Supporting Information for:

Stepwise Activation of „Non-innocent" Cp* Substituents – A Cp* Based Cascade Reaction

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S1. Experimental Section and analytical characterisation

General remarks:

All manipulations were performed under an atmosphere of dry nitrogen using standard glovebox and Schlenk techniques. Solvents were purified and degassed by standard procedures. The starting materials **1a** and **1b** were prepared according to published methods.[1]

Solution NMR spectra were recorded on a Bruker AVANCE 400 and 600 spectrometer. Mass spectra were performed using a Finnigan MAT 95 (EI-MS) and were measured on a FT-IR-spectrometer (Varian FTS 2000).

Synthesis of 2: In a 100 mL Schlenk tube a solution of [Cp*As{W(CO)$_5$}$_2$] (**1b**) (344 mg, 0.4 mmol) in CH$_2$Cl$_2$ (20 ml) was cooled to -30°C and 1,2,3,4,5-pentamethylcyclopentadienyl-phosphine (134 mg, 0.8 mmol) was added. The blue colour of **1b** turns to light brown after 16 hours stirring at room temperature. The solvent was removed under reduced pressure. The brown solid was dissolved in toluene (4 mL). **2** crystallizes as colourless crystals (110 mg, 30%) at 4°C.

^{1}H NMR δ_H (600MHz; CD$_2$Cl$_2$; Me$_4$Si): 0.72 (d, $^3J_{H,P}$ = 7 Hz, 3H, CH$_3$, Cp*), 1.44 (d, br, $^3J_{H,P}$ = 13 Hz, 3H, CH$_3$, Cp*), 1.51 (d, $^3J_{H,P}$ = 18 Hz, 3H, CH$_3$, Cp*), 1.58 (s, 3H, CH$_3$, Cp*), 1.59 (s, 3H, CH$_3$,Cp*), 1.80 (d, $^4J_{H,P}$ = 8 Hz, 3H, CH$_3$, Cp*), 1.83 (d, $^3J_{H,P}$ = 4 Hz, 3H, CH$_3$, Cp*), 1.85 (s, 3H, CH$_3$, Cp*), 1.86 (s, 3H, CH$_3$, Cp*), 1.90 (s, 3H, CH$_3$, Cp*), 2.05 (m, 1H, CH, Cp*), 5.23 (d, $^1J_{P,H}$ = 293 Hz, 1H, PH), 5.30 (dd, $^1J_{P,H}$ = 288 Hz, $^3J_{P,H}$ = 12 Hz, 1H, PH).

^{31}P{^{1}H} NMR δ_P (243 MHz; CD$_2$Cl$_2$; H$_3$PO$_4$): -51.0 to -42.2 (br, 2P, P-H), -10.1 (s, br, 2P, P-H).

^{31}P NMR δ_P (243 MHz; CD$_2$Cl$_2$; H$_3$PO$_4$): -51.0 to -42.2 (br, 2P, P-H), -10.1 (d, br, $^1J_{P,H}$ = 288 Hz, 2P, P-H).

^{13}C{H} NMR δ_C (151 MHz; CD$_2$Cl$_2$; Me$_4$Si): 10.7 (d, 4 Hz, 1C, CH$_3$, Cp*), 11.1 (m, 2C, CH$_3$, Cp*), 11.5 (m, br, 2C, CH$_3$, Cp*), 12.0 (s, 1C, CH$_3$, Cp*), 12.1 (d, 7 Hz, 1C, CH$_3$, Cp*), 13.1 (s, 1C, CH$_3$, Cp*), 14.1 (d, 9 Hz, 1C, CH$_3$, Cp*), 15.7 (s, 1C, CH$_3$, Cp*), 56.4 (s, 1C, Cp*), 59.9 (s 1C, Cp*), 63.4 (m, br, 1C, Cp*), 67.3 (m, br, 1C, Cp*), 137.8 (s, 2C, Cp*), 138.4 (s, 1C, Cp*), 139.1 (s, 1C, Cp*), 140.4 (s, br, 2C, Cp*), 196.9 (d, $^2J_{C,P}$ = 7 Hz, 4C, cis-CO), 197.4 (m, br, 4C, cis-CO), 198.2 (d, br, $^2J_{C,P}$ = 24 Hz, 1C, trans-CO), 198.8 (d, $^2J_{C,P}$ = 26 Hz, 1C, trans-CO).

MS (EI, 70eV) *m/z*: 1058.1 [M$^+$, 1], 923.8 [M$^+$-Cp*, 20], 893.8 [M$^+$,-Cp*-CO, 48].

IR (KBr): v_{max}/cm^{-1} 2965w, 2918w, 2870w, 2069m (CO), 1914vs (CO).

Synthesis of 3: In a 100 ml Schlenk tube a solution of **2** at room temperature was stirred for 72 h. The colour of **2** turns form colourless to light orange. Cp*H was formed. The solvent was removed under reduced pressure. The orange solid was dissolved in toluene CD_2Cl_2 and a ^{31}P NMR was recorded.

$^{31}P\{^1H\}$ NMR δ_P (162 MHz; CD_2Cl_2; H_3PO_4): Isomer **(A)** -54.8 (d, $^2J_{P,P} = 5$ Hz, $^1J_{P,W} = 220$ Hz, 1P, P-H), -16.3 (d, $^2J_{P,P} = 5$ Hz, $^1J_{P,W} = 223$ Hz, 1P, P-H), Isomer **(B)** -49.5 (d, $^2J_{P,P} = 11$ Hz, $^1J_{P,W} = 216$ Hz, 1P, P-H), 27.5 (d, $^2J_{P,P} = 11$ Hz, $^1J_{P,W} = 206$ Hz, 1P, P-H).

^{31}P NMR δ_P (162 MHz; CD_2Cl_2; H_3PO_4): Isomer **(A)** -54.8 (dm, $^1J_{P,H} = 303$ Hz, 1P, P-H), -16.3 (dm, $^1J_{P,H} = 288$ Hz, 1P, P-H), -49.5 (dm, $^1J_{P,H} = 298$ Hz, 1P, P-H), Isomer **(B)** -49.5 (dm, $^1J_{P,H} = 299$ Hz, 1P, P-H), 27.5 (dm, $^1J_{P,H} = 321$ Hz, 1P, P-H).

MS (EI, 70eV) m/z: 923.8 [M^+, 18], 893.8 [M^+, -CO, 55].

Synthesis of 4: In a 100 mL Schlenk tube a solution of [Cp*P{W(CO)$_5$}$_2$] (**1a**) (326 mg, 0.4 mmol) in CH_2Cl_2 (20 mL) was cooled to -30°C and 1,2,3,4,5-pentamethylcyclopentadienyl-phosphine (134 mg, 0.8 mmol) was added. The blue colour of **1a** turns to light brown after 16 hours, stirring at room temperature. The solvent was removed under reduced pressure. The brown solid was dissolved in toluene (4 mL). **4** crystallises as colourless crystals (98 mg, 28%) at 4°C.

^1H NMR δ_H (600MHz; CD_2Cl_2; Me_4Si): 0.83 (d, $^3J_{H,P} = 9$ Hz, 3H, CH_3, Cp*), 1.63 (d, $^3J_{H,P} = 19$ Hz, 3H, CH_3, Cp*), 1.67 (s, br, 3H, CH_3, Cp*), 1.79 (d, $^3J_{P,H} = 19$ Hz, 3H, CH_3, Cp*), 1.86 (d, br, $^4J_{H,H} = 7$ Hz, 3H, CH_3, Cp*), 3.79 (ddd, $^1J_{P,H} = 168$ Hz, $^3J_{P,H} = 47$ Hz, $^4J_{H,H} = 8$ Hz, 1H, PH), 4.51 (dddd, $^1J_{P,H} = 326$ Hz, $^2J_{P,H} = 12$ Hz, $^3J_{P,H} = 34$ Hz, $^4J_{H,H} = 8$ Hz, 1H, PH).

$^{31}P\{^1H\}$ NMR δ_P (243 MHz; CD_2Cl_2; H_3PO_4): -65.3 (dd, $^1J_{P,P} = 84$ Hz, $^2J_{P,P} = 153$ Hz, $^2J_{P,W} = 10$ Hz, 1P), 6.9 (dd, $^1J_{P,P} = 153$ Hz, $^2J_{P,P} = 153$ Hz, $^1J_{P,W} = 217$ Hz, $^2J_{P,W} = 7$ Hz, 1P), 10.2 (dd, $^1J_{P,P} = 153$ Hz, $^1J_{P,P} = 84$ Hz, $^1J_{P,W} = 216$ Hz, $^2J_{P,W} = 7$ Hz, 1P).

^{31}P NMR δ_P (243 MHz; CD_2Cl_2; H_3PO_4): -65.3 (ddddq, $^1J_{P,P} = 84$ Hz, $^2J_{P,P} = 153$ Hz, $^1J_{P,H} = 168$ Hz, $^3J_{P,H} = 34$ Hz, $^3J_{P,H} = 9$ Hz, 1P), 6.9 (ddddqm, $^1J_{P,P} = 153$ Hz, $^2J_{P,P} = 153$ Hz, $^1J_{P,H} = 326$ Hz, $^2J_{P,H} = 12$ Hz, $^3J_{P,H} = 19$ Hz, 1P), 10.2 (ddm, $^1J_{P,P} = 153$ Hz, $^1J_{P,P} = 84$ Hz, 1P).

$^{13}C\{H\}$ NMR δ_C (151 MHz; CD_2Cl_2; Me_4Si): 10.8 (s, br, 1C, CH_3, Cp*), 11.8 (s, br, 1C, CH_3, Cp*), 11.9 (d, $^2J_{C,P} = 11$ Hz, 1C, CH_3, Cp*), 15.7 (m, br, 1C, CH_3, Cp*), 17.7 (d, $^2J_{C,P} = 14$ Hz, 1C, CH_3, Cp*), 62.4 (ddd, $^1J_{C,P} = 14$ Hz, $^2J_{C,P} = 9$ Hz, $^3J_{C,P} = 2$ Hz, 1C, C-P, Cp*), 63.9 (dd, $^1J_{C,P} = 9$ Hz, $^2J_{C,P} = 9$ Hz, 1C, C-P, Cp*), 77.2 (m, 1C, C-P, Cp*), 137.2 (dt, $^2J_{C,P} = 2$ Hz, $^3J_{C,P} = 7$ Hz, 1C, Cp*), 148.5 (m, 1C, Cp*), 195.2 (d, $^2J_{C,P} = 6$ Hz, 4C, cis-CO), 196.0 (dd, $^2J_{C,P} = 6$ Hz, $^3J_{C,P} = 2$ Hz, 4C, cis-CO), 197.3 (d, $^2J_{C,P} = 29$ Hz, 1C, trans-CO), 198.1 (d, $^2J_{C,P} = 26$ Hz, 1C, trans-CO).

MS (EI, 70eV) m/z: 1201.8 [M^+ + W(CO)$_5$, 1], 1066.9 [M^+ + W(CO)$_5$ - Cp*, 1], 878.3 [M^+, 15], 850.3 [M^+ - CO, 25], 742.8 [M^+ - Cp*, 55].

- S4 -

IR (KBr): v_{max}/cm^{-1} 2966w, 2919w, 2854w, 2073s (CO), 2068s (CO), 1990m (CO), 1933vs (CO).

^{1}H NMR δ_H (600MHz; CD$_2$Cl$_2$; Me$_4$Si): 0.80 (d, $^3J_{H,P}$ = 7 Hz, 3H, CH$_3$, Cp*), 1.48 (d, $^3J_{H,P}$ = 20 Hz, 3H, CH$_3$, Cp*), 1.54 (d, $^3J_{P,H}$ = 19 Hz, 3H, CH$_3$, Cp*), 1.66 (s, br, 3H, CH$_3$, Cp*), 1.85 (s, br, 3H, CH$_3$, Cp*), 3.79 (dddd, $^1J_{P,H}$ = 168 Hz, $^2J_{P,H}$ = 2 Hz, $^3J_{P,H}$ = 4 Hz, $^4J_{H,H}$ = 14 Hz, 1H, PH), 4.44 (ddd, $^1J_{P,H}$ = 320 Hz, $^3J_{P,H}$ = 6 Hz, $^4J_{H,H}$ = 14 Hz, 1H, PH).

^{31}P{^{1}H} NMR δ_P (243 MHz; CD$_2$Cl$_2$; H$_3$PO$_4$): -70.6 (dd, $^1J_{P,P}$ = 130 Hz, $^2J_{P,P}$ = 14 Hz, $^2J_{P,W}$ = 10 Hz, 1P), -5.8 (dd, $^1J_{P,P}$ = 204 Hz, $^1J_{P,P}$ = 130 Hz, $^1J_{P,W}$ = 224 Hz, $^2J_{P,W}$ = 7 Hz, 1P), 20.8 (dd, $^1J_{P,P}$ = 204 Hz, $^2J_{P,P}$ = 14 Hz, $^1J_{P,W}$ = 220 Hz, $^2J_{P,W}$ = 7 Hz, 1P).

^{31}P NMR δ_P (243 MHz; CD$_2$Cl$_2$; H$_3$PO$_4$): -70.6 (ddddq, $^1J_{P,P}$ = 130 Hz, $^2J_{P,P}$ = 14 Hz, $^1J_{P,H}$ = 168 Hz, $^4J_{P,H}$ = 14 Hz, $^3J_{P,H}$ = 7 Hz, 1P), -5.8 (ddm, $^1J_{P,P}$ = 204 Hz, $^1J_{P,P}$ = 130 Hz, 1P), 20.8 (ddm, $^1J_{P,P}$ = 204 Hz, $^2J_{P,P}$ = 14 Hz, 1P).

^{13}C{H} NMR δ_C (151 MHz; CD$_2$Cl$_2$; Me$_4$Si): 9.8 (d, $^2J_{C,P}$ = 4 Hz, 1C, CH$_3$, Cp*), 9.9 (d, $^3J_{C,P}$ = 4 Hz, 1C, CH$_3$, Cp*), 12.6 (s, br, CH$_3$, Cp*), 14.1 (d, $^2J_{C,P}$ = 10 Hz, 1C, CH$_3$, Cp*), 16.5 (d, $^2J_{C,P}$ = 13 Hz, 1C, CH$_3$, Cp*), 58.2 (dd, $^1J_{C,P}$ = 9 Hz, $^2J_{C,P}$ = 2 Hz, 1C, C-P, Cp*), 59.1 (dd, $^1J_{C,P}$ = 18 Hz, $^2J_{C,P}$ = 2 Hz, 1C, C-P, Cp*), 61.2 (dd, $^1J_{C,P}$ = 10 Hz, $^2J_{C,P}$ = 2 Hz, 1C, C-P, Cp*), 133.5 (dt, $^1J_{C,P}$ = 10 Hz, $^2J_{C,P}$ = 2 Hz, 1C, C-P, Cp*), 138.9 (dd, $^1J_{C,P}$ = 7 Hz, $^2J_{C,P}$ = 3 Hz, 1C, C-P, Cp*), 195.7 (d, $^2J_{C,P}$ = 6 Hz, 4C, cis-CO), 195.8 (d, $^2J_{C,P}$ = 6 Hz, 4C, cis-CO), 197.7 (d, $^2J_{C,P}$ = 8 Hz, 1C, trans-CO), 197.8 (d, $^2J_{C,P}$ = 8 Hz, 1C, trans-CO).

Cp*H (CD$_2$Cl$_2$): δ_H: 0.91 (m, 3H), 1.66 (m, 6H), 1.73 (m, 6H), 2.32 (m. 1H).

^{1}H NMR spectrum of 2 at 25°C and -70°C.
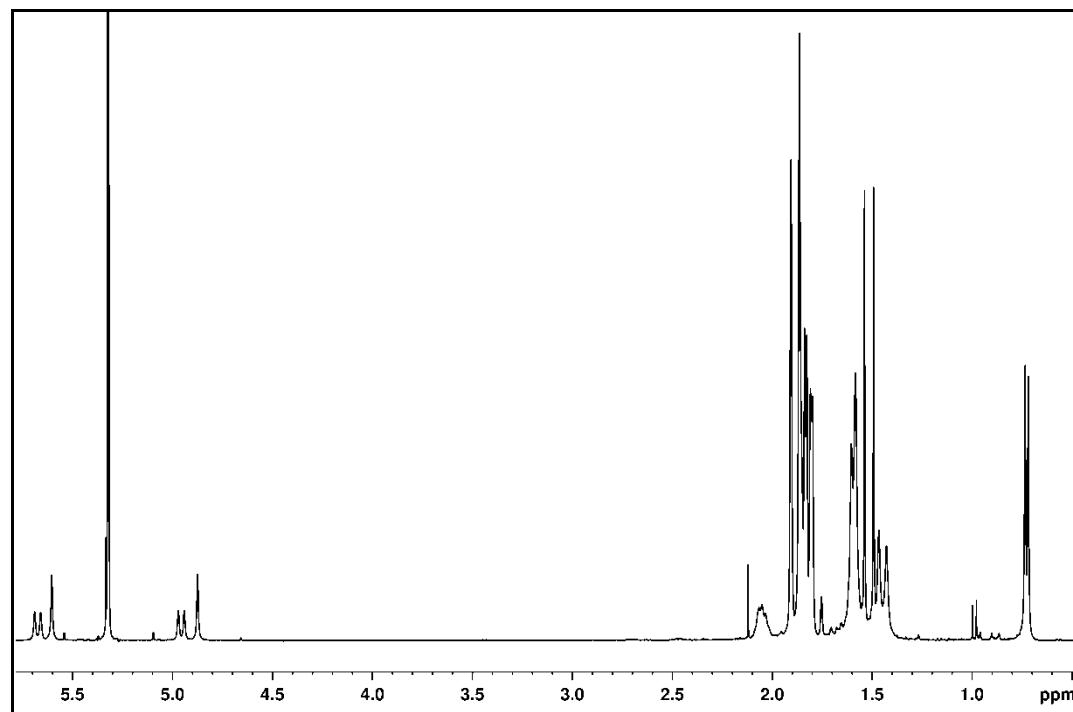
Fig. 1: ^{1}H NMR spectrum of **2** at 300 K in CD$_2$Cl$_2$.
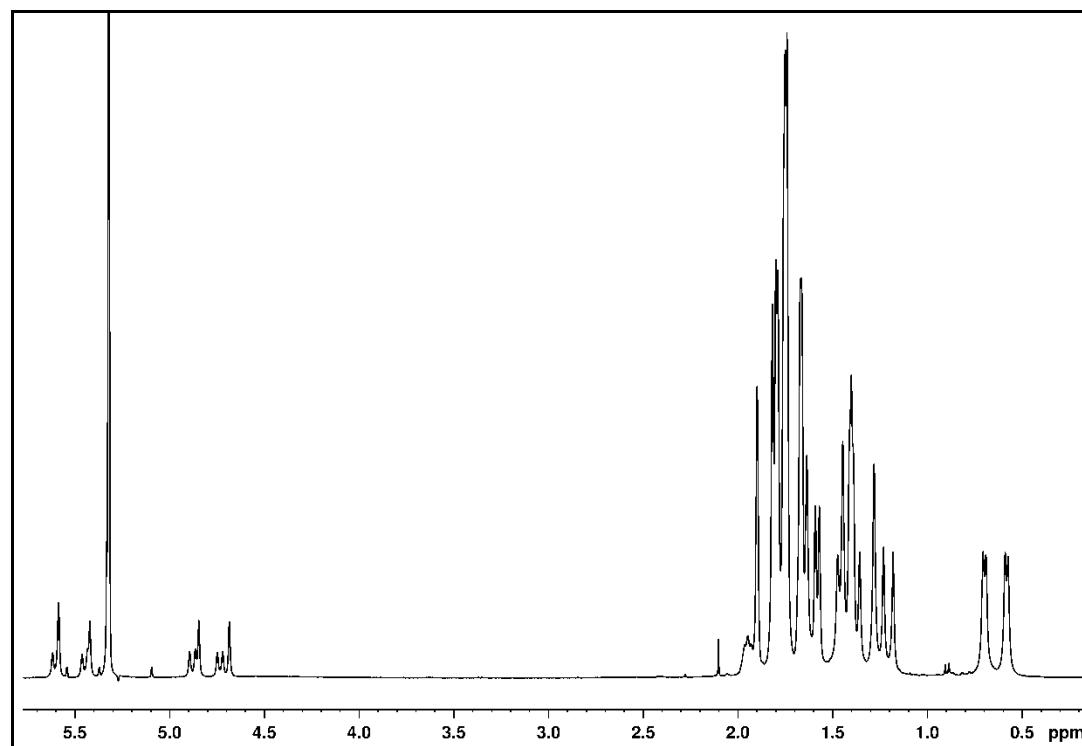

Fig. 2: ^{1}H NMR spectrum of **2** at 193 K in CD$_2$Cl$_2$.

S2. Crystallographic details

Crystal structure analysis: The crystal structure analysis of **2** and **4** were performed on a Agilant Gemini R Ultra and a Oxford Diffraction SuperNova CCD diffractometer using $Cu_{K\alpha}$ radiation ($\lambda = 1.54178$ Å). The structures were solved by charge-flipping methods with the program Superflip[2], and full matrix least squares refinement on F^2 in SHELXL-97[3] was performed with anisotropic displacements for non-H atoms. Hydrogen atoms at the carbon atoms were located in idealised positions and refined isotropically according to the riding model. The position of the hydrogen atoms bonded to phosphorus were calculated on idealised positions using the standard riding model

Crystal data for **2**: $C_{30}H_{33}As_1O_{10}P_2W_2$, $M = 1058.11$, triclinic, space group $P\bar{1}$, $a = 9.8692(5)$, $b = 12.9844(6)$, $c = 15.2994(6)$ Å, $\alpha = 80.608(4)$, $\beta = 72.490(4)$, $\gamma = 69.895(4)°$, $V = 1751.86(15)$ Å^3, $T = 123(1)$ K, $Z = 2$, $\mu(Cu_{K\alpha}) = 14.317$ mm^{-1}, 28010 reflections measured, 6116 unique ($R_{int} = 0.0436$) which were used in all calculations. The final R_1 [$I > 2\sigma(I)$] was 0.0243.

Crystal data for **4**: $C_{20}H_{17}O_{10}P_3W_2$, $M = 877.93$, triclinic, space group $P\bar{1}$, $a = 9.4184(5)$, $b = 10.4395(5)$, $c = 15.6135(8)$ Å, $\alpha = 71.461(5)$, $\beta = 89.764(4)$, $\gamma = 64.716(5)°$, $V = 1300.46(14)$ Å^3, $T = 123(1)$ K, $Z = 2$, $\mu(Cu_{K\alpha}) = 18.315$ mm^{-1}, 8886 reflections measured, 4805 unique ($R_{int} = 0.0508$) which were used in all calculations. The final R_1 [$I > 2\sigma(I)$] was 0.0457.

The position of the hydrogen atoms bonded to phosphorus was calculated on idealised positions using the standard riding model.

S3. Computational studies

The geometries of the compounds have been fully optimized with gradient-corrected density functional theory (DFT) in form of Becke's three-parameter hybrid method B3LYP[4] with standard 6-31G* all electron basis set as implemented in Gaussian 03 program package.[5] ECP basis set of Hay and Wadt was used for W.[6] All structures correspond to minima on their respective potential energy surfaces.

Scheme 1S. Labeling of compounds, theoretically studied in present work.

D (As) 1

2 (As) 1

E (As) 1

3 (As) 1

4 (As) 1

D (As) 2

2 (As) 2

E (As) 2

3 (As) 2

4 (As) 2

D (As) 3

2 (As) 3

F (As) 1

3 (As) 3

4 (As) 3

D (As) 3

2 (As) 4

F (As) 2

3 (As) 4

4 (As) 4
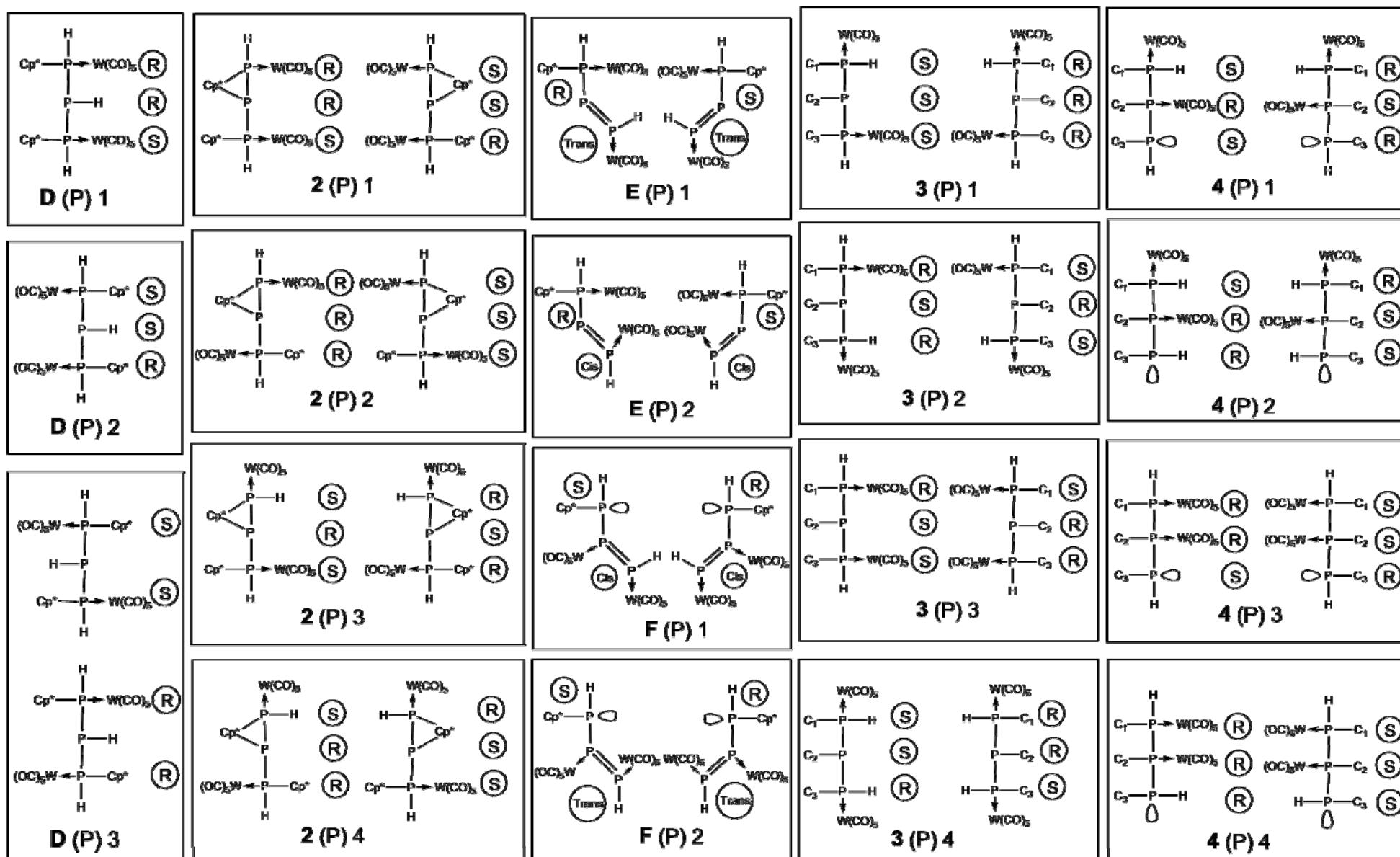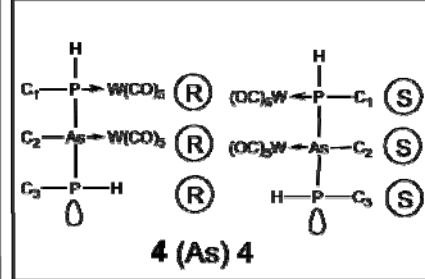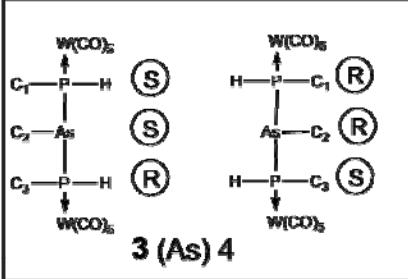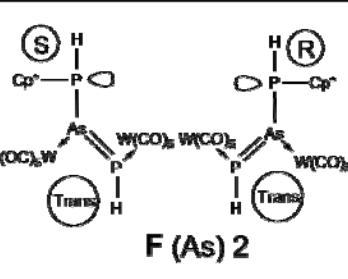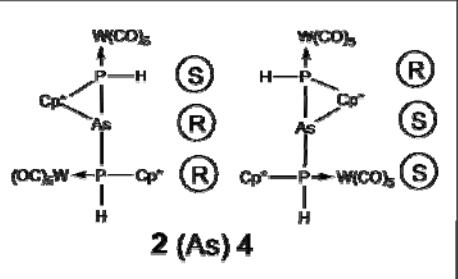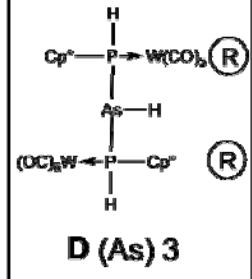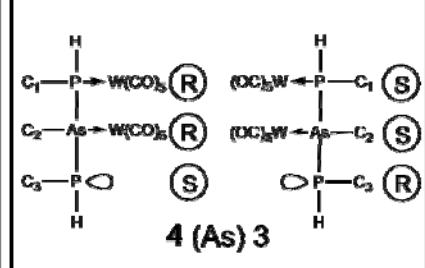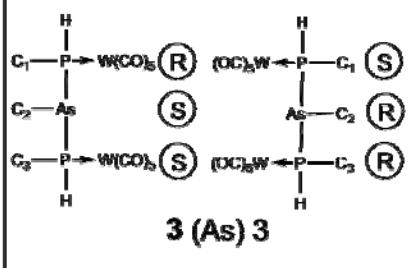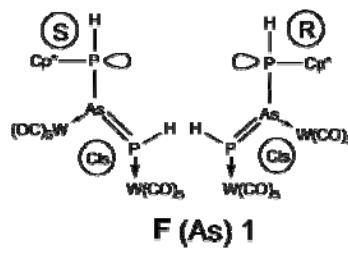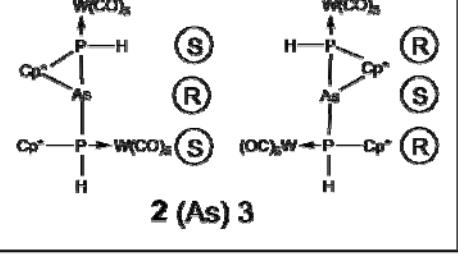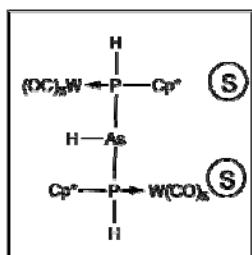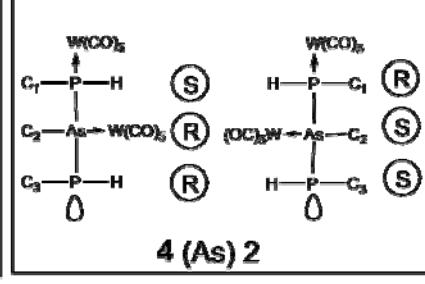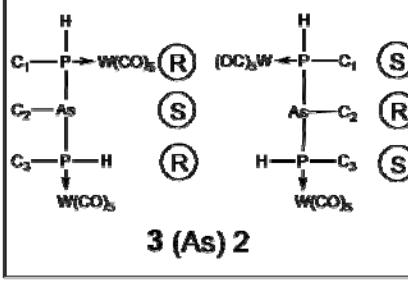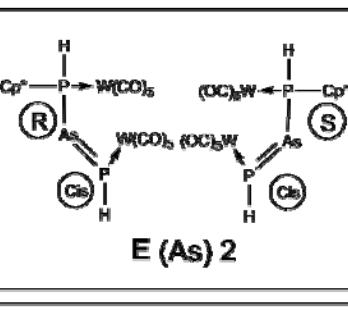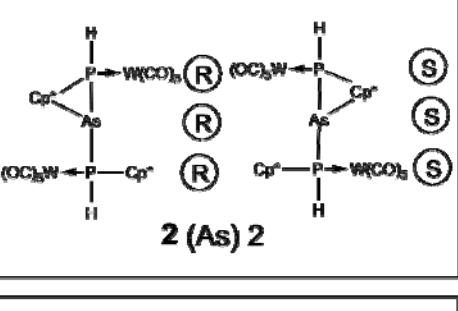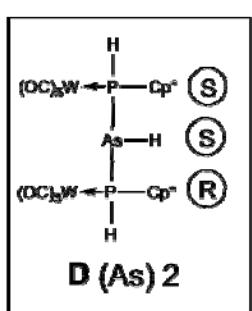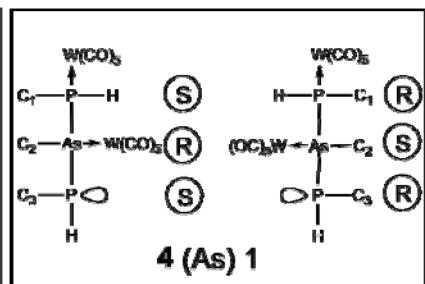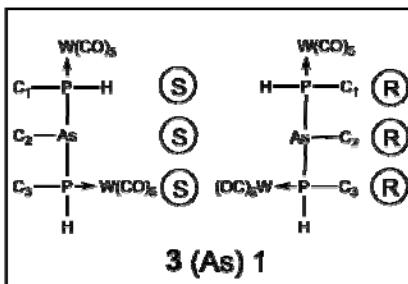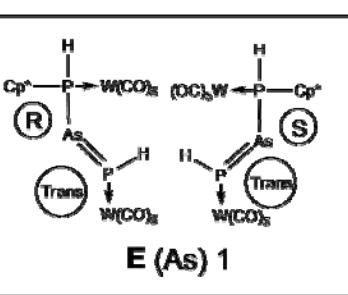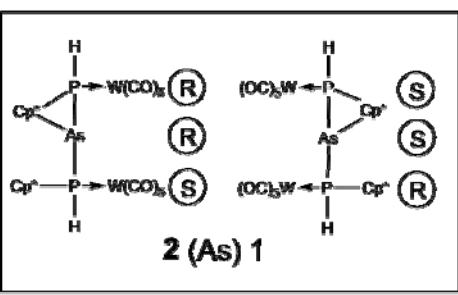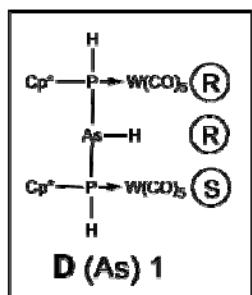
Table 1S. Total energies E^o_0, sum of electronic and thermal enthalpies H^o_{298} (Hartree) and standard entropies S^o_{298} (cal mol^{-1}K^{-1}) for studied compounds. B3LYP/6-31G*(ECP on W) level of theory.
Labeling of compounds is shown on Scheme 1S.

Compound	E^o_0	H^o_{298}	S^o_{298}
HCp*	-390.8243631	-390.438853	104.873
D(P)1	-3075.23898	-3074.615891	326.692
D(P)2	-3075.23233	-3074.609508	327.279
D(P)3	-3075.240122	-3074.616708	324.972
2(P)1	-3075.243897	-3074.617957	316.906
2(P)2	-3075.238241	-3074.61194	313.257
2(P)3	-3075.227717	-3074.601002	313.879
2(P)4	-3075.225716	-3074.599572	317.224
D(As)1	-4967.310848	-4966.68914	332.859
D(As)2	-4967.304049	-4966.682423	332.611
D(As)3	-4967.312167	-4966.689954	328.484
2(As)1	-4967.322475	-4966.697095	319.26
2(As)2	-4967.317233	-4966.691744	318.731
2(As)3	-4967.308139	-4966.682196	316.573
2(As)4	-4967.303452	-4966.677945	320.017
E(P)1	-2684.536571	-2684.160739	277.627
E(P)2	-2684.536983	-2684.160688	270.543
F(P)1	-2684.530369	-2684.155001	275.33
F(P)2	-2684.529881	-2684.154366	277.681
3(P)1	-2684.545455	-2684.168957	259.377
3(P)2	-2684.544953	-2684.168489	259.519
3(P)3	-2684.542438	-2684.166015	258.511
3(P)4	-2684.53502	-2684.158351	256.14
4(P)1	-2684.5459999	-2684.16979	256.329
4(P)2	-2684.545683	-2684.169322	254.513
4(P)3	-2684.542846	-2684.166541	253.569
4(P)4	-2684.540651	-2684.164408	253.236
E(As)1	-4576.61201	-4576.236797	281.447
E(As)2	-4576.612718	-4576.237028	273.442
F(As)1	-4576.603219	-4576.228407	279.756
F(As)2	-4576.602898	-4576.228044	284.677
3(As)1	-4576.620658	-4576.244719	263.3
3(As)2	-4576.620238	-4576.244227	261.34
3(As)3	-4576.618113	-4576.242341	261.893
3(As)4	-4576.611584	-4576.235262	257.837
4(As)1	-4576.618596	-4576.243186	260.683
4(As)2	-4576.617941	-4576.24242	260.129
4(As)3	-4576.616088	-4576.240487	259.019
4(As)4	-4576.613808	-4576.238278	258.78

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Table 2S. Relative energies (E^{rel}, kJ mol^{-1}) of **D** and **2** isomers.

Compound	E^{rel}		Compound	E^{rel}
D(P)1	12.9		**D**(As)1	30.5
D(P)2	30.4		**D**(As)2	48.4
D(P)3	9.9		**D**(As)3	27.1
2(P)1	0.0		**2**(As)1	0.0
2(P)2	14.8		**2**(As)2	13.8
2(P)3	42.5		**2**(As)3	37.6
2(P)4	47.7		**2**(As)4	49.9

Table 3S. Relative energies (E^{rel}, kJ mol^{-1}) of **E, F, 3** and **4** isomers.

Compound	E^{rel}		Compound	E^{rel}
E(P)1	24.8		**E**(As)1	22.7
E(P)2	23.7		**E**(As)2	20.8
F(P)1	41.0		**F**(As)1	45.8
F(P)2	42.3		**F**(As)2	46.6
3(P)1	1.4		**3**(As)1	0.0
3(P)2	2.7		**3**(As)2	1.1
3(P)3	9.4		**3**(As)3	6.7
3(P)4	28.8		**3**(As)4	23.8
4(P)1	0.0		**4**(As)1	5.4
4(P)2	0.8		**4**(As)2	7.1
4(P)3	8.3		**4**(As)3	12.0
4(P)4	14.0		**4**(As)4	18.0

Table 4S. Optimized geometries of theoretically studied compounds. xyz coordinates in angstroms. B3LYP/6-31G*(ECP on W) level of theory.

HCp[*], C_5Me_5H

```
C   1.6640656391  -1.0860831185   1.8823193293
C   0.7122261754  -0.4460147781   0.9254980761
C  -1.5219301122  -1.4549681176   1.662061462
C   2.2468145144  -0.0298661829  -1.0719633748
C  -0.1081428253   0.9265292385  -0.8322201293
C  -0.127184557    1.910824939   -1.9556042092
C  -1.1353131811   0.2614915422  -0.2680642788
C  -2.5883236132   0.3291956322  -0.6227864335
C  -0.6234691331  -0.5948653924   0.8286095889
H   1.8727492654  -0.9149013365  -1.58847296
H   3.1450395397  -0.3111276466  -0.5217337847
H   2.5377113085   0.704982546   -1.8229928389
H   0.2975102297   2.8720771674  -1.6515642703
H  -1.1364317607   2.0986957829  -2.3176033149
H   0.4660066252   1.5645812394  -2.8070882739
H  -3.190178475    0.6597896199   0.2276255889
H  -2.9728280933  -0.6513647408  -0.9150498841
H  -2.7761366735   1.0152410732  -1.4461962064
H  -2.0565790459  -2.1843240422   1.0480982463
H  -2.2828149303  -0.8583050419   2.1717374806
H  -0.9707948542  -2.0052437279   2.4219183433
H   2.2156128314  -0.3370589585   2.4581407692
H   2.4126544788  -1.6923295726   1.3637968607
H   1.1552250956  -1.7354306931   2.5924937396
C   1.1729205117   0.5360495744  -0.1288465574
H   1.5915997186   1.4224250474   0.3678870822
```

D(P)1

```
W   -1.24343635    1.0471554975    0.1695169048
C    1.9390607878   0.6959560394    2.4591258593
P    0.1957592619  -2.114126509    2.387566122
H   -0.9003180616  -2.4163268779   1.54657679
C    1.953564125   -4.8583533597   2.9255818388
W    1.1690267573  -4.5103203735   -0.9436365993
C    0.9486516662  -5.0706879906   -2.8748509997
C    3.001956263   -5.4535178655   -0.9172866333
C   -0.6980070505  -3.6455127938   -1.0037489435
C    2.0639524259  -2.7784506611   -1.5966590492
C    0.2605935969  -6.27634249     -0.3845968646
C   -2.7314841448   1.990688476    -0.8207227595
C   -2.6043147936  -0.386836945    0.7486174796
C    0.0298983323   2.5448014398   -0.4518711079
C   -0.802535639   -0.0074701096  -1.5460744823
C   -1.7160557854   2.1294221947   1.8579984903
C    0.8111370024  -5.8477629158   3.089193042
```

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C	1.2706024249	-7.0908908339	2.7976038164
C	2.6963499633	-7.0158794945	2.4120636601
C	3.1212979931	-5.7280817317	2.4782427275
C	2.2805934038	-4.1051082036	4.2295393767
C	-0.5649806907	-5.4497123274	3.5365082527
C	0.5203360952	-8.3893782578	2.8507774427
C	3.4922326992	-8.2338746281	2.043372563
C	4.5119255533	-5.1987368981	2.2819884388
C	2.6010087159	1.7893788406	1.6247917927
C	2.2633092457	2.99337921	2.1525404265
C	1.3783208816	2.7968206511	3.3204139395
C	1.1697994447	1.4709531384	3.5193452349
C	2.9860446564	-0.2518919973	3.0743207258
C	3.5305595863	1.5038584559	0.4815334143
C	2.6949683282	4.355945994	1.6954528311
C	0.8408389407	3.9475741344	4.1203036056
C	0.3698881903	0.8138330659	4.6052312532
H	3.5661088301	-0.7726429685	2.3048986725
H	2.5270615425	-1.0021028226	3.7259105691
H	3.6834834082	0.3367420736	3.6812554218
H	-0.5100482374	0.2836777764	4.2172554461
H	0.0080815944	1.5484152846	5.3295768729
H	0.9613012344	0.0705839738	5.156390589
H	4.376650632	0.8752929992	0.7922396121
H	3.9462030685	2.4279159388	0.0718225926
H	3.0401015714	0.9785832027	-0.348846567
H	3.209653801	4.8998595978	2.498238743
H	1.8301970694	4.964342917	1.4019719939
H	3.3680667717	4.3102950187	0.8361601196
H	1.6521531319	4.5864632439	4.4922887665
H	0.2549299328	3.6148111487	4.9802082125
H	0.1891809373	4.5837128765	3.5078331849
H	2.5504507703	-4.8362975753	5.000155297
H	1.4296368883	-3.5240211742	4.5955580269
H	3.1281934198	-3.4239379912	4.0984453627
H	5.1838221107	-5.9788692558	1.916161639
H	4.9343476184	-4.8145774767	3.2211643057
H	4.5569424952	-4.37604765	1.5568682647
H	4.51808237	-7.9879931222	1.7588130636
H	3.0320738431	-8.7634350495	1.1991464204
H	3.5370438855	-8.9481762883	2.8761824669
H	0.4271320025	-8.8322039072	1.8516034487
H	-0.4906893893	-8.2646521635	3.2471522254
H	1.0402548252	-9.1220899186	3.4811354183
H	-1.1254312629	-4.9202493319	2.752654437
H	-0.5360067154	-4.7834986317	4.4080557206
H	-1.1622292761	-6.3238771537	3.8106469794
O	0.8302785637	-5.3874925542	-3.9817924878
O	-1.7590817642	-3.1897565243	-1.0459167335
O	4.0205663378	-5.9985997382	-0.9485515368
O	-0.2718833451	-7.2782275419	-0.166535242

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O    2.5790320833   -1.8139507636   -1.9752828048
O   -2.039355574    2.7534062241    2.7758846638
O    0.6860444482    3.410586425    -0.8459435647
O   -0.5582227807   -0.5776370062   -2.5202244177
O   -3.3945200493   -1.1670018753    1.0680945345
O   -3.5812666496    2.5307734917   -1.3926457859
P    1.5717795448   -3.6769632004    1.4672926803
H    2.7480423752   -2.8935212678    1.5555500313
P    0.7176639353   -0.1969966959    1.2959978052
H    1.6542324443   -0.6969526737    0.3610569373
```

D(P)2
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W    1.4398558324   -0.3442354627    0.3791152806
P    0.4201791528    0.6398820079    2.5394306718
C   -0.8786892481    2.0493214397    2.4906624006
P    2.8128629468   -0.4891875667    5.0732241052
W    5.3651631166   -0.2310443569    5.3714843209
H    2.5405024909   -1.4680449323    4.0970874761
C    1.6153041942   -1.1122643203    6.4405293562
H   -0.3281311429   -0.2903434736    3.2983343
C    2.2420047866   -1.174188197    -1.2831501528
C    2.8597917342    1.1578409672    0.3930600783
C   -0.0460892583   -1.7611532215    0.4461695231
C    0.3129109335    0.7705639181   -0.9440462135
C    2.6803253133   -1.6152453471    1.4053735604
C   -0.3794045089    3.2280432907    1.6665689233
C   -1.185160633    3.3688239256    0.5848218076
C   -2.2237410966    2.3150443681    0.5946560004
C   -2.0586358825    1.5188708681    1.6805146192
C   -1.338617121    2.4911503188    3.8958442851
C    0.7777062028    4.0935450993    2.0723127961
C   -1.1068301863    4.404444686    -0.4982659477
C   -3.2777345662    2.220455848    -0.4688424045
C   -2.910666169    0.3636042106    2.1189703094
H    1.7457567459    3.5893428447    1.9576739615
H    0.7085150547    4.4027643747    3.1237080601
H    0.8190221605    5.0051464208    1.4694985462
H   -0.5536104064    3.0231044979    4.4399896549
H   -1.6572387617    1.6402244687    4.5066713487
H   -2.1891209082    3.1732906077    3.7860393388
H   -3.2325472688    0.4665004612    3.163847409
H   -2.3931749594   -0.6019144363    2.0404949223
H   -3.8143051371    0.2875332655    1.5080671693
H   -3.9950762744    1.4195771364   -0.2719586012
H   -2.823487355    2.0273049792   -1.4488590663
H   -3.8392948006    3.1594013964   -0.5574499259
H   -2.0535837774    4.9508753837   -0.597994591
H   -0.9058444593    3.9358082909   -1.4700251844
H   -0.3167722042    5.1367767391   -0.3138039455
O   -0.8913671431   -2.5488862561    0.5061040363
O    3.6309487583    2.016094515    0.3887204423
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O   3.3961138696   -2.384655925    1.8927578586
O   2.6994939091   -1.6532722174   -2.2323021609
O  -0.2435213851    1.3095580012   -1.8022496946
C   7.3828058984   -0.0840879625    5.4143620181
C   5.4052380568   -0.4684417554    7.4107173425
C   5.4553511425    0.028461999     3.3248648169
C   5.1718032353    1.8028454138    5.6423716447
C   5.4931623409   -2.2752220521    5.1354041639
C   1.2237447447    0.0137422945    7.3864169098
C  -0.1264654252    0.1505362847    7.3561505322
C  -0.7068194603   -0.8369017279    6.4186895979
C   0.2860374325   -1.5725288828    5.8567679947
C   2.3252073963   -2.2753007257    7.1742529041
C   2.210039165     0.7718389119    8.2234537363
C  -0.979291589     1.1029457438    8.1443252666
C  -2.1895857733   -0.9871062528    6.2285692005
C   0.1568911301   -2.7541118487    4.941197442
O   5.0635123728    2.9399998241    5.8168324353
O   5.5442617924    0.178774507     2.1837656742
O   8.5374724382   -0.0042579894    5.4311277813
O   5.4748917679   -0.5971049244    8.5590782433
O   5.5518655664   -3.422539166     5.0171960645
H  -2.6589677587   -0.0379984432    5.9378304481
H  -2.6775279444   -1.3003433889    7.1613434961
H  -2.4361415607   -1.7274992797    5.46333975
H  -0.3840015884    1.7594015741    8.7838455241
H  -1.6862015256    0.5637872875    8.7886977643
H  -1.5816579191    1.7410701793    7.4842891126
H   2.7955177523    0.105407236     8.8691002577
H   1.708060018     1.496170595     8.8705863809
H   2.9365927563    1.3273095269    7.6154293273
H   0.7213798343   -2.6363107612    4.0067702024
H  -0.8856652469   -2.9354520691    4.6657279608
H   0.531886019    -3.6726928365    5.4130392104
H   3.2273856687   -1.9398279212    7.6887921969
H   2.6086706258   -3.0786655868    6.4857481991
H   1.6389377329   -2.6923125087    7.9201124345
P   1.9303955945    1.3455456325    4.0824941412
H   1.0195553286    1.5814111238    5.1483751582
```

D(P)3
```
W  -1.605217615   -1.4193590008   -1.1896000959
C   1.0572514431    1.4755814323   -0.8634058175
P   1.7541217046   -1.0730009944    1.1637856021
H   3.0233746445   -0.5045286102    0.8827809195
W   4.2661517577   -3.5375611854   -1.1731593203
C   5.6474396669   -3.8760961277   -2.6088705102
C   4.7753976573   -1.5539632667   -1.180735928
C   3.8164477472   -5.5582187963   -1.1916648495
C   2.9003410349   -3.189752747    -2.6720400398
C   5.7499761088   -3.8532082179    0.226106269
```

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C   -3.3948094656   -2.2504927243   -1.6309065529
C   -2.6542286187    0.2508428918   -0.5787061409
C   -0.7514475781   -3.1891236043   -1.7930451269
C   -1.757727631    -2.1262980528    0.7322492907
C   -1.4879451222   -0.6771865753   -3.1156544012
C    0.8014832386    1.8388130462   -2.3247214846
C   -0.2319749521    2.7176071537   -2.3687693168
C   -0.7254002169    2.980682      -0.9995507245
C   -0.0075153886    2.2530120669   -0.1075344016
C    2.478271979     1.8856811691   -0.4260897631
C    1.657174242     1.3506022756   -3.4580858113
C   -0.8258095945    3.3817373418   -3.5768201664
C   -1.8447859981    3.9412902806   -0.72345948
C   -0.1436441703    2.2123614072    1.3855531627
H    3.2549433421    1.3109464857   -0.9379106688
H    2.6231679202    1.7706243909    0.6520740266
H    2.6213761124    2.9450125796   -0.6676950141
H    0.7931707567    2.48605315      1.8900909571
H   -0.4153719886    1.2127938732    1.7515290786
H   -0.9155080526    2.9035002307    1.7346448014
H    2.7253009667    1.4859142625   -3.2433440184
H    1.4376743558    1.895780925    -4.3799126448
H    1.5121912849    0.2842855293   -3.6781824704
H   -1.8893315284    3.13009601     -3.680729227
H   -0.3262758899    3.0813930778   -4.5009102878
H   -0.7666136583    4.475287136    -3.5004609026
H   -2.0550148144    4.0332712962    0.3447562264
H   -2.772224693     3.6201907704   -1.2132018242
H   -1.6094129765    4.942671728    -1.1070147217
O    6.4352088322   -4.0724103483   -3.4347312235
O    3.6043791757   -6.691307533    -1.2426855067
O    5.0864731199   -0.4377312158   -1.2025252176
O    6.65423454     -4.0092499919    0.9281322477
O    2.1806548768   -2.9696312575   -3.5500444277
O   -1.4527572381   -0.2755576778   -4.1971803204
O   -0.3381932374   -4.2201878195   -2.1173165603
O   -1.8797488561   -2.5288294477    1.8106284465
O   -3.3467958229    1.107828305    -0.2316051096
O   -4.4175194436   -2.7293101467   -1.8872849529
P    2.402385405    -3.1775848618    0.5894615508
C    2.369012863    -4.1230313263    2.2520648201
P    0.7299353904   -0.408100086    -0.7465061239
H    1.6951185717   -0.8308836591   -1.6895071671
C    2.3873087311   -5.6047642295    1.8943035702
C    3.53177648     -6.1480890232    2.3828013659
C    4.3276986445   -5.1053367323    3.0662840056
C    3.6806791847   -3.9151764592    2.9899417677
C    1.1437982925   -3.7691970939    3.1184395721
C    1.2384155152   -6.2986906161    1.2219801061
C    3.9783075069   -7.5792138951    2.3113253313
C    5.637516792    -5.4043547589    3.7351076184
```

```
C    4.1033973304   -2.5891148462    3.550043306
H    1.13248586     -3.5844432605    0.1221723703
H    0.3238775255   -6.2381743338    1.8279362523
H    1.4543001931   -7.3578655129    1.0609454139
H    0.9928014336   -5.8703202217    0.2416061455
H    4.967519232    -7.6609840634    1.8427347129
H    3.2882604595   -8.1990765309    1.7340619435
H    4.0671929768   -8.0193409975    3.313445689
H    6.3901949561   -5.7266291142    3.0050200106
H    5.5325973602   -6.2145705471    4.4680741545
H    6.0421474714   -4.5326324358    4.2555224315
H    3.3073153841   -2.1248016242    4.1467475851
H    4.3705408238   -1.8689435591    2.7632258072
H    4.980888741    -2.6894749354    4.1947726989
H    1.1505191694   -4.409706224     4.007893403
H    0.2027724445   -3.9347955603    2.5862421239
H    1.1600119766   -2.7274201533    3.4491569121
```

D(As)1

```
W    -1.2704002322    1.1061158963    0.1680307206
C     1.9242061814    0.7555962247    2.4504079932
As    0.1397009065   -2.1270857595    2.5105601905
H    -1.0189194958   -2.4542342962    1.5810944405
C     1.9853865567   -4.9284936112    2.9343318372
W     1.1761189192   -4.5425178928   -0.9336889509
C     0.9515152708   -5.0794600406   -2.8706269232
C     3.0004102781   -5.5030600034   -0.915468629
C    -0.6804358501   -3.6548749196   -0.983668864
C     2.0833241875   -2.8075839242   -1.5604226876
C     0.2514317359   -6.3045874149   -0.3880117414
C    -2.7547225554    2.0483155008   -0.82890895
C    -2.6400352432   -0.3185796437    0.7501033758
C     0.0047932586    2.5984786579   -0.4632531246
C    -0.8259226521    0.0316228561   -1.5347050303
C    -1.7322614059    2.1935627077    1.8553891487
C     0.8426287728   -5.9175155844    3.0962004315
C     1.2982806458   -7.1586818802    2.7903610734
C     2.7230716313   -7.0826218376    2.4007288361
C     3.1503838617   -5.7962441419    2.4779981803
C     2.3173576351   -4.1788707124    4.2394504767
C    -0.5305392096   -5.5177061472    3.5506227276
C     0.5449910175   -8.4558705519    2.830945954
C     3.5157437882   -8.2979958746    2.016726513
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C     2.5806254867    1.8477640149    1.6119954715
C     2.2480713135    3.0523086365    2.1421072238
C     1.3743586506    2.8563087097    3.3184300912
C     1.1672097629    1.5305556032    3.5191421791
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H    0.9575501723    0.1082680244    5.1373265891
H    4.3630958728    0.9532971323    0.7739352041
H    3.893695041     2.4836916533    0.0298168612
H    3.0104113204    1.0093546007   -0.3512322236
H    3.2076441082    4.954786235     2.4740556775
H    1.8071449044    5.0269140417    1.4052582125
H    3.3313815795    4.368780626     0.8078545997
H    1.6561383574    4.6557075328    4.473245259
H    0.2796433917    3.6732120283    4.9975670237
H    0.1716271108    4.632464991     3.521639086
H    2.6056435039   -4.9099681777    5.0034619242
H    1.4626118158   -3.6123063506    4.6200004442
H    3.1535558993   -3.4844082322    4.1037442545
H    5.2140268343   -6.0417497172    1.9144972667
H    4.9612637219   -4.8832827465    3.2241997243
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O    4.0142350377   -6.0567461488   -0.9509956199
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O    2.6019182339   -1.837362715    -1.9193090965
O   -2.0460460425    2.8174717466    2.7768663216
O    0.6613250502    3.4617024495   -0.8623388991
O   -0.5749268251   -0.5553827     -2.4970248617
O   -3.4390448618   -1.0904692536    1.0675569801
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P    1.5879613789   -3.7398703431    1.4861171446
H    2.7549727079   -2.9414897419    1.5760020894
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C   -0.0973908236   -1.7106706027   0.3385178715
C    0.33537732     0.8321492307   -1.0009656418
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C    0.7027276689    4.1068869481   2.0616565326
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H    0.6350018799    4.3854930091   3.1217059292
H    0.7328744015    5.0358133643   1.4850778889
H   -0.6364692685    2.9830285917   4.410713132
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O    2.7217117316   -1.6284126087   -2.2576527725
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C    5.5400553392   -2.3192094268   5.1923915726
C    1.26765256     0.0052945359   7.4356265335
C   -0.0809390265    0.1550051891   7.4012910782
C   -0.6671531478   -0.8215803269   6.4565066894
C    0.320310411    -1.5645704261   5.8951244355
C    2.3398928064   -2.2965275822   7.2284097561
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O     5.5523724273    0.1143007771   2.2280433634
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O     5.5205031021   -0.6376882688   8.6097432417
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H    -2.6456360359   -1.2672831949   7.1889133827
H    -2.4017371204   -1.6906559242   5.4904842673
H    -0.3281414754    1.7599977419   8.8351281035
H    -1.6435366897    0.5789612306   8.8277233534
H    -1.5191563973    1.7609576749   7.5292272907
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H     0.7523225357   -2.6230236991   4.0411140375
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C    -0.7388783762   -3.1189567022   -1.8518210396
C    -1.744541837    -2.0999689407    0.7033932001
C    -1.5821835307   -0.6214355012   -3.1385746065
C     0.6752272417    1.8680665448   -2.4112328076
C    -0.3548370929    2.7516606428   -2.3665331543
C    -0.7139822815    3.0310567117   -0.9592842957
C     0.0838090449    2.3088183752   -0.1328988354
C     2.5274547565    1.891351861    -0.6857139026
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C	-1.4990965699	-3.6209288754	1.4917238618
H	2.5252476145	-2.1183386442	-0.3327648106
H	2.4833653245	-4.5257648987	-2.1983717429
H	3.2811177605	-5.8471113814	-1.3407984129
H	3.5969539852	-4.1800235563	-0.8758078145
H	1.1544325621	-8.1635331098	0.2984863413
H	2.2335139618	-7.6027410898	1.5744622651
H	2.7363457913	-7.4812603783	-0.1123287554
H	-0.0039086104	-7.0046077585	2.9419824179
H	-0.9799244756	-7.5421620214	1.5750223886
H	-1.5526943516	-6.225388482	2.6084872061
H	-2.1929530211	-3.366844746	0.6784006791
H	-1.2170339881	-2.6746591415	1.9711580578
H	-2.0617579576	-4.1983308199	2.2296032697
H	-0.4539290237	-4.299965907	-1.7829476049
H	0.6901956839	-2.9689897623	-2.0428270765
H	-0.821301935	-2.6933050171	-1.1546651063
C	0.7633057332	2.2825424357	-0.0158595993
C	1.7837666976	1.2141000532	0.4774585897
H	-0.1439031899	2.2943230011	0.6060909146

2(As)3

W	-2.1474661116	-1.1984711336	-0.7248579348
C	0.4890978385	1.7523524057	-1.003401107
As	2.3940120497	-0.6721796011	-1.5904059882
W	2.1504315758	-4.428295209	-2.5986819493
C	2.0233801806	-5.6169397354	-4.228078471
C	1.2415249978	-2.9872704311	-3.752119456
C	3.0610610732	-6.0361425224	-1.6832849817
C	0.3184977528	-5.1012337229	-1.9359310199
C	3.996931142	-3.7403528427	-3.1935845832
C	-4.0056926222	-1.863835672	-0.3024625693
C	-2.1388110172	-0.1006977729	1.0092689579
C	-2.1177972337	-2.3733272315	-2.4270096634
C	-1.4721208066	-2.7904896535	0.3945388727
C	-3.0632602747	0.3098754109	-1.7830316134
C	2.6791467373	2.0092425022	-1.8337776606
C	1.386869207	2.3311851574	-2.0828839022
C	-0.7651475257	2.580390519	-0.7133483079
C	1.6502288779	2.8168697921	1.0508132396
C	4.0858736322	1.2411868921	0.1685237337
C	3.8854841069	2.3023885536	-2.6756111361
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H	-1.4470830332	2.6015635967	-1.5677982408
H	-0.4848270394	3.616818185	-0.4932758748

H	1.6018449995	3.3554580955	-3.9744140329
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H	0.0801776003	2.4736828797	-3.7889614799
H	0.7115893798	3.0720371428	1.5526369504
H	1.9694438977	3.6802115586	0.4576952834
H	2.3992789331	2.6449874412	1.8304649719
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H	4.0358573308	0.7350304469	1.1351872907
H	4.350497245	2.2875521013	0.3675917618
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H	4.3760188402	1.3702333868	-2.9872702079
H	4.6309130422	2.8848418456	-2.1194746266
O	1.9498976598	-6.2994421768	-5.161240165
O	3.5586227034	-7.0071438164	-1.3010087384
O	0.7316135984	-2.235581254	-4.4696230988
O	5.0359192024	-3.3632269277	-3.5335413066
O	-0.7051682028	-5.4883821343	-1.5666752319
O	-3.6226008935	1.1323847193	-2.3726706877
O	-2.1340258002	-3.0432312504	-3.3652349924
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O	-5.0796295939	-2.2290776971	-0.0706805281
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C	3.4848787852	-3.137964006	0.9061435639
P	0.0648112444	-0.0668945763	-1.549352383
H	-0.0561757507	0.1417448734	-2.9428728467
C	3.1845130559	-4.5140606575	1.4943714121
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C	3.3520307936	-2.0432998043	1.9798494984
C	1.9054694004	-4.8433086634	2.2056370542
C	4.493741277	-6.7004102759	1.821667325
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C	5.655628224	-2.1544250368	-0.2699036948
H	1.0810561589	-2.7448301948	0.2267869976
H	1.9481182641	-5.8407021664	2.6512639984
H	1.0320177699	-4.8235181693	1.5429296209
H	1.6964247134	-4.1328029701	3.0171371682
H	4.6708240317	-7.3794253047	0.9790287592
H	3.6312557952	-7.0806572387	2.3748636816
H	5.3698616823	-6.7675073565	2.4799528352
H	6.5410655034	-6.0340775828	-0.3453934118
H	7.1968703774	-5.4766751089	1.191558423
H	7.3179243225	-4.4484120267	-0.2428594303
H	5.8506800043	-1.3418652314	0.4439704006
H	5.112581478	-1.7112173026	-1.1152828881
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W    3.0389680745    -0.39154675     -1.3022473359
C    1.7301785481    0.4621062388    2.3953714633
W   -3.2186179971    -1.5649331841   -0.1081689493
C   -1.8287749086    4.1194399225    -0.7348231913
C   -3.0556350855    3.5484214806    -0.7761258578
C   -1.2563218001    5.1527505713    -1.6588307946
C   -4.1684542317    3.8070433514    -1.7457877193
H   -4.4335313892    2.8947506924    -2.2994493656
H   -3.906472976     4.5733620999    -2.4795862932
H   -5.0806705481    4.1341815739    -1.2306124858
H   -1.9649425931    5.4476409222    -2.4367630018
H   -0.3541527416    4.7708908721    -2.1565999953
H   -0.9587715094    6.059031163     -1.1160024517
C    1.863462304     -1.0387168406   2.5780029381
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C    3.872906975     -0.0588509296   3.1826209293
C    3.0926019367    0.9961503996    2.8324744527
C    0.5646696165    1.0392940917    3.2122303723
C    0.7154876057    -1.9816351209   2.3921165591
C    3.693252635     -2.660312566    3.3583159766
C    5.2837977168    -0.0348816023   3.6917718159
C    3.4283869945    2.4554525535    2.9265482462
H    5.3768864667    -0.5947109009   4.6308638127
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H    1.0531626928    -3.0158236891   2.287019742
H    4.3436645324    2.6097524822    3.5046482321
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O    -3.8981797494    -1.6448144352    -3.2517514313
O    -6.2739970636    -0.7131176347     0.3930510844
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C     4.7657711791    -0.063854883     -0.2287529103
C     2.8371654327    -2.2443614218    -0.4121189513
C     3.25668713      1.4448530315     -2.1997374832
O     2.7639502807    -3.30429257       0.0404662424
O     0.4352592545    -0.9430388747    -3.1073397607
O     3.3814505416     2.4806454267     -2.6996346816
O     4.812464613     -1.7061026797    -3.5867347458
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C    -0.9991483946     3.4795127845      0.3600838462
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H     0.6202390554     3.8491988509      1.7790660471
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P    -0.3669787571     0.8918360716     -0.9414291224
W     2.64240825      -1.4962001365     -0.0101371265
P    -1.8950142792     0.5176355822      0.3765990639
H    -1.3179604807     0.4299165356      1.6729738256
W    -4.3040037207     0.1311028123      0.0303354421
C     3.4037594932     2.4724366926      1.3040618422
C     4.602413844      2.6007713623      0.6802571809
C     4.3987679931     2.6816210702     -0.7823926584
C     3.0744018199     2.6029805541     -1.0651365309
C     1.2881254921     3.607544504       0.4595281325
C     3.1267306054     2.4059105432      2.7781705848
C     5.9656555336     2.6677805856      1.303432983
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H    1.8175217272     4.5668410325     0.4748883484
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C    1.5934814139     4.3071234605    -0.0087064001
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C    2.5513499835     1.972059019      2.464786305
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F(P)1

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P	-0.9892090218	-1.2043622958	-0.4884388785
C	4.0542202987	-3.3980682304	-0.6344902064
C	5.2928519092	-2.9878951407	-0.2408302043
C	5.1694603256	-2.0132206598	0.8562532069
C	3.8547269562	-1.8172788523	1.1433430526
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3(P)3

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4(P)1

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H	3.2941339434	0.9316227628	-0.5674956558
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4(P)2
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C    1.335237267    3.9777852522   2.3005643008
C   -1.8653837207   3.8328378367   2.0846160985
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P   -0.2835876456   1.5671639621  -2.3739083239
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4(P)4

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C	2.864088959	3.0598071626	1.4421896879
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O   -2.915344154    1.6423423495    1.8914876082
O   -3.9163017624    0.9256195471   -2.5141896971
O   -6.6064991294   -0.7455019386    0.6946297425
O   -4.0343127063   -3.5733341639   -1.7076709827
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F(As)2
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H    0.7583894361    1.8812424406   -1.1908735759
P   -0.6427704898    1.9686611061   -0.9589124432
C   -0.5679843766    3.2391602176    0.4826190374
P    1.2527481193   -1.0333066654    0.1092910057
W    3.6967343682   -0.4887462121    0.0293244829
C   -0.3411179829    4.488830323    -0.3540477585
C   -1.519530487     5.1699905544   -0.4290296998
C   -2.5431741727    4.4843335663    0.3771010793
C   -2.0015003606    3.3773149249    0.9515253564
C    0.46978066      2.9645154214    1.5715082629
C    0.9987247603    4.8782446024   -0.9088061561
C   -1.8019554358    6.4415634434   -1.1741062625
C   -3.9469259056    4.9986827569    0.513133507
C   -2.6217238989    2.4444500296    1.9475528493
H    1.4706845807    4.0800250679   -1.4942616253
H    1.7033925887    5.1311553866   -0.1037786216
H    0.9210576129    5.7541892898   -1.5586408664
H   -0.9264842113    6.8064649296   -1.7170864944
H   -2.128624504     7.2380970516   -0.4925740855
H   -2.6108004956    6.3002374244   -1.9028614444
H    0.4533127768    3.7745639669    2.3111484605
H    1.4809987718    2.9080028382    1.1579384239
H    0.2677549645    2.0247206834    2.0952205974
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H   -2.2738014516    2.6619334218    2.9678097695
H   -2.3605702524    1.3981715636    1.7523481501
H   -3.7129935913    2.5159190488    1.950788061
H   -3.9652030334    5.9945798334    0.9756324458
H   -4.5678618507    4.3385684218    1.1241556631
H   -4.430772601     5.0961114497   -0.4671871106
H    0.8946778428   -2.3712014147    0.4065076553
C    5.7123175257   -0.2303671442    0.0281437578
C    3.9571903229   -2.1787926735    1.1906031946
C    3.4911610723    1.1942788432   -1.1412703156
C    3.5611477376    0.6865830263    1.7257486145
C    3.8670372996   -1.6439461134   -1.68447106
O    4.1098049456   -3.1219266232    1.8349393135
O    3.4998604101    1.3477517049    2.6681885175
O    3.9795643718   -2.2800509828   -2.6377490445
O    3.4260762034    2.1409966016   -1.8000472357
O    6.8592968225   -0.0904622938    0.0324688443
As  -0.7481961978   -0.2179444831   -0.0602170142
W   -2.9345883476   -1.6746364616   -0.075358771
C   -4.6321342245   -2.7704219343   -0.1727289975
C   -2.639665588    -1.9808143852   -2.1024493044
C   -3.2229607835   -1.3897394825    1.9512915841
C   -4.0244851008    0.0279528972   -0.4855289129
C   -1.8421560311   -3.3733969896    0.3348072962
O   -1.2357374301   -4.3288168217    0.5640201676
O   -3.3946132654   -1.2356220767    3.0815566563
O   -2.4821328352   -2.1623779032   -3.2293151791
O   -4.6519500454    0.9703774619   -0.7088332932
O   -5.603096953    -3.3962620076   -0.2309589323
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3(As)1
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C    2.0373906713    3.3293735363   -0.9954530828
C    0.6724608195    2.8905357325   -0.4744600227
C    0.6085055261    2.0183281792    0.8212862602
C   -0.9280829327    2.1559612697    1.1364937901
C   -1.1915466077    3.5959435737    0.7482297783
C   -0.3229959762    3.9777010236   -0.2207226728
As  -0.0561957401    1.3180157536   -1.7226120987
C    1.4843359596    2.5011333935    1.9829443384
P   -1.8865636829    1.1540849618   -0.273795964
C   -1.3767335781    1.7158691114    2.5286380867
C   -2.3484943821    4.3624481731    1.318319791
C   -0.3125213106    5.2625757265   -0.9950260046
W   -3.2486986816   -1.0018504647   -0.017641634
W    3.3643692987   -0.8196856475    0.0767321023
C    5.1033081729   -1.8634984511    0.0822289473
C    3.5312392031   -0.4919367896   -1.9535321988
C    3.1734095813   -1.107879668     2.1109568504
C    2.3399557816   -2.5832433412   -0.2754661963
C    4.4188284753    0.9048464193    0.4363195104
O    5.02871034      1.8673195055    0.6382893266
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O    6.0925753132   -2.4625453039    0.087669803
O    3.0687335684   -1.2581437891    3.2510428721
O    1.7793046885   -3.572966112    -0.4634762521
O    3.6184165771   -0.2921505692   -3.087130399
H    2.7136476956    2.4858851728   -1.1600643864
H    2.5258155326    4.0109089742   -0.2871602696
H    1.9369491301    3.8568205852   -1.9493672527
H    1.4003398228    1.8296434608    2.8440670219
H    1.1919839957    3.506758381     2.3044849729
H    2.5374764112    2.5322609      1.693082491
H    0.6221695915    5.8180395631   -0.8473592466
H   -1.1386410091    5.9202674283   -0.713514919
H   -0.3952421941    5.0692571872   -2.0736563192
H   -2.2415208723    4.4920582144    2.4028634137
H   -3.300630222     3.8372154291    1.1604609312
H   -2.4412185735    5.3561754637    0.8730114787
H   -1.0892400941    0.6805056171    2.7341068279
H   -2.463627989     1.781019378     2.6389973219
H   -0.9275318144    2.3498270314    3.3011401338
C   -4.4453817507   -2.6327542144    0.1066899658
C   -4.3183395707   -0.373861154    -1.6681201749
C   -2.2050879772   -1.6650924656    1.6248527371
C   -4.5144913252    0.0524819029    1.2149261537
C   -1.9331579898   -2.0172555589   -1.2432693551
O   -4.9226923341   -0.0251429629   -2.5878077688
O   -1.6236850606   -2.0545132481    2.5460515437
O   -5.2108141102    0.658542178     1.9115925298
O   -1.185115776    -2.5748737954   -1.9228864236
O   -5.1356294498   -3.5584825888    0.1739545716
P    1.089003444     0.3175141619    0.1108419831
H    0.0976606275   -0.5212632437    0.6733109553
H   -2.6841874864    2.2133811263   -0.7700062697
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3(As)2
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6        0.52137   4.15705  -1.36894
6       -0.08268   2.99909  -0.57699
6        0.7749    2.31544   0.54577
6       -0.37681   1.55014   1.29648
6       -1.50237   2.56794   1.23506
6       -1.37897   3.31383   0.11106
33      -0.10635   1.25769  -1.79526
6        1.54329   3.26841   1.46835
15      -0.99049   0.14251   0.08006
6       -0.0477    0.97544   2.67457
6       -2.57077   2.64082   2.28496
6       -2.33959   4.3334   -0.42728
1        1.46769   3.89996  -1.85304
1        0.7059    5.01853  -0.71435
1       -0.16519   4.4834   -2.15621
1        2.12751   2.71275   2.20878
1        0.86023   3.93705   2.00415
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1              2.24141   3.88909   0.89703
1             -1.89925   5.33846  -0.44587
1             -3.25946   4.37892   0.15946
1             -2.62307   4.09331  -1.46101
1             -2.14852   2.98748   3.23793
1             -3.02327   1.66393   2.48307
1             -3.37183   3.32877   2.00602
1              0.80227   0.29031   2.63569
1             -0.89758   0.42313   3.08714
1              0.19673   1.77607   3.38181
15             1.89678   1.20015  -0.52058
74             3.5425   -0.67133   0.05045
74            -3.29642  -0.95966  -0.02394
1              2.5689    2.25479  -1.18286
6              4.98514  -2.05485   0.3899
6              2.34844  -1.63054   1.42163
6              4.79574   0.23964  -1.31203
6              4.30102   0.50524   1.56183
6              2.73089  -1.84302  -1.44714
8              1.71043  -2.19827   2.20155
8              2.26659  -2.4931   -2.27904
8              4.71732   1.16225   2.41666
8              5.49951   0.75134  -2.07051
8              5.81601  -2.83674   0.57817
1              0.04631  -0.80612   0.25867
6             -5.06817  -1.93437  -0.14259
6             -3.411    -1.00614   2.02912
6             -3.19108  -0.92314  -2.08645
6             -2.3125   -2.77552  -0.00069
6             -4.28253   0.84498  -0.07257
8             -4.86234   1.84525  -0.11354
8             -3.14161  -0.90366  -3.23923
8             -1.76064  -3.78851   0.00942
8             -6.0795   -2.49292  -0.207
8             -3.48369  -1.03108   3.18347
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3(As)3

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C   1.4069934273   2.45540356   -1.7696440083
C   0.3446767155   1.8975587212  -0.8273911629
C   0.7439764181   1.5613267893   0.647918677
C  -0.7032349073   1.4075003338   1.2566274235
C  -1.4277479488   2.545310292    0.5571926862
C  -0.8889925354   2.7342830863  -0.6731501015
As  0.0126461172  -0.1585761675  -1.3315665865
C   1.557486748    2.6375225204   1.377510821
P  -1.5231200095  -0.1754431945   0.44381189
C  -0.8049860439   1.3364949408   2.7797777869
C  -2.5715849903   3.2757500435   1.1941488049
C  -1.3727891702   3.6491879756  -1.7598626332
W  -4.011616024   -0.6190619575   0.0304834322
W   4.1821091117  -0.455737046    0.0766357359
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C   6.154525545   -0.9071566975   -0.0595343969
C   3.9496552793   -0.69723549    -1.9593407399
C   4.3735437843   -0.1819181848   2.1111550782
C   3.773733996   -2.4593001953    0.3702221111
C   4.6383061289   1.5259239798    -0.2275127608
O   4.9159106385   2.6344752008    -0.4059498658
O   7.2784924354   -1.1701168274   -0.1305854233
O   4.4735925324   -0.0209466468    3.2506133186
O   3.554755463   -3.5802517061    0.5354974642
O   3.8094860768   -0.8186829764   -3.0987426302
H   2.286164154   1.8097710244    -1.8430396496
H   1.7475031544   3.4425967302    -1.4319940485
H   1.0028291575   2.5710030583    -2.7800851629
H   1.814300431   2.3119458346    2.3913817349
H   0.9986282302   3.5764934971    1.4526441162
H   2.4934119347   2.8437093042    0.8531849099
H   -0.6456654525   4.4422284483   -1.9760744337
H   -2.3234909245   4.1218091034   -1.5049308139
H   -1.5238010908   3.095338558    -2.6961054305
H   -2.22117549   3.8489692317    2.0632638316
H   -3.3452656038   2.5944149297   1.5621212429
H   -3.0443499885   3.9768991537   0.5029047354
H   -0.2017527683   0.5143995418   3.1803413191
H   -1.83850403   1.1766773805    3.1032218853
H   -0.456274575   2.2658255372    3.2434654346
H   -0.9416295712   -1.2029238825   1.229225238
C   -5.9554745607   -1.1020518927   -0.2748010496
C   -4.3238646133   1.204627486    -0.871817076
C   -3.7051836236   -2.4601650557   0.9086394072
C   -4.4956981928   0.1627761336    1.8692706064
C   -3.5381749169   -1.415224357    -1.817036595
O   -4.5317451969   2.2149344109    -1.3947898703
O   -3.5272965413   -3.4891382874   1.4005970995
O   -4.7724405575   0.6016195028    2.9036770886
O   -3.284893637   -1.8611441038    -2.8505629366
O   -7.0658366562   -1.3795276166   -0.4441529512
P   1.6751672455   -0.0768635822    0.3668469581
H   1.1533578407   -0.9098675435    1.3864236691
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3(As)4
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C    -0.2561505384    -1.1825287809    -0.7322253501
C    -0.5363466429    -0.5130703798    0.6107534843
C    0.5052989122    0.4932194349    1.20685721
C    -0.4028648073    1.1601821999    2.3041512189
C    -1.7278302626    1.2544117521    1.5777961217
C    -1.8265446836    0.2424284887    0.6803784281
As   -0.2017049173    -1.9386144979    2.1946275834
C    1.0683762427    1.5175697768    0.2122516849
P    -0.821241825    -0.2290874956    3.6671015912
C    0.1373712524    2.4276299698    2.9603239929
C    -2.769728623    2.2567107751    1.9764302892
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C	-3.0270208348	-0.1468403298	-0.131674447
H	0.6846701061	-1.7390877316	-0.7540688577
H	-0.2165064642	-0.434713731	-1.5351321899
H	-1.0529018012	-1.8904849966	-0.9805195371
H	1.7855466956	2.186853178	0.6952258882
H	0.268254486	2.1285035071	-0.220027259
H	1.5907187167	1.0158672372	-0.6090650066
H	-2.8291674692	-0.0911175605	-1.2094778596
H	-3.8891791335	0.4901223134	0.0808409536
H	-3.3226505465	-1.1840187424	0.0802562895
H	-2.4022130385	3.282069574	1.8436112823
H	-3.0421731461	2.1571486441	3.0364907179
H	-3.6856317752	2.1529960559	1.3894635494
H	1.0947843114	2.2454911965	3.4574245678
H	-0.554546814	2.8114037512	3.7153574621
H	0.2873159083	3.2194087065	2.2178399767
W	-0.7307021459	-0.1680773707	6.2441604945
P	1.8164719682	-0.7090844016	1.8755489752
W	4.1032576436	-0.3554830782	2.982867688
H	-2.1968033511	-0.3447993353	3.3636342206
H	2.0775413066	-1.3168492332	0.6268010778
C	-0.920108076	-0.1702019051	8.2562781194
C	-2.5513694156	0.7686526447	6.081327806
C	1.0956105628	-1.1130730202	6.4213110292
C	0.1656458403	1.6885710979	6.3752046213
C	-1.6566678267	-2.0095053666	6.1850537016
C	5.9984014055	-0.1741813767	3.6703036049
C	3.4446505621	0.6668690959	4.6439925053
C	4.8498180418	-1.3241299211	1.327065429
C	4.3015352807	1.4512579473	2.0217895777
C	3.9197455059	-2.1760899244	3.9572088719
O	3.1539175704	1.2793438617	5.5789351956
O	3.8392754267	-3.2020029869	4.4748835976
O	4.4266673003	2.4716436816	1.4919080816
O	5.2633287077	-1.8579959071	0.3898722134
O	7.0846823958	-0.0743473916	4.0550228917
O	2.1040439797	-1.65399739	6.5709732123
O	0.6186650679	2.7430428438	6.4947000184
O	-2.1836589176	-3.0369846638	6.1667618999
O	-3.5737801208	1.2979517175	5.9649031529
O	-1.0399505605	-0.1754485431	9.4073820805

4(As)1

6	-2.70208	3.23898	-0.1826
6	-1.26166	2.80737	0.08638
6	-0.23606	3.05768	-1.08743
6	1.09876	2.91587	-0.2882
6	0.77873	3.45913	1.07224
6	-0.56226	3.46338	1.26295
15	-1.16464	0.88777	0.51283
6	-0.44119	4.41836	-1.76309

33	0.9853	0.82859	-0.41938
6	2.39044	3.41438	-0.92493
6	1.84847	3.89864	2.02891
6	-1.32885	3.91533	2.47016
74	2.81973	-0.99649	0.07325
6	4.26339	-2.35348	0.46764
6	1.59173	-2.52793	-0.58795
6	4.0581	0.4877	0.7651
6	2.05172	-1.21579	1.97592
6	3.54272	-0.73621	-1.84185
8	1.62184	-1.32089	3.04182
8	4.75405	1.31956	1.16982
8	5.09325	-3.12709	0.6935
8	3.94494	-0.58118	-2.91266
8	0.93365	-3.40581	-0.94045
1	-3.0893	2.78327	-1.09744
1	-2.76461	4.32722	-0.29533
1	-3.36949	2.95309	0.63663
1	0.35528	4.61556	-2.48778
1	-0.43747	5.23083	-1.02707
1	-1.39293	4.45171	-2.30305
1	-2.0231	4.72689	2.21756
1	-0.67044	4.27595	3.26418
1	-1.9398	3.10266	2.88718
1	2.40822	4.75849	1.63894
1	2.5829	3.09988	2.19651
1	1.43924	4.18307	3.00155
1	2.56088	2.99055	-1.9194
1	3.25568	3.15872	-0.30696
1	2.36996	4.50682	-1.02815
74	-2.88276	-0.94734	0.04973
15	-0.20714	1.5907	-2.33213
1	0.95932	2.03653	-3.01929
1	-0.84169	0.98664	1.88714
6	-4.22665	-2.45164	-0.13355
6	-3.87174	-0.26244	1.71912
6	-1.90299	-1.59692	-1.65
6	-1.71439	-2.18687	1.21614
6	-4.08379	0.21207	-1.15618
8	-1.07147	-2.89463	1.86297
8	-4.42455	0.13739	2.65254
8	-4.99469	-3.31177	-0.22633
8	-4.78074	0.82465	-1.84536
8	-1.38021	-1.96649	-2.60957

4(As)2

C	-2.3904800692	3.4038275401	-0.8048746919
C	-1.0742824874	2.8991206408	-0.2247353888
C	0.2188047539	3.0299215615	-1.0938078541
C	1.2981059444	2.7480319771	0.0224445518
C	0.6745752528	3.4279549139	1.2314702295

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C    -0.6751434014    3.4379618432    1.1152420054
As   -0.9998091654    0.8001895962   -0.3731593694
C     0.4134815564    4.406165806    -1.746878875
P     1.1822321878    0.8437318116    0.4786298081
C     2.7327479533    3.1420296323   -0.3257870344
C     1.5120277446    3.8812826549    2.3899089728
C    -1.686430113     3.8797586162    2.1319269565
W     2.9445029819   -0.9604456943    0.0333593509
H     0.9100821247    0.9692709349    1.863033432
P    -0.1107719869    1.6550621556   -2.3929489462
W    -2.8908549405   -0.9729105043    0.0890959275
H     1.1543434931    1.0023409581   -2.4074993596
C     4.343004949    -2.4125755685   -0.1712514647
C     1.589297799    -2.1136286814   -1.0141259935
C     4.3008326405    0.1855222283    1.0728362137
C     2.3431676148   -1.813763287     1.8178612432
C     3.581874773    -0.1072187471   -1.7230721967
C    -4.3730556452   -2.2998290863    0.4408641924
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C    -2.4723046114   -1.8864278035   -1.7222079689
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O     5.0643700124    0.8292049786    1.6561298088
O     5.1420504544   -3.2413429928    -0.2828851816
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H    -2.5884351807    3.0024461662    -1.8041266624
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H     0.4851642203    5.1998842983    -0.9944966157
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4(As)3
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C    -1.5726136406   2.8309384763    0.9758308658
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C    -0.0635508228   2.7134557639    3.0484717127
C    -2.9163762517   2.9744067583    1.6248045597
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4(As)4

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O	4.9232480545	-3.2982779681	0.7563685901

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