	0	0	0	0	0	0	0
2.4076	1.1283	2.6858	O	0	0	0	0	0	0	0	0	0	0	0	0
3.7069	0.7958	-1.4066	O	0	0	0	0	0	0	0	0	0	0	0	0
3.2312	4.0145	-0.0567	O	0	0	0	0	0	0	0	0	0	0	0	0
-0.8975	3.1858	2.2146	O	0	0	0	0	0	0	0	0	0	0	0	0
-0.5087	4.6938	-1.7820	O	0	0	0	0	0	0	0	0	0	0	0	0
-1.7819	0.6071	-1.1439	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.9781	1.1399	-0.2160	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.3524	1.0773	-1.9503	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.4583	-1.9582	0.3082	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.7845	-2.6306	-0.2245	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.1492	-2.5802	0.8852	H	0	0	0	0	0	0	0	0	0	0	0	0
1.9649	0.7569	1.6740	C	0	0	0	0	0	0	0	0	0	0	0	0
2.7818	0.5217	-0.7692	C	0	0	0	0	0	0	0	0	0	0	0	0
2.2534	3.3750	-0.1480	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.3118	2.8432	1.2624	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.0255	3.8510	-1.1314	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.0908	-0.7682	-0.1239	C	0	0	0	0	0	0	0	0	0	0	0	0
-5.2535	-1.1940	-0.7746	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.1982	-0.1344	1.1226	C	0	0	0	0	0	0	0	0	0	0	0	0
-6.5066	-0.9870	-0.1966	C	0	0	0	0	0	0	0	0	0	0	0	0
-5.1499	-1.6886	-1.7350	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.4510	0.0667	1.7010	C	0	0	0	0	0	0	0	0	0	0	0	0
-3.2992	0.1884	1.6386	H	0	0	0	0	0	0	0	0	0	0	0	0
-6.6077	-0.3552	1.0430	C	0	0	0	0	0	0	0	0	0	0	0	0
-7.4032	-1.3179	-0.7133	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.5222	0.5599	2.6654	H	0	0	0	0	0	0	0	0	0	0	0	0
-7.5820	-0.1901	1.4939	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.7064	-1.8670	-2.2354	O	0	0	0	0	0	0	0	0	0	0	0	0
-2.4635	-1.0857	-0.9590	P	0	0	0	0	0	0	0	0	0	0	0	0
2.0735	-2.0532	0.0826	P	0	0	0	0	0	0	0	0	0	0	0	0
2.0405	-3.1215	1.3555	O	0	0	0	0	0	0	0	0	0	0	0	0
1.4093	-3.2124	-0.9346	O	0	0	0	0	0	0	0	0	0	0	0	0
3.6882	-2.2015	-0.3506	O	0	0	0	0	0	0	0	0	0	0	0	0
4.3208	-3.4695	-0.4518	C	0	0	0	0	0	0	0	0	0	0	0	0
5.3264	-3.2904	-0.8419	H	0	0	0	0	0	0	0	0	0	0	0	0
4.3906	-3.9585	0.5262	H	0	0	0	0	0	0	0	0	0	0	0	0
3.7779	-4.1359	-1.1309	H	0	0	0	0	0	0	0	0	0	0	0	0
2.2302	-2.6347	2.6860	C	0	0	0	0	0	0	0	0	0	0	0	0
1.4168	-1.9613	2.9633	H	0	0	0	0	0	0	0	0	0	0	0	0
2.2198	-3.5162	3.3334	H	0	0	0	0	0	0	0	0	0	0	0	0

```
   3.1912   -2.1199    2.7943 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.1549   -2.8299   -2.2922 C   0  0  0  0  0  0  0  0  0  0  0  0
   0.3602   -3.4780   -2.6649 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.8267   -1.7889   -2.3608 H   0  0  0  0  0  0  0  0  0  0  0  0
   2.0571   -2.9638   -2.9026 H   0  0  0  0  0  0  0  0  0  0  0  0
 1 16  1  0  0  0  0
 1 17  1  0  0  0  0
 1 34  1  0  0  0  0
 2 18  1  0  0  0  0
 2 19  1  0  0  0  0
 2 20  1  0  0  0  0
 3 10  1  0  0  0  0
 4 13  1  0  0  0  0
 5 16  2  0  0  0  0
 6 17  3  0  0  0  0
 7 18  2  0  0  0  0
 8 19  2  0  0  0  0
 9 20  2  0  0  0  0
10 11  1  0  0  0  0
10 12  1  0  0  0  0
10 33  1  0  0  0  0
13 14  1  0  0  0  0
13 15  1  0  0  0  0
13 33  1  0  0  0  0
21 22  4  0  0  0  0
21 23  4  0  0  0  0
21 33  1  0  0  0  0
22 24  4  0  0  0  0
22 25  1  0  0  0  0
23 26  4  0  0  0  0
23 27  1  0  0  0  0
24 28  4  0  0  0  0
24 29  1  0  0  0  0
26 28  4  0  0  0  0
26 30  1  0  0  0  0
28 31  1  0  0  0  0
32 33  2  0  0  0  0
34 35  1  0  0  0  0
34 36  1  0  0  0  0
34 37  1  0  0  0  0
35 42  1  0  0  0  0
36 46  1  0  0  0  0
37 38  1  0  0  0  0
38 39  1  0  0  0  0
38 40  1  0  0  0  0
38 41  1  0  0  0  0
42 43  1  0  0  0  0
42 44  1  0  0  0  0
42 45  1  0  0  0  0
46 47  1  0  0  0  0
46 48  1  0  0  0  0
46 49  1  0  0  0  0
```

Molecular coordinates of **$6b^{2-}$**

```
6b2-, Fe2S2 mit Phosphanoxidbruecke, P(OMe)3

Created by GaussView 5.0.8
 49 47  0  0  0  0  0  0  0  0  0    0
   -0.1629    2.2701   -0.0738 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -1.6619    0.0225    0.3754 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -0.1014    0.2915   -1.3571 S   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5985   -1.7804   -0.1977 P   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9144   -0.6285    1.8307 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.2242    0.8184    0.4965 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9758    2.2860    1.5176 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.6442    3.7901   -0.4042 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.9825    1.8117    1.0079 S   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5571    2.8145   -1.0237 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.3424   -0.7552   -0.8573 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.8336   -3.0483   -0.9758 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.9600   -1.6571   -1.1751 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.1976   -2.8293    0.9607 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.5632   -1.0561    2.8641 O   0  0  0  0  0  0  0  0  0  0  0  0
   -4.2727    1.3035    0.7046 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3615    2.6125    2.5681 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.1302    4.8346   -0.5837 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.0708    1.5989   -0.4611 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4043    3.2637   -1.6700 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.0189   -0.0856   -1.1851 P   0  0  0  0  0  0  0  0  0  0  0  0
    1.2615   -0.9570    0.2083 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.2843   -1.7032   -1.4003 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3928   -2.8700   -2.3215 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.7933   -2.7803   -1.4331 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.8142   -2.3108    2.1376 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.7803    2.2856   -1.2593 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.1124    1.8054   -0.1968 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.1091   -1.1185   -0.0929 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.5246   -0.1894   -2.6103 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2336   -2.9588   -3.0215 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9161   -1.8974   -2.4686 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6741   -3.6676   -2.5253 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.2099   -3.6703   -1.6927 H   0  0  0  0  0  0  0  0  0  0  0  0
   -5.4406   -2.5098   -2.2725 H   0  0  0  0  0  0  0  0  0  0  0  0
   -5.4152   -3.0204   -0.5633 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.3476   -1.3761    2.4551 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.6944   -3.0650    2.9198 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.8838   -2.1337    1.9655 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.9328   -1.2345    1.2935 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.1599   -1.8099   -0.7061 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.7997   -2.0265    2.0462 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.1278   -0.6908    1.7767 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.0223   -2.6062    0.0481 C   0  0  0  0  0  0  0  0  0  0  0  0
```

```
   5.2797   -1.7072   -1.7797 H   0  0  0  0  0  0  0  0  0  0  0  0
   5.8437   -2.7158    1.4273 C   0  0  0  0  0  0  0  0  0  0  0  0
   4.6535   -2.1081    3.1187 H   0  0  0  0  0  0  0  0  0  0  0  0
   6.8319   -3.1413   -0.4403 H   0  0  0  0  0  0  0  0  0  0  0  0
   6.5119   -3.3369    2.0170 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  7  1  0  0  0  0
 1  8  1  0  0  0  0
 1 10  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 2  6  1  0  0  0  0
 3 11  1  0  0  0  0
 4 12  1  0  0  0  0
 4 13  1  0  0  0  0
 4 14  1  0  0  0  0
 5 15  2  0  0  0  0
 6 16  2  0  0  0  0
 7 17  2  0  0  0  0
 8 18  2  0  0  0  0
 9 19  1  0  0  0  0
10 20  3  0  0  0  0
11 21  1  0  0  0  0
11 22  1  0  0  0  0
11 23  1  0  0  0  0
12 24  1  0  0  0  0
13 25  1  0  0  0  0
14 26  1  0  0  0  0
19 21  1  0  0  0  0
19 27  1  0  0  0  0
19 28  1  0  0  0  0
21 29  1  0  0  0  0
21 30  2  0  0  0  0
24 31  1  0  0  0  0
24 32  1  0  0  0  0
24 33  1  0  0  0  0
25 34  1  0  0  0  0
25 35  1  0  0  0  0
25 36  1  0  0  0  0
26 37  1  0  0  0  0
26 38  1  0  0  0  0
26 39  1  0  0  0  0
29 40  4  0  0  0  0
29 41  4  0  0  0  0
40 42  4  0  0  0  0
40 43  1  0  0  0  0
41 44  4  0  0  0  0
41 45  1  0  0  0  0
42 46  4  0  0  0  0
42 47  1  0  0  0  0
44 46  4  0  0  0  0
44 48  1  0  0  0  0
46 49  1  0  0  0  0
```

Molecular coordinates of **7**

```
7, Monoanion - CO

Created by GaussView 5.0.8
 33 31  0  0  0  0  0  0  0  0  0    0
   -2.0855    0.6327    0.0000 P   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3182   -0.1302    1.4774 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3182   -0.1302   -1.4773 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6968    0.4496    2.3238 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6885   -1.1523    1.5835 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.5233   -0.1776    1.6320 S   0  0  0  0  0  0  0  0  0  0  0  0
   -3.8057   -0.0530    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1367    2.1332    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6968    0.4496   -2.3238 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6886   -1.1523   -1.5835 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.5233   -0.1777   -1.6320 S   0  0  0  0  0  0  0  0  0  0  0  0
   -4.1023   -1.4220    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.8568    0.8700    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.4252   -1.8595    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.3037   -2.1572    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   -6.1810    0.4324    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.6132    1.9268    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   -6.4674   -0.9317    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.6426   -2.9224    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   -6.9886    1.1569    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   -7.4974   -1.2728    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.6776    1.1389   -0.0000 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    2.9170    1.3161    1.2503 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.9173    1.3156   -1.2502 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.9134    2.7755   -0.0002 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.7179    1.4646    2.0701 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.7183    1.4639   -2.0699 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.6388    3.8924   -0.0004 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.5859   -1.4680    0.0000 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    2.4409   -2.3564    1.2793 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.4409   -2.3565   -1.2792 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.0043   -2.9390    2.1039 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.0042   -2.9393   -2.1038 O   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1  3  1  0  0  0  0
  1  7  1  0  0  0  0
  1  8  2  0  0  0  0
  2  4  1  0  0  0  0
  2  5  1  0  0  0  0
  2  6  1  0  0  0  0
  3  9  1  0  0  0  0
  3 10  1  0  0  0  0
  3 11  1  0  0  0  0
  7 12  4  0  0  0  0
```

7	13	4	0	0	0	0
12	14	4	0	0	0	0
12	15	1	0	0	0	0
13	16	4	0	0	0	0
13	17	1	0	0	0	0
14	18	4	0	0	0	0
14	19	1	0	0	0	0
16	18	4	0	0	0	0
16	20	1	0	0	0	0
18	21	1	0	0	0	0
22	23	1	0	0	0	0
22	24	1	0	0	0	0
22	25	1	0	0	0	0
23	26	3	0	0	0	0
24	27	3	0	0	0	0
25	28	3	0	0	0	0
29	30	1	0	0	0	0
29	31	1	0	0	0	0
30	32	3	0	0	0	0
31	33	3	0	0	0	0

Molecular coordinates of **8**

```
8, Fe2-Komplex, Dianion umgelagert, -PPh3

Created by GaussView 5.0.8
 33 33  0  0  0  0  0  0  0  0  0    0
    1.2554   -1.0730    0.2635 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    2.2314    1.1295   -0.1038 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    0.6496    0.2138   -1.5379 S   0  0  0  0  0  0  0  0  0  0  0  0
    2.3160    2.7770   -0.6867 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.9676    1.4418    1.5959 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.9810   -2.3576   -0.6340 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.1881   -1.4217    1.7148 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8089   -2.0058    0.7948 S   0  0  0  0  0  0  0  0  0  0  0  0
    3.8931    0.6801   -0.4158 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0312    0.8784   -1.0886 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.3743    3.8787   -1.0781 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.9323    1.7758    2.7223 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.4848   -3.2058   -1.2494 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.8223   -1.7218    2.6411 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.8209   -1.9584   -0.7472 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.0314    0.4299   -0.5436 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4153   -0.3124   -1.3003 P   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9990    1.2275   -0.0574 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2607    1.7258   -1.7410 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2464   -2.3526   -1.5888 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.7131   -2.5807   -0.6259 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.6946    0.2234   -0.0668 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.0549   -0.3302   -2.6756 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.4509    0.3608    1.3073 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.9719    0.5091   -0.5629 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.4733    0.7709    2.1629 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4695    0.1229    1.7016 H   0  0  0  0  0  0  0  0  0  0  0  0
   -5.9909    0.9266    0.2938 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.1402    0.3993   -1.6292 H   0  0  0  0  0  0  0  0  0  0  0  0
   -5.7433    1.0580    1.6603 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.2733    0.8693    3.2254 H   0  0  0  0  0  0  0  0  0  0  0  0
   -6.9763    1.1506   -0.1051 H   0  0  0  0  0  0  0  0  0  0  0  0
   -6.5340    1.3841    2.3300 H   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1  3  1  0  0  0  0
  1  6  1  0  0  0  0
  1  7  1  0  0  0  0
  2  4  1  0  0  0  0
  2  5  1  0  0  0  0
  2  9  1  0  0  0  0
  3 10  1  0  0  0  0
  4 11  2  0  0  0  0
  5 12  2  0  0  0  0
  6 13  2  0  0  0  0
```

7	14	2	0	0	0	0
8	15	1	0	0	0	0
9	16	2	0	0	0	0
10	17	1	0	0	0	0
10	18	1	0	0	0	0
10	19	1	0	0	0	0
15	17	1	0	0	0	0
15	20	1	0	0	0	0
15	21	1	0	0	0	0
17	22	1	0	0	0	0
17	23	2	0	0	0	0
22	24	4	0	0	0	0
22	25	4	0	0	0	0
24	26	4	0	0	0	0
24	27	1	0	0	0	0
25	28	4	0	0	0	0
25	29	1	0	0	0	0
26	30	4	0	0	0	0
26	31	1	0	0	0	0
28	30	4	0	0	0	0
28	32	1	0	0	0	0
30	33	1	0	0	0	0

Molecular coordinates of **P1**

```
P1, Dianion_Oet + CO

Created by GaussView 5.0.8
 60 58  0  0  0  0  0  0  0  0  0    0
    2.5238   -0.9894    0.2475 P   0  0  0  0  0  0  0  0  0  0  0  0
    0.8708    0.4177   -0.0788 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    3.8764   -0.5935   -0.6147 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.7263    1.4468   -1.2643 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.2548    1.4077    1.3518 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.4898   -2.6465    0.0502 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.2480   -1.0337    1.7296 O   0  0  0  0  0  0  0  0  0  0  0  0
    5.1581   -1.1925   -0.3943 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.3450    2.0071   -2.0594 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.5951    1.8981    2.3439 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.2683   -3.2714   -1.2318 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.5945   -1.5232    2.9171 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.0731   -0.7625   -1.5299 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.5467   -0.8601    0.5731 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.0593   -2.2832   -0.3571 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.1687   -4.7706   -1.0102 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.3601   -2.8678   -1.6866 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.1129   -3.0333   -1.8916 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.2415   -0.8568    4.1188 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.5237   -1.3068    2.8674 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.7230   -2.6118    2.9504 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.1500    0.3268   -1.5647 H   0  0  0  0  0  0  0  0  0  0  0  0
    7.0760   -1.1818   -1.3893 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.6825   -1.1040   -2.4919 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.0758   -5.1616   -0.5374 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.0257   -5.2776   -1.9701 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.3139   -5.0078   -0.3728 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.7885   -1.2353    5.0418 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.3167   -1.0618    4.1514 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.0912    0.2239    4.0759 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.8323    4.0392    0.0710 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6753    3.1303   -0.2025 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    1.7601    4.7240    0.2425 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6636    4.5566   -0.2887 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5870    2.4486    1.1710 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0362    2.6194   -1.8782 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3236    5.5167   -0.3435 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2598    2.1346    2.0678 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3473    2.4422   -2.9832 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0187   -2.4300    0.5907 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2442   -2.3222   -0.7694 P   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4323   -3.1105    1.3408 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1335   -2.8987    0.1611 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6131   -0.8304    1.3928 S   0  0  0  0  0  0  0  0  0  0  0  0
```

```
  -1.8019   -0.8322   -1.7433 C   0  0  0  0  0  0  0  0  0  0  0  0
  -3.8801   -1.9508    0.0217 C   0  0  0  0  0  0  0  0  0  0  0  0
  -2.3754   -3.6079   -1.5653 O   0  0  0  0  0  0  0  0  0  0  0  0
  -2.3242   -0.9285   -2.6994 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.0007   -0.6963   -2.0535 S   0  0  0  0  0  0  0  0  0  0  0  0
  -2.1607    0.0657   -1.2395 H   0  0  0  0  0  0  0  0  0  0  0  0
  -4.1245   -0.8283    0.8267 C   0  0  0  0  0  0  0  0  0  0  0  0
  -4.9235   -2.8512   -0.2265 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.3903   -0.6246    1.3772 C   0  0  0  0  0  0  0  0  0  0  0  0
  -3.3249   -0.1290    1.0413 H   0  0  0  0  0  0  0  0  0  0  0  0
  -6.1894   -2.6415    0.3206 C   0  0  0  0  0  0  0  0  0  0  0  0
  -4.7171   -3.7106   -0.8558 H   0  0  0  0  0  0  0  0  0  0  0  0
  -6.4247   -1.5265    1.1259 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.5619    0.2467    2.0008 H   0  0  0  0  0  0  0  0  0  0  0  0
  -6.9909   -3.3466    0.1178 H   0  0  0  0  0  0  0  0  0  0  0  0
  -7.4098   -1.3589    1.5524 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  3  1  0  0  0  0
 1  6  1  0  0  0  0
 1  7  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 3  8  1  0  0  0  0
 4  9  3  0  0  0  0
 5 10  3  0  0  0  0
 6 11  1  0  0  0  0
 7 12  1  0  0  0  0
 8 13  1  0  0  0  0
 8 14  1  0  0  0  0
 8 15  1  0  0  0  0
11 16  1  0  0  0  0
11 17  1  0  0  0  0
11 18  1  0  0  0  0
12 19  1  0  0  0  0
12 20  1  0  0  0  0
12 21  1  0  0  0  0
13 22  1  0  0  0  0
13 23  1  0  0  0  0
13 24  1  0  0  0  0
16 25  1  0  0  0  0
16 26  1  0  0  0  0
16 27  1  0  0  0  0
19 28  1  0  0  0  0
19 29  1  0  0  0  0
19 30  1  0  0  0  0
31 32  1  0  0  0  0
31 33  2  0  0  0  0
32 34  1  0  0  0  0
32 35  1  0  0  0  0
32 36  1  0  0  0  0
34 37  2  0  0  0  0
35 38  2  0  0  0  0
```

36	39	2	0	0	0	0
40	41	1	0	0	0	0
40	42	1	0	0	0	0
40	43	1	0	0	0	0
40	44	1	0	0	0	0
41	45	1	0	0	0	0
41	46	1	0	0	0	0
41	47	2	0	0	0	0
45	48	1	0	0	0	0
45	49	1	0	0	0	0
45	50	1	0	0	0	0
46	51	4	0	0	0	0
46	52	4	0	0	0	0
51	53	4	0	0	0	0
51	54	1	0	0	0	0
52	55	4	0	0	0	0
52	56	1	0	0	0	0
53	57	4	0	0	0	0
53	58	1	0	0	0	0
55	57	4	0	0	0	0
55	59	1	0	0	0	0
57	60	1	0	0	0	0

Molecular coordinates of **P2**

```
P2, Fe2-Komplex, P(OEt)3, Dianion + CO

Created by GaussView 5.0.8
 60 58  0  0  0  0  0  0  0  0  0    0
    2.5496   -0.5943   -0.2056 P   0  0  0  0  0  0  0  0  0  0  0  0
    0.7713   -1.5591    0.4307 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    3.7258   -0.1087    0.9125 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.7641   -2.6818   -0.9138 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.8460   -2.8781    1.5789 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.5743   -1.4222   -1.2841 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.6425    0.8420   -1.0836 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.9293   -0.8023    2.1461 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.7576   -3.4422   -1.7954 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.9976   -3.7673    2.3255 O   0  0  0  0  0  0  0  0  0  0  0  0
    4.0933   -2.7026   -0.9453 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.8686    1.4021   -1.5732 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.4386    0.1902    3.1797 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.9879   -1.2431    2.4787 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.6654   -1.6052    1.9914 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.4001   -3.4640   -2.2271 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.3698   -3.2564   -0.3371 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.0079   -2.5777   -0.3465 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.8718    1.4002   -3.0971 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.7216    0.8442   -1.1831 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.9350    2.4278   -1.1879 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.3552    0.6821    2.8368 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.6766    0.9500    3.3667 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.6511   -0.3249    4.1237 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.8300   -4.4450   -1.9934 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.4831   -3.6132   -2.8011 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.1146   -2.9107   -2.8450 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.7858    1.8713   -3.4813 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.8202    0.3738   -3.4657 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.0100    1.9493   -3.4872 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.8292    3.9940   -0.6702 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.2041    5.2541   -1.1365 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3262    3.8398    0.1091 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.4355    3.1272   -0.9129 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.4313    6.3757   -0.8307 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.1002    5.3602   -1.7405 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8972    2.2016    0.7866 P   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0949    4.9699    0.4102 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.7199    6.2301   -0.0558 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.7243    7.3556   -1.1961 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.5569    1.6174    1.7416 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0375    1.1965   -0.7520 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1638    2.4217    1.5732 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9870    4.8316    1.0124 H   0  0  0  0  0  0  0  0  0  0  0  0
```

```
  -1.3269    7.0986    0.1833 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.5997    2.2832    2.6106 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.4540    1.7886    1.1404 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.4700   -0.1169    2.3402 S   0  0  0  0  0  0  0  0  0  0  0  0
  -0.1132    1.3525   -1.3156 H   0  0  0  0  0  0  0  0  0  0  0  0
  -1.2682   -0.6219   -0.6353 S   0  0  0  0  0  0  0  0  0  0  0  0
  -1.8691    1.6305   -1.3134 H   0  0  0  0  0  0  0  0  0  0  0  0
  -3.6477   -1.0760   -0.3498 Fe  0  0  0  0  0  0  0  0  0  0  0  0
  -4.1774   -2.7594   -0.3065 C   0  0  0  0  0  0  0  0  0  0  0  0
  -4.9046    0.1600   -0.2498 C   0  0  0  0  0  0  0  0  0  0  0  0
  -3.6167   -1.0175   -2.1486 C   0  0  0  0  0  0  0  0  0  0  0  0
  -3.3427   -1.0314    1.4493 C   0  0  0  0  0  0  0  0  0  0  0  0
  -4.6406   -3.8267   -0.2881 O   0  0  0  0  0  0  0  0  0  0  0  0
  -5.8136    0.8835   -0.2030 O   0  0  0  0  0  0  0  0  0  0  0  0
  -3.5986   -0.9706   -3.3016 O   0  0  0  0  0  0  0  0  0  0  0  0
  -3.1990   -1.0446    2.5840 O   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  3  1  0  0  0  0
 1  6  1  0  0  0  0
 1  7  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 3  8  1  0  0  0  0
 4  9  2  0  0  0  0
 5 10  2  0  0  0  0
 6 11  1  0  0  0  0
 7 12  1  0  0  0  0
 8 13  1  0  0  0  0
 8 14  1  0  0  0  0
 8 15  1  0  0  0  0
11 16  1  0  0  0  0
11 17  1  0  0  0  0
11 18  1  0  0  0  0
12 19  1  0  0  0  0
12 20  1  0  0  0  0
12 21  1  0  0  0  0
13 22  1  0  0  0  0
13 23  1  0  0  0  0
13 24  1  0  0  0  0
16 25  1  0  0  0  0
16 26  1  0  0  0  0
16 27  1  0  0  0  0
19 28  1  0  0  0  0
19 29  1  0  0  0  0
19 30  1  0  0  0  0
31 32  4  0  0  0  0
31 33  4  0  0  0  0
31 34  1  0  0  0  0
32 35  4  0  0  0  0
32 36  1  0  0  0  0
33 37  1  0  0  0  0
33 38  4  0  0  0  0
```

35	39	4	0	0	0	0
35	40	1	0	0	0	0
37	41	1	0	0	0	0
37	42	1	0	0	0	0
37	43	2	0	0	0	0
38	39	4	0	0	0	0
38	44	1	0	0	0	0
39	45	1	0	0	0	0
41	46	1	0	0	0	0
41	47	1	0	0	0	0
41	48	1	0	0	0	0
42	49	1	0	0	0	0
42	50	1	0	0	0	0
42	51	1	0	0	0	0
52	53	1	0	0	0	0
52	54	1	0	0	0	0
52	55	1	0	0	0	0
52	56	1	0	0	0	0
53	57	2	0	0	0	0
54	58	2	0	0	0	0
55	59	3	0	0	0	0
56	60	3	0	0	0	0

Molecular coordinates of **P1**$^{-}$

```
P1-, Fe(CO)4 direkt an Fe

Created by GaussView 5.0.8
 60 58  0  0  0  0  0  0  0  0  0    0
    2.3719   -1.3527    0.2269 P   0  0  0  0  0  0  0  0  0  0  0  0
    0.8401    0.3121   -0.0876 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    3.7415   -1.1280   -0.6283 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.8549    1.1563   -1.3204 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.4471    1.1564    1.3883 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.9909   -2.9302   -0.0297 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.0285   -1.5412    1.7103 O   0  0  0  0  0  0  0  0  0  0  0  0
    4.9352   -1.9252   -0.4607 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.5363    1.5776   -2.1407 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.8793    1.5394    2.3822 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.6681   -3.4883   -1.3333 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.2932   -2.0291    2.8606 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.8988   -1.5551   -1.5724 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.3577   -1.7132    0.5243 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.6710   -2.9867   -0.4968 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.3129   -4.9490   -1.1391 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.8412   -2.9258   -1.7702 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.5440   -3.3778   -1.9819 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.1118   -1.7192    4.0985 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.3128   -1.5477    2.8950 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.1470   -3.1061    2.7355 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.1405   -0.4908   -1.5319 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.8261   -2.1275   -1.4689 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.4647   -1.7696   -2.5516 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.1383   -5.5005   -0.6799 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.0871   -5.3997   -2.1099 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.4265   -5.0511   -0.5100 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.5920   -2.0928    4.9861 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.0952   -2.1947    4.0486 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.2493   -0.6413    4.2070 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.6559    3.8645    0.0693 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.0155    3.2187   -0.1476 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    2.6992    4.3368    0.2086 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6504    4.8535   -0.2009 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0686    2.8378    1.2757 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6502    2.8906   -1.8178 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0660    5.9285   -0.2345 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.7688    2.7310    2.1837 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1032    2.8491   -2.8743 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4156   -2.1435    0.6881 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5913   -1.9959   -0.7136 P   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9281   -2.6828    1.4885 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.5963   -2.7691    0.3342 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.7830   -0.5657    1.3858 S   0  0  0  0  0  0  0  0  0  0  0  0
```

```
  -2.0202   -0.5428   -1.6741 C   0  0  0  0  0  0  0  0  0  0  0  0
  -4.2201   -1.5049    0.0009 C   0  0  0  0  0  0  0  0  0  0  0  0
  -2.7368   -3.2769   -1.5000 O   0  0  0  0  0  0  0  0  0  0  0  0
  -2.5398   -0.5823   -2.6348 H   0  0  0  0  0  0  0  0  0  0  0  0
  -0.2174   -0.5449   -2.0144 S   0  0  0  0  0  0  0  0  0  0  0  0
  -2.3089    0.3751   -1.1623 H   0  0  0  0  0  0  0  0  0  0  0  0
  -4.4030   -0.3850    0.8245 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.3215   -2.3072   -0.3187 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.6700   -0.0803    1.3197 C   0  0  0  0  0  0  0  0  0  0  0  0
  -3.5566    0.2377    1.0904 H   0  0  0  0  0  0  0  0  0  0  0  0
  -6.5881   -1.9963    0.1745 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.1636   -3.1710   -0.9552 H   0  0  0  0  0  0  0  0  0  0  0  0
  -6.7640   -0.8827    0.9947 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.8000    0.7864    1.9590 H   0  0  0  0  0  0  0  0  0  0  0  0
  -7.4362   -2.6234   -0.0812 H   0  0  0  0  0  0  0  0  0  0  0  0
  -7.7493   -0.6394    1.3791 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  3  1  0  0  0  0
 1  6  1  0  0  0  0
 1  7  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 3  8  1  0  0  0  0
 4  9  3  0  0  0  0
 5 10  3  0  0  0  0
 6 11  1  0  0  0  0
 7 12  1  0  0  0  0
 8 13  1  0  0  0  0
 8 14  1  0  0  0  0
 8 15  1  0  0  0  0
11 16  1  0  0  0  0
11 17  1  0  0  0  0
11 18  1  0  0  0  0
12 19  1  0  0  0  0
12 20  1  0  0  0  0
12 21  1  0  0  0  0
13 22  1  0  0  0  0
13 23  1  0  0  0  0
13 24  1  0  0  0  0
16 25  1  0  0  0  0
16 26  1  0  0  0  0
16 27  1  0  0  0  0
19 28  1  0  0  0  0
19 29  1  0  0  0  0
19 30  1  0  0  0  0
31 32  1  0  0  0  0
31 33  3  0  0  0  0
32 34  1  0  0  0  0
32 35  1  0  0  0  0
32 36  1  0  0  0  0
34 37  3  0  0  0  0
35 38  3  0  0  0  0
```

36	39	3	0	0	0	0
40	41	1	0	0	0	0
40	42	1	0	0	0	0
40	43	1	0	0	0	0
40	44	1	0	0	0	0
41	45	1	0	0	0	0
41	46	1	0	0	0	0
41	47	2	0	0	0	0
45	48	1	0	0	0	0
45	49	1	0	0	0	0
45	50	1	0	0	0	0
46	51	4	0	0	0	0
46	52	4	0	0	0	0
51	53	4	0	0	0	0
51	54	1	0	0	0	0
52	55	4	0	0	0	0
52	56	1	0	0	0	0
53	57	4	0	0	0	0
53	58	1	0	0	0	0
55	57	4	0	0	0	0
55	59	1	0	0	0	0
57	60	1	0	0	0	0

Molecular coordinates of **P1^0**

```
P10, neutral, Fe(CO)4 direkt an Fe

Created by GaussView 5.0.8
 60 58  0  0  0  0  0  0  0  0  0    0
    1.9663   -1.6507    0.0389 P   0  0  0  0  0  0  0  0  0  0  0  0
    1.1397    0.3904    0.3947 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    3.4053   -1.5129   -0.6930 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.4957    1.1192   -0.5623 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.0339    0.5566    1.9532 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.1590   -2.7756   -0.8115 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.3871   -2.5281    1.3285 O   0  0  0  0  0  0  0  0  0  0  0  0
    4.3326   -2.6190   -0.8751 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.4048    1.5293   -1.1200 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.5641    0.6924    2.9542 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.8496   -2.6391   -2.2383 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.5487   -3.4445    2.0865 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.4945   -2.1165   -1.7073 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.6567   -2.9562    0.1111 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.8099   -3.4428   -1.3689 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.4014   -3.9935   -2.7427 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.0490   -1.9098   -2.3558 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.7509   -2.2932   -2.7518 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.4149   -4.0813    3.1534 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.7293   -2.8709    2.5220 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.1466   -4.1891    1.3960 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.9963   -1.2847   -1.2089 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.2200   -2.9224   -1.8501 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.1571   -1.7779   -2.6892 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.1757   -4.7513   -2.5987 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.1783   -3.9205   -3.8106 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.5117   -4.3033   -2.2327 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.8115   -4.7757    3.7450 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.2434   -4.6382    2.7096 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.8230   -3.3232    3.8251 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.0181    3.3810   -1.7675 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.2052    3.0091   -0.1655 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    1.4806    3.6597   -2.7706 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.4438    4.0134    0.6743 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.4177    2.5783    1.5101 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2084    4.0670   -0.5210 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.2166    4.6817    1.1899 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8134    2.5605    2.5819 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.0851    4.7767   -0.7069 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5391   -1.7869    0.7717 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5145   -1.1543   -0.6627 P   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2334   -2.2684    1.4637 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8935   -2.5597    0.3549 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.5894   -0.5631    1.7648 S   0  0  0  0  0  0  0  0  0  0  0  0
```

```
  -2.1127    0.6361   -0.7666 C   0  0  0  0  0  0  0  0  0  0  0  0
  -4.2758   -1.1587   -0.1673 C   0  0  0  0  0  0  0  0  0  0  0  0
  -2.2782   -1.9121   -1.9421 O   0  0  0  0  0  0  0  0  0  0  0  0
  -2.7427    1.0701   -1.5454 H   0  0  0  0  0  0  0  0  0  0  0  0
  -0.3714    0.9880   -1.2340 S   0  0  0  0  0  0  0  0  0  0  0  0
  -2.3453    1.0942    0.1925 H   0  0  0  0  0  0  0  0  0  0  0  0
  -4.7139   -0.6448    1.0606 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.2034   -1.6977   -1.0648 C   0  0  0  0  0  0  0  0  0  0  0  0
  -6.0690   -0.6671    1.3814 C   0  0  0  0  0  0  0  0  0  0  0  0
  -4.0031   -0.2330    1.7701 H   0  0  0  0  0  0  0  0  0  0  0  0
  -6.5586   -1.7173   -0.7392 C   0  0  0  0  0  0  0  0  0  0  0  0
  -4.8487   -2.1020   -2.0062 H   0  0  0  0  0  0  0  0  0  0  0  0
  -6.9915   -1.2017    0.4812 C   0  0  0  0  0  0  0  0  0  0  0  0
  -6.4049   -0.2696    2.3325 H   0  0  0  0  0  0  0  0  0  0  0  0
  -7.2748   -2.1369   -1.4368 H   0  0  0  0  0  0  0  0  0  0  0  0
  -8.0459   -1.2178    0.7334 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  3  1  0  0  0  0
 1  6  1  0  0  0  0
 1  7  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 3  8  1  0  0  0  0
 4  9  3  0  0  0  0
 5 10  3  0  0  0  0
 6 11  1  0  0  0  0
 7 12  1  0  0  0  0
 8 13  1  0  0  0  0
 8 14  1  0  0  0  0
 8 15  1  0  0  0  0
11 16  1  0  0  0  0
11 17  1  0  0  0  0
11 18  1  0  0  0  0
12 19  1  0  0  0  0
12 20  1  0  0  0  0
12 21  1  0  0  0  0
13 22  1  0  0  0  0
13 23  1  0  0  0  0
13 24  1  0  0  0  0
16 25  1  0  0  0  0
16 26  1  0  0  0  0
16 27  1  0  0  0  0
19 28  1  0  0  0  0
19 29  1  0  0  0  0
19 30  1  0  0  0  0
31 32  1  0  0  0  0
31 33  3  0  0  0  0
32 34  1  0  0  0  0
32 35  1  0  0  0  0
32 36  1  0  0  0  0
34 37  3  0  0  0  0
35 38  3  0  0  0  0
```

36	39	3	0	0	0	0
40	41	1	0	0	0	0
40	42	1	0	0	0	0
40	43	1	0	0	0	0
40	44	1	0	0	0	0
41	45	1	0	0	0	0
41	46	1	0	0	0	0
41	47	2	0	0	0	0
45	48	1	0	0	0	0
45	49	1	0	0	0	0
45	50	1	0	0	0	0
46	51	4	0	0	0	0
46	52	4	0	0	0	0
51	53	4	0	0	0	0
51	54	1	0	0	0	0
52	55	4	0	0	0	0
52	56	1	0	0	0	0
53	57	4	0	0	0	0
53	58	1	0	0	0	0
55	57	4	0	0	0	0
55	59	1	0	0	0	0
57	60	1	0	0	0	0

Molecular coordinates of **P2^0**

```
P20, neutral, Fe(CO)4 ueber S gebunden

Created by GaussView 5.0.8
 60 59  0  0  0  0  0  0  0  0  0    0
    1.7920    1.8134   -0.1547 P   0  0  0  0  0  0  0  0  0  0  0  0
    1.3485   -0.3138    0.2621 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    2.5667    2.7666    0.9128 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.6164   -0.9199   -0.8608 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.4136   -0.6000    1.6865 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.7495    2.1249   -1.4433 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.4826    2.6539   -0.6173 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.5235    2.7521    2.3684 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.4655   -1.2633   -1.5474 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.0741   -0.8194    2.5933 O   0  0  0  0  0  0  0  0  0  0  0  0
    4.1963    2.1018   -1.3973 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.5857    4.0147   -1.1256 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.7096    4.1741    2.8592 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.5746    2.3275    2.6966 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.3379    2.1101    2.7124 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.7105    2.2302   -2.8171 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.5367    1.1652   -0.9457 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.5345    2.9281   -0.7683 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8148    4.5712   -1.2816 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.1131    3.9828   -2.0804 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.1734    4.6092   -0.4219 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.6478    4.5987    2.4943 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.8862    4.8125    2.5306 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.7317    4.1815    3.9527 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.8041    2.2310   -2.8143 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.3670    1.3964   -3.4323 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.3669    3.1629   -3.2702 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.7606    5.5925   -1.6691 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3964    3.9734   -1.9874 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3388    4.5979   -0.3235 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.3420    2.1278   -0.6336 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.5708    2.7278   -0.8980 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.2881    0.8476   -0.0668 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.4300    2.6647   -0.8706 H   0  0  0  0  0  0  0  0  0  0  0  0
   -6.7550    2.0542   -0.5983 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.6052    3.7190   -1.3364 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.7198   -0.0187    0.3187 P   0  0  0  0  0  0  0  0  0  0  0  0
   -5.4800    0.1776    0.2323 C   0  0  0  0  0  0  0  0  0  0  0  0
   -6.7080    0.7810   -0.0334 C   0  0  0  0  0  0  0  0  0  0  0  0
   -7.7111    2.5222   -0.8050 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.7234    1.1637    1.2973 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.8527   -0.1089   -1.2932 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9699   -1.3655    0.9342 O   0  0  0  0  0  0  0  0  0  0  0  0
   -5.4269   -0.8120    0.6717 H   0  0  0  0  0  0  0  0  0  0  0  0
```

```
  -7.6275    0.2563    0.2009 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.3181    1.4383    2.1718 H   0  0  0  0  0  0  0  0  0  0  0  0
  -1.5483    2.0596    0.6983 H   0  0  0  0  0  0  0  0  0  0  0  0
  -0.1481    0.4974    1.9541 S   0  0  0  0  0  0  0  0  0  0  0  0
  -1.7602    0.8894   -1.7261 H   0  0  0  0  0  0  0  0  0  0  0  0
  -0.1706   -0.8395   -1.3446 S   0  0  0  0  0  0  0  0  0  0  0  0
  -2.4670   -0.7151   -1.9623 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.2188   -2.8612   -0.1980 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   1.5021   -3.7411    0.7036 C   0  0  0  0  0  0  0  0  0  0  0  0
  -1.1828   -3.9345   -0.5926 C   0  0  0  0  0  0  0  0  0  0  0  0
   1.0507   -3.3190   -1.7613 C   0  0  0  0  0  0  0  0  0  0  0  0
  -0.5366   -2.5562    1.4910 C   0  0  0  0  0  0  0  0  0  0  0  0
   2.3075   -4.3444    1.2525 O   0  0  0  0  0  0  0  0  0  0  0  0
  -2.0405   -4.6514   -0.8217 O   0  0  0  0  0  0  0  0  0  0  0  0
   1.5367   -3.6603   -2.7343 O   0  0  0  0  0  0  0  0  0  0  0  0
  -0.8900   -2.6729    2.5627 O   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  3  1  0  0  0  0
 1  6  1  0  0  0  0
 1  7  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 2 50  1  0  0  0  0
 3  8  1  0  0  0  0
 4  9  3  0  0  0  0
 5 10  3  0  0  0  0
 6 11  1  0  0  0  0
 7 12  1  0  0  0  0
 8 13  1  0  0  0  0
 8 14  1  0  0  0  0
 8 15  1  0  0  0  0
11 16  1  0  0  0  0
11 17  1  0  0  0  0
11 18  1  0  0  0  0
12 19  1  0  0  0  0
12 20  1  0  0  0  0
12 21  1  0  0  0  0
13 22  1  0  0  0  0
13 23  1  0  0  0  0
13 24  1  0  0  0  0
16 25  1  0  0  0  0
16 26  1  0  0  0  0
16 27  1  0  0  0  0
19 28  1  0  0  0  0
19 29  1  0  0  0  0
19 30  1  0  0  0  0
31 32  4  0  0  0  0
31 33  4  0  0  0  0
31 34  1  0  0  0  0
32 35  4  0  0  0  0
32 36  1  0  0  0  0
33 37  1  0  0  0  0
```

33	38	4	0	0	0	0
35	39	4	0	0	0	0
35	40	1	0	0	0	0
37	41	1	0	0	0	0
37	42	1	0	0	0	0
37	43	2	0	0	0	0
38	39	4	0	0	0	0
38	44	1	0	0	0	0
39	45	1	0	0	0	0
41	46	1	0	0	0	0
41	47	1	0	0	0	0
41	48	1	0	0	0	0
42	49	1	0	0	0	0
42	50	1	0	0	0	0
42	51	1	0	0	0	0
52	53	1	0	0	0	0
52	54	1	0	0	0	0
52	55	1	0	0	0	0
52	56	1	0	0	0	0
53	57	3	0	0	0	0
54	58	3	0	0	0	0
55	59	3	0	0	0	0
56	60	3	0	0	0	0