Supporting Information

Single- and double-bridged PNP Ligands in Chromium-catalysed Ethylene Oligomerisation

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Experimental details

Syntheses of air or moisture sensitive complexes were carried out using standard Schlenk line, vacuum or cannula techniques under a nitrogen atmosphere. These complexes were further manipulated and stored in a standard nitrogen filled glove box. All glassware was dried overnight in the oven at 150 ℃. All reactions were stirred with magnetic stirrer bars. NMR spectra were recorded on Bruker DRX-400 MHz, AV-400 MHz and AV-500 MHz spectrometers. Chemical shifts for ^{1}H and ^{13}C were reported in ppm and referenced to the deuterated NMR solvents. ^{31}P NMR spectra are referenced externally using H_3PO_4 (85%). Elemental analyses were carried out by the Science and Technical Support Unit at London Metropolitan University or MEDAC LTD. Unless otherwise stated, all spectra were recorded at 298 K. GC analysis was carried out using an Agilent 6890 Series (Plus) system with an Agilent 19091N-133 column (HP INNOWAX, 300 mm x 0.250 mm). Method details: Injector 310 ˚C. Column: 30 ˚C 15 min isothermal; ramp 5 ˚C/min to 100 ˚C, 10 min. isothermal; ramp 10 ˚C/min to 260 ˚C, 10 minute isothermal. Total run time 65 min. FID detector 325 ˚C. Carrier gas: Helium.

Solvent and Reagents

THF and diethyl ether were refluxed under a nitrogen atmosphere and dried over sodium metal with a benzophenone ketyl indicator. Toluene and pentane were obtained from Romil and dried

by passing through a column that contains commercially available Q-5 reagent (13 % CuO on alumina) and activated alumina (pellets, 3 mm) under a nitrogen atmosphere. Dichloromethane was dried by passing through a column that contains alumina and stored under molecular sieves. All NMR solvents were degassed and stored over molecular sieves.

Phosphorous trichloride, triethylamine, *n*-propylamine, isopropylamine and *N,N'*-dimethylethylenediamine were degassed using the freeze-pump-thaw technique and dried over 3 Å molecular sieves (dried in a 150 ˚C beforehand) in a Schlenk vessel. Pre-dried deuterated solvents and $[CrCl_3(THF)_3]$ were obtained commercially. MAO was purchased from Sigma-Aldrich and was used without any purification. The following compounds were prepared according to literature procedures: 2-chloro-1,3-dimethyl-1,3,2-diazaphospholane[1] and $[ClP(\mu\text{-}N^tBu)]_2$,[2] and $[Li(OEt_2)]_4[\{Cr(C_4H_8)_2\}_2]$ (**6**).[6]

Ligand and complex syntheses

Bis(1,3-dimethyl-[1,3,2]-diazaphospholidin-2-yl)propylamine (1)

n-propylamine (1.44 ml, 17.3 mmol) in DCM (20 ml) was added dropwise with stirring at 0 ℃ to a mixture of 2-Chloro-1,3-dimethyl-1,3,2-diazaphosphacyclopentane (5.30 g, 34.7 mmol) and triethylamine (6.50 ml, 42.9 mmol) in DCM (100 ml) under a nitrogen atmosphere. The reaction mixture was allowed to warm to room temperature before it was refluxed for 24 hrs. DCM was then removed under high vacuum and the residue was extracted using 5 portions (5 x 20 ml) of dry pentane. The pentane was then removed under high vacuum and the product was purified via vacuum distillation. The product obtained was a viscous colourless oil (1.70 g, 5.84 mmol, 34 % yield). ^{1}H NMR (C_6D_6, 298K) δ(ppm): 3.13 (m, 4H, CH_2), 2.81 (m, 4H, CH_2), 2.78 (m, 2H, NCH_2), 2.56 (m, 12H, NCH_3), 1.48 (m, 2H, CH_2), 0.81 (t, 3H, J = 7.4 Hz, CH_3); ^{13}C NMR (C_6D_6, 298K) δ(ppm): 53.0 (d, J 3.9 Hz, 4C, CH$_2$), 45.3 (m, 1C, NCH$_2$) 34.3 (d, J 12 Hz, 4C, NCH$_3$), 26.1 (s, 1C, CH$_2$), 12.6 (s, 1C, CH$_3$); ^{31}P NMR (C_6D_6, 298K) δ(ppm): 112.3.

Bis(1,3-dimethyl-[1,3,2]-diazaphospholidin-2-yl)isopropylamine (2)

Isopropylamine (1.12 ml, 13.2 mmol) in DCM (20 ml) was added dropwise with stirring at 0 ℃ to a mixture of 2-chloro-1,3-dimethyl-1,3,2-diazaphospholane (4.00 g, 26.4 mmol) and triethylamine (5.00 ml, 33.0 mmol) in DCM (80 ml) under a nitrogen atmosphere. The reaction mixture was allowed to warm to room temperature before it was refluxed for 24 hrs. DCM was

then removed under high vacuum and the residue was extracted using 5 portions (5 x 20 ml) of dry pentane. The pentane was then removed under high vacuum and the product was purified via vacuum distillation. The product obtained was a viscous colourless oil (1.05 g, 3.61 mmol, 21 % yield). ^{1}H NMR (C_7D_8, 298K) δ(ppm): 3.41 (sep/tr, J = 6.8 and 1.5 Hz, 1H, iPr), 3.16 (m, 4H, CH_2), 2.77 (m, 4H, CH_2), 2.53 (d, J = 12.6 Hz, 12H, NCH_3), 1.31 (d, J = 6.8 Hz, 6H, CCH_3); ^{13}C NMR (C_7D_8, 298K) δ(ppm): 53.3 (m, 4C, *C*H$_2$), 44.9 (t, *J* 9.5 Hz, N*C*H) 34.3 (d, *J* 18.8 Hz, N*C*H$_3$), 25.7 (t, *J* 7.9 Hz, 2C, C*C*H$_3$); ^{31}P NMR (C_7D_8, 298K) δ(ppm): 109.6.

Bis(1,3-dimethyl-1,3,2-diazaphospholane) (3)

2-Chloro-1,3-dimethyl-1,3,2-diazaphospholane (0.537 g; 4.3 mmol) was dissolved in THF (20 mL). To this was added Mg (0.157 g; 6.5 mmol), followed by one crystal of iodine. The reaction mixture was stirred overnight, which resulted in a yellow liquid and a dark brown precipitate. The solvent was removed under vacuum and the residue was extracted with pentane (2 x 5ml) to give a yellow solution. The solvent was removed to leave a yellow oil. Yield: 0.42 g (84% yield). ^{1}H NMR (C_6D_6, 298K) δ(ppm): 3.08 (m, 4H, CH_2), 2.81 (m, 4H, CH_2), 2.52 (d, 12H, *J* = 12 Hz), CH_3). ^{13}C NMR (C_6D_6, 298K) δ(ppm): 52.9 (d, *J* 4.0 Hz, 4C, CH_2), 34.2 (d, *J* 12 Hz, 4C, N*C*H$_3$). ^{31}P NMR (C_6D_6, 298K) δ(ppm): 115.4.

1,3-diphenyl-2,4-di(tert-butyl)cyclodiphosphazane (4)

To a 20mL THF solution of [ClP(μ-N^{t}Bu)]$_2$ (0.550g, 2.0 mmol), phenyl lithium (1.9 M, 1.05 mL, 2.0 mmol) was added dropwise at -78˚C. The reaction mixture is left to stir and gradually warmed to room temperature. The solvent was evaporated under vacuo and the product was extracted with toluene (20 mL) and evaporated. Yield: 0.509g (71 %); ^{1}H NMR (CDC*l*$_3$, 300MHz): δ(ppm) 7.64 - 7.72 (m, 4 H, Ar*H*), 7.34 - 7.40 (m, 6 H, Ar*H*), 1.19 (s, 18H, C(CH_3)$_3$); ^{31}P{^{1}H} NMR (CDC*l*$_3$, 162 MHz): δ(ppm) 155.4. This compound was previously prepared by a different method and the NMR data correspond to those previously reported.[3]

[{Bis(1,3-dimethyl-[1,3,2]-diazaphospholidin-2-yl)propylamine}CrCl$_2$(μ-Cl)]$_2$ [(**1**)CrCl$_3$]$_2$

Bis(1,3-dimethyl-[1,3,2]-diazaphospholidin-2-yl)propylamine (1) (0.320 g, 1.10 mmol) and [CrCl$_3$(THF)$_3$] (0.412 g, 1.1 mmol) were added to dry toluene (40.0 ml, 376 mmol) in a Schlenk tube. The mixture was then left to stir overnight (approximately 18 hours) at 80 °C. The resulting mixture was then filtered and washed with three portions of dry pentane (approximately 15.0 ml for each wash). The dark blue solid was then left to dry under vacuum

(0.183 g, 0.407 mmol, 74.0 % yield). Elemental analysis for $C_{11}H_{27}N_5P_2CrCl_3$: calcd: C 29.38, H 6.052, N 15.57; found: C 28.92, H 6.22, N 14.98. The remaining residue was redissolved in DCM and filtered into a new Schlenk tube and layered using an equal amount of dry pentane. Crystals suitable for X-ray analysis were formed after a period of 2 days.

[{Bis(1,3-dimethyl-[1,3,2]-diazaphospholidin-2-yl)isopropylamine}$CrCl_2$(μ-Cl)]$_2$

[(**2**)$CrCl_3$]$_2$

Bis(1,3-dimethyl-[1,3,2]-diazaphospholidin-2-yl)isopropylamine (**2**) (0.320 g, 1.10 mmol) and [$CrCl_3(THF)_3$] (0.412 g, 1.1 mmol) were added to dry toluene (40.0 ml, 376 mmol) in a Schlenk tube. The mixture was then left to stir overnight (approximately 18 hours) at 80 °C. The resulting mixture was then filtered and washed with three portions of dry pentane (approximately 15.0 ml for each wash). The dark blue solid was then left to dry under vacuum (0.243 g, 0.541 mmol, 98.0 % yield). Elemental analysis for $C_{11}H_{27}N_5P_2CrCl_3$: calcd: C 29.38, H 6.052, N 15.57; found: C 29.10, H 6.20, N 15.05. The remaining residue was redissolved in DCM and filtered into a new Schlenk tube and layered using an equal amount of dry pentane. Crystals suitable for X-ray analysis were formed after a period of 2 days.

General Oligomerisation Procedure

A 300 mL Parr reactor was dried in the oven overnight and cooled to room temperature before each run. The reactor was flushed with a gentle stream of nitrogen for 15 minutes. The ligand (50.0 μmol) and [$CrCl_3(THF)_3$] (0.0187 g, 50.0 μmol) were added to dry toluene (20 ml) in a Schlenk flask. The mixture was left to stir until no further colour change was observed (approximately 10 min.). The reaction was prepared by transferring toluene (100 ml) via cannula into the reactor. This was followed by injecting the required amount of MAO into the reactor (500 equiv.). The mixture of toluene and MAO was left to stir for 30 minutes before the catalyst solution was injected into the reactor. An aliquot of 8 ml containing 20 μmol catalyst was taken from the catalyst solution and injected into the Parr reactor. The reactor was pressurized with ethylene and left to stir at room temperature. After 60 minutes, the reactor was exposed to air, quenched with dilute hydrochloric acid (2M). The organic phase was separated and analysed by GC using n-nonane as the standard.

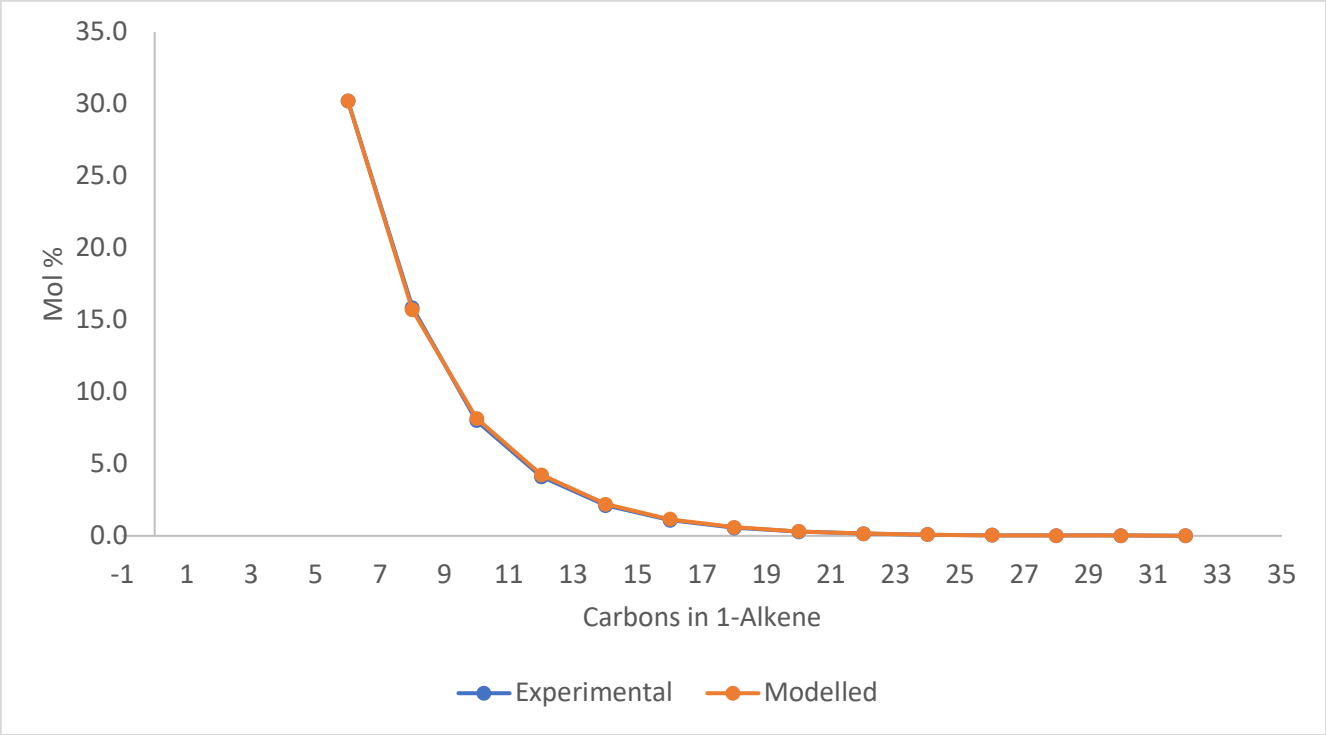


Figure S1. Oligomer distribution obtained with catalyst system **4**/Cr (run 8, Table 1) Conditions: Catalyst prepared *in situ* from 20 μmol PNP ligand **4** and 20 μmol $[CrCl_3(THF)_3]$; MAO 500 equiv.; 100 ml toluene; 60 min. $\alpha = 0.52$.

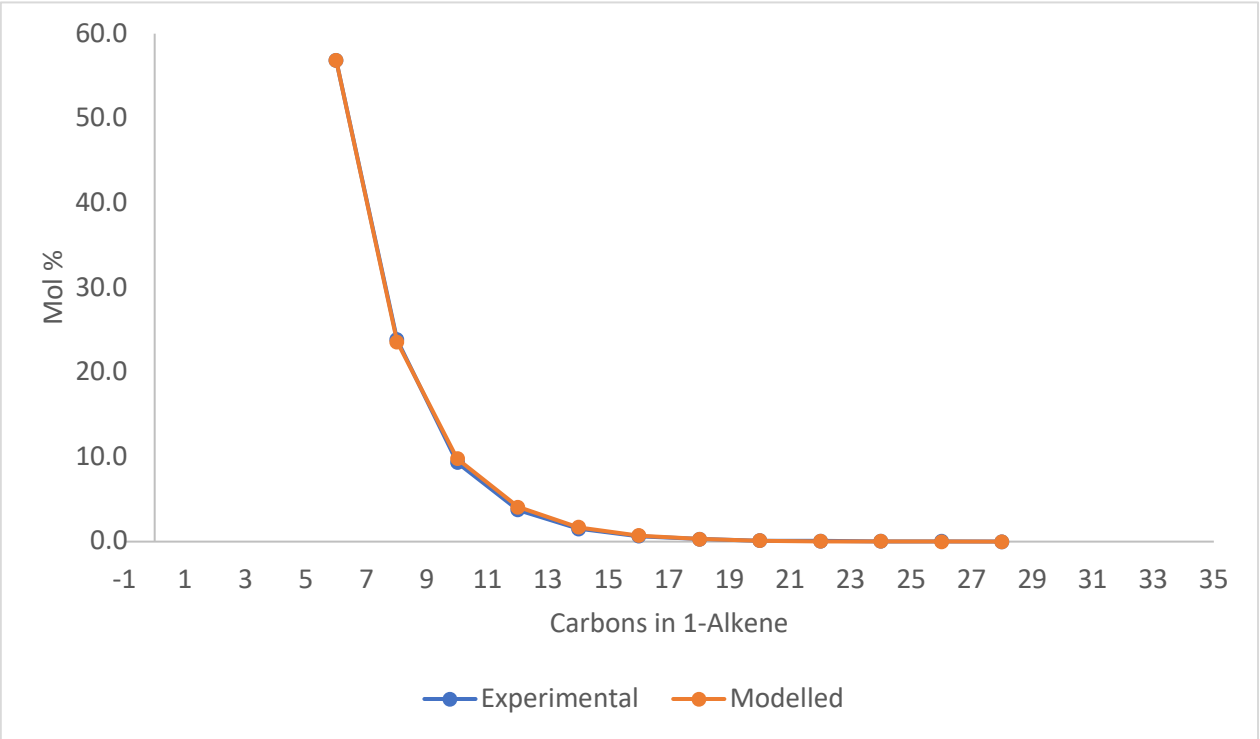


Figure S2. Oligomer distribution obtained with catalyst system **4**/Cr (run 9, Table 1) Conditions: Catalyst prepared *in situ* from 5 μmol PNP ligand **4** and 5 μmol $[CrCl_3(THF)_3]$; MAO 500 equiv.; 100 ml toluene; 60 min. $\alpha = 0.42$.

X-Ray Analysis

The X-ray crystal structure of [(**1**)$CrCl_3$]$_2$

Crystal data for [(**1**)$CrCl_3$]$_2$: $C_{22}H_{54}Cl_6Cr_2N_{10}P_4 \cdot 2(CH_2Cl_2)$, M = 1069.18, monoclinic, $P2_1/c$ (no. 14), a = 11.9522(3), b = 13.5271(4), c = 14.8191(5) Å, β = 104.592(3)°, V = 2318.65(12) Å^3, Z = 2 [C_i symmetry], D_c = 1.531 g cm^{-3}, μ(Mo-Kα) = 1.215 mm^{-1}, T = 173 K, dark blue blocks, Agilent Xcalibur 3 E diffractometer; 4651 independent measured reflections (R_{int} = 0.0281), F^2 refinement,[4,5] R_1(obs) = 0.0410, wR_2(all) = 0.1015, 3858 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$, completeness to θ_{full}(25.2°) = 98.8%], 258 parameters. CCDC 2108180.

The structure of [(**1**)$CrCl_3$]$_2$ was found to sit across a centre of symmetry at the middle of the Cr_2Cl_2 ring. The C20-based included dichloromethane solvent molecule was found to be disordered, and three orientations were identified of *ca*. 69, 17 and 14% occupancy. The geometries of all three orientations were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientation were refined anisotropically (those of the minor occupancy orientations were refined isotropically).

The X-ray crystal structure of [(**2**)$CrCl_3$]$_2$

Crystal data for [(**2**)$CrCl_3$]$_2$: $C_{22}H_{54}Cl_6Cr_2N_{10}P_4 \cdot 2(CH_2Cl_2)$, M = 1069.18, monoclinic, $P2_1/c$ (no. 14), a = 9.3625(3), b = 12.7925(3), c = 19.2108(5) Å, β = 96.406(3)°, V = 2286.52(11) Å^3, Z = 2 [C_i symmetry], D_c = 1.553 g cm^{-3}, μ(Mo-Kα) = 1.232 mm^{-1}, T = 173 K, dark blue blocks, Agilent Xcalibur 3 E diffractometer; 4609 independent measured reflections (R_{int} = 0.0214), F^2 refinement,[4,5] R_1(obs) = 0.0467, wR_2(all) = 0.1121, 3857 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$, completeness to θ_{full}(25.2°) = 99.0%], 284 parameters. CCDC 2108181.

The structure of [(**2**)$CrCl_3$]$_2$ was found to sit across a centre of symmetry at the middle of the Cr_2Cl_2 ring. The C10-based isopropyl group and the C20-based included dichloromethane solvent were both found to be disordered. For the former two orientations were identified of *ca*. 74 and 26% occupancy, whilst for the latter four orientations were identified of *ca*. 62, 19, 11 and 8% occupancy. In each case the geometries of each set of orientations were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientations were refined anisotropically (those of the minor occupancy orientations were refined isotropically).

The X-ray crystal structure of $[Li(OEt_2)]_4[\{Cr(C_4H_8)_2\}_2]$ (**6**)

Crystal data for **6**: $C_{32}H_{72}Cr_2Li_4O_4$, M = 652.65, orthorhombic, *Pccn* (no. 56), a = 9.9307(3), b = 17.6625(6), c = 22.0161(10) Å, V = 3861.7(3) Å^3, Z = 4 [C_2 symmetry], D_c = 1.123 g cm^{-3}, μ(Mo-Kα) = 0.592 mm^{-1}, T = 173 K, brown blocks, Agilent Xcalibur 3 E diffractometer; 3948 independent measured reflections (R_{int} = 0.0269), F^2 refinement,[4,5] R_1(obs) = 0.0619, wR_2(all) = 0.1775, 2610 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$, completeness to θ_{full}(25.2°) = 99.1%], 250 parameters. CCDC 2115885.

The structure of **6** was found to sit across a C_2 axis that bisects the Li1···Li1A, Cr1···Cr1A and Li2···Li2A vectors. The C1/C4 and C5/C8 butyl groups, and the O10- and O20-based coordinated diethylether solvent molecules were all found to be disordered, and in each case two orientations were identified of *ca*. 64:36, 83:17, 69:31 and 56:44% occupancy respectively. In each case the geometries of each pair of orientations were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientations were refined anisotropically (those of the minor occupancy orientations were refined isotropically). (This extensive disorder persists when the structure is solved and refined at lower symmetries.) This structure was originally reported in 1971 [CSD refcode TMCRLI], though that study was at room temperature and gave a poorer quality result with a final *R*-factor greater than 15%.[6]

Figures

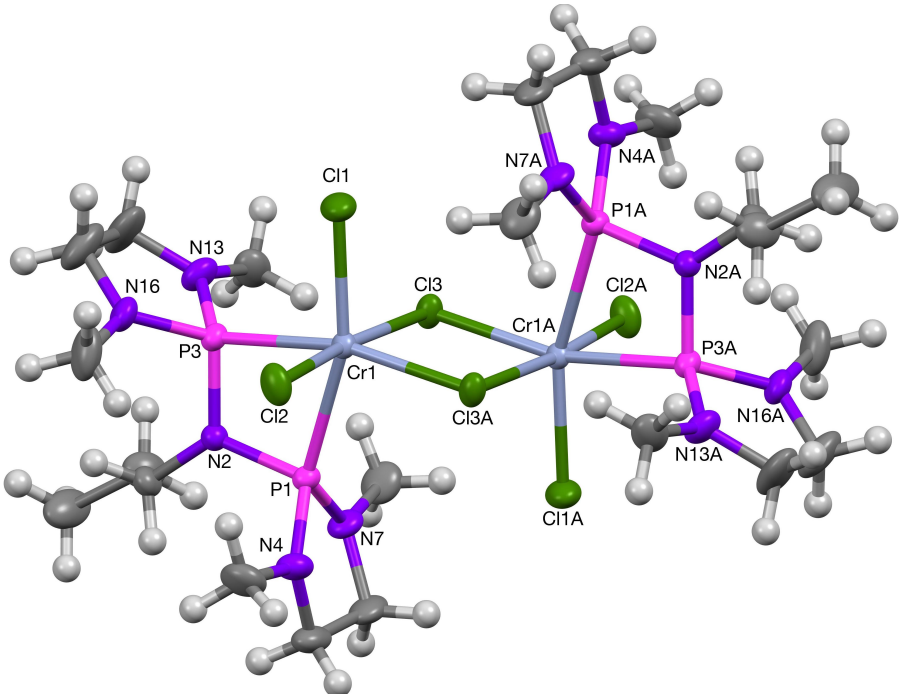


Figure S3. The crystal structure of the C_i-symmetric complex [(**1**)$CrCl_3$]$_2$ (50% probability ellipsoids).

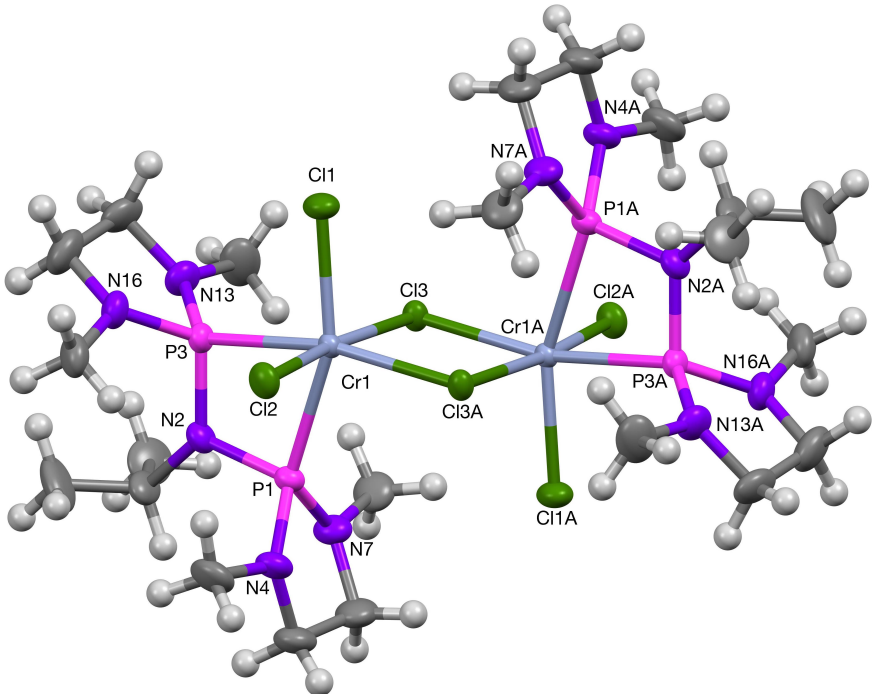


Figure S4. The crystal structure of the C_i-symmetric complex [(**2**)$CrCl_3$]$_2$ (50% probability ellipsoids).

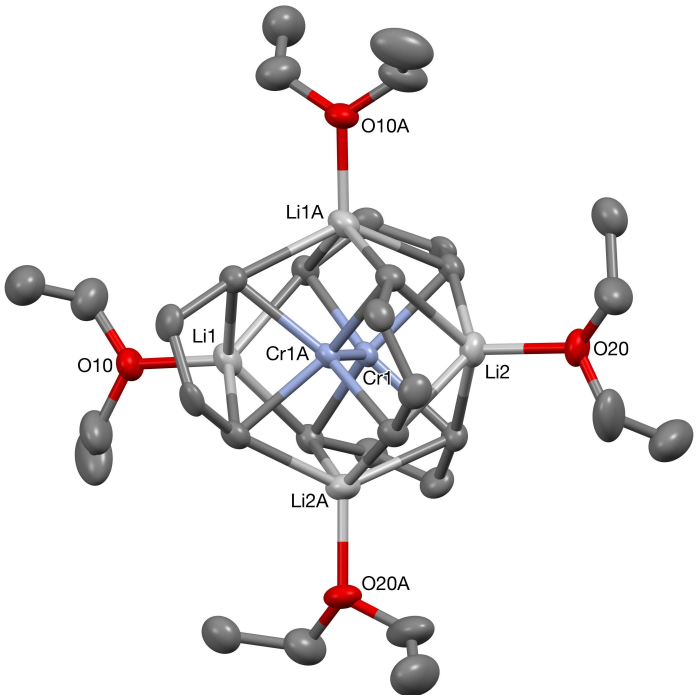


Figure S5. The crystal structure of the C_2-symmetric complex **6** (30% probability ellipsoids).

Additional Spectra

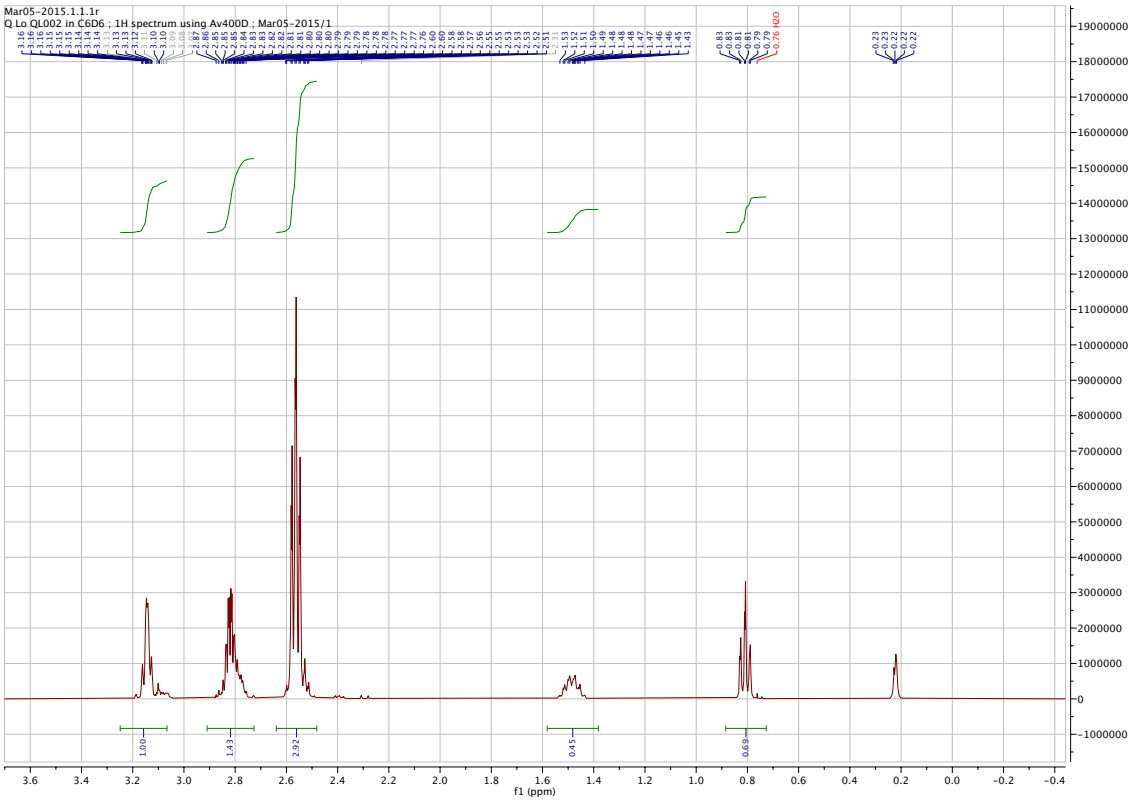


Figure S6. ^{1}H NMR spectrum of **1** in C_6D_6 at 298K (δ = 0.22 ppm: silicon grease).

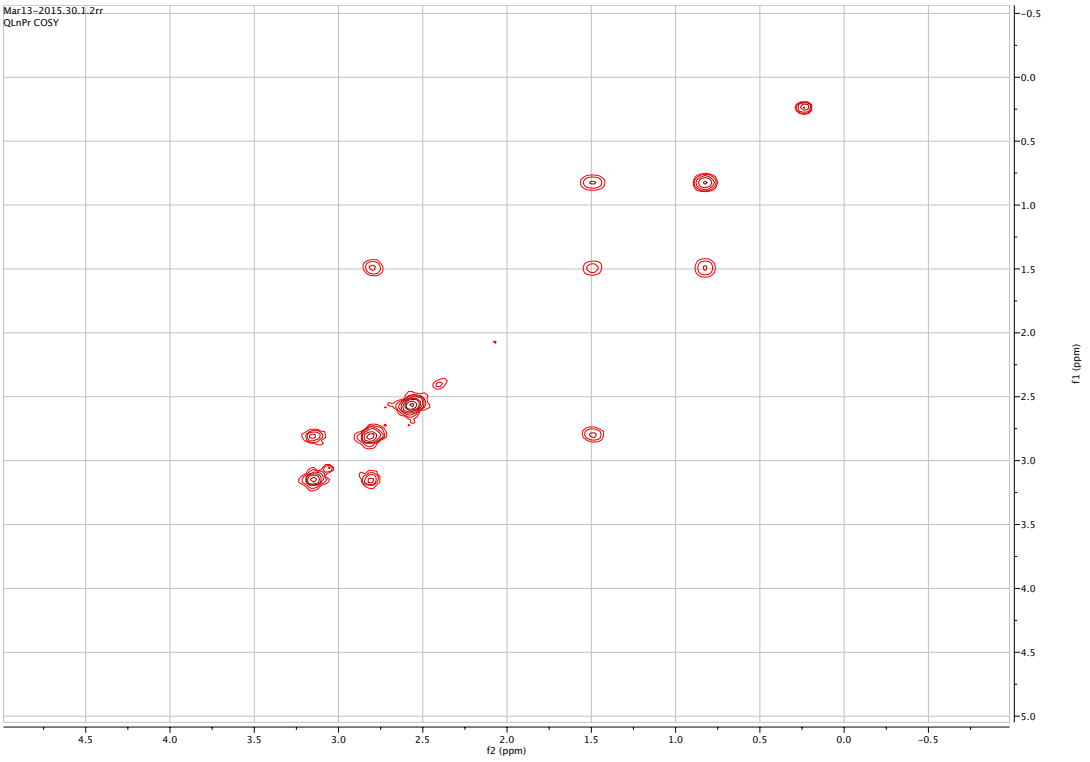


Figure S7. COSY NMR spectrum of **1** in C_6D_6 at 298K (δ = 0.22 ppm: silicon grease).

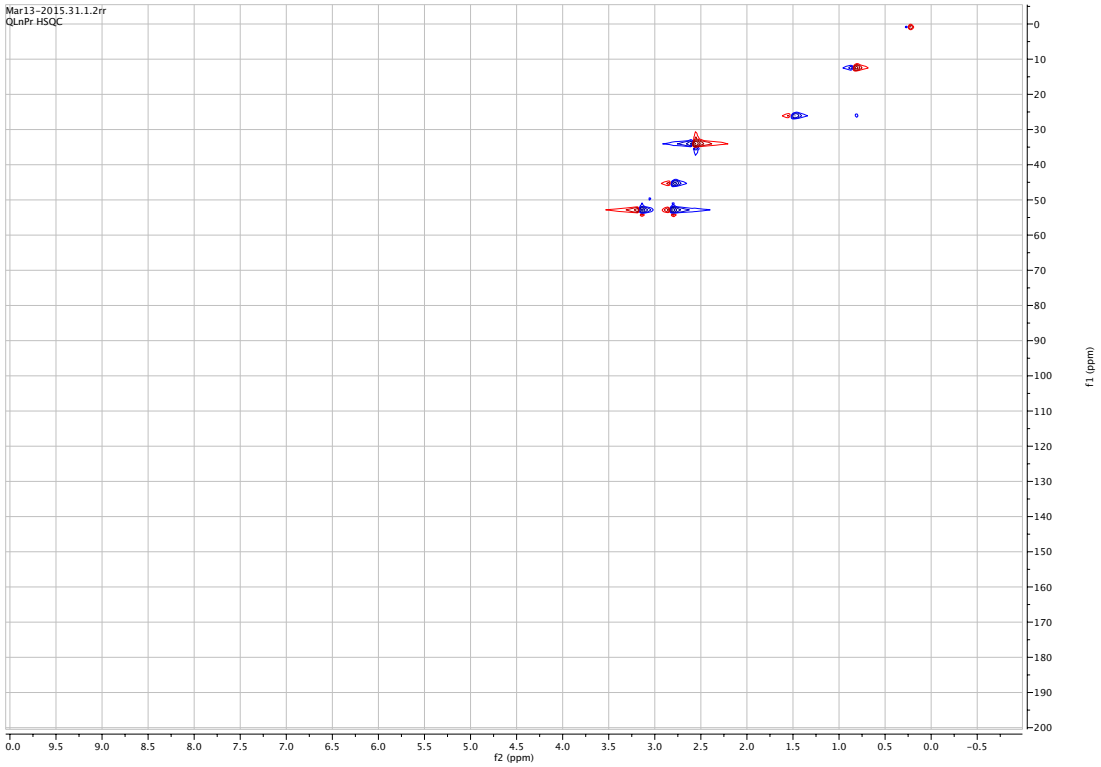


Figure S8. HSQC NMR spectrum of **1** in C_6D_6 at 298K.

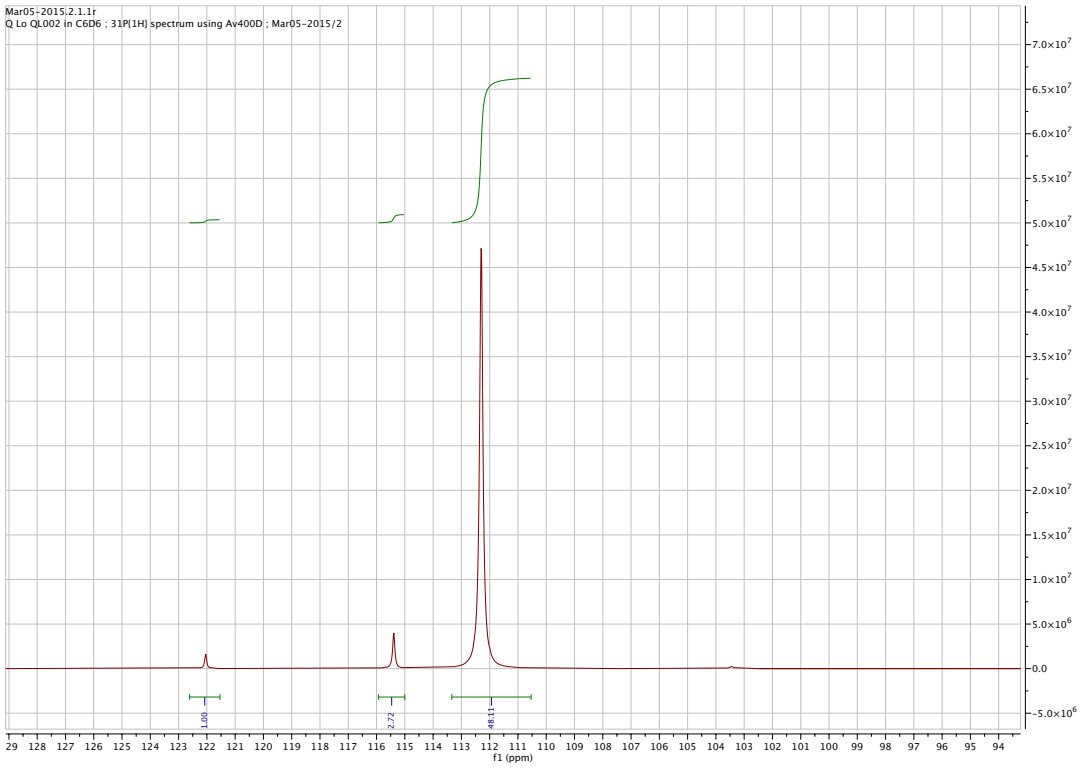


Figure S9. ^{31}P NMR spectrum of **1** in C_6D_6 at 298K (the signal at δ = 115.4 ppm is bis(1,3-dimethyl-1,3,2-diazaphospholane).

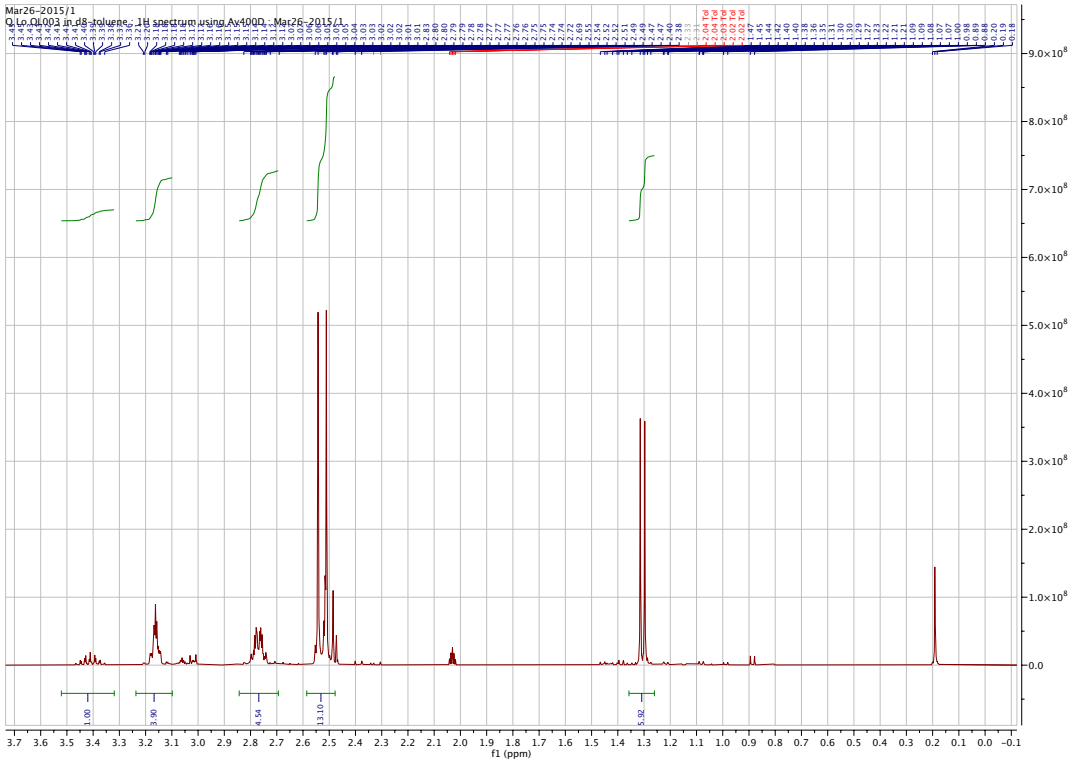


Figure S10. ^{1}H NMR spectrum of **2** in C_7D_8 at 298K (δ = 0.19 ppm: silicon grease).

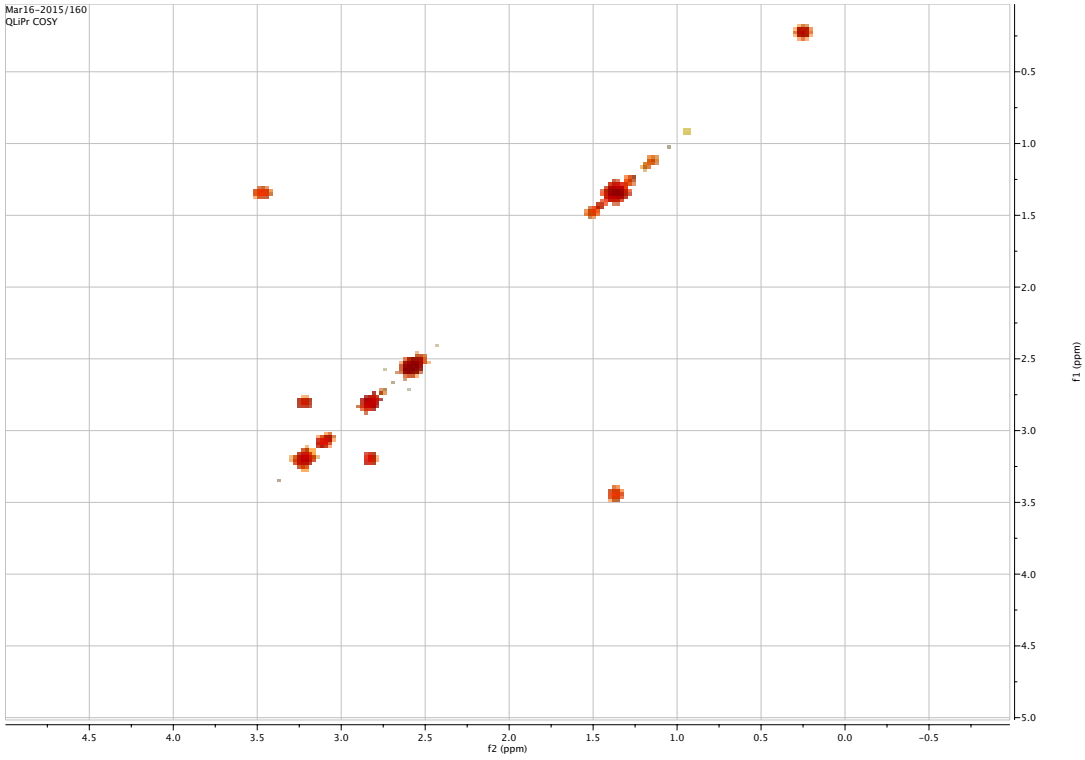


Figure S11. COSY NMR spectrum of **2** in C_7D_8 at 298K (δ = 0.19 ppm: silicon grease).

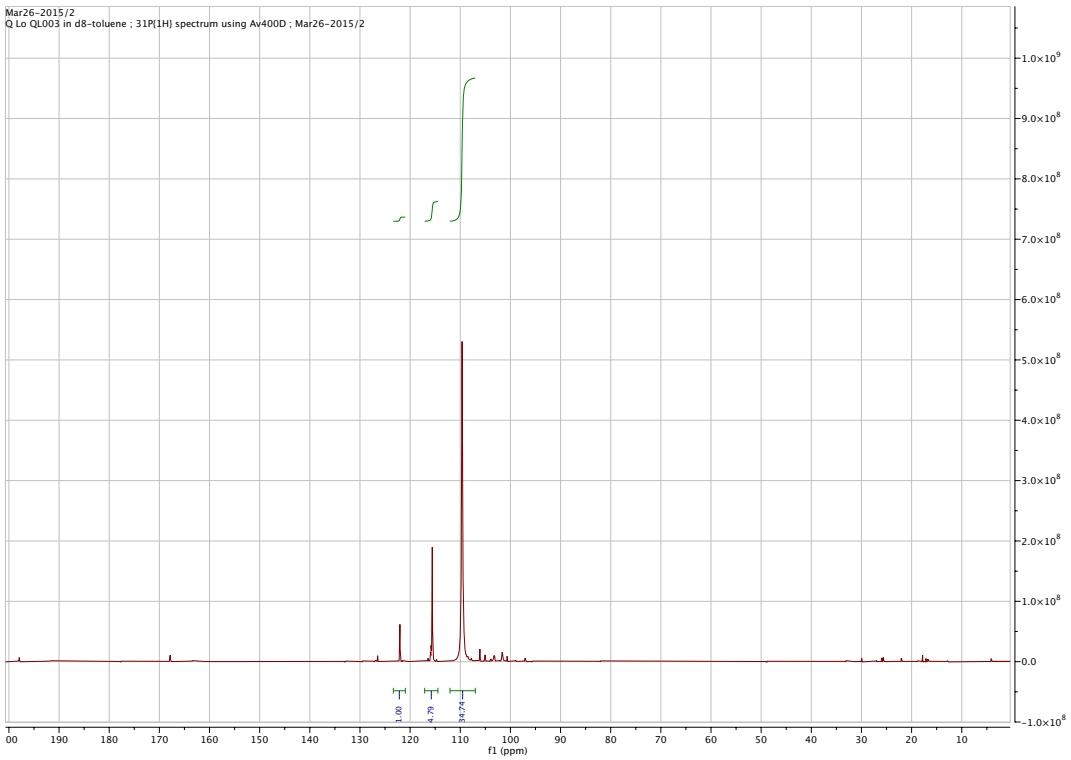


Figure S12. ^{31}P NMR spectrum of **2** in C_7D_8 at 298K (the signal at δ = 115.4 ppm is bis(1,3-dimethyl-1,3,2-diazaphospholane **3**).

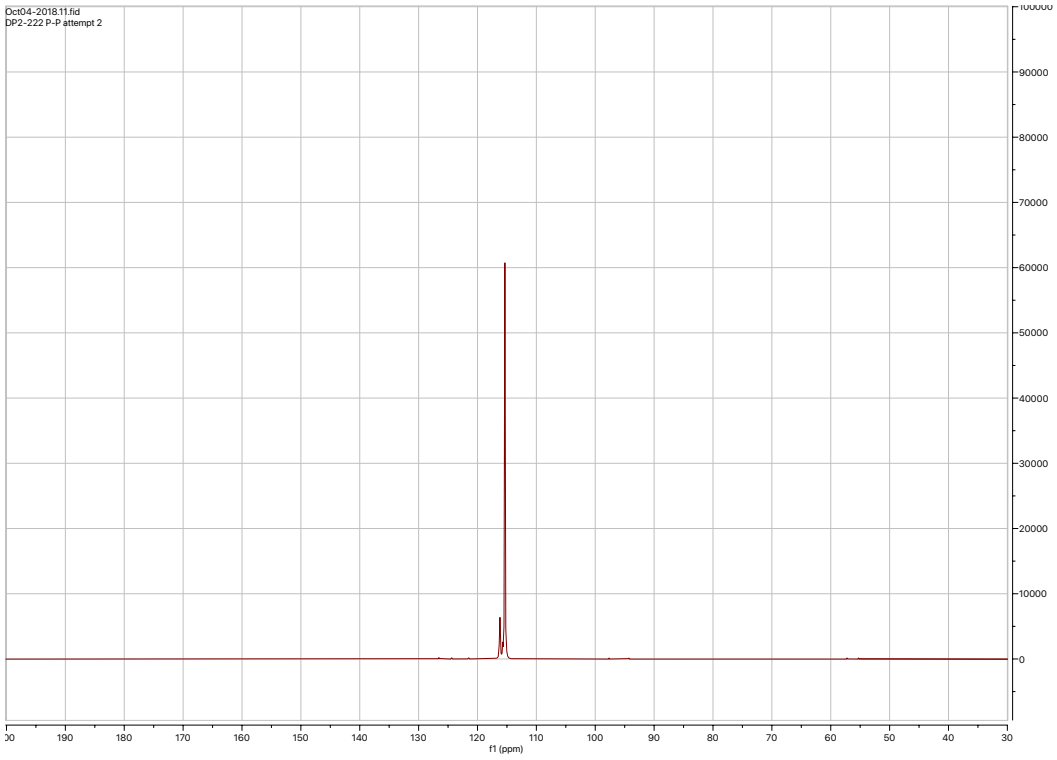
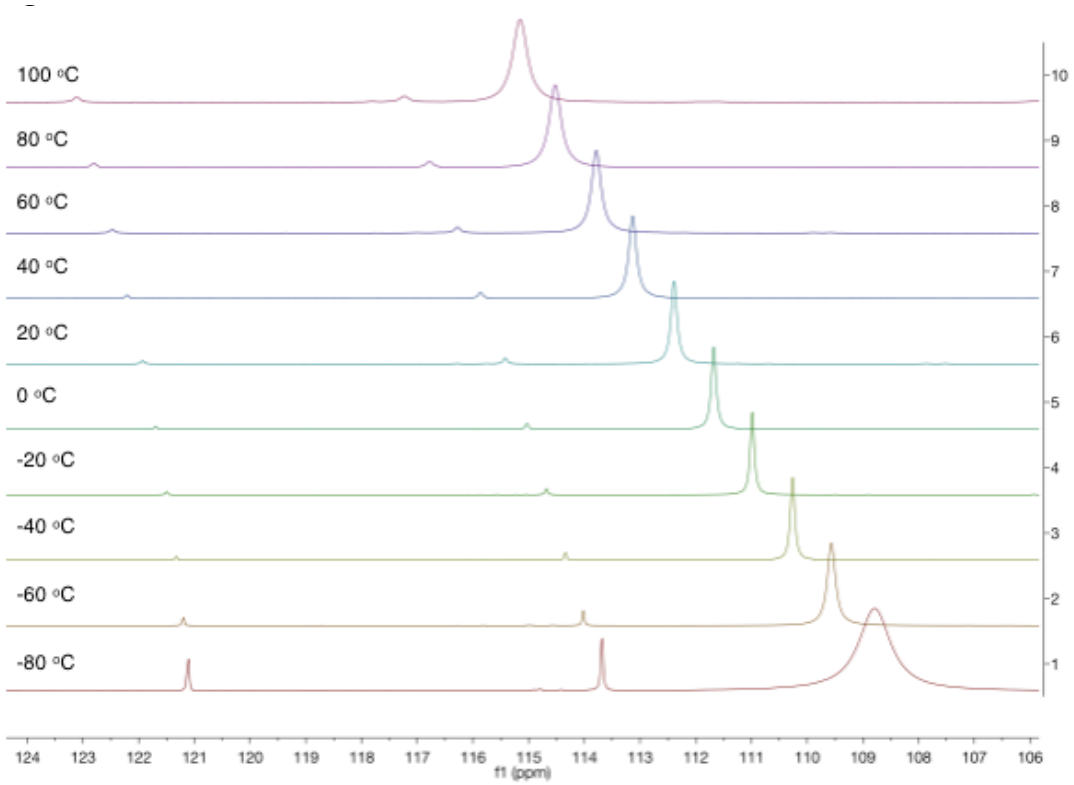
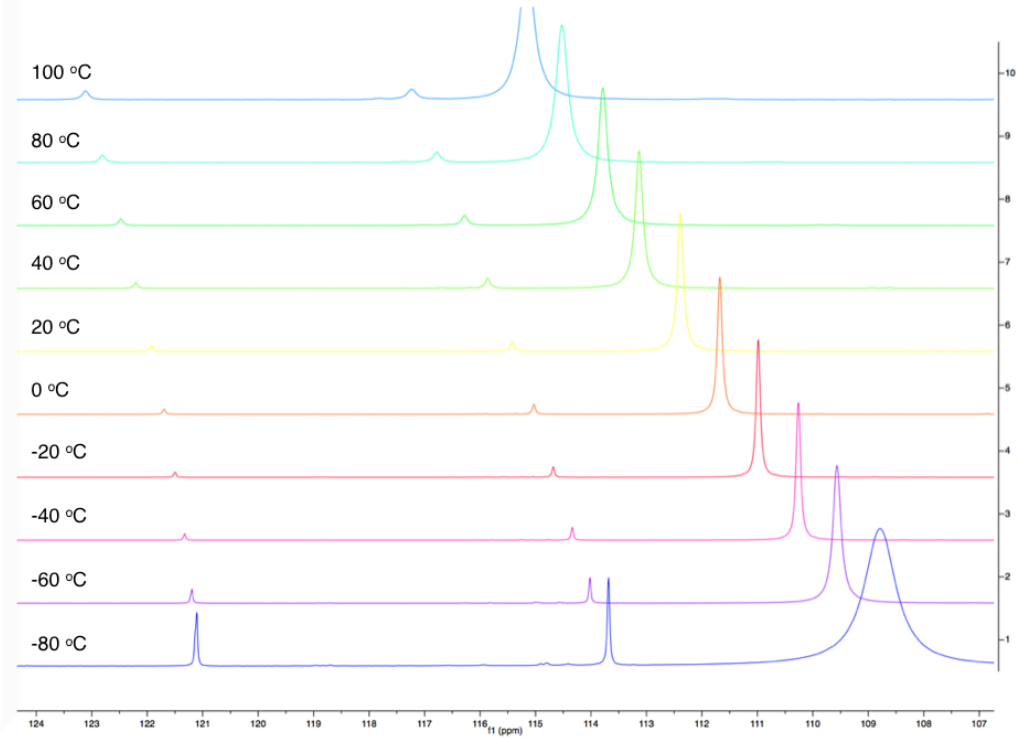


Figure S13. ^{31}P NMR spectrum of bis(1,3-dimethyl-1,3,2-diazaphospholane) **3** in C_6D_6 at 298K.



Figures S14. VT ^{31}P NMR analysis of **1** in C_7D_8 from -80 to +100 ˚C. No change in the integration of the individual peaks was observed.



Figures S15. VT ^{31}P NMR analysis of **2** in C_7D_8 from -80 to +100 ˚C. No change in the integration of the individual peaks was observed.

Computational Details

All calculations were performed using Gaussian 09 (Revision D01)[7] carried out without symmetry constraints using the M06L density functional,[8] combined with the Stuttgart-Dresden (SDD) double-ζ valence basis set.[9] For geometry optimisations, an effective core potential (ECP) was applied on the Cr atoms while the other atoms used the 6-31G(d) basis set (referred to as BS1). Solvation and dispersion effects were included in a polarisable continuum model (PCM, toluene)[10] and with Grimme's empirical dispersion correction (GD3),[11] respectively. The validity of a structure was assessed with analytical frequency calculations that would only display one imaginary frequency if the structure were a transition state and none if the structure was at minimum. Energies were obtained by carrying out a single-point energy calculation on the optimised geometries using an advanced basis set consisting of the quadruple-ζ valence def2-QZVP basis set[12,13] with SDD ECP on the chromium atoms, and the 6-311+G(2d,p) basis set on all other atoms (referred to as BS2). All computational results are listed below as xyz files and are also collected in the repository, accessible via: https://doi.org/10.14469/hpc/10510.

XYZ files:

58
Complex ^{4}I
Cr -1.80822 5.44345 -1.04868
P -1.45149 3.89997 -2.88622
N -2.83428 4.39017 -3.77151
P -3.43581 5.69126 -2.82606
N -1.43507 2.23747 -2.60627
C -0.63356 1.50315 -3.58188
H -0.24061 0.58776 -3.12395
H -1.22804 1.21356 -4.46623
C 0.47048 2.47310 -3.95614
H 0.90841 2.24668 -4.93609
H 1.28235 2.45587 -3.20801
N -0.18145 3.77920 -4.00387
C -2.56231 1.57909 -1.98468
H -3.38769 1.37564 -2.68734
H -2.23944 0.62853 -1.54584
H -2.95065 2.20657 -1.17150
C 0.64578 4.92325 -4.32555
H 1.45694 5.08753 -3.59770
H 1.09684 4.78120 -5.31445
H 0.02871 5.82800 -4.37118
C -3.34739 3.84696 -5.03034

H	-3.00645	2.80469	-5.10771
H	-4.44460	3.81956	-4.95812
C	-2.90331	4.63763	-6.25075
H	-3.25754	5.67499	-6.15327
H	-1.80503	4.68617	-6.25768
C	-3.42293	4.02845	-7.53978
H	-4.51918	3.98983	-7.55001
H	-3.10455	4.60684	-8.41261
H	-3.05708	3.00273	-7.67115
N	-3.56872	7.16706	-3.62693
C	-4.89002	7.37645	-4.21140
H	-5.09395	8.45070	-4.28789
H	-4.96562	6.94082	-5.22414
C	-5.82896	6.68184	-3.24324
H	-6.78076	6.40512	-3.71322
H	-6.05046	7.32904	-2.37667
N	-5.11581	5.47382	-2.83935
C	-2.42078	7.82953	-4.20178
H	-2.15805	7.45458	-5.20506
H	-2.61308	8.90583	-4.27569
H	-1.55134	7.69075	-3.54432
C	-5.76918	4.58500	-1.90200
H	-5.95915	5.05405	-0.92275
H	-6.73030	4.25928	-2.31590
H	-5.15502	3.69029	-1.74800
C	-3.05284	7.11213	-0.36097
H	-2.91242	7.92011	-1.08052
H	-4.08528	6.77503	-0.25160
C	-2.13729	6.90386	0.66117
H	-2.43787	6.40430	1.57865
H	-1.27246	7.55600	0.75888
C	-0.38425	5.09390	0.68992
H	0.25669	5.95261	0.87256
H	-0.94018	4.74619	1.55763
C	-0.11965	4.22594	-0.35984
H	-0.45996	3.19053	-0.32718
H	0.73245	4.40407	-1.01933

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Complex ^{6}I

Cr	-1.77824	5.47383	-1.01601
P	-1.25465	4.05828	-2.96281
N	-2.76014	4.43398	-3.70914
P	-3.60785	5.53453	-2.68149
N	-1.01577	2.38457	-2.84506
C	-0.24193	1.84460	-3.96160
H	0.29747	0.94654	-3.63753
H	-0.89014	1.56235	-4.81050
C	0.69923	2.97030	-4.34141
H	1.06025	2.87791	-5.37349

H	1.57926	2.98823	-3.67477
N	-0.09733	4.18501	-4.20671
C	-2.02476	1.53700	-2.24771
H	-2.86060	1.31268	-2.93214
H	-1.57297	0.58912	-1.93469
H	-2.43666	2.02244	-1.35379
C	0.58174	5.44527	-4.42748
H	1.40109	5.62620	-3.71119
H	0.99938	5.46387	-5.44077
H	-0.13625	6.27072	-4.35026
C	-3.23767	3.87965	-4.98039
H	-2.75072	2.90437	-5.12479
H	-4.31528	3.68316	-4.87420
C	-2.96603	4.77496	-6.17850
H	-3.46659	5.74245	-6.02434
H	-1.88884	4.98827	-6.22301
C	-3.44336	4.14424	-7.47366
H	-4.52073	3.93848	-7.44458
H	-3.25463	4.79704	-8.33175
H	-2.93273	3.19200	-7.66388
N	-4.08616	6.97090	-3.43814
C	-5.41865	6.87799	-4.02769
H	-5.86842	7.87625	-4.08352
H	-5.38644	6.46271	-5.05204
C	-6.17219	5.96073	-3.08492
H	-7.03647	5.48752	-3.56812
H	-6.53690	6.51833	-2.20451
N	-5.20293	4.93886	-2.70517
C	-3.13068	7.87380	-4.03930
H	-2.86678	7.59682	-5.07353
H	-3.53798	8.89143	-4.04994
H	-2.20811	7.88546	-3.44578
C	-5.62554	3.95631	-1.72939
H	-5.85689	4.39628	-0.74448
H	-6.52122	3.44069	-2.09394
H	-4.84002	3.20281	-1.59811
C	-0.27243	7.29164	-0.75368
H	0.57690	6.84386	-0.23886
H	-0.09736	7.61098	-1.78069
C	-1.42375	7.60629	-0.09576
H	-2.20903	8.19517	-0.57017
H	-1.52995	7.43328	0.97503
C	-1.11307	4.32341	0.92546
H	-0.63912	3.43380	0.51025
H	-0.45409	5.03675	1.41990
C	-2.46796	4.43524	1.00754
H	-2.94368	5.24680	1.55699
H	-3.12707	3.64202	0.65670

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Transition Structure TSI-II

Cr	-1.84726	5.40283	-1.11463
P	-1.49238	3.84802	-2.93275
N	-2.86894	4.34514	-3.82813
P	-3.49423	5.63225	-2.87454
N	-1.46216	2.18922	-2.64656
C	-0.62286	1.46277	-3.59608
H	-0.22414	0.55918	-3.12015
H	-1.18908	1.15508	-4.49248
C	0.47090	2.45169	-3.94832
H	0.94808	2.22233	-4.90892
H	1.25481	2.46395	-3.17074
N	-0.20794	3.74257	-4.03729
C	-2.58664	1.51198	-2.04085
H	-3.39397	1.28749	-2.75780
H	-2.25190	0.57048	-1.59173
H	-3.00232	2.13463	-1.23826
C	0.62111	4.89962	-4.30974
H	1.37852	5.07863	-3.52921
H	1.13783	4.75886	-5.26581
H	-0.00592	5.79392	-4.40191
C	-3.35557	3.83105	-5.11005
H	-2.98793	2.80102	-5.21906
H	-4.45255	3.77557	-5.05299
C	-2.91582	4.67383	-6.29691
H	-3.29764	5.69796	-6.16905
H	-1.81902	4.74962	-6.28662
C	-3.40185	4.09758	-7.61386
H	-4.49643	4.03146	-7.64178
H	-3.08656	4.71480	-8.46090
H	-3.00738	3.08702	-7.77590
N	-3.62713	7.11736	-3.65231
C	-4.95200	7.34517	-4.22001
H	-5.15413	8.42151	-4.26590
H	-5.03804	6.93664	-5.24301
C	-5.88295	6.62808	-3.26069
H	-6.84299	6.37106	-3.72476
H	-6.08662	7.25093	-2.37202
N	-5.17370	5.40315	-2.89998
C	-2.48104	7.80817	-4.19535
H	-2.21549	7.47754	-5.21320
H	-2.67664	8.88618	-4.22277
H	-1.61198	7.64368	-3.54315
C	-5.81517	4.52078	-1.94649
H	-5.95993	4.98734	-0.95844
H	-6.79624	4.22108	-2.33154
H	-5.21718	3.61099	-1.82071
C	-2.78008	7.01970	-0.30462
H	-2.78354	7.85673	-1.00601
H	-3.76492	6.83458	0.13449

C	-1.62872	6.90014	0.58326
H	-1.84539	6.95710	1.64943
H	-0.80219	7.56859	0.32846
C	-0.70311	5.27926	0.84504
H	0.09515	5.81257	1.35979
H	-1.35355	4.78161	1.56919
C	-0.28283	4.42188	-0.25842
H	-0.49309	3.35402	-0.16782
H	0.70131	4.62179	-0.69298

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Complex II

Cr	-1.86092	5.39798	-1.11280
P	-1.48879	3.84226	-2.95275
N	-2.87286	4.34397	-3.83464
P	-3.52285	5.62273	-2.88590
N	-1.44772	2.18200	-2.68498
C	-0.61887	1.46929	-3.65403
H	-0.21173	0.56123	-3.19427
H	-1.19596	1.17065	-4.54660
C	0.46792	2.46528	-4.00846
H	0.93268	2.24939	-4.97835
H	1.26200	2.46948	-3.24144
N	-0.21418	3.75620	-4.07231
C	-2.55555	1.49310	-2.06232
H	-3.36679	1.25365	-2.76984
H	-2.20323	0.55927	-1.61050
H	-2.97059	2.11635	-1.26020
C	0.61529	4.91961	-4.31741
H	1.36226	5.08894	-3.52436
H	1.14441	4.79394	-5.26854
H	-0.01321	5.81337	-4.40476
C	-3.35202	3.83283	-5.12147
H	-2.98353	2.80302	-5.23059
H	-4.44918	3.77673	-5.06981
C	-2.90619	4.67836	-6.30407
H	-3.28939	5.70200	-6.17646
H	-1.80963	4.75493	-6.28775
C	-3.38484	4.10441	-7.62474
H	-4.47921	4.03734	-7.65863
H	-3.06563	4.72367	-8.46882
H	-2.98861	3.09454	-7.78681
N	-3.66287	7.10711	-3.66279
C	-4.98329	7.32027	-4.24674
H	-5.19850	8.39411	-4.29112
H	-5.05028	6.91523	-5.27250
C	-5.91813	6.58820	-3.30258
H	-6.86805	6.31988	-3.78085
H	-6.14219	7.20560	-2.41536
N	-5.19914	5.37097	-2.93393

C	-2.51927	7.81605	-4.18756
H	-2.24285	7.49967	-5.20705
H	-2.72547	8.89225	-4.20423
H	-1.65364	7.65243	-3.53073
C	-5.83671	4.49279	-1.97312
H	-5.98663	4.96953	-0.99061
H	-6.81434	4.18191	-2.35783
H	-5.23172	3.58926	-1.83662
C	-2.62984	6.97815	-0.16117
H	-2.78179	7.90298	-0.72482
H	-3.48727	6.77646	0.49369
C	-1.29374	6.89361	0.56751
H	-1.30810	7.50039	1.48058
H	-0.48289	7.31495	-0.05180
C	-0.86247	5.43470	1.04679
H	-0.03257	5.60005	1.74402
H	-1.69023	5.02088	1.63962
C	-0.44254	4.46851	-0.05684
H	-0.61806	3.41212	0.16819
H	0.59306	4.61856	-0.38704

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Complex ^{4}III

Cr	-1.82014	5.53841	-0.99554
P	-1.51140	3.90552	-2.77879
N	-2.82085	4.53057	-3.71011
P	-3.46577	5.82621	-2.78692
N	-1.66303	2.25946	-2.41521
C	-0.97406	1.39407	-3.36887
H	-0.66907	0.46597	-2.87107
H	-1.62238	1.12559	-4.22151
C	0.21378	2.21963	-3.82065
H	0.59878	1.89625	-4.79566
H	1.04018	2.15572	-3.09067
N	-0.30375	3.57922	-3.92999
C	-2.83154	1.74016	-1.74058
H	-3.67671	1.55755	-2.42601
H	-2.58316	0.79430	-1.24547
H	-3.15847	2.44791	-0.96752
C	0.61376	4.60822	-4.37250
H	1.42271	4.80960	-3.65155
H	1.06662	4.30056	-5.32188
H	0.06615	5.54021	-4.55407
C	-3.35898	3.96104	-4.95021
N	-3.69638	7.29800	-3.58689
C	-5.04380	7.43258	-4.14055
H	-5.30311	8.49531	-4.20704
H	-5.10543	7.00119	-5.15627
C	-5.93060	6.67935	-3.17093
H	-6.85495	6.32816	-3.64636

H	-6.20851	7.30674	-2.30721
N	-5.12884	5.53437	-2.76578
C	-2.63753	8.00564	-4.27520
H	-2.43710	7.60199	-5.28134
H	-2.91810	9.05945	-4.37963
H	-1.71260	7.96723	-3.69473
C	-5.76530	4.45774	-2.04605
H	-6.20901	4.78610	-1.09357
H	-6.56322	4.02030	-2.66035
H	-5.03547	3.66800	-1.83628
C	-3.36767	5.29796	0.46811
H	-4.29458	4.98829	-0.01186
H	-3.00617	4.60811	1.23343
C	-3.02145	6.65308	0.51655
H	-2.40915	7.05542	1.32064
H	-3.63500	7.39591	0.00601
C	-0.23902	5.14707	0.91919
H	0.52746	5.90356	0.76204
H	-0.91774	5.31394	1.75340
C	-0.26479	4.00684	0.20052
H	-0.96606	3.20148	0.41692
H	0.48506	3.80020	-0.56351
C	-2.96572	4.74167	-6.19267
H	-3.33466	5.77435	-6.09872
H	-1.86932	4.80943	-6.23505
H	-2.99596	2.92625	-5.02466
C	-0.99623	7.60854	-0.93130
H	-1.73432	8.30620	-1.32748
H	-0.63054	7.85846	0.06241
C	-0.25050	6.79791	-1.79252
H	0.70514	6.38117	-1.46798
H	-0.33376	6.90757	-2.87193
H	-4.45425	3.90871	-4.85328
C	-3.51286	4.10763	-7.45822
H	-3.23318	4.68197	-8.34681
H	-3.13101	3.08781	-7.58967
H	-4.60798	4.04777	-7.43373

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Complex ^{6}III

Cr	-1.86127	5.92527	-1.09183
P	-1.68805	4.08006	-2.74877
N	-3.04256	4.58511	-3.66743
P	-3.75119	5.99469	-2.93272
N	-1.79601	2.42365	-2.37553
C	-1.05699	1.58419	-3.31692
H	-0.73320	0.66257	-2.81814
H	-1.67986	1.29927	-4.18428
C	0.11422	2.44302	-3.74798
H	0.53082	2.12119	-4.71105

H	0.92605	2.40522	-2.99935
N	-0.43955	3.78534	-3.87458
C	-3.01979	1.88144	-1.82565
H	-3.79003	1.69196	-2.59305
H	-2.80949	0.93730	-1.31014
H	-3.43800	2.57906	-1.09097
C	0.47330	4.84952	-4.23194
H	1.24669	5.03893	-3.46685
H	0.97715	4.59879	-5.17253
H	-0.08808	5.77766	-4.39707
C	-3.53746	3.89134	-4.86180
N	-3.88713	7.31114	-3.99910
C	-5.13852	7.30751	-4.75009
H	-5.39380	8.33073	-5.05081
H	-5.06888	6.69299	-5.66735
C	-6.14368	6.72718	-3.77562
H	-7.02367	6.31210	-4.28419
H	-6.49313	7.50020	-3.06841
N	-5.42119	5.65986	-3.09512
C	-2.72334	7.90756	-4.61247
H	-2.39273	7.37877	-5.52284
H	-2.93490	8.94938	-4.88084
H	-1.88912	7.90742	-3.89894
C	-6.11771	4.94106	-2.05118
H	-6.34071	5.55882	-1.16393
H	-7.06552	4.55398	-2.44261
H	-5.51891	4.07724	-1.73569
C	-3.11577	4.77146	0.64383
H	-4.06467	4.54077	0.16068
H	-2.45204	3.93093	0.84745
C	-2.85107	6.01637	1.10822
H	-1.96458	6.21967	1.70892
H	-3.57080	6.82853	1.00844
C	0.52015	4.57568	1.24197
H	1.16067	5.43775	1.42583
H	-0.05904	4.21793	2.09254
C	0.45937	3.98210	0.05006
H	-0.16444	3.10738	-0.13819
H	1.05934	4.32547	-0.79410
C	-2.99981	4.45496	-6.16719
H	-3.26077	5.52165	-6.23152
H	-1.90206	4.40666	-6.14809
H	-3.26458	2.82918	-4.77495
C	-0.95553	8.05444	-0.67585
H	-1.68105	8.70101	-1.17105
H	-0.92487	8.10459	0.41160
C	-0.00041	7.38517	-1.37840
H	0.81485	6.86390	-0.87814
H	0.07596	7.47073	-2.46190
H	-4.63650	3.93877	-4.83774

C	-3.55170	3.71280	-7.37048
H	-3.16336	4.12205	-8.30852
H	-3.28594	2.64872	-7.33891
H	-4.64663	3.77546	-7.40987

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Transition Structure TSIII-IV

Cr	-1.85798	5.51806	-1.02255
P	-1.44475	3.92150	-2.82681
N	-2.79463	4.45960	-3.74169
P	-3.54199	5.65612	-2.76394
N	-1.48978	2.24931	-2.53167
C	-0.70381	1.48198	-3.49666
H	-0.33625	0.56229	-3.02638
H	-1.31202	1.19669	-4.37319
C	0.42181	2.41484	-3.89386
H	0.84293	2.15924	-4.87397
H	1.24178	2.38877	-3.15557
N	-0.20039	3.73162	-3.96341
C	-2.69993	1.63459	-2.02759
H	-3.45549	1.47150	-2.81478
H	-2.46218	0.66705	-1.57090
H	-3.14279	2.27196	-1.25240
C	0.61493	4.83626	-4.42120
H	1.44608	5.07419	-3.73976
H	1.03367	4.58719	-5.40341
H	-0.00549	5.73111	-4.54179
C	-3.27355	3.89056	-5.00468
N	-3.88361	7.11613	-3.53471
C	-5.24078	7.16696	-4.07278
H	-5.57885	8.20827	-4.12240
H	-5.28920	6.74332	-5.09235
C	-6.05493	6.34356	-3.09512
H	-6.97786	5.95753	-3.54557
H	-6.33101	6.94255	-2.20931
N	-5.18383	5.23168	-2.73130
C	-2.86111	7.92386	-4.16197
H	-2.64219	7.61155	-5.19616
H	-3.17975	8.97239	-4.17924
H	-1.93446	7.86306	-3.58082
C	-5.69692	4.27250	-1.77617
H	-5.97877	4.73407	-0.81612
H	-6.58081	3.77451	-2.19171
H	-4.94147	3.50411	-1.57958
C	-3.23364	6.21777	0.31762
H	-4.26601	6.23879	-0.03648
H	-3.14539	5.77440	1.31289
C	-2.45370	7.43358	0.07658
H	-2.11016	7.95981	0.96710
H	-2.93480	8.12650	-0.61688

C	-0.56170	4.62878	0.80978
H	0.45319	4.60489	0.41587
H	-0.78637	5.41248	1.53352
C	-1.44318	3.63562	0.54778
H	-2.41618	3.58929	1.03373
H	-1.16490	2.79349	-0.08426
C	-2.96155	4.75537	-6.21404
H	-3.43623	5.73961	-6.08374
H	-1.87799	4.93864	-6.24803
H	-2.80713	2.90206	-5.12062
C	-0.67645	7.46888	-0.63365
H	-0.81014	8.50680	-0.93770
H	-0.10354	7.41013	0.29299
C	-0.21493	6.56752	-1.68155
H	0.70021	6.00669	-1.47748
H	-0.23498	6.96108	-2.69928
H	-4.35745	3.72519	-4.90979
C	-3.43677	4.11482	-7.50516
H	-3.21693	4.74728	-8.37083
H	-2.94982	3.14596	-7.67093
H	-4.51955	3.93973	-7.48904

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Complex IV

Cr	-2.00498	5.26414	-0.89623
P	-1.42023	3.73157	-2.89404
N	-2.80449	4.33638	-3.74354
P	-3.48545	5.59290	-2.79915
N	-1.47437	2.04295	-2.75737
C	-0.75387	1.36297	-3.83383
H	-0.38773	0.39279	-3.47779
H	-1.40411	1.17803	-4.70708
C	0.37888	2.30869	-4.18017
H	0.75349	2.14998	-5.19923
H	1.22617	2.18128	-3.48447
N	-0.19890	3.64479	-4.07360
C	-2.64579	1.39109	-2.21283
H	-3.47082	1.30731	-2.94049
H	-2.38458	0.38386	-1.86965
H	-3.01410	1.95246	-1.34440
C	0.69091	4.76760	-4.29449
H	1.53422	4.79202	-3.58597
H	1.09543	4.71939	-5.31211
H	0.13463	5.70717	-4.20021
C	-3.31554	3.81798	-5.01896
N	-3.77884	7.04133	-3.59590
C	-5.17162	7.18957	-4.01622
H	-5.44155	8.25180	-4.02121
H	-5.32245	6.79322	-5.03633
C	-5.96633	6.40268	-2.99317

H	-6.94034	6.08187	-3.38257
H	-6.14166	7.00319	-2.08374
N	-5.14138	5.23364	-2.70792
C	-2.77727	7.81770	-4.29340
H	-2.78086	7.62040	-5.37664
H	-2.95636	8.88803	-4.13545
H	-1.77961	7.58485	-3.90879
C	-5.61334	4.31371	-1.69284
H	-5.72059	4.78174	-0.70061
H	-6.58595	3.90524	-1.98881
H	-4.91478	3.47104	-1.61071
C	-3.07110	6.63562	0.21266
H	-4.15996	6.63006	0.04534
H	-2.91337	6.41432	1.28266
C	-2.44055	7.97758	-0.15635
H	-2.71568	8.78122	0.54536
H	-2.81103	8.29581	-1.14539
C	-0.56400	4.68707	1.12774
H	0.46495	4.88623	0.83392
H	-1.00770	5.37751	1.84188
C	-1.23228	3.60875	0.67246
H	-2.23687	3.37532	1.03655
H	-0.75936	2.86410	0.03245
C	-3.02382	4.72422	-6.20307
H	-3.53422	5.68694	-6.05375
H	-1.94672	4.94437	-6.22189
H	-2.85459	2.83348	-5.17986
C	-0.92398	7.81107	-0.23613
H	-0.42111	8.75719	-0.49523
H	-0.54225	7.53243	0.75964
C	-0.60668	6.70796	-1.23502
H	0.41401	6.30282	-1.16186
H	-0.75812	7.05382	-2.26975
H	-4.39754	3.65110	-4.90959
C	-3.46761	4.09985	-7.51320
H	-3.27000	4.76420	-8.36014
H	-2.94039	3.15666	-7.70207
H	-4.54236	3.88058	-7.50810

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Transition Structure TSIV-V

Cr	-1.98785	5.68314	-1.15073
P	-1.49388	3.89838	-2.96504
N	-2.97129	4.30036	-3.75978
P	-3.79057	5.49420	-2.82689
N	-1.33539	2.21625	-2.81617
C	-0.55016	1.63055	-3.90470
H	-0.05806	0.71583	-3.55383
H	-1.19056	1.36191	-4.76393
C	0.44600	2.70772	-4.28120

H	0.82073	2.58333	-5.30495
H	1.31407	2.69827	-3.59925
N	-0.29874	3.95736	-4.17614
C	-2.42692	1.41834	-2.29589
H	-3.21548	1.23173	-3.04463
H	-2.04467	0.45173	-1.95000
H	-2.88573	1.92137	-1.43802
C	0.43286	5.18625	-4.40613
H	1.27226	5.32574	-3.70446
H	0.83352	5.19307	-5.42659
H	-0.24424	6.04615	-4.31276
C	-3.43497	3.73111	-5.03052
N	-4.18282	6.90080	-3.65953
C	-5.51581	6.86395	-4.24924
H	-5.90709	7.88349	-4.34390
H	-5.51035	6.40603	-5.25525
C	-6.31963	6.03200	-3.26595
H	-7.20373	5.57778	-3.73063
H	-6.65756	6.65000	-2.41659
N	-5.40731	4.97930	-2.82365
C	-3.16849	7.77783	-4.19293
H	-2.84463	7.50231	-5.21028
H	-3.53767	8.80971	-4.21292
H	-2.28842	7.75119	-3.53414
C	-5.88591	4.07836	-1.79368
H	-6.11690	4.59458	-0.84764
H	-6.79355	3.57337	-2.14237
H	-5.13097	3.30914	-1.59475
C	-2.61350	7.47102	-0.34414
H	-3.49716	7.88325	-0.85321
H	-2.90376	7.25997	0.69900
C	-1.42953	8.42849	-0.37744
H	-1.61058	9.35011	0.19727
H	-1.24121	8.75792	-1.41350
C	-1.09409	4.84095	0.77807
H	-0.28165	4.14089	0.59716
H	-0.90082	5.57788	1.55435
C	-2.41162	4.45472	0.48540
H	-3.24164	4.92117	1.01608
H	-2.59151	3.44635	0.11059
C	-3.10082	4.59623	-6.23582
H	-3.56121	5.58669	-6.10481
H	-2.01462	4.76154	-6.26017
H	-2.97657	2.73818	-5.14174
C	-0.18653	7.70824	0.12964
H	0.72881	8.29441	-0.04518
H	-0.24161	7.56983	1.22070
C	-0.08541	6.36248	-0.54532
H	0.84864	5.82126	-0.37127
H	-0.17549	6.48743	-1.66427

H	-4.52070	3.57355	-4.94885
C	-3.57889	3.96780	-7.53170
H	-3.33867	4.59700	-8.39445
H	-3.11136	2.98902	-7.69581
H	-4.66541	3.81560	-7.52478

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Complex V

Cr	-1.76094	5.95419	-1.48547
P	-1.28634	4.06769	-3.22538
N	-2.88063	4.34645	-3.84842
P	-3.58921	5.65915	-3.01053
N	-1.03690	2.42207	-2.92599
C	-0.39954	1.72997	-4.04696
H	0.18010	0.87915	-3.67012
H	-1.14703	1.34013	-4.76051
C	0.47973	2.78125	-4.69099
H	0.69602	2.55192	-5.74204
H	1.44227	2.87163	-4.15823
N	-0.29245	4.01619	-4.60737
C	-1.95438	1.65629	-2.10834
H	-2.85832	1.34454	-2.65838
H	-1.45103	0.75680	-1.73717
H	-2.26471	2.24717	-1.24024
C	0.34306	5.22133	-5.09874
H	1.27067	5.47190	-4.55864
H	0.58749	5.10026	-6.16055
H	-0.34929	6.06786	-5.01688
C	-3.49694	3.60149	-4.95504
N	-4.07437	6.98439	-3.92270
C	-5.49332	6.95315	-4.26511
H	-5.86708	7.97727	-4.37617
H	-5.67199	6.41748	-5.21459
C	-6.13744	6.23177	-3.09560
H	-7.09632	5.77362	-3.36663
H	-6.31143	6.92105	-2.25212
N	-5.18591	5.18242	-2.74130
C	-3.16244	7.75776	-4.73373
H	-3.04639	7.35431	-5.75276
H	-3.51830	8.79159	-4.80798
H	-2.17295	7.78392	-4.25944
C	-5.53694	4.27411	-1.66905
H	-5.60907	4.77133	-0.68934
H	-6.50248	3.80813	-1.89476
H	-4.78808	3.47683	-1.60425
C	-2.23104	7.79982	-0.78034
H	-2.30982	8.48642	-1.64120
H	-3.23872	7.73633	-0.33777
C	-1.21486	8.30564	0.24201
H	-1.57868	9.21625	0.74378

H	-0.28737	8.60520	-0.27294
C	-1.05989	4.71542	0.76750
H	-0.49027	3.88150	0.33082
H	-1.18304	4.47389	1.83577
C	-2.40266	4.84916	0.06852
H	-3.11744	5.46488	0.63140
H	-2.87065	3.88206	-0.15123
C	-3.43179	4.33738	-6.28366
H	-3.96943	5.29310	-6.19210
H	-2.38272	4.59107	-6.49235
H	-2.97533	2.63745	-5.03319
C	-0.85832	7.25530	1.28978
H	-0.18253	7.69049	2.03583
H	-1.76685	6.96395	1.83864
C	-0.21459	5.99929	0.67621
H	0.76808	5.79813	1.12041
H	0.07505	6.22362	-0.38533
H	-4.53819	3.38102	-4.67796
C	-4.02193	3.51594	-7.41503
H	-3.97760	4.05549	-8.36619
H	-3.48013	2.57107	-7.54534
H	-5.07325	3.26813	-7.22376

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Transition Structure TSV-VI

Cr	-2.11153	5.27431	-1.10871
P	-1.73808	3.80380	-2.96987
N	-3.16949	4.23219	-3.81589
P	-3.93397	5.39506	-2.80257
N	-1.55116	2.13573	-2.84116
C	-0.67183	1.58564	-3.87086
H	-0.18744	0.67693	-3.49486
H	-1.22897	1.32002	-4.78650
C	0.32739	2.69462	-4.13673
H	0.79576	2.60362	-5.12456
H	1.12868	2.69163	-3.37703
N	-0.45508	3.92656	-4.07582
C	-2.60242	1.30064	-2.30299
H	-3.39148	1.07126	-3.03838
H	-2.17572	0.35572	-1.94885
H	-3.06610	1.79936	-1.44335
C	0.27132	5.17479	-4.20190
H	1.01197	5.32455	-3.39808
H	0.79775	5.19720	-5.16286
H	-0.43119	6.01720	-4.19039
C	-3.60804	3.75133	-5.12868
N	-4.23864	6.89919	-3.50521
C	-5.56139	6.98041	-4.11805
H	-5.90088	8.02246	-4.12881
H	-5.55127	6.61435	-5.16075

C	-6.42726	6.10359	-3.23378
H	-7.31978	5.73949	-3.75774
H	-6.75867	6.65389	-2.33677
N	-5.57517	4.97246	-2.88209
C	-3.17373	7.73384	-4.01459
H	-2.88398	7.48249	-5.04820
H	-3.48061	8.78588	-3.98668
H	-2.28819	7.62759	-3.37376
C	-6.13065	3.95696	-2.01194
H	-6.39349	4.34201	-1.01373
H	-7.03560	3.54034	-2.46876
H	-5.41210	3.13825	-1.89362
C	-2.54695	7.34408	-0.44163
H	-3.30507	7.56421	-1.20281
H	-2.97901	7.66301	0.51725
C	-1.22481	8.06846	-0.69233
H	-1.40175	9.14492	-0.83429
H	-0.77351	7.71830	-1.64286
C	-0.81071	5.33949	0.62812
H	-1.20929	5.23451	1.64415
H	-1.93561	6.18574	0.26709
C	-0.69635	4.12958	-0.15022
H	-1.12726	3.20388	0.23992
H	0.22629	3.96803	-0.71408
C	-3.23151	4.69048	-6.26393
H	-3.69485	5.67226	-6.08383
H	-2.14461	4.85336	-6.23830
H	-3.15812	2.76173	-5.29172
C	-0.21681	7.83584	0.43293
H	0.64189	8.50740	0.31292
H	-0.68375	8.10403	1.39348
C	0.28292	6.39373	0.47859
H	1.01283	6.26829	1.29049
H	0.83236	6.18687	-0.45440
H	-4.69720	3.60425	-5.08429
C	-3.66335	4.15178	-7.61510
H	-3.39128	4.83684	-8.42417
H	-3.19092	3.18491	-7.82754
H	-4.74938	4.00326	-7.65817

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Complex VI

Cr	-1.95197	5.18203	-1.18021
P	-1.64989	3.76837	-3.02511
N	-3.09022	4.26255	-3.83353
P	-3.74740	5.48493	-2.81893
N	-1.54713	2.09232	-2.92314
C	-0.72638	1.50901	-3.98194
H	-0.27629	0.57418	-3.62770
H	-1.32210	1.27917	-4.88314

C	0.31891	2.56956	-4.26898
H	0.74865	2.46645	-5.27315
H	1.14400	2.51549	-3.53735
N	-0.39489	3.84013	-4.16761
C	-2.61257	1.30569	-2.34298
H	-3.45134	1.13223	-3.03762
H	-2.22035	0.33316	-2.02576
H	-3.00134	1.81411	-1.45175
C	0.39567	5.04835	-4.29591
H	1.18189	5.13165	-3.52673
H	0.87518	5.07230	-5.28122
H	-0.25483	5.92884	-4.22370
C	-3.60913	3.75890	-5.10772
N	-4.02735	6.97837	-3.56136
C	-5.38503	7.09600	-4.08835
H	-5.67670	8.15192	-4.12786
H	-5.46303	6.68270	-5.11043
C	-6.22729	6.30427	-3.10800
H	-7.17692	5.97367	-3.54704
H	-6.45787	6.90798	-2.21234
N	-5.41158	5.14266	-2.77089
C	-2.97364	7.73002	-4.20636
H	-2.80799	7.42777	-5.25347
H	-3.21676	8.79882	-4.19050
H	-2.03213	7.59378	-3.66020
C	-5.93811	4.22717	-1.77919
H	-6.06875	4.69451	-0.78865
H	-6.91146	3.84859	-2.11063
H	-5.26633	3.36733	-1.67534
C	-3.06977	7.32609	0.07128
H	-3.91294	7.49697	-0.60683
H	-3.32094	7.77223	1.04097
C	-1.76919	7.92878	-0.45455
H	-1.97644	8.98015	-0.69330
H	-1.48412	7.49015	-1.43741
C	-0.60991	5.26588	0.39670
H	-1.15281	5.11277	1.33760
H	-3.02818	6.23967	0.30820
C	-0.30571	4.12704	-0.38653
H	-0.60079	3.12912	-0.05583
H	0.57632	4.13105	-1.03276
C	-3.23396	4.62795	-6.29761
H	-3.66368	5.63122	-6.15739
H	-2.14228	4.75842	-6.30688
H	-3.21782	2.74067	-5.24550
C	-0.57804	7.81493	0.50108
H	0.09156	8.67214	0.36013
H	-0.94260	7.88384	1.53682
C	0.21653	6.52709	0.31249
H	1.03806	6.49143	1.04614

H	0.71068	6.55680	-0.67492
H	-4.70163	3.66964	-5.01415
C	-3.71635	4.03440	-7.60826
H	-3.45143	4.67149	-8.45787
H	-3.27263	3.04674	-7.78426
H	-4.80629	3.91048	-7.61437

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Complex VII

Cr	-2.04001	5.32193	-0.82074
P	-1.46029	3.74690	-2.83745
N	-2.98160	4.16199	-3.58278
P	-3.58140	5.57215	-2.80235
N	-1.29816	2.05665	-2.92292
C	-0.63951	1.64223	-4.16580
H	-0.16708	0.66408	-4.01816
H	-1.36114	1.53995	-4.99608
C	0.37977	2.72545	-4.45401
H	0.58563	2.81522	-5.52952
H	1.33606	2.51885	-3.94483
N	-0.19356	3.96252	-3.93525
C	-2.31991	1.16861	-2.40762
H	-3.27600	1.22179	-2.95712
H	-1.95549	0.13770	-2.46404
H	-2.51164	1.38549	-1.35194
C	0.67140	5.12231	-3.94196
H	1.68958	4.85552	-3.61814
H	0.73732	5.56482	-4.94575
H	0.29098	5.88772	-3.25600
C	-3.50507	3.60579	-4.84005
N	-3.46954	6.98402	-3.73635
C	-4.72443	7.35675	-4.37822
H	-4.78821	8.44753	-4.46997
H	-4.78809	6.92447	-5.39416
C	-5.79844	6.79009	-3.47786
H	-6.74029	6.61901	-4.01273
H	-6.00644	7.46071	-2.62713
N	-5.26329	5.50546	-3.03453
C	-2.25931	7.35745	-4.43830
H	-2.32033	7.10000	-5.50756
H	-2.07680	8.43561	-4.35014
H	-1.39782	6.83161	-4.01713
C	-6.16735	4.64094	-2.30936
H	-6.43042	5.01761	-1.30810
H	-7.09450	4.54689	-2.88627
H	-5.74010	3.63823	-2.21604
C	-2.92433	6.37910	0.71610
H	-3.96791	6.08317	0.91008
H	-2.32791	6.05896	1.59307
C	-2.75846	7.87174	0.50074

H	-2.96678	8.46611	1.40504
H	-3.47067	8.21832	-0.26726
C	0.38435	5.14879	0.01145
H	0.84100	5.07374	-0.97497
H	0.51333	6.09309	0.53469
C	-0.21993	4.09490	0.58527
H	-0.59649	4.14130	1.60539
H	-0.26115	3.12708	0.08584
C	-2.97490	4.27124	-6.10093
H	-3.32227	5.31452	-6.12560
H	-1.87715	4.31480	-6.05567
H	-3.26486	2.53356	-4.84739
C	-1.34356	8.08391	-0.01173
H	-1.13672	9.14088	-0.24594
H	-0.63245	7.80834	0.78475
C	-1.17884	7.19430	-1.23563
H	-0.14648	7.17153	-1.61790
H	-1.81596	7.60720	-2.02750
H	-4.60121	3.67741	-4.80255
C	-3.43187	3.54293	-7.35190
H	-3.07183	4.03968	-8.25820
H	-3.05988	2.51044	-7.37091
H	-4.52622	3.49716	-7.41219
C	-3.93020	3.49609	-0.22737
H	-4.64917	4.30257	-0.10694
H	-4.02926	2.87834	-1.11839
C	-3.03886	3.21679	0.73284
H	-2.37143	2.35920	0.66786
H	-2.99869	3.79831	1.65211

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Transition Structure TSVII-VIII

Cr	-2.06681	5.22814	-0.72675
P	-1.54073	3.70077	-2.81115
N	-3.00750	4.18705	-3.61504
P	-3.66938	5.52469	-2.76286
N	-1.43083	2.00664	-2.91418
C	-0.73134	1.58546	-4.13258
H	-0.30203	0.58845	-3.98020
H	-1.41607	1.52520	-4.99797
C	0.33659	2.63612	-4.35371
H	0.61212	2.72085	-5.41410
H	1.25224	2.40111	-3.78520
N	-0.24016	3.88717	-3.87741
C	-2.51695	1.15739	-2.46707
H	-3.44170	1.27009	-3.05983
H	-2.19933	0.11156	-2.53068
H	-2.74958	1.35881	-1.41652
C	0.62879	5.04174	-3.87799
H	1.60702	4.81258	-3.42547

H	0.80225	5.40103	-4.90179
H	0.17516	5.85968	-3.30702
C	-3.47740	3.69451	-4.91873
N	-3.62049	6.98254	-3.64152
C	-4.90195	7.35837	-4.22896
H	-5.01182	8.44951	-4.23028
H	-4.96604	7.00768	-5.27543
C	-5.94210	6.67998	-3.36426
H	-6.87945	6.50908	-3.90753
H	-6.17509	7.28021	-2.46777
N	-5.34670	5.39482	-3.01861
C	-2.43620	7.45071	-4.33243
H	-2.61390	7.48757	-5.41780
H	-2.13938	8.45424	-3.99844
H	-1.59429	6.76619	-4.17244
C	-6.19961	4.41490	-2.38544
H	-6.51355	4.68907	-1.36586
H	-7.10400	4.29315	-2.99319
H	-5.69626	3.44264	-2.35544
C	-2.96134	6.50404	0.62839
H	-4.00357	6.21098	0.82964
H	-2.39560	6.37037	1.56790
C	-2.85173	7.93807	0.14836
H	-3.20046	8.66770	0.89640
H	-3.48674	8.08494	-0.74257
C	0.17460	5.59354	-0.09362
H	0.83985	5.43564	-0.94078
H	0.42634	6.45132	0.52547
C	-0.44832	4.48077	0.48543
H	-0.72101	4.52577	1.53817
H	-0.21552	3.49044	0.09411
C	-2.83386	4.37064	-6.11997
H	-3.09767	5.43799	-6.11209
H	-1.74028	4.32501	-6.02011
H	-3.29546	2.61084	-4.94910
C	-1.40597	8.20012	-0.23714
H	-1.27939	9.18902	-0.70596
H	-0.77333	8.21257	0.66496
C	-0.94299	7.12261	-1.19048
H	0.04744	7.31140	-1.61262
H	-1.63542	7.06660	-2.04232
H	-4.56869	3.82550	-4.94574
C	-3.27921	3.73226	-7.42309
H	-2.83507	4.23447	-8.28823
H	-2.98699	2.67521	-7.46843
H	-4.36930	3.77539	-7.53905
C	-3.92079	3.61718	-0.20457
H	-4.69051	4.36962	-0.05216
H	-4.01737	2.99486	-1.09182
C	-2.99590	3.36222	0.74114

H	-2.29411	2.53535	0.65197
H	-2.98043	3.91448	1.67805

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Complex VIII

Cr	-2.34981	5.08717	-0.72609
P	-1.61437	3.72256	-2.82292
N	-2.97217	4.26621	-3.74013
P	-3.82223	5.45059	-2.81440
N	-1.50378	2.03139	-2.78479
C	-0.61529	1.48766	-3.81082
H	-0.17898	0.54561	-3.45838
H	-1.15931	1.28044	-4.74938
C	0.43054	2.56505	-4.01230
H	0.90716	2.49884	-4.99851
H	1.22349	2.49878	-3.24687
N	-0.30938	3.81606	-3.91254
C	-2.63210	1.22019	-2.38479
H	-3.35687	1.06075	-3.20156
H	-2.28219	0.24057	-2.04030
H	-3.15833	1.69647	-1.54904
C	0.41162	5.04559	-4.15482
H	1.25100	5.20438	-3.45823
H	0.81379	5.03891	-5.17553
H	-0.27192	5.89974	-4.07658
C	-3.30885	3.80607	-5.09315
N	-3.98831	6.97997	-3.52684
C	-5.23146	7.13283	-4.27853
H	-5.52961	8.18769	-4.28149
H	-5.11235	6.80922	-5.32881
C	-6.22337	6.25462	-3.54421
H	-7.05402	5.94044	-4.18862
H	-6.64870	6.77820	-2.67093
N	-5.44712	5.08692	-3.15197
C	-2.85589	7.76717	-3.96049
H	-2.52900	7.51516	-4.98329
H	-3.11371	8.83249	-3.93400
H	-2.00778	7.61635	-3.28313
C	-6.13943	3.96316	-2.56662
H	-6.55860	4.17267	-1.56927
H	-6.96370	3.66450	-3.22521
H	-5.45674	3.10792	-2.49174
C	-3.01904	6.74834	0.27646
H	-4.09856	6.88754	0.11144
H	-2.87442	6.50855	1.34375
C	-2.24859	8.00930	-0.09153
H	-2.52830	8.83989	0.57669
H	-2.53486	8.33800	-1.10432
C	0.37781	5.49803	-0.51018
H	0.74644	4.87639	-1.33936

H	1.26758	5.79223	0.06998
C	-0.61256	4.69583	0.32471
H	-0.71628	5.10854	1.33773
H	-0.32477	3.64111	0.40637
C	-2.84822	4.75163	-6.19011
H	-3.31962	5.73408	-6.03740
H	-1.76549	4.91015	-6.08882
H	-2.84689	2.81807	-5.23167
C	-0.74047	7.79689	-0.04800
H	-0.21737	8.74784	-0.20673
H	-0.45487	7.45659	0.95873
C	-0.26877	6.76455	-1.08511
H	0.40091	7.21975	-1.82836
H	-1.14483	6.48779	-1.73224
H	-4.39801	3.65983	-5.13913
C	-3.18582	4.22312	-7.57203
H	-2.85572	4.91196	-8.35591
H	-2.70277	3.25574	-7.75689
H	-4.26661	4.07863	-7.69189
C	-4.10542	3.86716	0.24197
H	-4.79553	4.68901	0.42702
H	-4.40198	3.14612	-0.51869
C	-3.04801	3.62926	1.05645
H	-2.43530	2.73632	0.95137
H	-2.83106	4.26602	1.91044

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Complex VIII agostic

Cr	-2.18724	4.80420	-0.67433
P	-1.60244	3.37925	-2.83102
N	-2.90288	4.13210	-3.68760
P	-3.58943	5.35534	-2.68934
N	-1.66764	1.68767	-2.96276
C	-0.87491	1.16539	-4.07583
H	-0.54508	0.14599	-3.84268
H	-1.46099	1.12584	-5.01135
C	0.28436	2.13046	-4.19754
H	0.72196	2.12555	-5.20423
H	1.08551	1.88358	-3.47936
N	-0.29486	3.43797	-3.92348
C	-2.85940	0.95003	-2.60571
H	-3.65393	1.01231	-3.36882
H	-2.60518	-0.10576	-2.46148
H	-3.26171	1.32171	-1.65737
C	0.57641	4.58390	-4.04343
H	1.45741	4.52631	-3.38336
H	0.93643	4.66791	-5.07686
H	0.02562	5.50354	-3.81137
C	-3.28749	3.83207	-5.07197
N	-3.55946	6.93485	-3.28868

C	-4.76889	7.30061	-4.01891
H	-4.92780	8.38275	-3.94700
H	-4.69651	7.03705	-5.08987
C	-5.86518	6.51104	-3.33109
H	-6.73379	6.35261	-3.98251
H	-6.21165	7.02692	-2.41908
N	-5.24959	5.22649	-3.02393
C	-2.33499	7.64046	-3.58137
H	-1.95725	7.44624	-4.59910
H	-2.49349	8.71986	-3.47220
H	-1.55614	7.34751	-2.86513
C	-6.07634	4.19279	-2.44397
H	-6.43791	4.43661	-1.43204
H	-6.94918	4.02459	-3.08570
H	-5.51541	3.25181	-2.40139
C	-2.68775	4.79051	-6.08839
H	-3.00501	5.81556	-5.84459
H	-1.59391	4.77395	-5.98499
H	-2.96933	2.80294	-5.29082
H	-4.38597	3.84458	-5.12666
C	-3.09870	4.44212	-7.50708
H	-2.66652	5.13878	-8.23224
H	-2.76806	3.43260	-7.78100
H	-4.18879	4.47365	-7.62658
C	-3.84953	3.47394	0.24530
H	-4.59392	4.23892	0.46043
H	-4.10905	2.75249	-0.52789
C	-2.76726	3.28935	1.04676
H	-2.10292	2.43649	0.92201
H	-2.59159	3.91801	1.91737
C	-2.81273	6.43753	0.42196
C	0.45067	6.94784	-0.00887
C	-0.69300	7.86960	0.39804
C	-1.79295	7.22070	1.23610
H	-3.29568	7.11836	-0.30117
H	-3.61254	6.06717	1.08323
H	1.06426	6.70588	0.86941
H	1.10871	7.48673	-0.70335
H	-0.26151	8.72126	0.93936
H	-1.15525	8.29676	-0.50821
H	-1.34177	6.58597	2.01621
H	-2.31731	8.01898	1.78595
H	0.76195	5.28090	-1.39524
H	-0.83464	5.92899	-1.37894
H	-0.35583	4.75126	1.30857
H	0.07702	3.54702	0.03061
C	0.02722	5.62910	-0.65895
C	-0.38878	4.51253	0.24364

Transition Structure TSVIII-IX

Cr	-2.27574	5.14570	-0.83454
P	-1.55411	3.68678	-2.89088
N	-2.93513	4.24941	-3.76388
P	-3.69989	5.48123	-2.83538
N	-1.45997	1.99239	-2.93398
C	-0.59902	1.49798	-4.00932
H	-0.17526	0.52826	-3.72265
H	-1.16310	1.35719	-4.94879
C	0.46254	2.56511	-4.16635
H	0.92580	2.54402	-5.16106
H	1.26357	2.44135	-3.41619
N	-0.25202	3.82165	-3.98483
C	-2.59438	1.16602	-2.57704
H	-3.35565	1.11119	-3.37376
H	-2.25051	0.14843	-2.36144
H	-3.07333	1.55051	-1.67101
C	0.51475	5.04224	-4.09992
H	1.31607	5.12893	-3.34659
H	0.97687	5.09165	-5.09321
H	-0.14804	5.91113	-4.00596
C	-3.33780	3.78183	-5.09587
N	-3.84571	6.99203	-3.58506
C	-5.13446	7.17941	-4.24609
H	-5.38601	8.24629	-4.26272
H	-5.11163	6.81731	-5.29020
C	-6.10239	6.37258	-3.40666
H	-7.00058	6.08693	-3.96810
H	-6.42193	6.94001	-2.51551
N	-5.35643	5.17394	-3.04275
C	-2.71837	7.73276	-4.10338
H	-2.45687	7.44793	-5.13591
H	-2.94306	8.80580	-4.08767
H	-1.83715	7.57257	-3.47170
C	-6.04714	4.16626	-2.26683
H	-6.29041	4.49549	-1.24391
H	-6.98176	3.90338	-2.77499
H	-5.43668	3.25790	-2.20981
C	-3.08002	6.76559	0.14296
H	-4.15780	6.82909	-0.07586
H	-2.98132	6.56988	1.22396
C	-2.37324	8.05731	-0.24416
H	-2.71656	8.90220	0.37452
H	-2.64306	8.32196	-1.28045
C	0.22740	5.58244	-0.34138
H	0.58706	4.85186	-1.08074
H	1.11979	5.88666	0.23065
C	-0.70776	4.89994	0.66590
H	-0.98457	5.58692	1.47222
H	-0.17536	4.05252	1.09792

C	-2.88887	4.69585	-6.22421
H	-3.34622	5.68689	-6.08585
H	-1.80211	4.84314	-6.14730
H	-2.91302	2.77763	-5.23658
C	-0.85344	7.94974	-0.15702
H	-0.39460	8.90825	-0.42801
H	-0.55485	7.75684	0.88446
C	-0.29797	6.83777	-1.06075
H	0.51714	7.20845	-1.69611
H	-1.07146	6.58457	-1.82700
H	-4.43188	3.66811	-5.09654
C	-3.26110	4.13784	-7.58552
H	-2.94188	4.80433	-8.39289
H	-2.79071	3.16160	-7.75676
H	-4.34540	4.00043	-7.67903
C	-3.57113	3.80724	0.07550
H	-4.38366	4.37000	0.53447
H	-3.88276	3.04590	-0.63898
C	-2.39522	3.57389	0.82727
H	-1.80401	2.68793	0.60140
H	-2.35705	3.87839	1.87012

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Transition Structure TSVIII-IX agostic

Cr	-2.23680	4.88282	-0.78526
P	-1.63773	3.40305	-2.85176
N	-2.93630	4.13311	-3.72193
P	-3.64919	5.33646	-2.71923
N	-1.68665	1.71089	-2.97321
C	-0.85138	1.19322	-4.05750
H	-0.51421	0.17975	-3.80937
H	-1.41000	1.14084	-5.00909
C	0.29882	2.17342	-4.15283
H	0.77130	2.16066	-5.14337
H	1.07765	1.94558	-3.40397
N	-0.30763	3.47628	-3.91527
C	-2.89812	0.97576	-2.67514
H	-3.62773	0.99746	-3.50246
H	-2.65016	-0.07039	-2.46418
H	-3.38060	1.38881	-1.78283
C	0.55677	4.63382	-3.97232
H	1.37780	4.60046	-3.23733
H	1.00142	4.71233	-4.97202
H	-0.02772	5.54686	-3.80271
C	-3.30713	3.83215	-5.10944
N	-3.66863	6.90562	-3.32844
C	-4.90400	7.24233	-4.02588
H	-5.08786	8.32032	-3.95040
H	-4.85738	6.97790	-5.09794
C	-5.96120	6.42809	-3.30320

H	-6.84632	6.24989	-3.92638
H	-6.28808	6.93823	-2.38078
N	-5.31058	5.15493	-3.01091
C	-2.46451	7.65620	-3.58655
H	-2.05603	7.48893	-4.59694
H	-2.65983	8.72814	-3.46446
H	-1.69587	7.37458	-2.85234
C	-6.08426	4.14214	-2.32416
H	-6.35140	4.42436	-1.29307
H	-7.00888	3.95468	-2.88172
H	-5.51931	3.20294	-2.29524
C	-2.72740	4.81624	-6.11337
H	-3.07930	5.82912	-5.86671
H	-1.63456	4.83316	-5.99751
H	-2.95774	2.81458	-5.33498
H	-4.40530	3.81363	-5.16833
C	-3.11124	4.46498	-7.53886
H	-2.69398	5.18068	-8.25418
H	-2.74501	3.46877	-7.81614
H	-4.20037	4.46224	-7.67029
C	-3.49937	3.58836	0.18325
H	-4.23482	4.13040	0.77826
H	-3.92862	2.87555	-0.52194
C	-2.25929	3.23182	0.80228
H	-1.77141	2.32858	0.43674
H	-2.16276	3.35634	1.87846
C	-2.77048	6.64241	0.16627
C	0.55258	6.68362	0.23319
C	-0.48650	7.79316	0.34890
C	-1.79307	7.41316	1.04675
H	-3.09027	7.30678	-0.65651
H	-3.68473	6.40070	0.73222
H	0.97568	6.45410	1.22083
H	1.39030	7.03963	-0.38094
H	-0.01710	8.64001	0.86585
H	-0.73010	8.16018	-0.66342
H	-1.57165	6.86298	1.97504
H	-2.27618	8.34415	1.38441
H	0.81401	4.81486	-0.88732
H	-0.59462	5.73806	-1.26776
H	-0.81938	5.00051	1.57412
H	-0.01916	3.60034	0.82328
C	0.02489	5.38539	-0.38424
C	-0.66092	4.46090	0.64039

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Complex IX

Cr	-1.21220	5.49745	-1.85566
P	-1.39239	3.86840	-3.67416
N	-2.99000	4.34616	-4.07215

P	-3.36061	5.65343	-3.01713
N	-1.28246	2.21451	-3.38436
C	-0.81373	1.46634	-4.54945
H	-0.27976	0.56731	-4.22059
H	-1.65408	1.14792	-5.19094
C	0.09795	2.43561	-5.27809
H	0.19641	2.18983	-6.34246
H	1.10763	2.43938	-4.83406
N	-0.54762	3.73873	-5.13605
C	-2.17275	1.56075	-2.44953
H	-3.15294	1.31599	-2.89106
H	-1.71331	0.63425	-2.08754
H	-2.33774	2.21234	-1.58173
C	0.13925	4.88724	-5.69371
H	1.14176	5.03500	-5.26196
H	0.24378	4.76121	-6.77736
H	-0.45267	5.79368	-5.51903
C	-3.86320	3.72252	-5.07280
N	-3.89707	7.04938	-3.78711
C	-5.35285	7.10840	-3.88990
H	-5.67537	8.15457	-3.94256
H	-5.72147	6.59189	-4.79470
C	-5.83765	6.42124	-2.62782
H	-6.86097	6.03892	-2.72843
H	-5.81321	7.11320	-1.76797
N	-4.91563	5.30544	-2.43360
C	-3.09193	7.74621	-4.76539
H	-3.19639	7.33388	-5.78202
H	-3.37734	8.80401	-4.79069
H	-2.03629	7.68849	-4.47574
C	-5.09689	4.49339	-1.24728
H	-4.98039	5.06762	-0.31285
H	-6.09924	4.05076	-1.25596
H	-4.36941	3.67298	-1.24171
C	-1.22215	7.53586	-1.84977
H	-0.40301	7.89224	-2.48837
H	-2.13930	8.10394	-2.02409
C	-0.85820	7.35196	-0.40877
H	0.01009	7.95562	-0.10381
H	-0.39939	6.32485	-0.26913
C	-2.21761	5.42395	2.11985
H	-1.83992	5.02232	3.07095
H	-3.31356	5.44604	2.21670
C	-1.85765	4.46902	0.98791
H	-2.33533	4.85468	0.06126
H	-2.35997	3.50348	1.14574
C	-3.87854	4.45370	-6.40495
H	-4.23452	5.48227	-6.24562
H	-2.84661	4.53744	-6.77429
H	-3.52241	2.68694	-5.21437

C	-2.00334	7.50141	0.59364
H	-2.20571	8.57431	0.70668
H	-2.92790	7.07668	0.16177
C	-1.71423	6.86277	1.95682
H	-2.16645	7.46684	2.75278
H	-0.63034	6.90819	2.14357
H	-4.87404	3.66826	-4.64228
C	-4.75925	3.75178	-7.42221
H	-4.77205	4.28671	-8.37686
H	-4.40620	2.73210	-7.61910
H	-5.79547	3.67812	-7.06970
C	-0.02893	4.15125	-0.75417
H	-0.26903	3.14750	-1.13580
H	1.04371	4.30168	-0.95253
C	-0.35482	4.25058	0.73577
H	0.20920	5.08557	1.17856
H	-0.01884	3.36024	1.28966

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Complex IX agostic

Cr	-2.11340	5.22821	-1.09357
P	-1.55318	3.64605	-3.03918
N	-2.98042	4.21369	-3.84682
P	-3.71051	5.43170	-2.89185
N	-1.48166	1.95784	-3.09859
C	-0.67007	1.46523	-4.21266
H	-0.24091	0.49098	-3.95076
H	-1.27396	1.33278	-5.12817
C	0.39402	2.52517	-4.40382
H	0.81912	2.50848	-5.41514
H	1.22087	2.38579	-3.68557
N	-0.29341	3.79290	-4.17772
C	-2.59553	1.13559	-2.67243
H	-3.39222	1.06663	-3.43220
H	-2.23881	0.12267	-2.45587
H	-3.02895	1.53912	-1.75194
C	0.53065	4.98510	-4.18081
H	1.30503	4.97773	-3.39505
H	1.02870	5.08487	-5.15206
H	-0.09680	5.87452	-4.04339
C	-3.43454	3.76923	-5.17161
N	-3.87967	6.95252	-3.58999
C	-5.20768	7.17765	-4.15310
H	-5.45033	8.24548	-4.10879
H	-5.26024	6.85788	-5.20922
C	-6.12692	6.34507	-3.27874
H	-7.05906	6.07956	-3.79181
H	-6.38675	6.88359	-2.35189
N	-5.36891	5.12876	-2.99639
C	-2.75885	7.70747	-4.10240

H	-2.54489	7.48845	-5.16106
H	-2.95476	8.78110	-4.00117
H	-1.85743	7.47912	-3.51807
C	-6.00212	4.10425	-2.19024
H	-6.19678	4.42864	-1.15611
H	-6.95474	3.82235	-2.65190
H	-5.36687	3.21178	-2.16409
C	-3.07490	4.73583	-6.28830
H	-3.57150	5.70008	-6.10339
H	-1.99377	4.93175	-6.24743
H	-2.97669	2.78862	-5.36205
H	-4.52163	3.61032	-5.12310
C	-3.47443	4.19981	-7.65066
H	-3.22125	4.90543	-8.44803
H	-2.96370	3.25429	-7.87081
H	-4.55352	4.01097	-7.70609
C	-3.04144	3.82912	0.02807
H	-3.76161	4.42668	0.61139
H	-3.61162	3.09860	-0.56239
C	-2.01656	3.17201	0.93863
H	-1.38746	2.46948	0.36633
H	-2.52494	2.56201	1.70199
C	-2.39177	7.04182	-0.23943
C	0.63696	6.05205	1.17288
C	0.02913	7.32140	0.57835
C	-1.46292	7.55844	0.85307
H	-2.24987	7.66506	-1.14857
H	-3.45234	7.16389	0.03355
H	0.58592	6.10575	2.27060
H	1.70558	6.03468	0.92333
H	0.61535	8.17248	0.94795
H	0.18908	7.31314	-0.51731
H	-1.73202	7.12444	1.82757
H	-1.62598	8.64091	0.97615
H	0.74734	3.94658	0.62920
H	-0.30967	4.85149	-0.34827
H	-1.76201	5.04190	1.97212
H	-0.65813	3.79708	2.51964
C	-0.00699	4.74067	0.72744
C	-1.13017	4.21326	1.61990

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Transition Structure TSIX-X

Cr	-1.28981	5.73826	-1.91218
P	-1.39646	3.97480	-3.68212
N	-3.00453	4.40053	-4.10643
P	-3.36502	5.79221	-3.16143
N	-1.23587	2.35673	-3.22718
C	-0.81165	1.49560	-4.32951
H	-0.25469	0.63774	-3.93503

H	-1.67511	1.10789	-4.89777
C	0.05689	2.39300	-5.18979
H	0.11673	2.03945	-6.22662
H	1.08367	2.44982	-4.79008
N	-0.60008	3.69663	-5.15588
C	-2.06838	1.79123	-2.18737
H	-3.06688	1.49497	-2.55015
H	-1.57847	0.90891	-1.76029
H	-2.19933	2.52414	-1.37955
C	0.04609	4.78468	-5.86238
H	1.05584	5.00442	-5.48060
H	0.12677	4.53337	-6.92623
H	-0.56360	5.69224	-5.78227
C	-3.88106	3.72102	-5.06532
N	-3.88390	7.13725	-4.02428
C	-5.33753	7.21483	-4.13184
H	-5.64224	8.26101	-4.25029
H	-5.71724	6.64792	-5.00125
C	-5.83065	6.61848	-2.82679
H	-6.86109	6.24917	-2.90008
H	-5.79095	7.36503	-2.01407
N	-4.92783	5.50126	-2.56558
C	-3.05425	7.79262	-5.00889
H	-3.13438	7.34080	-6.01126
H	-3.33424	8.84960	-5.08350
H	-2.00552	7.74418	-4.69060
C	-5.12201	4.75314	-1.34031
H	-4.97165	5.36187	-0.43225
H	-6.13983	4.34794	-1.31600
H	-4.42597	3.90629	-1.30818
C	-1.45970	7.74846	-1.66110
H	-0.72438	8.25001	-2.29899
H	-2.45881	8.18360	-1.73263
C	-1.01966	7.24635	-0.37442
H	-0.03280	7.58788	-0.03463
H	-0.40733	5.89257	-0.49831
C	-2.13667	5.07353	2.16107
H	-1.75943	4.66684	3.11039
H	-3.23431	5.05094	2.23866
C	-1.70894	4.15678	1.02142
H	-2.23284	4.47879	0.09794
H	-2.08739	3.14359	1.21384
C	-3.90722	4.38819	-6.43093
H	-4.23604	5.43151	-6.31324
H	-2.88086	4.43044	-6.82190
H	-3.53708	2.68138	-5.15893
C	-2.06315	7.23370	0.73602
H	-2.28786	8.28809	0.95424
H	-3.00850	6.81986	0.34164
C	-1.68092	6.52691	2.03891

H	-2.10888	7.08047	2.88392
H	-0.59144	6.59819	2.17678
H	-4.88944	3.68596	-4.62702
C	-4.82236	3.66100	-7.39854
H	-4.83749	4.14855	-8.37826
H	-4.49950	2.62375	-7.55019
H	-5.85404	3.63259	-7.02651
C	0.13888	4.51124	-0.69031
H	-0.04331	3.64510	-1.33904
H	1.19618	4.77751	-0.82384
C	-0.19320	4.13668	0.75248
H	0.30708	4.83590	1.43731
H	0.22509	3.14940	0.98982

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Transition Structure TSIX-X agostic

Cr	-2.62850	5.03818	-0.89872
P	-2.07548	3.46853	-2.73571
N	-3.16782	4.20720	-3.83364
P	-3.77559	5.55111	-2.94833
N	-2.34570	1.81566	-2.52852
C	-1.50651	0.99004	-3.39509
H	-1.33101	0.01641	-2.92268
H	-1.98580	0.81178	-4.37377
C	-0.22717	1.78984	-3.54560
H	0.32836	1.51840	-4.45184
H	0.43916	1.63400	-2.67842
N	-0.66166	3.18102	-3.63654
C	-3.66292	1.32902	-2.17887
H	-4.33275	1.24319	-3.05095
H	-3.58257	0.34470	-1.70455
H	-4.12672	2.01292	-1.45629
C	0.37525	4.18964	-3.72620
H	1.05557	4.18529	-2.85774
H	0.97191	4.02204	-4.63043
H	-0.07875	5.18453	-3.80773
C	-3.44642	3.82685	-5.22048
N	-3.49488	7.06758	-3.61984
C	-4.60745	7.55091	-4.43005
H	-4.62424	8.64700	-4.41969
H	-4.52707	7.22049	-5.48142
C	-5.83000	6.95425	-3.75644
H	-6.68928	6.88651	-4.43503
H	-6.12993	7.55784	-2.88163
N	-5.41768	5.61132	-3.35873
C	-2.16338	7.58830	-3.82465
H	-1.72509	7.28879	-4.79111
H	-2.18111	8.68356	-3.77959
H	-1.50016	7.23244	-3.02148
C	-6.38810	4.78950	-2.66509

H	-6.71013	5.22237	-1.70409
H	-7.27392	4.66006	-3.29718
H	-5.96532	3.79546	-2.47768
C	-2.67798	4.66130	-6.23316
H	-2.93173	5.72221	-6.08719
H	-1.60314	4.56919	-6.02101
H	-3.19245	2.76349	-5.33476
H	-4.53060	3.91825	-5.38173
C	-2.98108	4.24347	-7.66014
H	-2.42678	4.85158	-8.38190
H	-2.71007	3.19491	-7.83399
H	-4.04871	4.34880	-7.88910
C	-1.50147	3.69261	0.46954
H	-1.53176	3.74041	1.57021
H	-2.15434	2.84439	0.20839
C	-0.06929	3.43031	0.01780
H	-0.05706	3.23162	-1.06415
H	0.30052	2.50462	0.48705
C	-3.71851	6.63866	-0.19231
C	-0.17061	6.72782	1.12989
C	-1.50392	7.39407	0.81992
C	-2.67141	6.41620	0.77964
H	-3.65706	7.53722	-0.81051
H	-4.74345	6.35999	0.06835
H	-0.31124	6.04477	1.98234
H	0.55010	7.47774	1.47795
H	-1.73242	8.16591	1.56817
H	-1.44083	7.91986	-0.14624
H	-2.03075	5.15739	0.65687
H	-3.00704	6.10073	1.77680
H	1.24213	6.54494	-0.50187
H	-0.31992	5.87176	-0.87462
H	1.20250	4.54075	1.37019
H	1.86207	4.32276	-0.23493
C	0.43172	5.95255	-0.05767
C	0.93293	4.55123	0.30383

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Complex X

Cr	-1.89893	5.83083	-1.66700
P	-1.86176	3.95494	-3.23432
N	-3.29562	4.50938	-3.99949
P	-3.63905	6.01858	-3.23201
N	-1.99493	2.37525	-2.64649
C	-1.49943	1.37473	-3.58847
H	-1.14927	0.49185	-3.04060
H	-2.28670	1.04709	-4.29038
C	-0.36984	2.07931	-4.31514
H	-0.16612	1.63328	-5.29674
H	0.56263	2.03933	-3.72463

N	-0.83069	3.45306	-4.48676
C	-3.06516	2.00507	-1.74679
H	-4.01014	1.78160	-2.27016
H	-2.77374	1.12196	-1.16659
H	-3.25465	2.82237	-1.03717
C	0.07219	4.38295	-5.13308
H	1.03869	4.47459	-4.61187
H	0.26705	4.05464	-6.16097
H	-0.38974	5.37568	-5.18375
C	-4.05645	3.84046	-5.05784
N	-3.78878	7.33012	-4.27377
C	-5.16887	7.57633	-4.68092
H	-5.29873	8.63822	-4.91985
H	-5.44401	6.98942	-5.57610
C	-5.98746	7.15744	-3.47396
H	-7.02233	6.90842	-3.74033
H	-6.01280	7.96288	-2.71923
N	-5.31328	5.96888	-2.96075
C	-2.70617	7.77382	-5.12079
H	-2.65161	7.22769	-6.07724
H	-2.82157	8.84145	-5.33977
H	-1.75225	7.64198	-4.59406
C	-5.83910	5.37181	-1.75032
H	-5.80977	6.05446	-0.88491
H	-6.87872	5.06514	-1.91175
H	-5.26206	4.47288	-1.50227
C	-2.62448	7.65083	-0.91126
H	-2.22621	8.48523	-1.49309
H	-3.70596	7.70080	-0.75958
C	-1.80102	6.99543	0.03781
H	-0.78042	7.37213	0.17713
H	0.44487	5.97008	-1.84877
C	-0.89940	4.18468	1.63222
H	-0.16397	3.78731	2.34626
H	-1.74435	3.47969	1.64945
C	-0.28573	4.16673	0.24308
H	-1.07858	4.45247	-0.49065
H	-0.07426	3.13235	-0.06724
C	-3.73926	4.36803	-6.44819
H	-3.95710	5.44616	-6.47952
H	-2.65881	4.26725	-6.62457
H	-3.83567	2.76490	-5.00226
C	-2.39528	6.25415	1.21790
H	-2.97425	6.96679	1.82715
H	-3.15143	5.52093	0.86583
C	-1.38458	5.54821	2.12141
H	-1.83342	5.40383	3.11204
H	-0.52933	6.22115	2.28531
H	-5.12545	3.96031	-4.82696
C	-4.52961	3.64593	-7.52369

H	-4.29563	4.03291	-8.52042
H	-4.30970	2.57124	-7.52624
H	-5.60987	3.75933	-7.36958
C	1.23156	5.31636	-1.41668
H	1.25335	4.39852	-2.01953
H	2.17661	5.84750	-1.57126
C	0.95725	5.02264	0.04564
H	0.86375	5.96780	0.59669
H	1.81697	4.50321	0.49014

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Complex X agostic

Cr	-2.61700	5.32567	-1.03010
P	-2.08079	3.61478	-2.69814
N	-3.18729	4.29960	-3.82020
P	-3.84340	5.66788	-3.00041
N	-2.34667	1.96214	-2.45555
C	-1.53443	1.12813	-3.34044
H	-1.35784	0.15301	-2.87111
H	-2.03841	0.95071	-4.30705
C	-0.24946	1.91172	-3.52368
H	0.27305	1.63982	-4.44952
H	0.44238	1.73480	-2.68080
N	-0.65922	3.31154	-3.58146
C	-3.66171	1.47811	-2.09153
H	-4.34063	1.38790	-2.95625
H	-3.57538	0.49425	-1.61683
H	-4.12026	2.16069	-1.36479
C	0.39871	4.30000	-3.63479
H	1.07806	4.24437	-2.76651
H	0.99407	4.15662	-4.54412
H	-0.03134	5.30820	-3.67420
C	-3.44537	3.86711	-5.19627
N	-3.62400	7.14466	-3.77282
C	-4.74840	7.52884	-4.61666
H	-4.80781	8.62147	-4.68161
H	-4.65219	7.13059	-5.64303
C	-5.94965	6.93312	-3.90464
H	-6.80269	6.78537	-4.57846
H	-6.27650	7.58474	-3.07519
N	-5.48850	5.63788	-3.41212
C	-2.31581	7.72044	-3.96840
H	-1.81605	7.37159	-4.88732
H	-2.38996	8.81345	-4.00845
H	-1.67828	7.46013	-3.10953
C	-6.42951	4.84053	-2.65291
H	-6.76566	5.33779	-1.72864
H	-7.31079	4.62925	-3.26916
H	-5.97188	3.88085	-2.38753
C	-2.65348	4.65621	-6.22755

H	-2.90354	5.72313	-6.12969
H	-1.58350	4.56754	-5.99143
H	-3.19943	2.79805	-5.26727
H	-4.52629	3.96005	-5.37777
C	-2.93215	4.18287	-7.64204
H	-2.35935	4.75756	-8.37667
H	-2.66575	3.12627	-7.76822
H	-3.99436	4.28626	-7.89609
C	-1.16064	3.21825	0.84013
H	-1.04531	3.21851	1.93143
H	-1.78542	2.36292	0.55988
C	0.17683	3.19580	0.12181
H	-0.00275	3.06587	-0.95720
H	0.73636	2.30555	0.43809
C	-3.72520	6.98390	-0.32472
C	-0.27630	6.47864	1.17404
C	-1.45544	7.37636	0.82431
C	-2.73071	6.59392	0.60288
H	-3.57497	7.87317	-0.94247
H	-4.77523	6.74257	-0.14600
H	-0.59934	5.75258	1.93646
H	0.53100	7.05668	1.64358
H	-1.61753	8.11209	1.62800
H	-1.22359	7.97060	-0.07589
H	-1.74295	4.13773	0.62353
H	-3.05478	5.99696	1.46596
H	0.94455	6.42287	-0.60227
H	-0.50272	5.48547	-0.76693
H	1.37971	4.49801	1.36278
H	1.94554	4.33596	-0.28926
C	0.30283	5.73804	-0.03003
C	1.03805	4.44205	0.31872

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