Electronic Supplementary Material (ESI) for Dalton Transactions.

Charge-Assisted Phosph(V)azane Anion receptors

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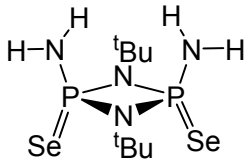
Synthetic Procedures

General Experimental Methods

All experiments involving phosphorus(III) containing species were carried out on a Schlenk-line under nitrogen atmosphere or with the aid of a N_2-filled glove box (Saffron type α). Toluene and THF were dried under nitrogen over sodium or sodium/benzophenone, respectively, whereas acetonitrile and CH_2Cl_2 was dried over calcium hydride. ^{1}H, $^{13}C\{^{1}H\}$, $^{31}P\{^{1}H\}$, $^{19}F\{^{1}H\}$ NMR spectra were recorded on a Bruker Avance 400 QNP or Bruker Avance 500 MHz cryo spectrometer. All spectra were recorded with $SiMe_4$ (^{1}H), H_3PO_4 (^{31}P, 85% in D_2O) and C_6H_5F (^{19}F, 0.1 M in $CDCl_3$) as external standards and referenced to the residual solvent signal. All reagents were purchased from commercial sources and used as received without further purification unless stated differently. $[P(\mu\text{-}N^tBu)NH^tBu]_2$, $[P(\mu\text{-}N^tBu)NH_2]_2$, $[Se{=}P(\mu\text{-}N^tBu)NH^tBu]_2$, $[^tBuNH(Me\text{-})P(\mu\text{-}N^tBu)_2PNH^tBu]I$, $(Ph_3P)_2Pd(CH_3CN)_2(BF_4)_2$ and $(Ph_3P)Cu(CH_3CN)_3(BF_4)$ were synthesized according to previously published procedures.[1–6] Elemental analysis was obtained using a Perkin Elmer 240 Elemental Analyser. Low resolution electrospray ionisation (LR-ESI) mass spectrometry was undertaken on a Micromass Quattro LC mass spectrometer (cone voltage 10-30 eV; desolvation temp. 313 K; ionization temp. 313 K) infused from a Harvard syringe pump at a rate of 10 μL min^{-1}

Synthesis of new compounds



Synthesis of 1: Inside a N_2 filled glovebox a Schlenk tube was charged with $[P(\mu\text{-}N^tBu)NH_2]_2$ (236 mg, 1 mmol) and selenium (316 mg, 4 mmol, 4 equivalents) and transferred to a Schlenk line. 20 ml of THF were added and the resulting suspension was stirred overnight. Afterwards unreacted selenium was filtered off under ambient conditions and the solvent was removed *in vacuo* to yield **3** as a white powder (390 mg, 99%).

^{1}H NMR (25°C, d_6-Acetone, 500.12 MHz): δ [ppm] = 5.04 (s, 4H, NH_2), 1.67 (s, 18H, ^{t}Bu).

^{31}P NMR (25°C, d_6-Acetone, 202.48 MHz): δ [ppm] = 33.8 (s, with two satellite doublets arising from [(^{77}Se=)H_2N-P(μ-N tBu)P-NH_2(=Se)], $^1J_{PSe}$ = 878 Hz, $^2J_{PP}$ = 20 Hz).

Elemental analysis (%): calcd. for **1**, C 24.4% H 5.6% N 14.2% found C 24.0% H 5.6% N 13.9%.

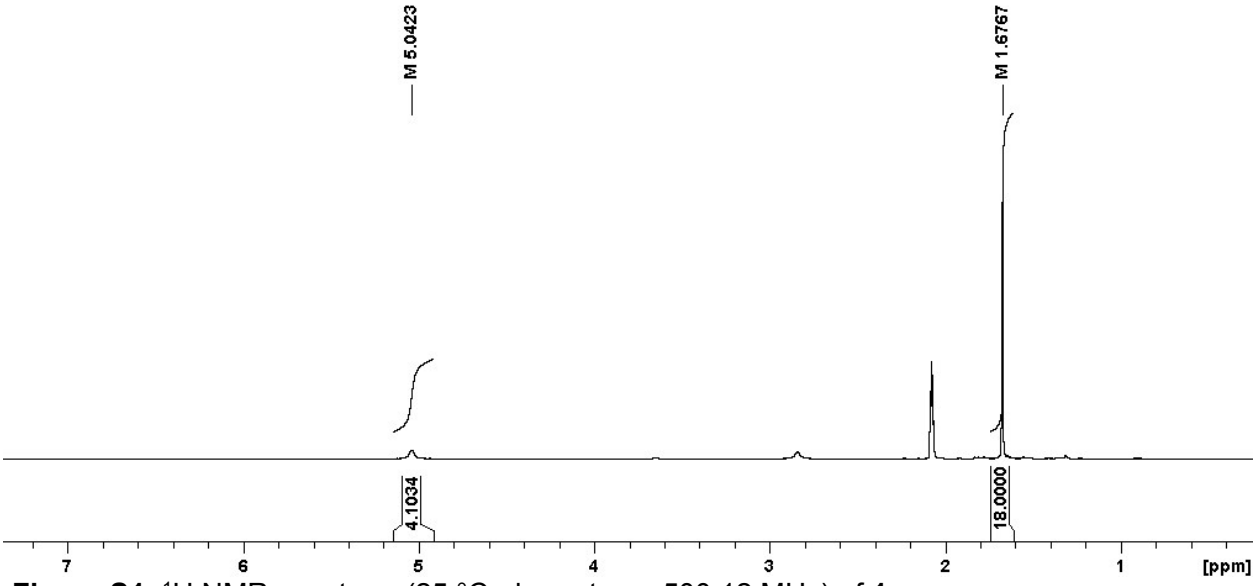


Figure S1: ^{1}H NMR spectrum (25 °C, d_6-acetone, 500.12 MHz) of **1**.

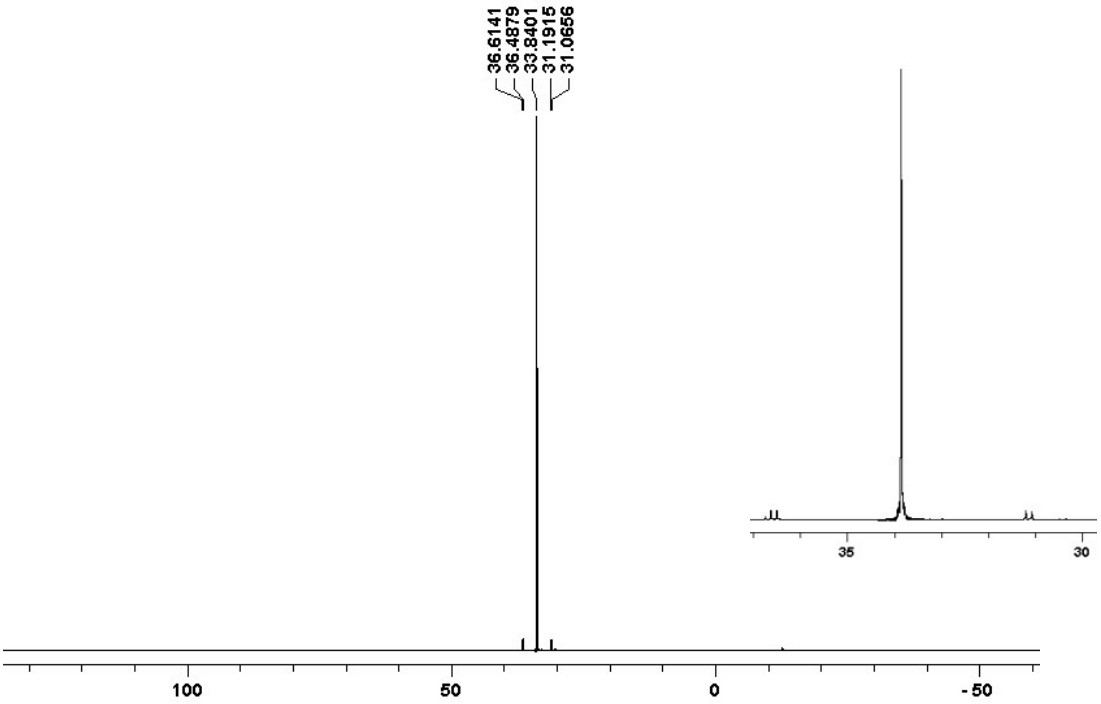
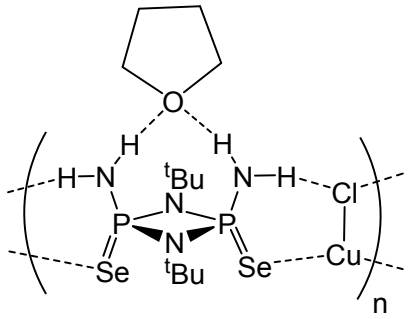


Figure S2: $^{31}P\{^{1}H\}$ NMR spectrum (25°C, d_6-acetone, 202.48 MHz) of **1**.



Synthesis of 2: Inside a N_2 filled glovebox a Schlenk tube was charged with **1** (100 mg, 0.25 mmol) and CuCl (25 mg, 0.25 mmol, 1 eq).The Schlenk tube was transferred to a Schlenk line and 10ml of THF were added. The resulting orange/brown mixture was stirred at room temperature for 1 h. Afterwards the solution was reduced to approximately 5 ml *in vacuo* and stored at 4°C for 3 days which lead to the formation of orange crystals suitable for X-ray crystallography. The crystals were isolated by filtration and dried *in vacuo* to yield **2** as an orange/brown crystalline solid (113 mg, 0.20 mmol, 80%). Crystal lose THF when dried under vacuum. The following spectroscopic and analytical data refers to this material.

^{1}H NMR (25°C, d_8-thf, 500.12 MHz): δ [ppm] = 5.81 (s, 4H, NH_2), 1.71 (s, 18H, ^{t}Bu).

^{31}P NMR (25°C, d_8-thf, 202.48 MHz): δ [ppm] = 30.36 (s).

Elemental analysis (%) calcd. for 2 (-THF): calcd C 30.1% H 6.0% N 8.8, found C 30.4% H 6.5% N 8.9%.

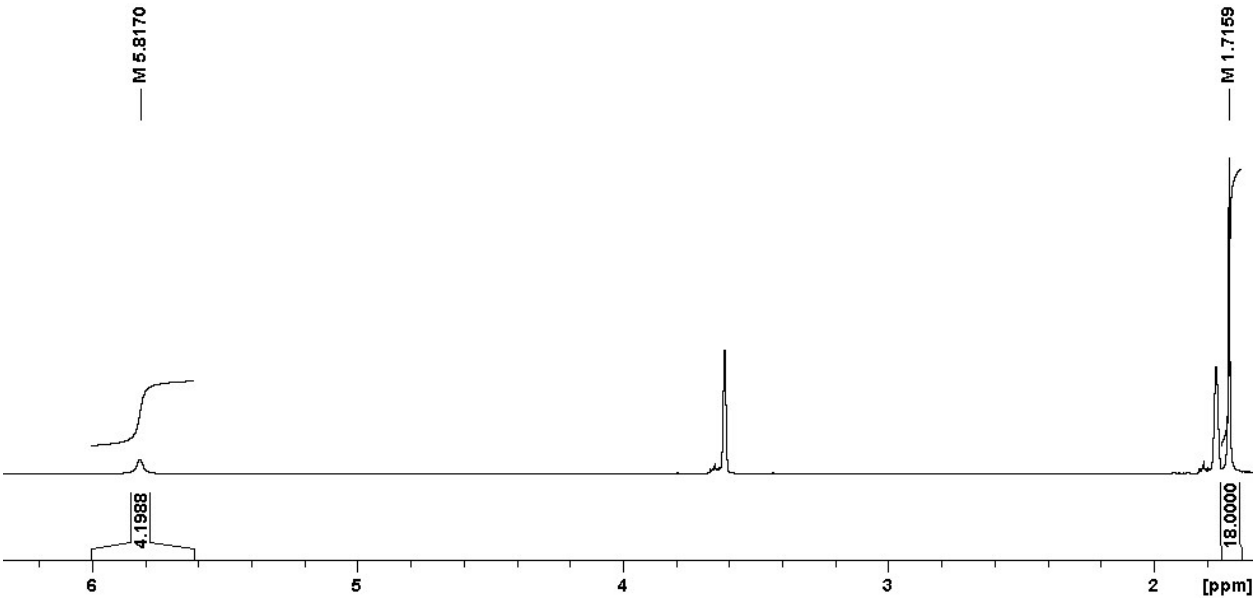


Figure S3: ^{1}H NMR spectrum (25°C, d_8-thf, 500.12 MHz) of **2**.

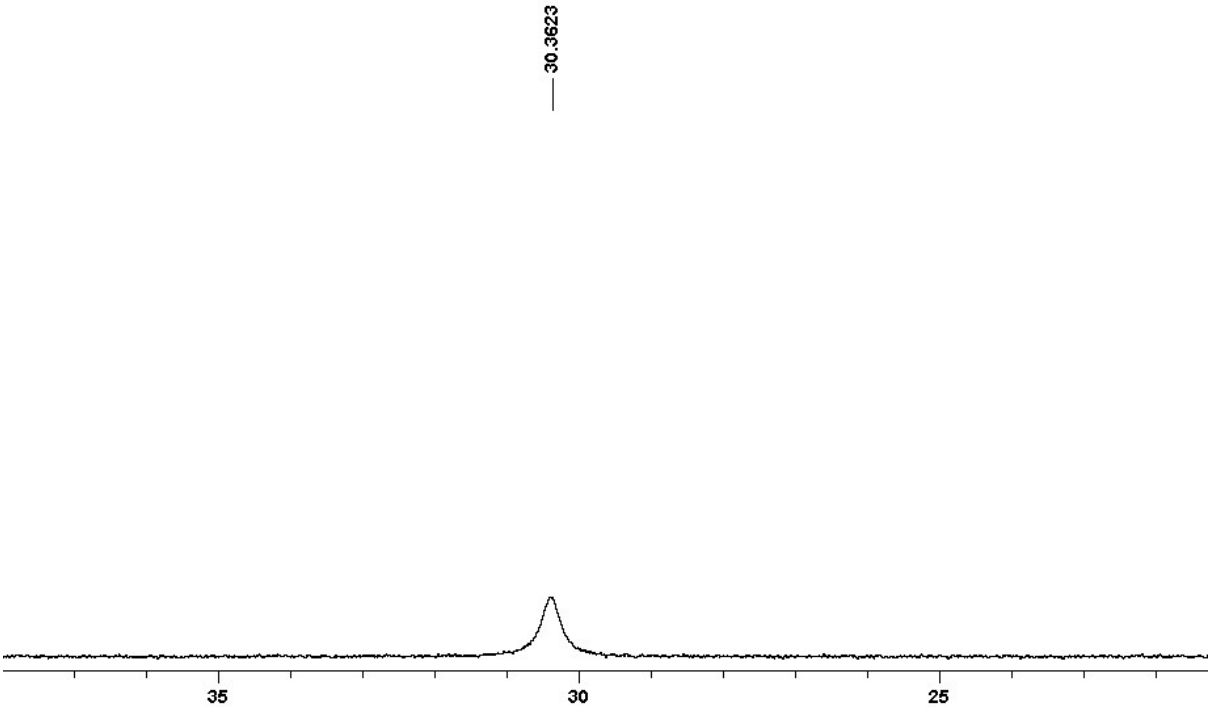
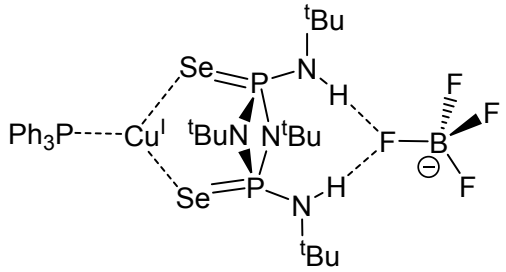


Figure S4: ^{31}P NMR spectrum (25°C, d_8-thf, 202.48 MHz) of **2**.



Synthesis of 4: To solution of **3** (50 mg, 0.1 mmol) in 1 ml CH_2Cl_2 was added $(Ph_3P)Cu(CH_3CN)_3(BF_4)$ (55 mg, 0.1 mmol, 1 eq) in 1ml CH_3CN. After 10 minutes the resulting

mixture was transferred to a crystallization tube and layered with approximately 10 ml of Et_2O. After 10 days at room temperature large colorless crystals formed which were suitable for X-ray crystallography. The crystals were isolated by filtration and dried *in vacuo* to yield **4** (69 mg, 0.75 mmol, 75%).

^{1}H NMR (25°C, CD_2Cl_2, 500.12 MHz): δ [ppm] =7.46 (t, $^3J_{HH}$= 7.4, 3H, PPh_3), 7.40 – 7.20 (m, 12H, PPh_3), 5.33 (s, 2H, NH), 1.71 (s, 18H, $^tBu_{endo}$), 1.54 (s, 18H, $^tBu_{exo}$).

^{31}P NMR (25°C, CD_2Cl_2, 202.48 MHz): δ [ppm] =18.64 (s, with two satellite doublets arising from [(^{77}Se=)HRN-P(μ-N^{t}Bu)P-NRH (=Se)], $^1J_{PSe}$ = 732 Hz, $^2J_{PP}$ = 25 Hz).

^{19}F NMR (25°C, CD_2Cl_2, 395.99 MHz): δ [ppm] = -150.59 (s), -150.63 (s).

Elemental analysis (%): calcd. for **4,** C44.4% H 5.8% N 6.1% found C 45.6% H 6.1% N 5.5%.

LRESI-MS (+ve ion): simul. (**4** - BF_4)$^+$ 848.13, found 848.10.

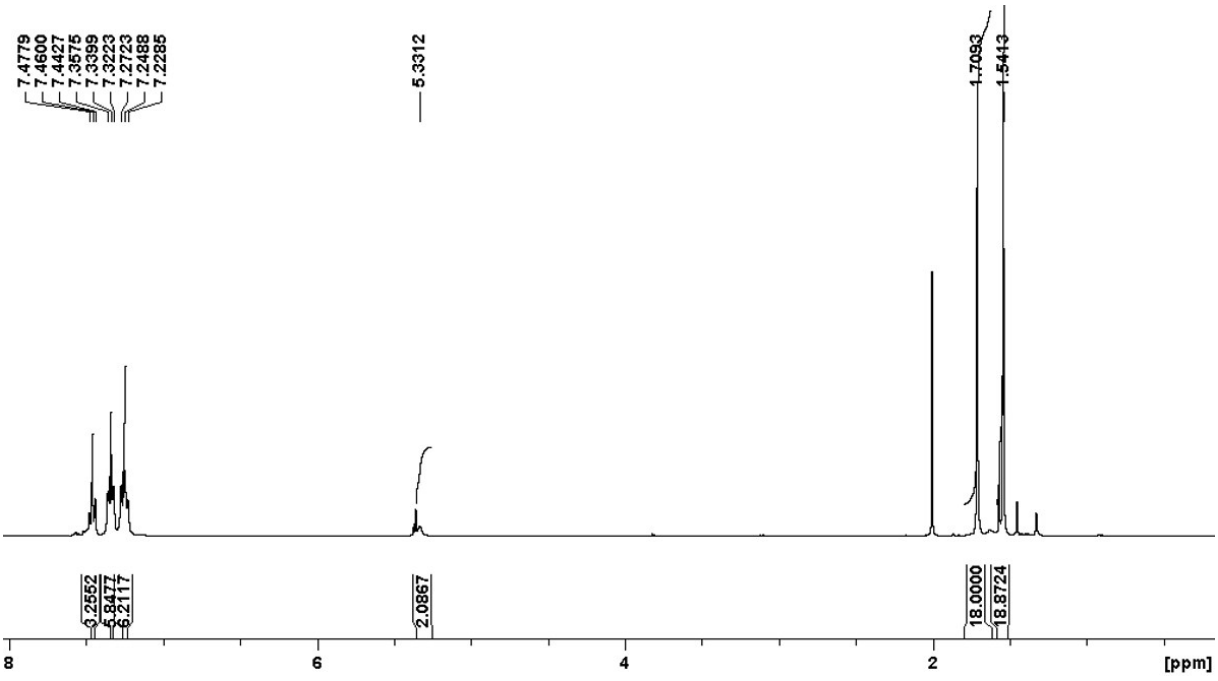


Figure S5: ^{1}H NMR spectrum (25°C, CD_2Cl_2, 500.12 MHz) of **4**: excess acetonitrile at 2.1ppm.

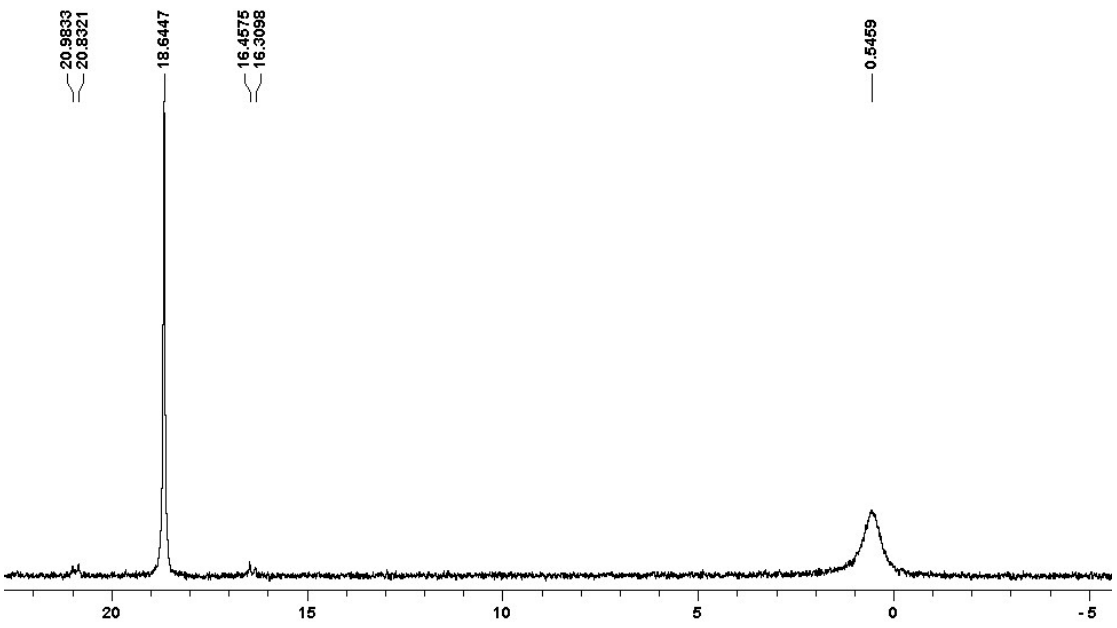


Figure S6: ^{31}P NMR spectrum (25°C, CD_2Cl_2, 202.48 MHz) of **4**.

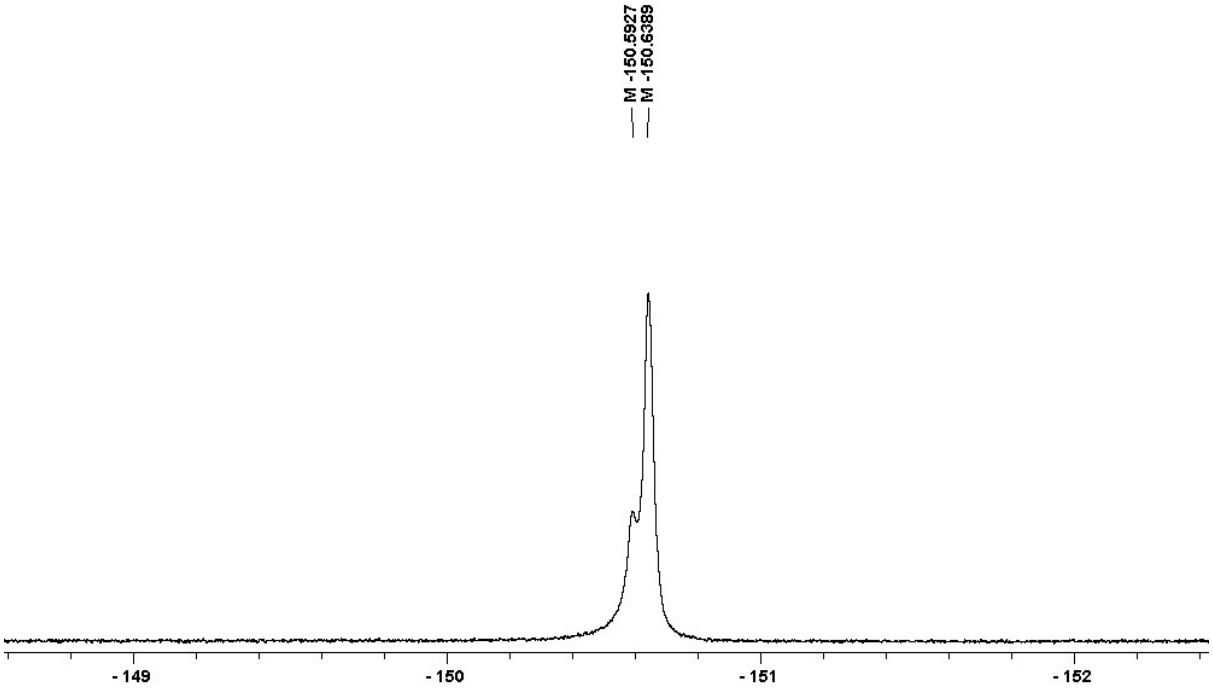
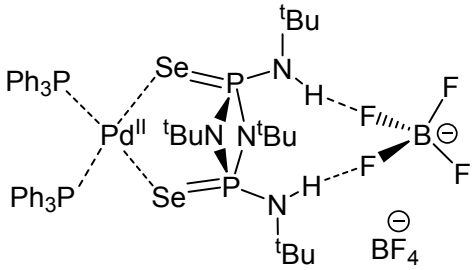


Figure S7: ^{19}F NMR spectrum (25°C, CD_2Cl_2, 375.99 MHz) of **4**.



Synthesis of 5: To solution of **3** (50 mg, 0.1 mmol) in 1 ml CH_2Cl was added $(Ph_3P)_2Pd(CH_3CN)_2(BF_4)_2$ (92 mg, 0.1 mmol, 1 eq) in 1ml CH_2Cl_2. After 10 minutes the resulting orange mixture was transferred to a crystallization tube and layered with approximately 10 ml of pentane. After 3 days at room temperature large orange crystals formed which were suitable for X-ray crystallography. The crystals were isolated by filtration and dried *in vacuo* to yield **5**·CH_2Cl_2. (126 mg, 0.95 mmol, 95%).

^{1}H NMR (25°C, CD_2Cl_2, 500.12 MHz): δ [ppm] = 7.62-7.51 (m, 6H, PPh_3), 7.40 -7.27 (m, 24H, PPh_3), 5.62 (s, 2H, NH), 1.69 (s, 18H, ^{t}Bu$_{endo}$), 1.19 (s, 18H, ^{t}Bu$_{exo}$).

^{31}P NMR (25°C, CD_2Cl_2, 202.48 MHz): δ [ppm] = 27.3 (AA'XX'), 17.61 (AA'XX').

^{19}F NMR (25°C, CD_2Cl_2, 395.99 MHz): δ [ppm] = -150.05 (s), -150.10 (s).

Elemental analysis (%): calcd. for **5**·CH_2Cl_2, C 45.6% H 5.0% N 4.0%, found C46.0% H 5.2% N 3.7%.

LRESI-MS: simul (**5**-BF_4)$^+$ 1255.23, found 1225.17.

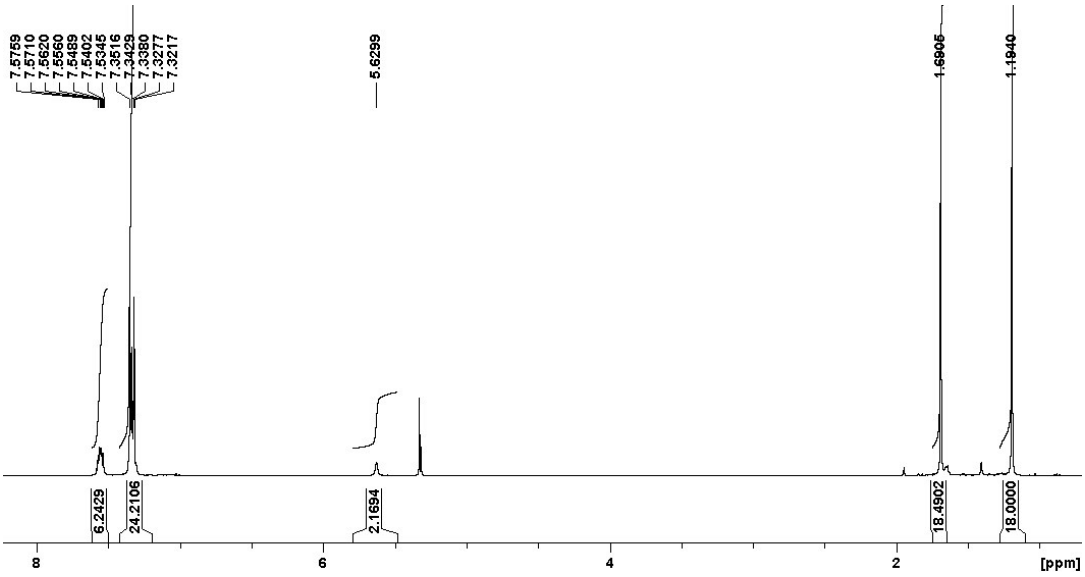


Figure S8: ^{1}H NMR spectrum (25°C, CD_2Cl_2, 500.12 MHz) of **5**·CH_2Cl_2

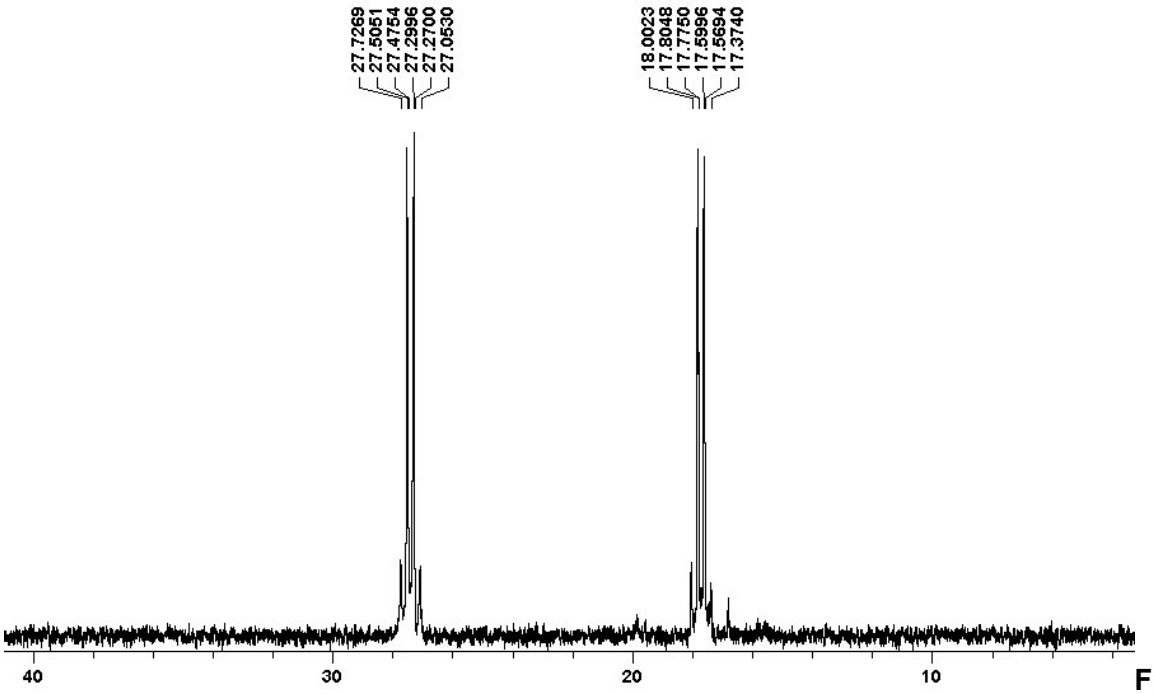


Figure S9: ^{31}P NMR spectrum (25°C, CD_2Cl_2, 202.48 MHz) of **5**·CH_2Cl_2

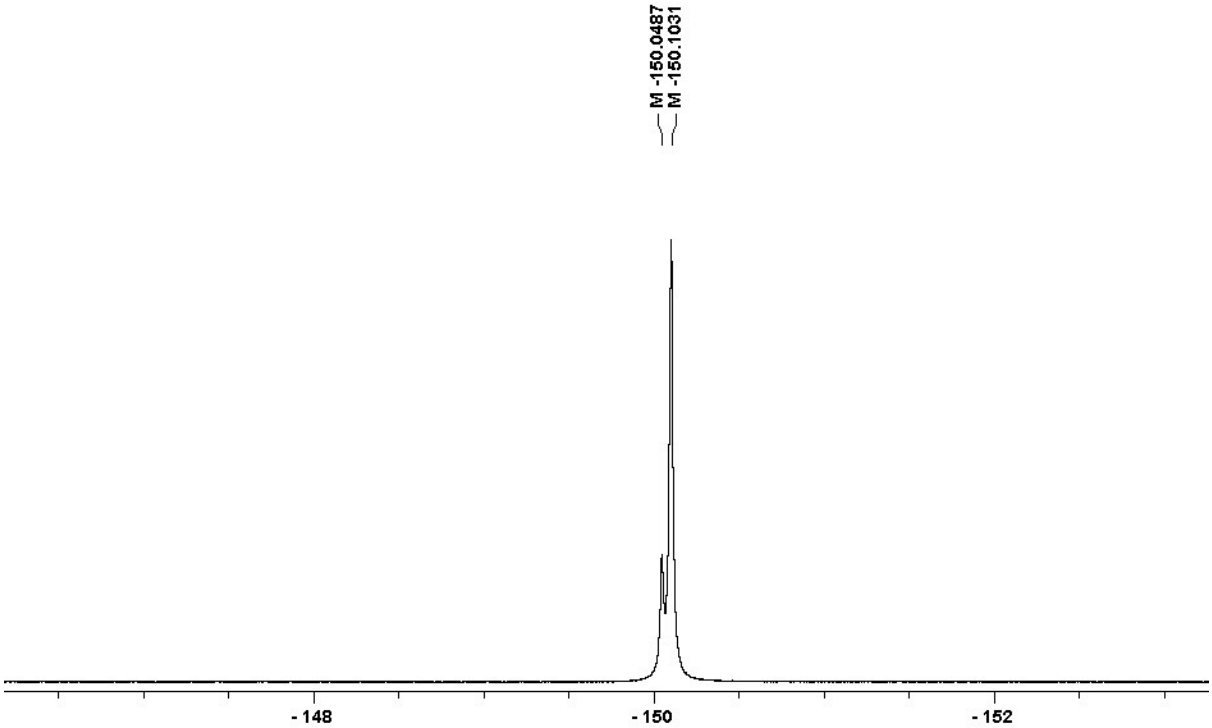


Figure S10: ^{19}F NMR spectrum (25°C, CD_2Cl_2, 375.99 MHz) of **5**·CH_2Cl_2

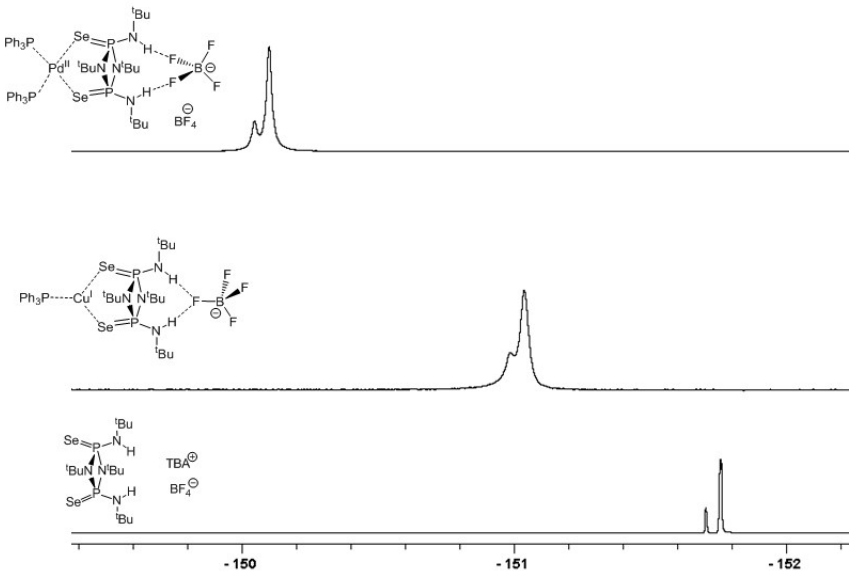


Figure S11: ^{19}F NMR spectra (25°C, CD_2Cl_2, 375.99 MHz) of **3** (in the presence 2 equiv of $TBABF_4$), **4** (in the presence equiv of $TBABF_4$)and **5** (from bottom to top). $TBABF_4$ was added so that all receptors are in presence of two equivalents tetrafluoroborate. The chemical shift for the BF_4^- anion in the presence of **3** is the same as that of the free anion, suggesting that no binding of the anion occurs to **3**

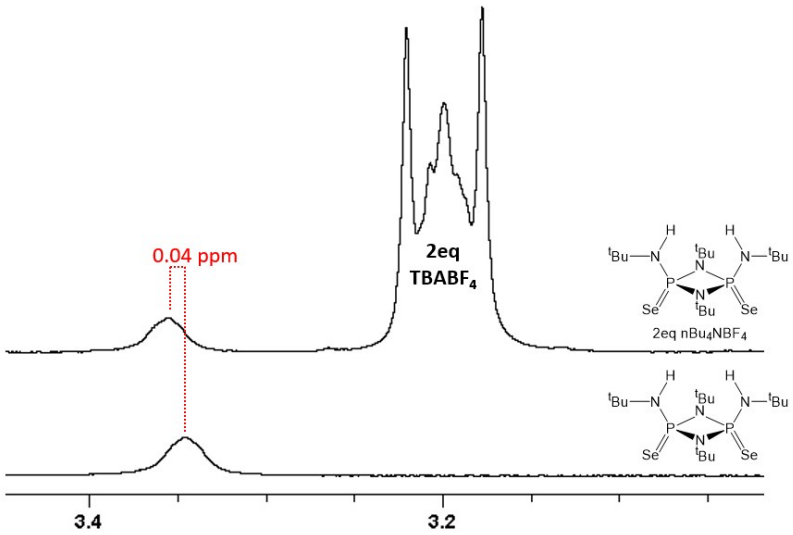


Figure S12: Overlaid ^1H NMR spectra (25°C, CD_2Cl_2, 400 MHz) of **3** (bottom) and **3** in presence of two equivalents $TBABF_4$

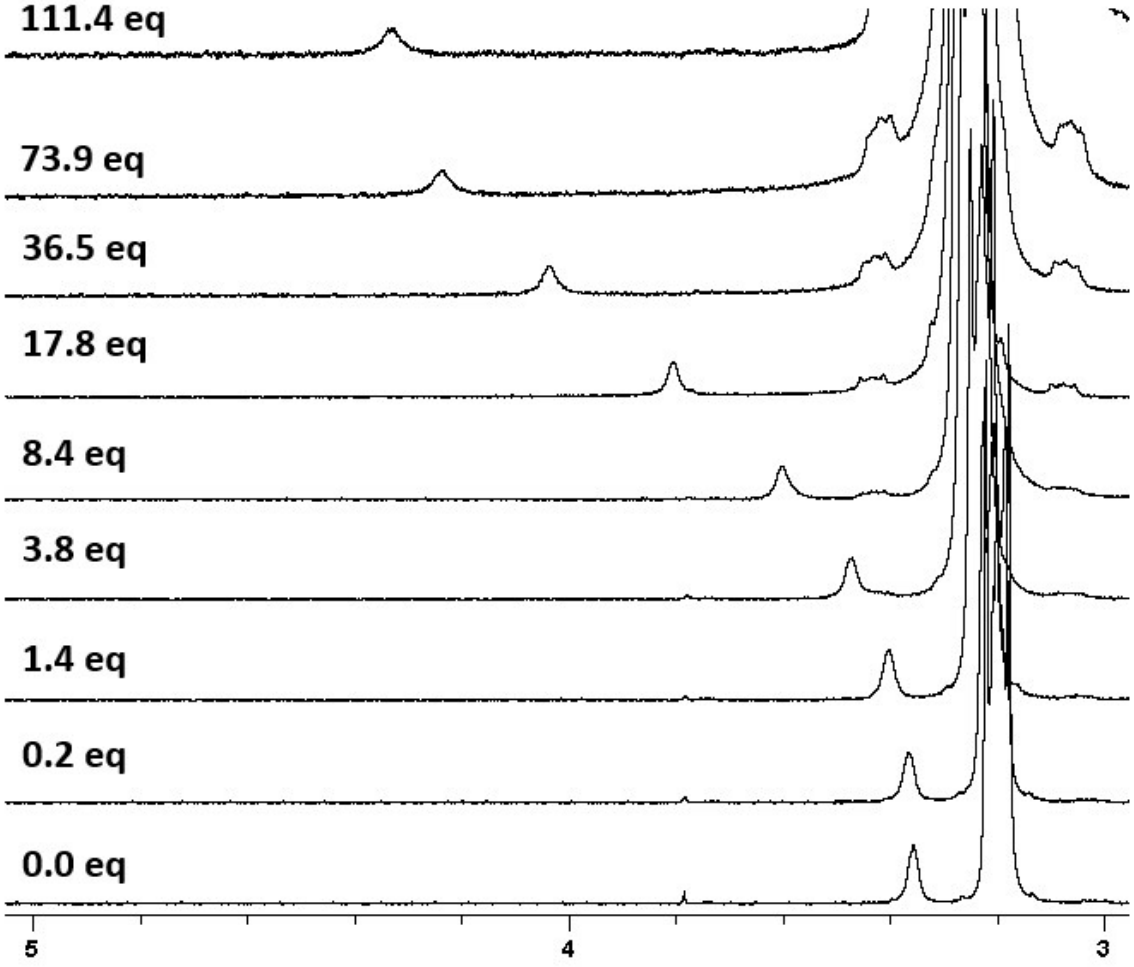


Figure S13: ^{1}H NMR titration (25°C, CD_2Cl_2, 400 MHz) of **3** with increasing amounts of $TBANO_3$ in presence of two equivalents $TBABF_4$

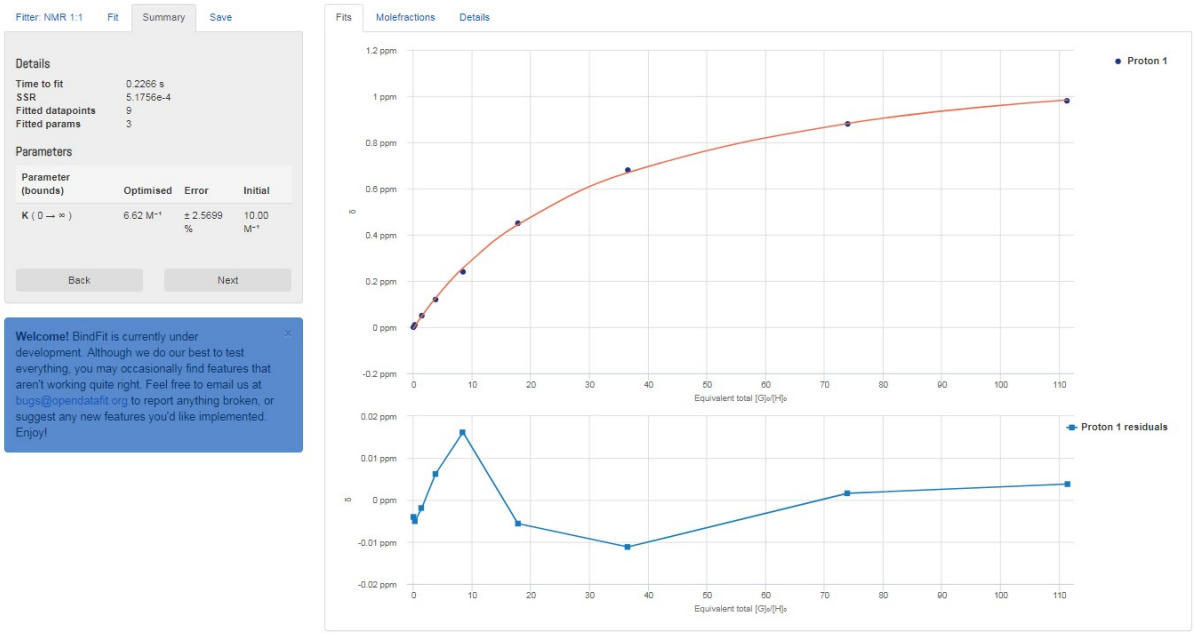


Figure S14: Binding isotherm (1:1 system) fitted to the ^{1}H NMR chemical shift of the NH protons in **3** vs. the equivalents of $TBANO_3$ added (top). The residual plot from the fit (bottom).[7]

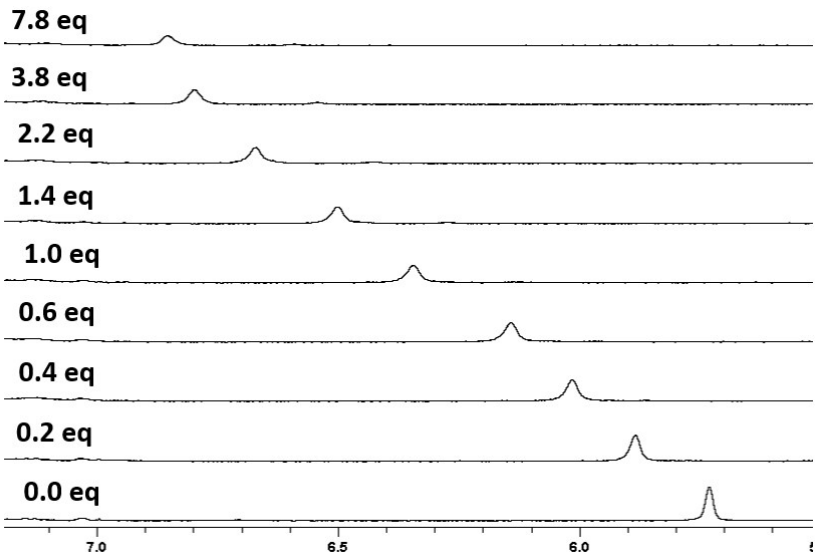


Figure S15: ^{1}H NMR titration (25°C, CD_2Cl_2, 400 MHz) of **5** with increasing amounts of $TBANO_3$

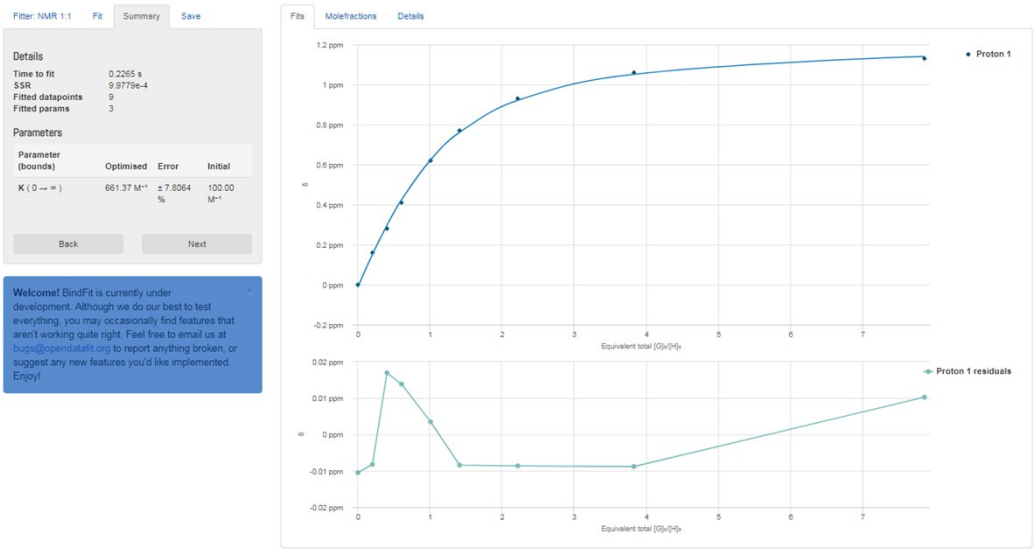
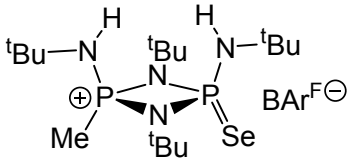


Figure S16: Binding isotherm (1:1 system) fitted to the ^{1}H NMR chemical shift of the NH protons in **5** vs. the equivalents of $TBANO_3$ added (top). The residual plot from the fit (bottom). [7]



Synthesis of 6: Inside a N_2 filled glovebox, a Schlenk flask was filled with 491mg [^{t}BuNH(Me-)P(μ-N^{t}Bu)$_2$PNH^{t}Bu]I (1mmol, 1 equivalent) and 200mg Selenium (excess) and transferred to a Schlenk line. 50ml of THF were added and the resulting suspension was stirred at room temperature for 72h. Afterwards the suspension was filtered in air to remove unreacted selenium. All volatiles were removed *in vacuo* yielding a white solid which was redissolved in 50ml of 1:1 THF/CH_2Cl_2. SodiumBAr^{F} (886 mg, 1mmol, 1 equivalent) was added to the solution and the mixture was stirred for 2h at room temperature yielding a white suspension. The suspension was filtered and all solvent was removed in vacuum yielding **6** as a white solid (1.23g, 0.95mmol, 95%)

^{1}H NMR (25°C, $CDCl_3$, 400 MHz): δ [ppm] = 7.69 (s, 8H, Bar^{F}), 7.53 (s, 4H, Bar^{F}), 3.43 (s, 1H, SePN**H**), 3.30 (d, J_{PH} = 18Hz, 1H, MePN**H**)**,** 2.15 (d, J_{PH} = 20 Hz, 3H, **Me**P)**,** 1.59 (s, 18H, ^{t}Bu), 1.58 (s, 9H, ^{t}Bu), 1.47 (s, 9H, ^{t}Bu)

^{31}P NMR (25°C, $CDCl_3$, 202.48 MHz): δ [ppm] = 25.3 (s), 25.1 (s)

^{19}F NMR (25°C, $CDCl_3$, 395.99 MHz): δ [ppm] = 62.4 (s).

Elemental analysis (%): calcd. for **6** C 45.1%, H 4.1%, N 4.3%, found C 44.7, H 4.1%, N 4.1%.

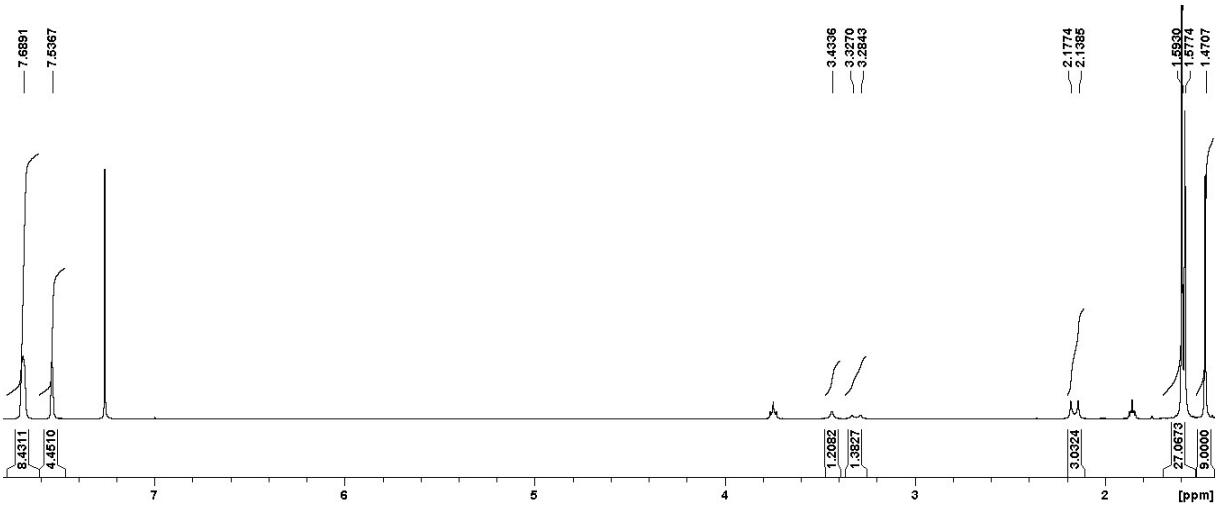


Figure S17: ^{1}H NMR spectrum (25°C, $CDCl_3$, 500.12 MHz) of **6;** residual THF at 1.45 and 3.73 ppm

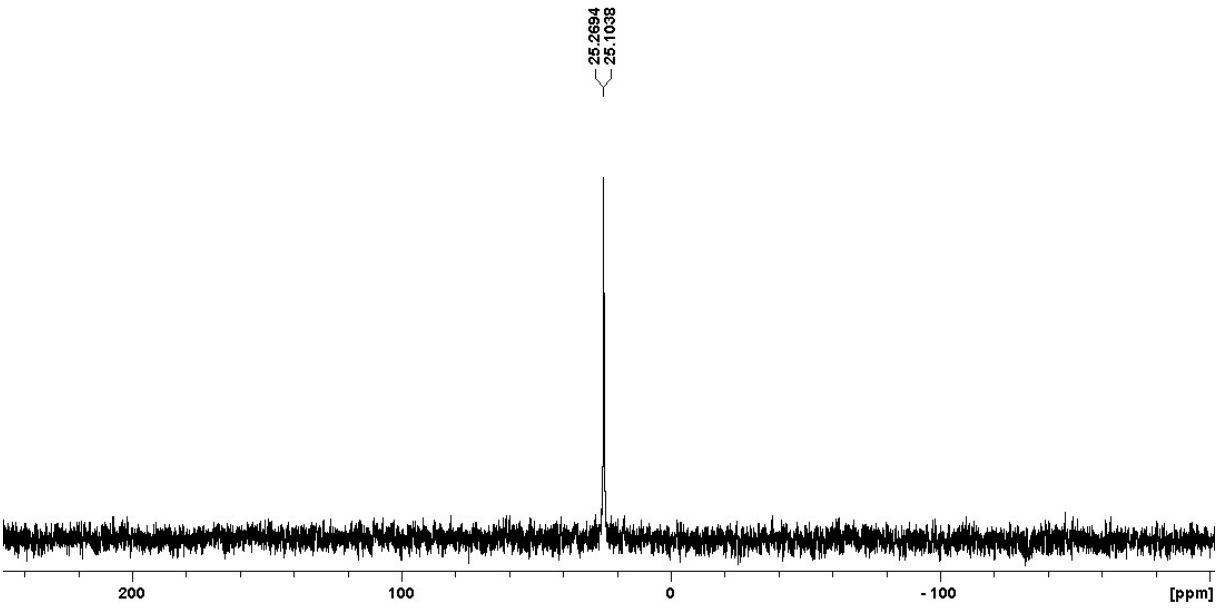


Figure S18: ^{31}P NMR spectrum (25°C, $CDCl_3$, 202.48 MHz) of **6**

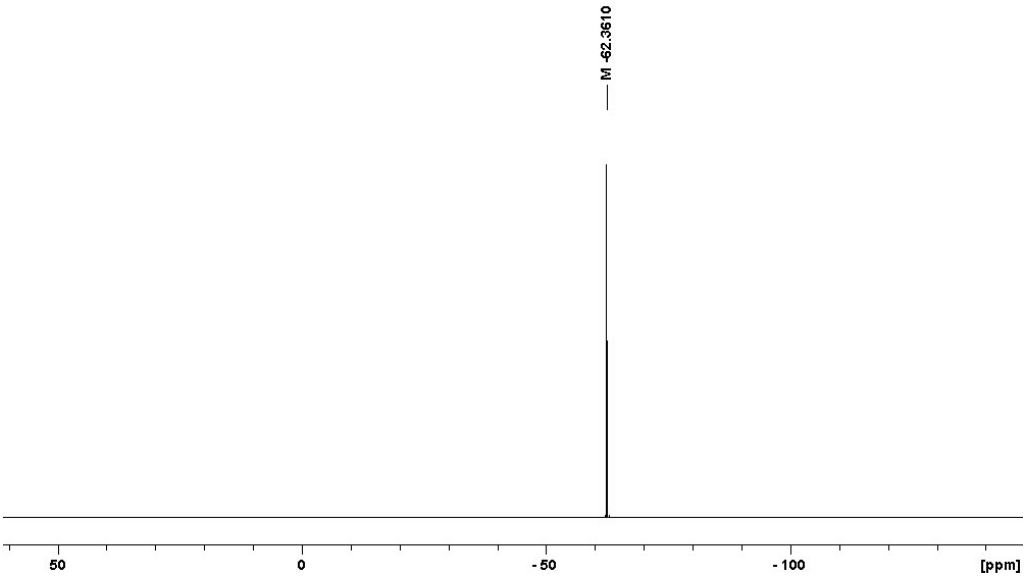


Figure S19: ^{19}F NMR spectrum (25°C, $CDCl_3$, 375.99 MHz) of **6**

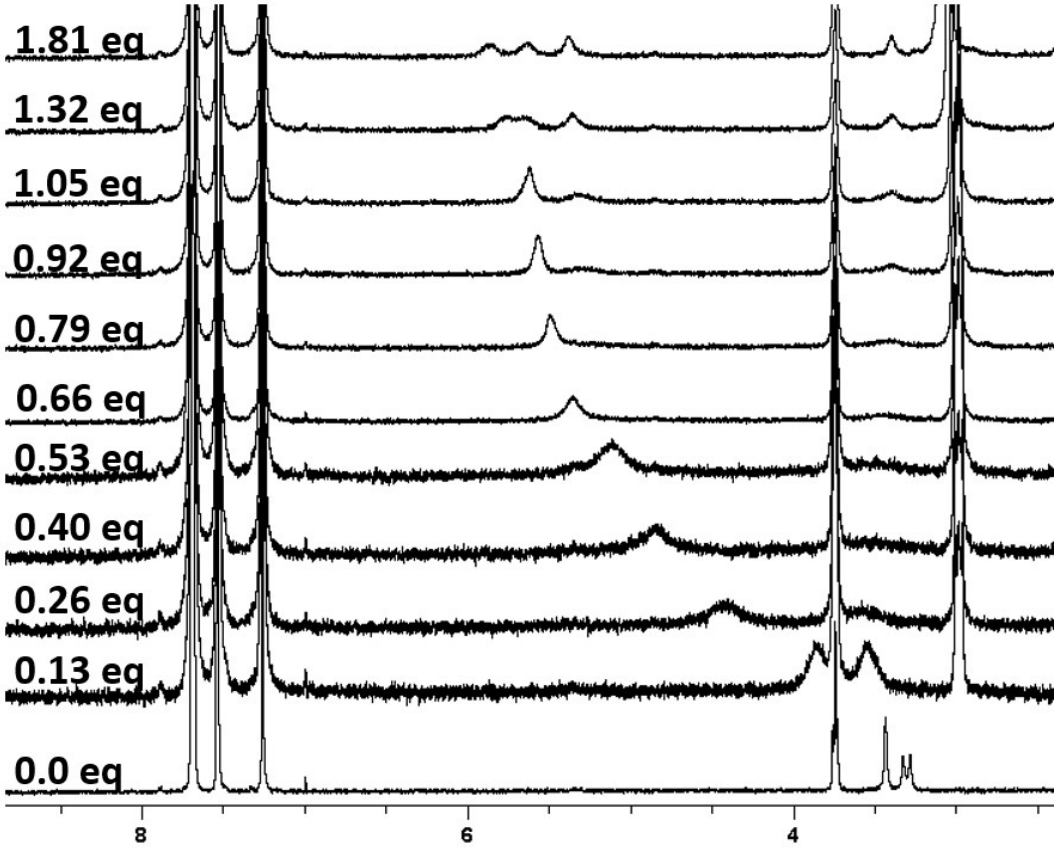


Figure S20: ^1H NMR titration (25°C, CD_2Cl_2, 400 MHz) of **6** with increasing amounts of $TBABF_4$.

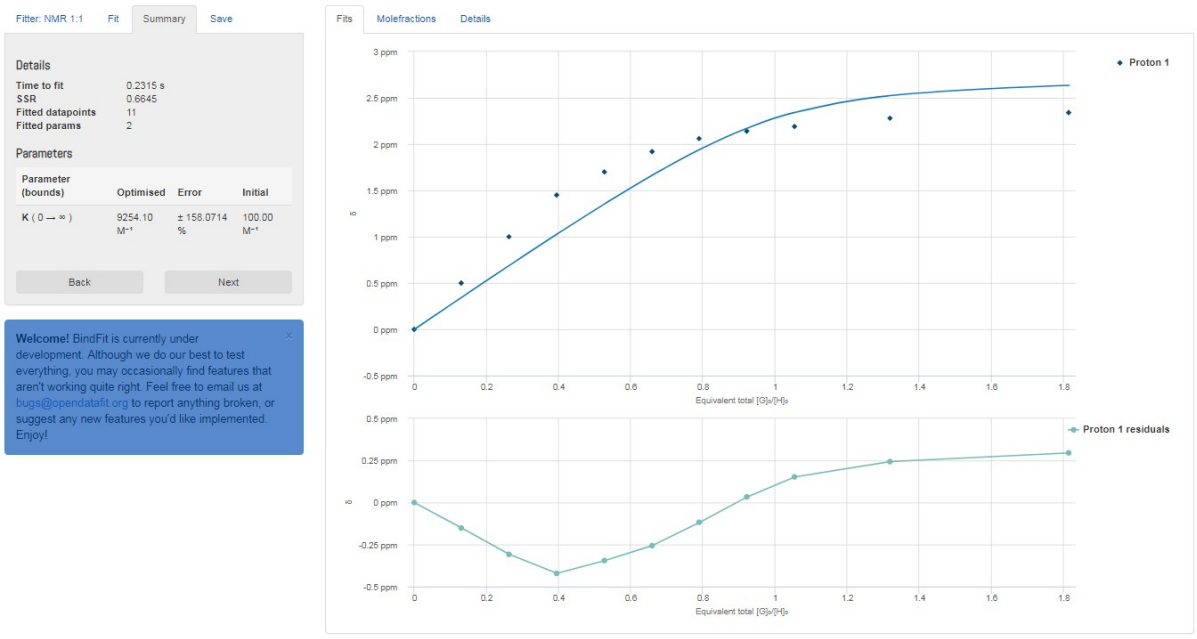


Figure S21: Binding isotherm (1:1 system) fitted to the ^{1}H NMR chemical shift of the NH protons in **6** vs. the equivalents of $TBABF_4$ added (top). The residual plot from the fit (bottom).[7]

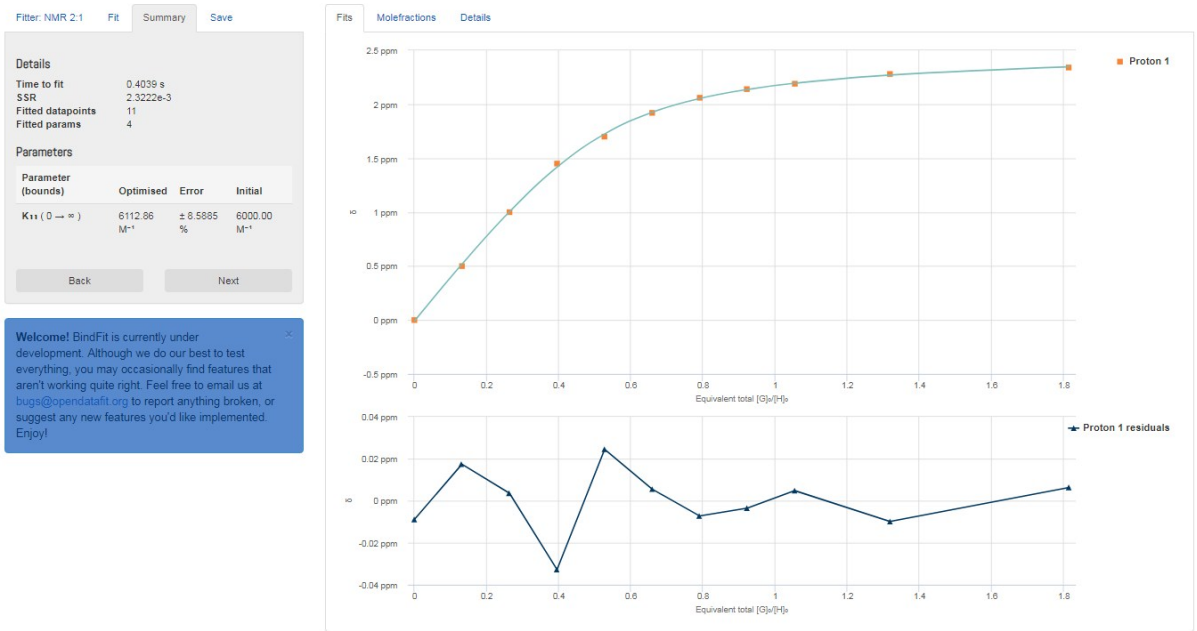


Figure S22: Binding isotherm (2:1 system, non cooperative) fitted to the ^{1}H NMR chemical shift of the NH protons in **6** vs. the equivalents of $TBABF_4$ added (top). The residual plot from the fit (bottom); note that attempting other fits (1:2, 2:1 cooperative failed).[7]

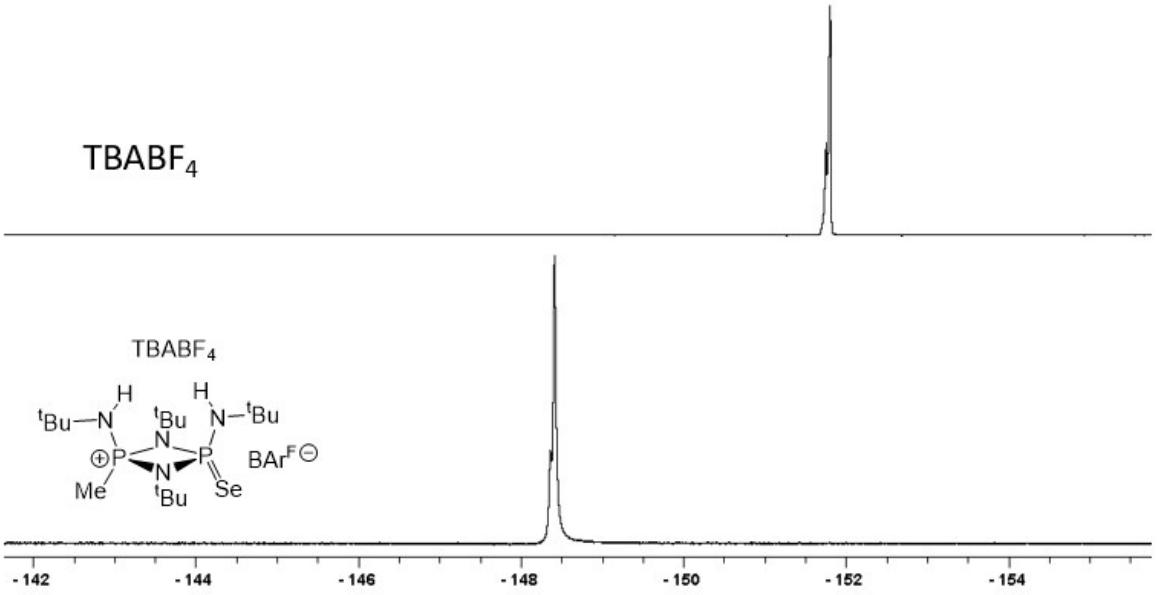


Figure S23: ^{19}F NMR spectra (25°C, $CDCl_3$, 375.99 MHz) of **6** (in the presence 1 equiv of $TBABF_4$) and $TBABF_4$.

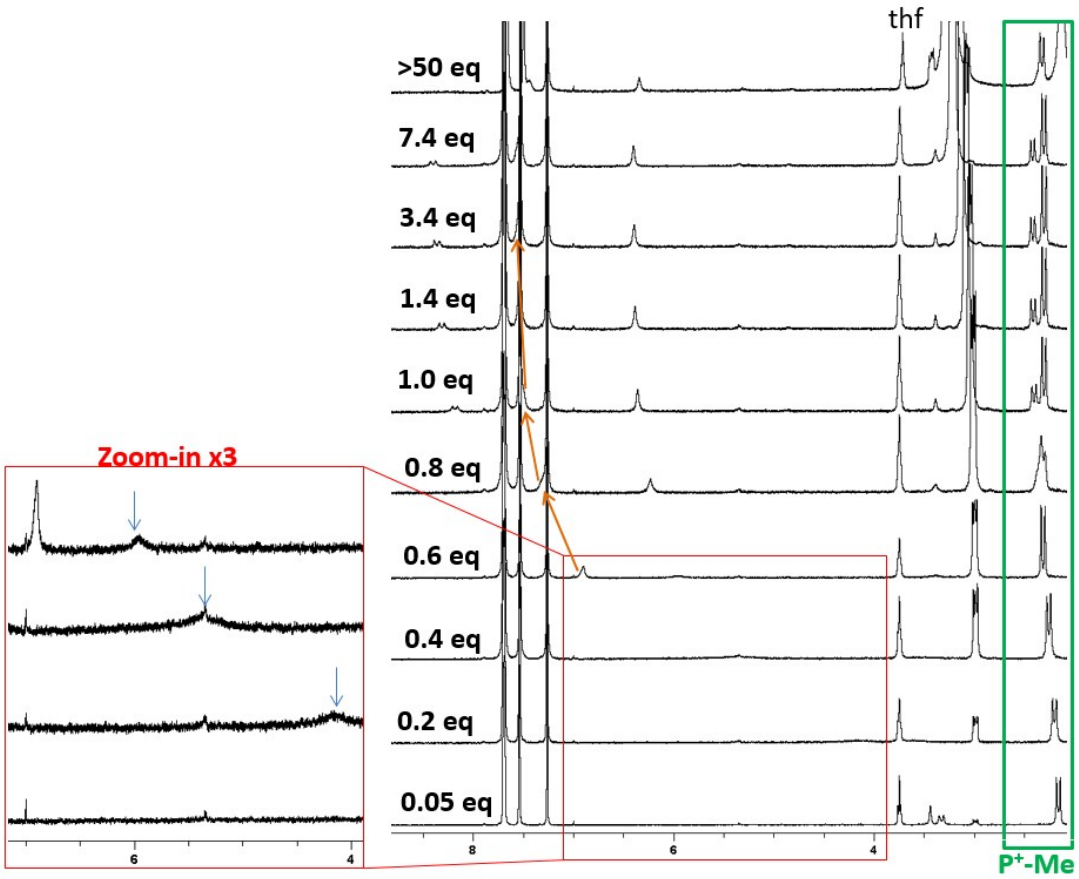


Figure S24: ^1H NMR titration (25°C, CD_2Cl_2, 400 MHz) of **6** with increasing amounts of $TBANO_3$

1 Tristram Chivers, Mark Krahn, and Masood Parvez and G. Schatte, , DOI:10.1021/IC001093O.
2 T. Roth, H. Wadepohl, D. S. Wright and L. H. Gade, *Chemistry - A European Journal*, 2013, **19**, 13823–13837.
3 C. G. M. Benson, V. Vasilenko, R. García-Rodríguez, A. D. Bond, S. González Calera, L. H. Gade, D. S. Wright *Dalton Trans.*, 2015, **44**, 14242–14247.
4 G. R. Lief, C. C. Carrow, D. F. Moser and L. Stahl, *Phosphorus, Sulfur, and Silicon and the Related Elements*, 2001, **168**, 157–162.
5 S. Oi, K. Kashiwagi and Y. Inoue, *Tetrahedron Letters*, 1998, **39**, 6253–6256.
6 J. Manzur, A. Vega, A. M. García, C. Acuña, M. Sieger, B. Sarkar, M. Niemeyer, F. Lissner, T. Schleid and W. Kaim, *European Journal of Inorganic Chemistry*, 2007, **2007**, 5500–5510.
7 P. Thordarson, *Chem. Soc. Rev.*, 2011, **40**, 1305–1323.

Single-crystal X-ray diffraction and structure refinement

X-ray crystallographic data were collected using a D8-QUEST PHOTON-100 diffractometer equipped with an Incoatec IμS Cu microsource (Cu Kα, λ= 1.5418 Å). The temperature was held at 180(2) K using an Oxford Cryosystems N_2 cryostat. Data integration and reduction were undertaken with *SAINT* in the *APEX3* software suite. Multi-scan corrections were applied using SADABS. Structures were solved using *SHELXT* and refined using *SHELXL*.

1: The structure contains layers of polymers, interspersed with layers of THF molecules. One molecule (O1S) accepts hydrogen bonds from the NH_2 groups of the polymers and is (consequently) well defined. All non-H atoms sit on a mirror plane, so the molecule appears flat. It was felt unnecessary to split atoms across the mirror plane to define a more realistic geometry. This molecule is refined with anisotropic ADPs. The other molecules lie on two sites, both "perpendicular" to the mirror plane. One of these (O1T/O1U) is modelled as two components, both defined as complete molecules, with the site occupancy of all atoms constrained to 0.25. Hence, this gives 2*(2*0.25) = 1 molecule on the site. The other site (O1X) is defined as a complete molecule with SOF constrained to 0.5 for all atoms. The action of the mirror gives 2*0.5 = 1 molecule. All THF molecules have all 1,2 and 1,3 distances restrained, and the disordered molecules (O1T/O1U/O1X) have a single common isotropic ADP refined. The disorder model seems to do a fair job of modelling the electron density in the THF regions. Omitting all THF molecules and applying *SQUEEZE* produces *R*1 = 0.0354, *wR*2 = 0.1002, which is comparable to the provided atomic model. *SQUEEZE* corrects for 202 electrons per cell, which equals 5 THF molecules, compared to 6 molecules if each site in the unit cell is fully occupied. The atomic model is preferred since the THF molecules clearly are an integral part of this structure.

4: Rotational disorder of BF_4^- anion is handled by defining multiple F sites. Atoms F4 and F4A are closely-spaced sites for one F atom. These site occupancies are constrained to FVAR and 1-FVAR for one free variable. Atoms F1-F3,F1A-F3A,F1B-F3B are refined as three groups, each with their own FVAR representing the sof of the group, with all three FVARs constrained to sum to 1.0 (via a SUMP restraint). All B-F bond lengths are restrained to a common refined value and all isotropic displacement parameters of the F atoms are constrained to a common FVAR. All of this is a best effort to represent the rotationally disordered anion in some reasonable way to provide a reasonable R-factor. The H atoms of the NH groups are visible in difference Fourier maps, and their positions are close to the idealised positions. The idealised positions and a riding model are applied in the final refinement. *checkCIF*/*PLATON* warns that there are small voids remaining in the structure. There is no sign of any significant electron density in these voids. The highest residual peaks in the structure are less than 1 $eÅ^{-3}$ and are associated with BF_4^- anion.

5: Both BF_4^- anions are rotationally disordered to some degree. Both were modelled with two well-defined sets of F atoms, each set having a common site occupancy factor, and with the SOFs for the two sets constrained to sum to unity. A single common isotropic ADP was refined for all of the F atoms. All B---F distances are restrained to a common refined value and all F...F distances are restrained to 1.633 times that value. A disordered dichloromethane molecule (one per asymmetric unit = 4 per cell) is clearly visible, but it was difficult to define discrete molecules with a reasonable geometry. *SQUEEZE* has therefore been applied. *SQUEEZE* corrects for the expected 4 dichloromethane molecules per unit cell (172 electrons corrected vs 168 calculated).

Summary of crystallographic data

	1	**4**	**5** *SQUEEZE* applied
CCDC number	1890515	1890518	1890520
Cambridge data number	DW_B1_0182	DW_B1_0268	DW_B1_0262
Chemical formula	$C_{20}H_{46}ClCuN_4O_3P_2Se_2$	$C_{34}H_{53}BCuF_4N_4P_3Se_2$	$C_{53}H_{70}B_2Cl_2F_8N_4P_4PdSe_2$
Formula weight	709.46	918.98	1395.85
Temp / K	180(2)	180(2)	180(2)
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/m$	$P2_1/c$	$P2_1/n$
a / Å	10.2274(3)	11.3820(3)	10.8880(4)
b / Å	9.4057(3)	13.3316(3)	19.8347(7)
c / Å	16.1265(5)	28.1088(7)	28.1508(9)
α / °	90	90	90
β / °	96.507(2)	98.8212(14)	90.458(2)
γ / °	90	90	90
Unit-cell volume / Å^3	1541.31(8)	4214.79(18)	6079.3(4)
Z	2	4	4
Calc. density / g cm^{-3}	1.529	1.448	1.525
F(000)	724	1872	2824
Radiation type	Cu$K\alpha$	Cu$K\alpha$	Cu$K\alpha$
Absorption coefficient / mm^{-1}	5.697	4.169	6.170
Crystal size / mm^3	0.24 x 0.15 x 0.10	0.09 x 0.05 x 0.02	0.20 x 0.10 x 0.05
2-Theta range / °	5.52-133.42	6.36-133.46	5.45-133.62
Completeness to max 2-theta	0.990	0.996	0.993
No. reflections measured	17462	28136	46784
No. independent reflections	2890	7431	10690
R_{int}	0.0427	0.0606	0.0438
No. parameters / restraints	180 / 29	457 / 30	662 / 47
Final *R*1 values (I > 2σ(I))	0.0425	0.0410	0.0379
Final *wR*(F^2) values (all data)	0.0511	0.0638	0.0466
Goodness-of-fit on F^2	1.082	1.016	1.024
Largest difference peak & hole / eÅ^{-3}	0.787, -0.560	0.742, -0.625	1.210, -1.203

Single-crystal XRD data were solved and refined with *SHELXL/SHELXT/SQUEEZE*:

SHELXL: G. M. Sheldrick, *Acta Crystallogr. Sect. C,* 2015, **71**, 3–8
SHELXT: G. M. Sheldrick, *Acta Crystallogr. Sect. A,* 2015, **71**, 3–8.
SQUEEZE: A. L. Spek, *Acta Crystallogr. Sect. C,* 2015, **71**, 9–18.

Computations

1. Introduction

One of the most established computational approach to characterise the hydrogen bonding (H-bonding) interactions is Bader's Atoms in Molecules (AIM)[1]. In the AIM method, a bond or an interaction between a pair of atoms can be characterised by the properties of electron density at bond critical point (BCP). The BCP corresponds to the saddle point in the electron density in the space between the two interacting atoms. The strength of the H-bonding interaction can be classified according to the electron density, $\rho(r)$, at the BCP. ρ_{BCP} greater than 0.05 is a strong H-bonding interaction, between 0.02-0.05 is a moderate interaction and less than 0.02 is a weak interaction.[2]

Another popular approach to characterise the H-bonding interaction is *via* Natural Bond Orbital (NBO) analysis.[3] The NBO method transfers the delocalised molecular orbitals (MOs) to more localised orbitals, which is more related to the concept of a chemical bond. The H-bonding interaction can be computed by examining the delocalisation due to the intermolecular interactions between the filled and the antibonding orbital. The interaction strength can be quantified using $E^{(2)}$

$$E^{(2)} = q_i \frac{F(i,j)^2}{\epsilon_j - \epsilon_i}$$

where q_i is the donor orbital occupancy, $F(i,j)$ is the coupling NBO Fock matrix element and ϵ_i and ϵ_j are the orbital energies. The $E^{(2)}$ stabilisation energy has previously been shown to correlate with the strength of H-bonding interactions.[2,4,5]

The degree of charge transfer between the donor and the acceptor is another important measure of H-bonding interactions. For example, the charge transfer ranges from 0.003e for netural H_2O-NH_3 H-bond to 0.234e in very strong H-bond of $[F\text{-}H\text{-}F]^-$.[4] The NBO charge transfer in neutral H-bond has been successfully correlated with the associated energy.[6,7]

The present work investigates the ability of the $[^tBuNH(Se{=})P(\mu\text{-}N^tBu)]_2$ cyclodiphosphazane **3** to hydrogen bond depending on the receptor modulation via metal coordination in **4a**. The cyclodiphosphazane has also been made more electron deficient by increasing the oxidation state of the coordinating transition metal in **5a**. Furthermore, the P-N backbone has been made positively charge by replacing the Se atom with a methyl group for complex **6a**. The H-bonding ability has been tested by coordinating the metal-cyclodiphosphazane complexes to either BF_4^- or $BArF^-$ anions.

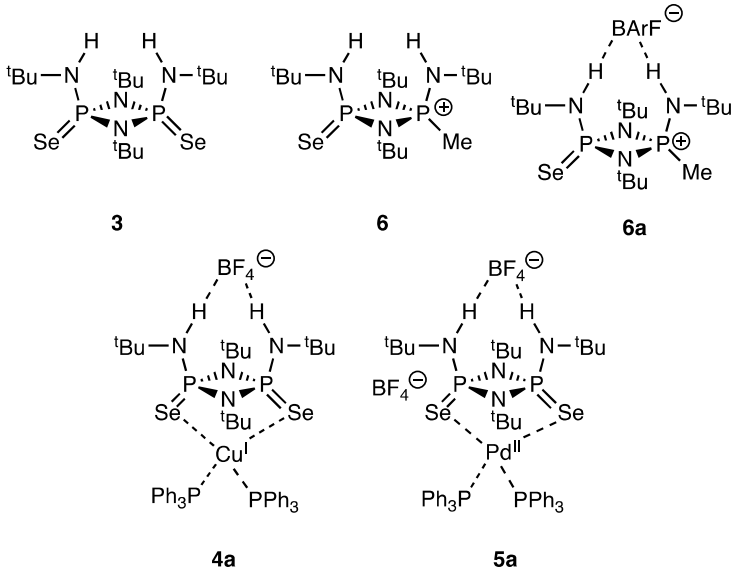


Figure S25. [tBuNH(Se=)P(μ-NtBu)]$_2$ cyclodiphosphazane complexes studied in the present work.

2. Computational Methods

All geometry optimisations were performed in Gaussian 16[8] package at B3LYP-D3/def2-sv(p) level of theory. The chosen method was the best compromise between the accuracy and the computational time. The frequency calculations were carried out on the optimised geometries to ensure the structures are optimised to the energy minimum. The topology analysis were done using the Multiwfn package.[9] The molecular orbitals were visualised using the IQmol[10] open source package. The overall charge of the complexes were kept neutral to allow the results to be comparable between them.

3. Results and Discussion

3.1. Optimised Geometries

The conformational searching for structures **4**, **5**, and **6** were performed by placing the anions at different locations around the cationic cyclodiphosphazane or cyclodiphosphazane-metal complex. The lowest free energy ion complexes are shown in Figure 2. The BF_4^- and the $BArF^-$ anions are located at the N-H receptors in the most stable structures for all four complexes. The relative free energy of all complexes are reported in ESI. Complexation of the transition metal increased the hydrogen bonding N-H bond lengths slightly in **4a** and **5a**.

The association free energies are calculated as: $G_a = G(anion - cyclophoshadizane\ complex) - G(anions) - G(cyclophosphadizane\ complex)$, Table 1. The large association energies are typical for an ionic salt in gas phase.[11] The association energy for complex **5a** is more than twice the value of **4a** and **6a**, because of the increased oxidation state of the transition metal and the additional BF_4^- anion.

Complex	ΔG_a / kJ mol^{-1}
4a	-373.61
5a	-871.34
6a	-246.06

Table 1. Stabilisation free energies of optimised complexes

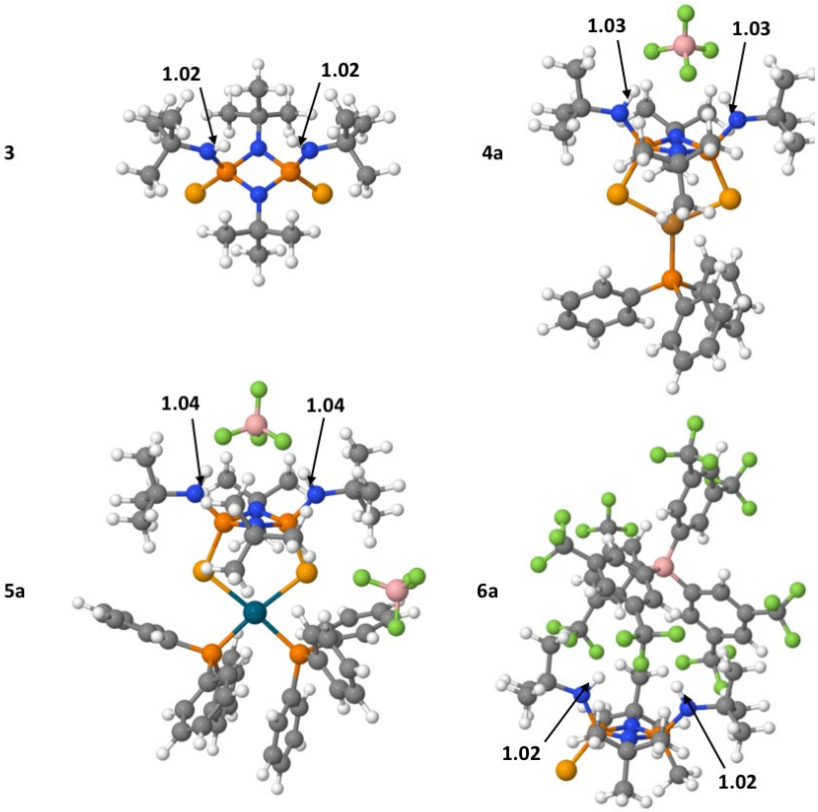


Figure S26. Optimised [tBuNH(Se=)P(μ-NtBu)]2 cyclodiphosphazane complexes

3.2. H-bonding Interactions

The NBO analysis for complex **4a** shows the majority of the H-bonding interaction comes from the donation of lone pair electrons from the BF_4^- fluorine atoms to the N-H σ* orbitals in the cyclodiphosphazane. N-H σ* interactions accounted for 40.51 kcal mol^{-1} out of 49.40 kcal mol^{-1} interaction strength. The fluorine lone pair donation to C-H σ* of cyclodiphophazane is not negligible at 8.15 kcal mol^{-1}. The fluorine lone pairs can also interact with the other σ* orbitals in the P-N ring but their overall contributions are very small compared to N-H σ* and C-H σ* interactions.

Interaction	$E^{(2)}$ / kcal mol$^-$	N(int)

	[1]	
n(F) → σ*(N35-H36)	21.62	11
n(F) → σ*(N33-H34)	18.89	11
Σn(F) → σ*(C-H)	8.15	20
Σn(F) → σ*(P-N)	0.25	4
Σn(F) → σ*(P-Se)	0.40	3
Σn(F) → σ*(N-C)	0.09	1
Total	**49.40**	**50**

Table 2 NBO interaction summary for complex **4a**. N(int) is number of such interactions found in the complex.

The NBO analysis for complex **5a** shows the overall H-bonding interaction energy has increased compared to the complex **4a** by 8.89 kcal mol^{-1}. The majority of the H-boning interaction energy also comes from the lone pair electron donation from the fluorine atom to N-H σ* orbitals. N-H σ* interactions accounts for 51.65 kcal mol^{-1} of the total $E^{(2)}$energy. The lone pair donation to C-H and the other σ* orbitals around the P-N backbone remained at about the same level as the complex **4a**. Therefore, the increase in H-bonding interactions in **5a** came from the enhanced ability of the N-H σ* orbitals to accept electrons from the fluorine lone pairs. The result also supports the increased H-H bond length in **5a**.

Interaction	**$E^{(2)}$ / kcal mol^{-1}**	**N(int)**
n(F) → σ*(N35-H36)	27.65	9
n(F) → σ*(N33-H34)	24.00	10
Σn(F) → σ*(C-H)	6.19	15
Σn(F) → σ*(P-N)	0.23	4
Σn(F) → σ*(P-Se)	0.15	2
Σn(F) → σ*(N-C)	0.07	1
Total	**58.29**	**41**

Table 3. NBO interaction summary for complex **5a**. N(int) is number of such interactions found in the complex.

The NBO analysis of complex **6a** shows a different behaviour from complex **4a** and **5a**. The overall H-bonding $E^{(2)}$ stabilisation is less than the like charged complex **4a** at 21.69 kcal mol^{-}

[1]. The N-H σ* interaction now accounts for 11.45 kcal mol^{-1} out of the 21.69 kcal mol^{-1} total. The total C-H σ* interactions sum to 8.35 kcal mol^{-1}. Therefore, the contribution of the C-H σ* interactions to the overall H-bonding between the anion and the cation has now increased. The number possible cyclodiphosphazane C-H interactions with the $BArF^-$ anion is significantly higher at 36 compared to 20 and 15 in the BF_4^- complexes and thus the contribution increases. The size of the $BArF^-$ anion is much larger than the pocket containing the N-H bonds in the cyclodiphosphazane. Therefore, the ^{t}Bu groups in the cyclodiphosphazane can now interact more readily with the anion than in **4a**. Furthermore, the decreased N-H σ* interaction also originates from the charge density of the anion but will be considered in more detail in section 3.4. The results support the observation that the N-H bond length in **6a** is shorter than **4a**. The donation of the π electrons from the phenyl to the C-H σ* is a new interaction mode, unobserved in complex **4a** and **5a**. The interaction accounted for 1.47 kcal mol^{-1} out of 21.69 kcal mol^{-1} total but nevertheless is the third strongest interaction between the anion and the cation.

Interaction	**$E^{(2)}$ / kcal mol^{-1}**	**N(int)**
n(F) → σ*(N32-H33)	7.44	3
n(F) → σ*(N34-H35)	4.01	4
Σπ(C-C) → σ*(C-H)	1.47	3
Σn(F) → σ*(C-H)	8.35	36
Σn(F) → σ*(P-N)	0.07	1
Σn(F) → σ*(P-C)	0.10	1
Σn(F) → σ*(C-C)	0.25	3
Total	**21.69**	**51**

Table 4. NBO interaction summary for complex **6a**. N(int) is number of such interactions found in the complex.

The topology analysis for the complex **4a** showed the average electron density at BCP was 0.033e for N-H···F interaction and 0.009e for C-H···F interaction. Therefore, the N-H···F interaction shows moderate H-bonding strength and the C-H···F interaction shows weak H-bonding strength. The average electron density at BCP increases for both N-H···F and C-H···F interactions in complex **5a**. The complex **5a** is able to from stronger H-bonds with the BF_4^- anion. Furthermore, the sum of the electron density over all BCP shows an increase from 0.119e in complex **4a** to 0.126e in **5b**, also reflecting on the increased H-bonding strength.

H-Bond Donor	**H-Bond Acceptor**	**$\Sigma(\rho_{BCP})$/e**	**$\mu(\rho_{BCP})$/e**

N-H	F	0.066	0.033
C-H	F	0.053	0.009
Total		0.119	

Table 5. Topology analysis for complex **4a**. $\Sigma(\rho_{BCP})$ is the sum of the electron density and $\mu(\rho_{BCP})$ is the average electron density at the BCP.

H-Bond Donor	**H-Bond Acceptor**	**$\Sigma(\rho_{BCP})$/e**	**$\mu(\rho_{BCP})$/e**
N-H	F	0.079	0.040
C-H	F	0.047	0.009
Total		0.126	

Table 6. Topology analysis for complex **5a**. Σ(ρBCP) is the sum of the electron density and μ(ρBCP) is the average electron density at the BCP.

For complex **6a**, the average electron density at the BCP for N-H and C-H interaction is less than **4a** at 0.018e and 0.006e, respectively. The H-bonding interaction strength is weaker, in agreement with the NBO results. However, the sum of the electron density is greater than complex **4a** at 0.155e. The difference arise because the NBO method is able to detect long range H-bonding interactions but the AIM method only detects the nearby interactions, Figure 3. The electron density at the BCP depends exponentially on the atom-atom distance and therefore decreases rapidly with the increasing separation.[12] The $\Sigma\rho_{BCP}$ for N-H interaction is less than the C-H interaction in **6a** whereas the NBO analysis shows the summed fluorine lone pair donation to σ*(N-H) is stronger than σ*(C-H). The AIM method only found the N-H interaction with the nearest fluorine atoms whereas the NBO detected the interaction with fluorine lone pairs further away. Nevertheless, the average BCP electron density correctly predicts the N-H interaction to be stronger as in complex **4a** and **5a**.

H-Bond Donor	**H-Bond Acceptor**	**$\Sigma(\rho_{BCP})$**	**$\mu(\rho_{BCP})$**
N-H	F	0.036	0.018

C-H	F	0.088	0.006
C-H	π(Ph)	0.032	0.006
Total		0.155	

Table 7. Topology analysis for complex **6a**. Σ(ρBCP) is the sum of the electron density and μ(ρBCP) is the average electron density at the BCP.

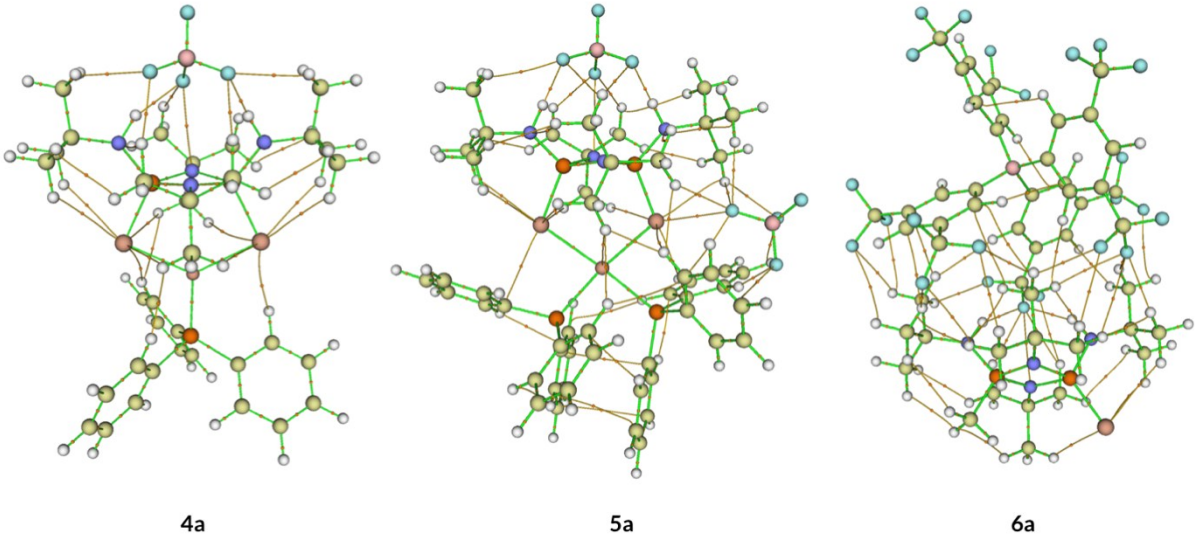


Figure S27. Visualisation of BCPs for complexes 4a, 5a and 6a.

3.3. Molecular Orbital Calculations

Complex	ΔE / kJ mol^{-1}
3	19.9
4a	16.3
5a	9.9
6a	17.7

Table 8. Summary of HOMO-LUMO energy gap in complexes **3**, **4a**, **5a** and **6a**

Complexing the transition metal to **3** decreases the HOMO-LUMO energy gap, Table 8. Increasing the oxidation state of the metal from Cu^{I} to Pd^{II} decreases the HOMO-LUMO energy gap further by 6.4 kJ mol^{-1}. Decreasing gap in the frontier molecular orbital indicates that

greater electron density from the BF_4^- anion is able to delocalise into the cyclophosphazane. The visualisation of the LUMO supports the greater electron density delocalisation from the BF_4^- anion and therefore increasing the H-bonding strength. The greatest contribution to the LUMO in **4a**, **5a**, and **6a** are all from the aromatic π-system. However, as the oxidation state of the transition metal is increased, the contribution of the N-H σ* orbital to the LUMO increases. For complex **6a**, the contribution of the N-H σ* orbital to LUMO is less than complex **5a**, but the contribution from the ^{t}Bu C-H gtoup is more significant, supporting the NBO and the AIM results.

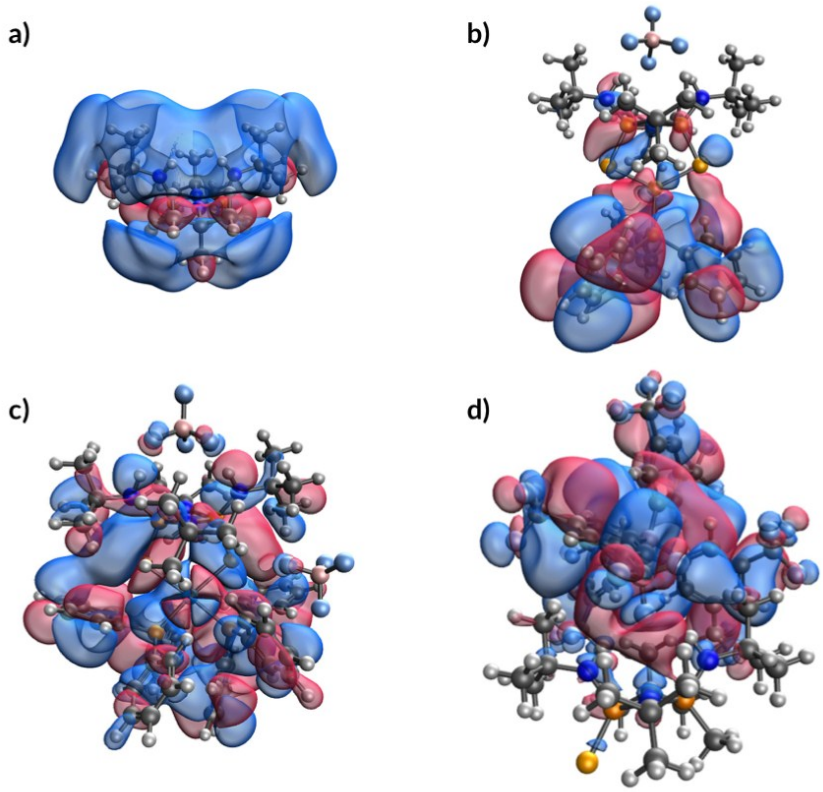


Figure S28. LUMO visualisation for complexes a) **3**, b) **4a**, c) **5a** and d) **6a**.

3.4 Charge Analysis

Atom	3	6	4a	5a	6a
N1	-1.02	-1.02	-1.04	-1.03	-1.03
H1	0.39	0.42	0.46	0.46	0.44
N2	-1.02	-1.01	-1.04	-1.04	-1.02
H2	0.39	0.40	0.46	0.47	0.42

Table 9. Partial charges of N-H bond atoms in H-bond donors

The NBO partial charge analysis for all five structures are presented in Table 9. The protic N-H bonds have a strong dipole moment because the nitrogen atom has negative charge whereas the hydrogen atom has a positive charge. The BF_4^- and $BArF^-$ anions will be repelled from the negative nitrogen but overall, the high partial charge of the proton is more likely to dominate, as reported in double ionic hydrogen bonding ionic liquid systems[4]. The partial charge of the nitrogen remains constant across all complexes compared to the neutral cyclodiphosphazane **3**. However, the coordination of the transition metal ions in complex **4a** and **5a** increases the partial charge of the hydrogen, increasing the dipole moment of the N-H bonds. Replacing the Se atom with a methyl group in **6** also increases the partial charge of the hydrogen in N-H receptors to a similar degree as coordinating the transition metal. The partial charge of the carbon in H-bonding C-H bond is less than the nitrogen at around -0.6 (see ESI NBO Partial Charge section). The weaker dipole moment of the C-H bond consequently results in weaker H-bonding interactions.

Increasing the oxidation state of the transition metal between complex **4a** and **5a** does not increase the partial charge of the hydrogen anymore. However, the partial charge of the phosphorus and the selenium atoms becomes significantly more positive, Table 10. Therefore, the favourable electrostatic attraction between the BF_4^- anion and the cyclodiphosphazane will increase.

4a		**5a**	
P2	0.10	Se31	0.27
P1	0.09	Se32	0.17
H36	0.07	P2	0.15
H34	0.07	P1	0.13
H20	0.04	H36	0.07
H24	0.03	H34	0.07
H11	0.03	H16	0.04
H49	0.03	H22	0.04
H16	0.03	H28	0.03
H57	0.02	H11	0.03
N4	0.01	H56	0.02
H44	0.01	C6	0.02
H56	0.01	H43	0.02
N3	0.01	H45	0.02
Se32	0.01	N4	0.02
Se31	0.01	N3	0.02

Table 10. The top 16 atoms showing largest change in partial charge when **3** coordinates with the anion to form **4a** and **5a**

Furthermore, the partial charges on the anion explains the weaker H-bonding interactions with the N-H receptors in complex **6a**. The partial charge of the anion fluorine atoms forming H-bond has been averaged, Table 11. The fluorine atoms in BF_4^- anions have significantly more average negative partial charge than the $BArF^-$ anions and therefore the interaction with the positive H atoms in the N-H receptors are electrostatically more favourable.

4a	**5a**	**6a**
-0.58	-0.58	-0.38

Table 11. The average partial charge of the fluorine atoms in the anion

The amount of charge transfer from the BF_4^- and $BArF^-$ anion has been calculated in Table 12. The charge transfer is fairly large for all three systems due to the presence of the oppositely charge ions. The increased charge transfer moving from **4a** to **5a** is likely to be attributed from the more favourable electrostatic attraction between the ion pairs. Compared to **4a**, the complex $BArF^-$ anion shows significantly less charge transfer because the negative charge is less localised in $BArF^-$ anion than the BF_4^- anion. The reduced NBO charge transfer means weaker H-bonding interactions are present in complex **6a**, supporting the previous findings.

4a	**5a**	**6a**
-0.12	-0.14	-0.08

Table 12. The charge transfer for the BF_4^- and $BArF^-$ anions in complex **4a**, **5a** and **6a**.

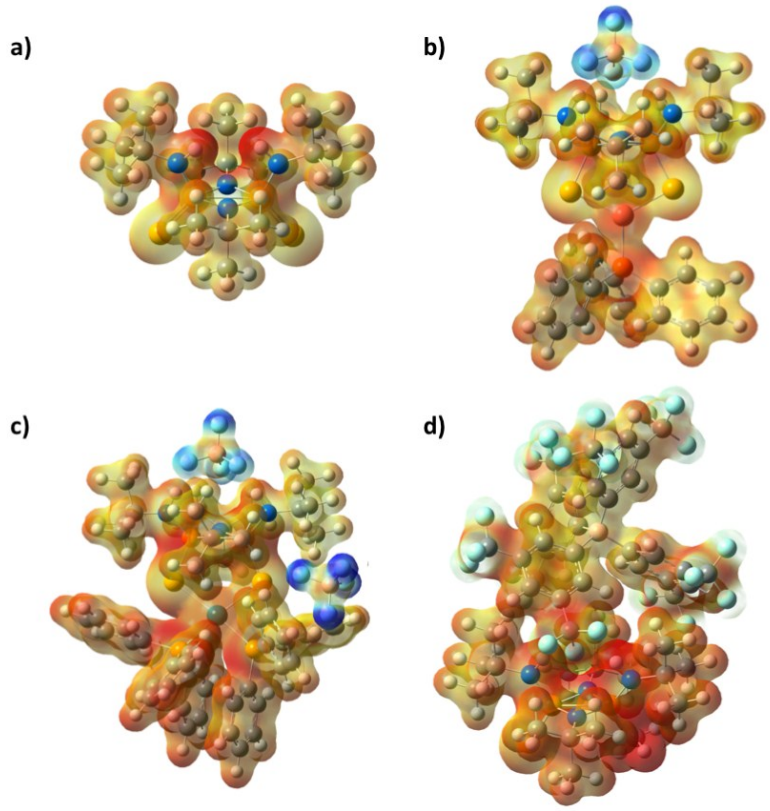


Figure S29. Visualisation of electrostatic potential surfaces for a) **3**, b) **4a**, c) **5a** and d) **6a**

The visualisation of the electrostatic potential surface for **3** shows the positive charge is localised mostly around the H atom of the N-H receptors, Figure 5. The coordination with the transition metal and the BF_4^- anion reduces the local charge around the N-H receptors. However, for complex **5a**, the surface around the transition metal and the cyclodiphophazane remain more positive than **4a** due to the increased oxidation state. The N-H receptors remain polarised in complex **6a** which is a consequence of the reduced charge transfer.

4. Conclusions

The NBO and the AIM analysis have shown that increasing the electron withdrawing ability of the Se atom *via* transition metal coordination in the cyclodiphosphazane increases the ability of the N-H receptors to hydrogen bond with the anion. Introducing a positive charge to cyclodiphosphazane by replacing the Se atom with a methyl group also improves the H-bonding ability of the N-H receptors. However, because the negative charge is more delocalised in $BArF^-$ than the BF_4^- anion, the H-bonding interactions in complex **6a** is weaker than **4a**.

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Relative Energies

	E/Hart	ΔE/kJ mol^{-1}	G/Hart	ΔG/kJ mol^{-1}
4a	-9436.557651	0.00	-9435.817124	0.00
4b	-9436.518277	103.38	-9435.777538	103.93
4c	-9436.516106	109.08	-9435.777619	103.72
4d	-9436.494674	165.35	-9435.75736	156.91

Table S1. Relative energies and free energies of all optimsed complex 4

	E/Hart	ΔE/kJ mol^{-1}	G/Hart	ΔG/kJ mol^{-1}
5a	-9384.024698	0	-9383.014148	0.00
5b	-9383.982862	109.84	-9382.972912	108.27
5c	-9384.022014	7.047	-9383.011191	7.76
5d	-9384.017558	18.75	-9383.007555	17.31
5e	-9383.986529	100.21	-9382.977264	96.84

Table S2. Relative energies and free energies of all optimsed complex 5

	E/Hart	ΔE/kJ mol^{-1}	G/Hart	ΔG/kJ mol^{-1}
6a	-7619.961055	0.00	-7619.102648	0.00
6b	-7619.956269	12.57	-7619.097322	13.98
6c	-7619.942997	47.41	-7619.090161	32.78
6d	-7619.94763	35.25	-7619.092317	27.12
6e	-7619.936509	64.45	-7619.083855	49.34
6f	-7619.942384	49.02	-7619.085994	43.73

Table S3. Relative energies and free energies of all optimsed complex 6

NBO Interaction Energy

4a

Donor	Acceptor	Bond Type	$E^{(2)}$ / kcal mol^{-1}
F 100	C 10 - H 11	LP	0.80
F 100	N 33 - H 34	LP	2.90
F 100	N 35 - H 36	LP	0.39
F 100	P 1 - N 4	LP	0.06
F 100	P 1 -Se 31	LP	0.14
F 100	P 2 - N 3	LP	0.05
F 100	P 2 - N 4	LP	0.07
F 100	P 2 -Se 32	LP	0.15
F 100	C 10 - H 11	LP	0.06
F 100	N 33 - H 34	LP	0.16
F 100	N 35 - H 36	LP	0.94
F 100	P 1 -Se 31	LP	0.11
F 100	P 1 - N 33	LP	0.07
F 100	C 10 - H 11	LP	0.06
F 100	N 33 - H 34	LP	12.20
F 100	N 33 - C 37	LP	0.09
F 100	N 35 - H 36	LP	0.09
F 100	C 10 - H 11	LP	0.16
F 100	N 33 - H 34	LP	0.51
F 100	N 35 - H 36	LP	0.12
F 101	N 35 - H 36	LP	0.57
F 101	C 19 - H 20	LP	0.83
F 101	N 35 - H 36	LP	3.57
F 101	C 55 - H 57	LP	0.52
F 101	C 19 - H 20	LP	1.37
F 101	C 55 - H 57	LP	0.15
F 101	C 55 - H 58	LP	0.06

F 101	C 19 - H 20	LP	0.07
F 101	N 35 - H 36	LP	15.24
F 101	C 55 - H 57	LP	0.05
F 101	N 33 - H 34	LP	0.13
F 101	N 35 - H 36	LP	0.36
F 101	C 55 - H 57	LP	0.08
F 102	C 23 - H 24	LP	1.18
F 102	N 33 - H 34	LP	0.47
F 102	C 46 - H 49	LP	0.59
F 102	C 23 - H 24	LP	1.20
F 102	N 33 - H 34	LP	0.79
F 102	C 23 - H 24	LP	0.14
F 102	N 33 - H 34	LP	1.28
F 102	C 46 - H 48	LP	0.06
F 102	C 46 - H 49	LP	0.64
F 102	C 23 - H 24	LP	0.08
F 102	N 33 - H 34	LP	0.21
F 102	N 35 - H 36	LP	0.11
F 99	N 35 - H 36	LP	0.06
F 99	N 33 - H 34	LP	0.06
F 99	C 23 - H 24	LP	0.05
F 99	N 33 - H 34	LP	0.18
F 99	N 35 - H 36	LP	0.17

Table S4. NBO interaction energies for complex 4a

5a

Donor	Acceptor	Bond Type	$E^{(2)}$/kcal mol^{-1}
F 134	C 14 - H 16	LP	0.55
F 134	N 33 - H 34	LP	4.30
F 134	C 14 - H 16	LP	1.39

F 134	N 33 - H 34	LP	0.24
F 134	C 46 - H 47	LP	0.09
F 134	P 1 - N 33	LP	0.06
F 134	N 33 - H 34	LP	18.21
F 134	N 33 - C 37	LP	0.07
F 134	N 33 - H 34	LP	0.23
F 135	N 35 - H 36	LP	0.81
F 135	C 14 - H 16	LP	0.11
F 135	N 35 - H 36	LP	4.75
F 135	C 55 - H 56	LP	0.19
F 135	C 55 - H 58	LP	0.07
F 135	C 14 - H 15	LP	0.08
F 135	C 14 - H 16	LP	0.39
F 135	P 2 - N 35	LP	0.06
F 135	N 35 - H 36	LP	21.15
F 135	N 33 - H 34	LP	0.06
F 135	N 35 - H 36	LP	0.25
F 135	C 55 - H 56	LP	0.05
F 136	C 19 - H 22	LP	1.19
F 136	C 27 - H 28	LP	0.87
F 136	N 33 - H 34	LP	0.18
F 136	N 35 - H 36	LP	0.10
F 136	P 1 - N 3	LP	0.05
F 136	P 1 -Se 31	LP	0.08
F 136	P 2 - N 3	LP	0.06
F 136	P 2 -Se 32	LP	0.07
F 136	N 33 - H 34	LP	0.25
F 136	N 35 - H 36	LP	0.16
F 136	C 19 - H 22	LP	0.41
F 136	C 27 - H 28	LP	0.56

F 136	N 33 - H 34	LP	0.30
F 136	N 35 - H 36	LP	0.18
F 136	C 19 - H 22	LP	0.14
F 136	C 27 - H 28	LP	0.10
F 136	N 33 - H 34	LP	0.08
F 136	N 35 - H 36	LP	0.06
F 133	N 33 - H 34	LP	0.15
F 133	N 35 - H 36	LP	0.19

Table S5. NBO interaction energies for complex 5a

6a

Donor	Acceptor	Bond Type	$E^{(2)}$/kcal mol^{-1}
C 72 - C 74	C 54 - H 55	π	0.44
C 77 - C 79	C 45 - H 48	π	0.82
C 78 - C 81	C 19 - H 20	π	0.21
F 115	N 32 - H 33	LP	0.18
F 115	N 34 - H 35	LP	0.09
F 113	C 49 - C 54	LP	0.06
F 113	C 49 - C 54	LP	0.10
F 114	C 14 - H 16	LP	0.09
F 114	C 14 - H 16	LP	0.16
F 115	P 1 - N 4	LP	0.07
F 115	P 1 - C 62	LP	0.10
F 115	C 10 - H 11	LP	0.09
F 115	C 14 - H 16	LP	0.06
F 115	N 32 - H 33	LP	3.08
F 115	N 34 - H 35	LP	2.10
F 115	C 10 - H 11	LP	0.26
F 115	C 14 - H 16	LP	0.06
F 115	N 34 - H 35	LP	1.01

F 115	C 14 - H 16	LP	0.06
F 115	N 32 - H 33	LP	4.18
F 115	N 34 - H 35	LP	0.81
F 116	C 45 - H 46	LP	0.44
F 116	C 45 - H 46	LP	0.06
F 116	C 45 - H 46	LP	0.34
F 117	C 19 - H 22	LP	0.09
F 117	C 50 - H 53	LP	1.18
F 117	C 54 - H 56	LP	0.43
F 117	C 50 - H 53	LP	0.67
F 117	C 54 - H 56	LP	0.13
F 117	C 19 - H 22	LP	0.16
F 118	C 19 - H 21	LP	0.24
F 118	C 27 - H 29	LP	0.26
F 118	C 19 - H 21	LP	0.11
F 118	C 27 - H 29	LP	0.11
F 118	C 19 - H 20	LP	0.06
F 118	C 19 - H 21	LP	0.30
F 118	C 27 - H 29	LP	0.08
F 130	C 36 - C 45	LP	0.09
F 131	C 41 - H 44	LP	0.05
F 131	C 45 - H 47	LP	0.19
F 131	C 45 - H 47	LP	0.45
F 132	C 23 - H 24	LP	0.10
F 132	C 41 - H 43	LP	0.30
F 132	C 41 - H 43	LP	0.58
F 132	C 23 - H 24	LP	0.09
F 132	C 41 - H 43	LP	0.05
F 134	C 19 - H 21	LP	0.34
F 134	C 23 - H 26	LP	0.11

F 134	C 19 - H 21	LP	0.29
F 134	C 19 - H 21	LP	0.16
F 134	C 23 - H 26	LP	0.20

Table S6. NBO interaction energies for complex 6a

Electron Density at BCP

4a

BCP idx	Type	ρ_{BCP} / e
49	C-H···F	0.009
85	C-H···F	0.011
68	N-H···F	0.031
85	C-H···F	0.011
74	C-H···F	0.007
130	C-H···F	0.005
129	N-H···F	0.035
144	C-H···F	0.009

Table S7. Electron density at BCP for complex 4a

5a

BCP idx	Type	ρ_{BCP} / e
23	C-H···F	0.006
43	N-H···F	0.041
74	C-H···F	0.010
60	C-H···F	0.009
121	C-H···F	0.010
94	C-H···F	0.011
140	N-H···F	0.038

Table S8. Electron density at BCP for complex 5a

6a

BCP idx	Type	ρ_{BCP} / e
240	C-H --- F	0.002
235	C-H --- F	0.008
221	C-H --- F	0.006
174	C-H --- F	0.008
152	N-H --- F	0.021
181	C-H --- F	0.005
158	C-H --- F	0.007
108	C-H --- F	0.007
100	C-H --- F	0.006
71	C-H --- F	0.005
61	C-H --- F	0.003
28	C-H --- F	0.005
4	C-H --- F	0.004
29	C-H --- F	0.011
96	N-H --- F	0.014
104	C-H --- F	0.004
218	C-H --- C	0.007
194	C-H --- C	0.008
159	C-H --- C	0.005
147	C-H --- C	0.005
27	C-H --- C	0.008
77	C-H --- F	0.003
139	C-H --- F	0.005

Table S9. Electron density at BCP for complex 6a

Partial Charge Analysis

3

Atom Type	Atom No.	Natural Charge/e
P	1	1.72735

P	2	1.72575
N	3	-1.13158
N	4	-1.13532
C	5	0.14683
C	6	-0.61509
H	7	0.22603
H	8	0.20433
H	9	0.22560
C	10	-0.60970
H	11	0.20467
H	12	0.21705
H	13	0.22227
C	14	-0.60970
H	15	0.21745
H	16	0.20349
H	17	0.22237
C	18	0.14477
C	19	-0.60644
H	20	0.20448
H	21	0.21172
H	22	0.20689
C	23	-0.60845
H	24	0.21219
H	25	0.23022
H	26	0.21309
C	27	-0.60818
H	28	0.21202
H	29	0.21284
H	30	0.23043
Se	31	-0.47333

Se	32	-0.47250
N	33	-1.01505
H	34	0.39271
N	35	-1.01562
H	36	0.39313
C	37	0.14748
C	38	-0.61186
H	39	0.20864
H	40	0.20632
H	41	0.23054
C	42	-0.61419
H	43	0.23158
H	44	0.20571
H	45	0.21077
C	46	-0.60710
H	47	0.20724
H	48	0.22286
H	49	0.20892
C	50	0.14740
C	51	-0.61445
H	52	0.23148
H	53	0.21151
H	54	0.20622
C	55	-0.60626
H	56	0.20584
H	57	0.20997
H	58	0.22234
C	59	-0.61230
H	60	0.20834
H	61	0.23063

H	62	0.20564

Table S10. NBO partial charge analysis for complex 3

4a

Atom Type	Atom No.	Natural Charge / e
P	1	1.82032
P	2	1.82106
N	3	-1.11999
N	4	-1.12172
C	5	0.14779
C	6	-0.61411
H	7	0.21348
H	8	0.21294
H	9	0.21357
C	10	-0.61023
H	11	0.23813
H	12	0.21282
H	13	0.20641
C	14	-0.61556
H	15	0.21921
H	16	0.22896
H	17	0.21288
C	18	0.14779
C	19	-0.61698
H	20	0.24194
H	21	0.21592
H	22	0.20568
C	23	-0.6206
H	24	0.2457
H	25	0.20571
H	26	0.2162

C	27	-0.61957
H	28	0.21786
H	29	0.21251
H	30	0.21117
Se	31	-0.4641
Se	32	-0.46147
N	33	-1.03666
H	34	0.46192
N	35	-1.04034
H	36	0.46274
C	37	0.14651
C	38	-0.60949
H	39	0.21315
H	40	0.20888
H	41	0.21764
C	42	-0.61129
H	43	0.21489
H	44	0.21872
H	45	0.21232
C	46	-0.61314
H	47	0.21586
H	48	0.21328
H	49	0.23795
C	50	0.14622
C	51	-0.61212
H	52	0.21697
H	53	0.21204
H	54	0.21531
C	55	-0.60981
H	56	0.21842

H	57	0.23305
H	58	0.2127
C	59	-0.61116
H	60	0.21385
H	61	0.21727
H	62	0.21214
Cu	63	0.30393
P	64	0.8784
C	65	-0.34245
C	66	-0.20418
C	67	-0.19198
C	68	-0.20633
H	69	0.22896
C	70	-0.20443
H	71	0.22768
C	72	-0.19956
H	73	0.22113
H	74	0.22265
H	75	0.22052
C	76	-0.34752
C	77	-0.19595
C	78	-0.20151
C	79	-0.20347
H	80	0.22565
C	81	-0.20521
H	82	0.22842
C	83	-0.20214
H	84	0.22292
H	85	0.22096
H	86	0.2206

C	87	-0.34884
C	88	-0.18689
C	89	-0.19692
C	90	-0.20468
H	91	0.22459
C	92	-0.20728
H	93	0.22702
C	94	-0.197
H	95	0.22367
H	96	0.22161
H	97	0.22117
B	98	1.43967
F	99	-0.55874
F	100	-0.59282
F	101	-0.5812
F	102	-0.58203

Table S11. NBO partial charge analysis for complex 4a

5a

Atom Type	Atom No.	Natural Charge/e
P	1	1.85686
P	2	1.87446
N	3	-1.11653
N	4	-1.11767
C	5	0.14347
C	6	-0.59296
H	7	0.20097
H	8	0.21709
H	9	0.21043
C	10	-0.62721
H	11	0.23096

H	12	0.21986
H	13	0.23723
C	14	-0.6083
H	15	0.21042
H	16	0.24754
H	17	0.19985
C	18	0.14681
C	19	-0.61513
H	20	0.20577
H	21	0.21594
H	22	0.24457
C	23	-0.60629
H	24	0.21941
H	25	0.21112
H	26	0.20957
C	27	-0.61238
H	28	0.2423
H	29	0.21588
H	30	0.20075
Se	31	-0.20114
Se	32	-0.30427
N	33	-1.03428
H	34	0.46378
N	35	-1.04455
H	36	0.468
C	37	0.15024
C	38	-0.61589
H	39	0.2181
H	40	0.20736
H	41	0.24155

C	42	-0.63231
H	43	0.25088
H	44	0.19633
H	45	0.22945
C	46	-0.60318
H	47	0.22175
H	48	0.21486
H	49	0.20799
C	50	0.145
C	51	-0.60983
H	52	0.21464
H	53	0.21371
H	54	0.21687
C	55	-0.60838
H	56	0.22914
H	57	0.22442
H	58	0.21387
C	59	-0.61063
H	60	0.21244
H	61	0.21572
H	62	0.21359
Pd	63	-0.17499
P	64	1.05066
C	65	-0.3599
C	66	-0.19599
C	67	-0.18367
C	68	-0.20673
H	69	0.22843
C	70	-0.20138
H	71	0.23658

C	72	-0.1894
H	73	0.2259
H	74	0.23482
H	75	0.22631
C	76	-0.35879
C	77	-0.18757
C	78	-0.18974
C	79	-0.20467
H	80	0.23292
C	81	-0.20302
H	82	0.22979
C	83	-0.19231
H	84	0.22542
H	85	0.22448
H	86	0.22338
C	87	-0.34569
C	88	-0.20272
C	89	-0.18376
C	90	-0.20598
H	91	0.23109
C	92	-0.19783
H	93	0.22734
C	94	-0.19587
H	95	0.2267
H	96	0.22517
H	97	0.22413
P	98	1.06732
C	99	-0.37715
C	100	-0.18929
C	101	-0.1646

C	102	-0.19477
H	103	0.22656
C	104	-0.18547
H	105	0.22484
C	106	-0.1648
H	107	0.22087
H	108	0.22706
H	109	0.22245
C	110	-0.34293
C	111	-0.20127
C	112	-0.18387
C	113	-0.2107
H	114	0.23513
C	115	-0.20534
H	116	0.23345
C	117	-0.19973
H	118	0.22324
H	119	0.22369
H	120	0.22083
C	121	-0.38359
C	122	-0.21665
C	123	-0.17293
C	124	-0.21132
H	125	0.21658
C	126	-0.18086
H	127	0.26533
C	128	-0.19296
H	129	0.2179
H	130	0.24943
H	131	0.22037

B	132	1.43933
F	133	-0.55609
F	134	-0.57813
F	135	-0.5796
F	136	-0.58835
B	137	1.43351
F	138	-0.59631
F	139	-0.59085
F	140	-0.59006
F	141	-0.57342

Table S12. NBO partial charge analysis for complex 5a

6a

Atom Type	Atom No.	Natural Charge/e
P	1	2.16555
P	2	1.7013
N	3	-1.13682
N	4	-1.12863
C	5	0.14332
C	6	-0.6087
H	7	0.19676
H	8	0.21849
H	9	0.23313
C	10	-0.60793
H	11	0.21773
H	12	0.22865
H	13	0.19952
C	14	-0.61227
H	15	0.22356
H	16	0.2192
H	17	0.22286

C	18	0.14669
C	19	-0.61628
H	20	0.20556
H	21	0.23483
H	22	0.2123
C	23	-0.61418
H	24	0.20372
H	25	0.21171
H	26	0.23976
C	27	-0.61336
H	28	0.21835
H	29	0.23401
H	30	0.22214
Se	31	-0.43114
N	32	-1.034
H	33	0.43657
N	34	-1.021
H	35	0.42136
C	36	0.14356
C	37	-0.60674
H	38	0.22988
H	39	0.21725
H	40	0.1993
C	41	-0.61329
H	42	0.19892
H	43	0.22842
H	44	0.23079
C	45	-0.61872
H	46	0.22088
H	47	0.23687

H	48	0.21906
C	49	0.14736
C	50	-0.61845
H	51	0.22416
H	52	0.21831
H	53	0.21949
C	54	-0.61114
H	55	0.20249
H	56	0.22412
H	57	0.23256
C	58	-0.61145
H	59	0.21872
H	60	0.22116
H	61	0.20685
C	62	-0.96978
H	63	0.26217
H	64	0.25627
H	65	0.27606
B	66	0.50382
C	67	-0.242
C	68	-0.15009
C	69	-0.17252
C	70	-0.16846
H	71	0.23991
C	72	-0.19983
H	73	0.2137
C	74	-0.18876
H	75	0.24094
C	76	-0.24919
C	77	-0.16569

C	78	-0.16992
C	79	-0.18357
H	80	0.23428
C	81	-0.18141
H	82	0.23171
C	83	-0.19364
H	84	0.23697
C	85	-0.25788
C	86	-0.15631
C	87	-0.17407
C	88	-0.16536
H	89	0.23102
C	90	-0.18367
H	91	0.21494
C	92	-0.18209
H	93	0.24131
C	94	-0.2662
C	95	-0.16793
C	96	-0.16937
C	97	-0.17002
H	98	0.22127
C	99	-0.17049
H	100	0.22673
C	101	-0.18213
H	102	0.24149
C	103	1.17555
C	104	1.17856
C	105	1.17877
C	106	1.17642
C	107	1.17673

C	108	1.17588
C	109	1.17644
C	110	1.1764
F	111	-0.36898
F	112	-0.37786
F	113	-0.38331
F	114	-0.36416
F	115	-0.41432
F	116	-0.36755
F	117	-0.39154
F	118	-0.38571
F	119	-0.36866
F	120	-0.3755
F	121	-0.37604
F	122	-0.38027
F	123	-0.37858
F	124	-0.37996
F	125	-0.3796
F	126	-0.37893
F	127	-0.37921
F	128	-0.37742
F	129	-0.36551
F	130	-0.37892
F	131	-0.3902
F	132	-0.39208
F	133	-0.36686
F	134	-0.37891

Table S13. NBO partial charge analysis for complex 6a

Cartesian Coordinates

3

P	1.29292	-0.14116	-0.20221
P	-1.2939	-0.14463	-0.2001
N	-0.00092	0.82335	-0.80252
N	-0.00064	-1.05271	0.49742
C	-0.00298	-2.43295	1.05149
C	-0.00439	-3.48421	-0.07336
H	0.88824	-3.37109	-0.70986
H	-0.00506	-4.50151	0.35857
H	-0.89761	-3.36968	-0.70893
C	1.25008	-2.59629	1.92799
H	1.27485	-1.83644	2.7286
H	1.24854	-3.59693	2.39463
H	2.17175	-2.50324	1.32993
C	-1.25794	-2.59394	1.92629
H	-1.26095	-3.59655	2.38862
H	-1.28028	-1.83844	2.73121
H	-2.17923	-2.49433	1.32848
C	-0.00016	2.17537	-1.41216
C	-0.01048	3.24109	-0.29696
H	0.88875	3.14411	0.33571
H	-0.02397	4.2589	-0.72601
H	-0.90261	3.11967	0.34152
C	1.25509	2.33716	-2.28519
H	2.17981	2.25751	-1.69133
H	1.29035	1.56329	-3.06905
H	1.24291	3.33257	-2.76334
C	-1.24395	2.33207	-2.30229
H	-2.17652	2.25532	-1.72058
H	-1.22569	3.32484	-2.7857
H	-1.26886	1.55364	-3.08194

Se	2.63427	-1.05295	-1.53726
Se	-2.63491	-1.03363	-1.55107
N	2.00524	0.70939	1.06073
H	1.30998	1.04932	1.72045
N	-2.00328	0.67125	1.0891
H	-1.32475	0.8658	1.82146
C	3.41	1.00369	1.46318
C	4.1802	-0.28647	1.79502
H	5.20399	-0.0431	2.1316
H	3.67215	-0.84448	2.60039
H	4.25065	-0.93873	0.91025
C	4.14055	1.80486	0.37154
H	4.20002	1.2292	-0.56549
H	3.61269	2.75335	0.16917
H	5.16841	2.04324	0.69883
C	3.30063	1.8688	2.73178
H	2.78234	1.32307	3.54245
H	4.30648	2.13734	3.09694
H	2.75144	2.80685	2.52811
C	-3.40577	0.99653	1.47268
C	-4.10179	1.81964	0.37576
H	-4.16897	1.24966	-0.56404
H	-5.12585	2.08349	0.69488
H	-3.54739	2.75465	0.18252
C	-3.29398	1.85507	2.74559
H	-2.80107	1.29477	3.56257
H	-2.71795	2.77864	2.55222
H	-4.2981	2.14589	3.09842
C	-4.20967	-0.27823	1.78591
H	-5.23315	-0.01679	2.10997
H	-4.27928	-0.9229	0.8953

H	-3.7249	-0.85248	2.59459

4a

P	1.72057	-1.23287	0.07382
P	1.75967	1.30409	0.02287
N	2.0118	0.0147	-1.07322
N	1.79749	0.05372	1.19589
C	1.62313	0.08177	2.6715
C	0.14647	-0.13418	3.04987
H	-0.20021	-1.12954	2.72862
H	0.01853	-0.05882	4.14448
H	-0.49728	0.62299	2.56937
C	2.5055	-1.01785	3.28357
H	3.54437	-0.91386	2.92998
H	2.48313	-0.94106	4.38485
H	2.14027	-2.02	3.00908
C	2.09998	1.44911	3.17992
H	2.03648	1.47215	4.28146
H	3.14396	1.63431	2.87938
H	1.46473	2.26145	2.79042
C	2.0157	-0.0123	-2.5653
C	2.82772	1.19347	-3.05992
H	3.82972	1.2033	-2.60172
H	2.93317	1.13652	-4.15728
H	2.3138	2.13947	-2.82482
C	2.70829	-1.3087	-3.00761
H	3.7091	-1.39164	-2.5535
H	2.10807	-2.18992	-2.72852
H	2.80901	-1.31139	-4.10694
C	0.58288	0.04486	-3.12731
H	0.06694	0.96571	-2.8089

H	0.61581	0.0268	-4.23129
H	-0.00895	-0.81904	-2.78156
Se	-0.23792	-2.14923	-0.13454
Se	-0.18885	2.26091	-0.11521
N	2.98033	-2.25512	0.26702
H	3.84774	-1.7109	0.37307
N	3.05693	2.30139	0.07286
H	3.93116	1.77714	-0.09411
C	3.15949	-3.73935	0.27081
C	2.35891	-4.38767	1.41305
H	2.51003	-5.4816	1.40219
H	2.69813	-4.00727	2.39102
H	1.27863	-4.19032	1.31462
C	2.75841	-4.35297	-1.0801
H	1.69493	-4.16637	-1.30678
H	3.37379	-3.93291	-1.89183
H	2.9152	-5.44592	-1.05667
C	4.66478	-3.95555	0.50602
H	4.9734	-3.53409	1.47936
H	4.89286	-5.03547	0.50724
H	5.25871	-3.46041	-0.27995
C	3.24007	3.78822	0.0838
C	2.78078	4.40683	-1.24794
H	1.7112	4.20986	-1.43295
H	2.93047	5.50105	-1.22935
H	3.36571	3.99528	-2.08689
C	4.75364	4.00739	0.2574
H	5.10705	3.56615	1.20581
H	5.32173	3.53773	-0.56204
H	4.97349	5.08898	0.27054
C	2.49933	4.4411	1.26138

H	2.67175	5.53157	1.24344
H	1.41178	4.26964	1.20992
H	2.87329	4.05193	2.22201
Cu	-1.30336	0.07994	-0.12904
P	-3.56428	0.0117	-0.0732
C	-4.20547	-0.44712	1.5871
C	-5.4099	0.0491	2.11177
C	-3.43357	-1.33865	2.35257
C	-5.84076	-0.35299	3.38035
H	-6.00977	0.75755	1.53291
C	-3.86967	-1.74196	3.61697
H	-2.48327	-1.71057	1.95568
C	-5.07406	-1.24962	4.13286
H	-6.77966	0.03904	3.78373
H	-3.26055	-2.43543	4.20482
H	-5.41249	-1.5597	5.12641
C	-4.42378	1.58674	-0.4646
C	-3.94145	2.74556	0.17168
C	-5.49234	1.69326	-1.36745
C	-4.53151	3.98577	-0.07689
H	-3.09592	2.67427	0.86439
C	-6.0754	2.94046	-1.62216
H	-5.87153	0.80425	-1.8785
C	-5.60009	4.08585	-0.97693
H	-4.14888	4.87952	0.42538
H	-6.90612	3.01439	-2.33091
H	-6.05725	5.05938	-1.17921
C	-4.27753	-1.23837	-1.21193
C	-3.49843	-1.62991	-2.31349
C	-5.54297	-1.81795	-1.02067
C	-3.98596	-2.57144	-3.22445

H	-2.49833	-1.20425	-2.44692
C	-6.02641	-2.76293	-1.92998
H	-6.14917	-1.5367	-0.15423
C	-5.25062	-3.13797	-3.0338
H	-3.37037	-2.87088	-4.07802
H	-7.01172	-3.21302	-1.77375
H	-5.63025	-3.88122	-3.74183
B	5.74183	-0.10817	-0.20467
F	7.03358	-0.08351	0.24672
F	4.82584	-0.23265	0.89408
F	5.40647	1.1097	-0.8697
F	5.50027	-1.18259	-1.07616

4b

P	2.6033	-1.18644	0.17592
P	2.10783	1.20839	-0.48823
N	2.99381	-0.14551	-1.13103
N	2.20513	0.28007	0.96879
C	1.63701	0.52386	2.34011
C	0.23676	-0.08602	2.48474
H	0.25477	-1.18094	2.37117
H	-0.17527	0.15092	3.4799
H	-0.45491	0.35077	1.75183
C	2.59855	-0.10964	3.35808
H	3.62383	0.28589	3.23902
H	2.25397	0.12682	4.37921
H	2.63006	-1.20593	3.26064
C	1.57661	2.03774	2.56838
H	1.19678	2.2343	3.58452
H	2.57568	2.49857	2.47606

H	0.8689	2.52506	1.88583
C	3.34574	-0.45951	-2.54675
C	3.83059	0.84257	-3.20262
H	4.65571	1.29669	-2.62787
H	4.18784	0.63001	-4.22498
H	3.01271	1.57644	-3.27908
C	4.49252	-1.48164	-2.52464
H	5.3398	-1.11738	-1.91791
H	4.15577	-2.44601	-2.11231
H	4.84847	-1.66449	-3.55336
C	2.15839	-1.03087	-3.34376
H	1.3127	-0.32604	-3.35046
H	2.47127	-1.21648	-4.38676
H	1.80957	-1.98149	-2.91082
Se	0.97744	-2.56899	-0.16206
Se	0.20932	1.52582	-1.40723
N	3.96315	-1.84659	0.86332
H	4.63999	-1.12714	1.10946
N	3.05102	2.55508	-0.32795
H	3.88587	2.3764	0.2256
C	4.35473	-3.23236	1.28075
C	3.43469	-3.76428	2.39362
H	3.73832	-4.78797	2.6746
H	3.49994	-3.13089	3.29392
H	2.38388	-3.79573	2.06423
C	4.35499	-4.19081	0.07839
H	3.35682	-4.2572	-0.38391
H	5.07643	-3.85777	-0.68608
H	4.64614	-5.2036	0.4074
C	5.78806	-3.10297	1.82415
H	5.82445	-2.4217	2.69427

H	6.15651	-4.08907	2.15362
H	6.47625	-2.72471	1.04626
C	2.82622	4.01084	-0.6591
C	2.71273	4.19886	-2.18015
H	1.8317	3.67437	-2.58405
H	2.59847	5.27174	-2.41299
H	3.61521	3.82521	-2.69385
C	4.09039	4.72601	-0.15279
H	4.19784	4.6122	0.9418
H	5.00041	4.33646	-0.64665
H	4.02088	5.80502	-0.36945
C	1.59374	4.58648	0.05607
H	1.48525	5.65275	-0.20917
H	0.65535	4.08549	-0.22398
H	1.68541	4.52194	1.15005
Cu	-0.56166	-0.69149	-0.68089
P	-2.78759	-0.86263	-0.29122
C	-3.11055	-0.70287	1.51334
C	-3.45245	0.52235	2.1018
C	-2.82041	-1.80773	2.33694
C	-3.50031	0.64398	3.49433
H	-3.64679	1.41184	1.50541
C	-2.89205	-1.68787	3.72557
H	-2.53084	-2.76503	1.89151
C	-3.22696	-0.45777	4.30829
H	-3.72728	1.62485	3.92009
H	-2.67218	-2.55532	4.35646
H	-3.2639	-0.36001	5.39814
C	-3.79601	0.41926	-1.13146
C	-3.3563	1.75066	-1.01519
C	-4.93439	0.13317	-1.90351

C	-4.0634	2.78586	-1.63064
H	-2.4782	2.00357	-0.41899
C	-5.626	1.17157	-2.5367
H	-5.28532	-0.89578	-2.01776
C	-5.1971	2.49695	-2.39754
H	-3.70693	3.80901	-1.48579
H	-6.51079	0.9409	-3.13897
H	-5.75046	3.30452	-2.88771
C	-3.5249	-2.47858	-0.74818
C	-2.80456	-3.31717	-1.61278
C	-4.77364	-2.90203	-0.26064
C	-3.32759	-4.55549	-1.99959
H	-1.82174	-2.99487	-1.97469
C	-5.29429	-4.14024	-0.64449
H	-5.33397	-2.26138	0.42686
C	-4.57353	-4.96702	-1.51608
H	-2.75743	-5.20169	-2.67418
H	-6.26677	-4.46392	-0.26049
H	-4.98342	-5.93749	-1.8133
B	-1.70653	3.66366	1.52367
F	-0.70334	4.34479	2.21603
F	-1.27498	2.3087	1.32958
F	-2.90454	3.63706	2.24067
F	-1.89757	4.23148	0.25085

4c

P	-2.22132	0.90862	-0.4789
P	-2.3736	-1.5287	0.21665
N	-2.71436	-0.60665	-1.18457
N	-2.34497	-0.00164	0.98925
C	-1.92351	0.38777	2.37888

C	-0.40494	0.26095	2.57685
H	0.13817	0.94173	1.90929
H	-0.13946	0.566	3.60263
H	-0.06329	-0.77486	2.4187
C	-2.36212	1.84077	2.60399
H	-3.45224	1.95168	2.465
H	-2.10519	2.13912	3.63389
H	-1.82819	2.53868	1.94164
C	-2.65527	-0.54152	3.35766
H	-2.44435	-0.21887	4.39138
H	-3.7485	-0.51269	3.20072
H	-2.3109	-1.58371	3.25658
C	-2.76634	-0.99772	-2.62085
C	-3.55987	-2.3088	-2.72389
H	-4.55025	-2.21513	-2.24598
H	-3.7046	-2.57384	-3.78549
H	-3.01515	-3.138	-2.2441
C	-3.51015	0.11542	-3.37694
H	-4.51247	0.28435	-2.94853
H	-2.95254	1.06688	-3.34085
H	-3.62198	-0.16746	-4.43799
C	-1.3652	-1.19446	-3.23116
H	-0.80213	-1.96998	-2.68766
H	-1.46205	-1.5068	-4.28626
H	-0.7838	-0.26026	-3.19339
Se	-0.27001	1.58929	-1.00911
Se	-0.52679	-2.64507	0.16486
N	-3.48091	1.97425	-0.52805
H	-4.30301	1.56714	-0.08241
N	-3.70678	-2.38038	0.72494
H	-4.50992	-1.76663	0.84542

C	-3.72848	3.39538	-0.94238
C	-3.982	4.22833	0.32554
H	-4.28244	5.25427	0.04785
H	-4.79748	3.78888	0.93081
H	-3.06649	4.29004	0.93267
C	-2.55671	3.99216	-1.72732
H	-1.66629	4.10153	-1.09078
H	-2.30835	3.38564	-2.61539
H	-2.85235	4.99781	-2.07332
C	-4.98941	3.36449	-1.82611
H	-5.84729	2.91926	-1.28639
H	-5.2756	4.39002	-2.11715
H	-4.81448	2.7772	-2.74382
C	-3.94884	-3.79884	1.14173
C	-3.60185	-4.77687	0.00742
H	-2.53781	-4.71087	-0.27135
H	-3.80474	-5.81215	0.33287
H	-4.21323	-4.5703	-0.88655
C	-5.45648	-3.88449	1.43604
H	-5.74348	-3.19503	2.2516
H	-6.05178	-3.64043	0.53731
H	-5.72164	-4.90734	1.75252
C	-3.16079	-4.14677	2.41627
H	-3.35217	-5.19566	2.70369
H	-2.07651	-4.02563	2.26067
H	-3.4681	-3.49951	3.25445
Cu	0.71636	-0.55762	-0.36354
P	2.97477	-0.54227	-0.20931
C	3.56951	0.20516	1.35382
C	4.56297	-0.37488	2.16082
C	2.95894	1.40749	1.74968

C	4.93796	0.24936	3.35494
H	5.04126	-1.31252	1.86386
C	3.3348	2.02394	2.94584
H	2.197	1.89556	1.13728
C	4.32362	1.44471	3.74865
H	5.71236	-0.20406	3.98223
H	2.82254	2.94408	3.23669
H	4.61539	1.92372	4.68893
C	3.77327	-2.196	-0.28069
C	3.2221	-3.20959	0.52478
C	4.87342	-2.49441	-1.0985
C	3.77146	-4.493	0.52389
H	2.35958	-2.9874	1.16237
C	5.41556	-3.78517	-1.10621
H	5.31075	-1.71908	-1.7334
C	4.86941	-4.78455	-0.29541
H	3.33705	-5.27073	1.15975
H	6.27227	-4.00793	-1.75
H	5.29642	-5.79227	-0.3028
C	3.75943	0.44077	-1.54272
C	3.06114	0.58679	-2.75235
C	5.00888	1.06234	-1.38572
C	3.61365	1.32642	-3.80144
H	2.07011	0.13289	-2.86178
C	5.55733	1.80566	-2.43444
H	5.54547	0.97653	-0.43607
C	4.86282	1.93589	-3.64303
H	3.05971	1.44077	-4.73819
H	6.52733	2.2952	-2.30383
H	5.29116	2.52656	-4.45881
B	0.50039	4.17949	1.47785

F	-0.82858	4.28063	0.96627
F	0.51054	3.15631	2.45824
F	1.36271	3.80788	0.4289
F	0.89021	5.38063	2.03946

4d

P	-3.06784	1.12258	0.08357
P	-2.87443	-1.40976	0.08144
N	-3.32835	-0.17098	-1.02914
N	-3.07381	-0.1505	1.24368
C	-2.70454	-0.12938	2.69573
C	-1.20636	0.14354	2.91034
H	-0.92809	1.14403	2.54793
H	-0.96553	0.0906	3.98611
H	-0.57818	-0.59407	2.38686
C	-3.53608	0.97059	3.37137
H	-4.61639	0.81923	3.19928
H	-3.34987	0.96013	4.4589
H	-3.25646	1.96759	2.99607
C	-3.07224	-1.49531	3.29175
H	-2.89466	-1.47876	4.38035
H	-4.13301	-1.74161	3.11353
H	-2.44538	-2.29534	2.86645
C	-3.29971	-0.16782	-2.52463
C	-3.98247	-1.45581	-3.00697
H	-4.99565	-1.55655	-2.5807
H	-4.06456	-1.44141	-4.10719
H	-3.39393	-2.34438	-2.72933
C	-4.09794	1.05346	-3.00263
H	-5.11614	1.05945	-2.57704
H	-3.59237	1.9909	-2.72121

H	-4.17697	1.03545	-4.10298
C	-1.86809	-0.10102	-3.08901
H	-1.26823	-0.96669	-2.76694
H	-1.90623	-0.10055	-4.19236
H	-1.35146	0.81567	-2.76331
Se	-1.23002	2.20115	-0.1723
Se	-0.89095	-2.1948	-0.119
N	-4.44225	2.03355	0.26109
H	-5.2587	1.45372	0.4442
N	-4.09962	-2.51763	0.22285
H	-5.00908	-2.06777	0.30463
C	-4.71911	3.51019	0.27239
C	-4.00134	4.19855	1.44533
H	-4.21509	5.28142	1.43284
H	-4.34968	3.79328	2.41
H	-2.90903	4.06721	1.38193
C	-4.32028	4.15949	-1.06248
H	-3.24249	4.04565	-1.2615
H	-4.88314	3.71269	-1.89861
H	-4.54718	5.23927	-1.03329
C	-6.24045	3.6349	0.46142
H	-6.56341	3.1786	1.41546
H	-6.53067	4.69864	0.48314
H	-6.78671	3.15138	-0.36908
C	-4.15001	-4.0198	0.24358
C	-3.64368	-4.608	-1.08349
H	-2.59739	-4.3209	-1.27727
H	-3.69178	-5.71012	-1.04651
H	-4.26637	-4.26613	-1.92693
C	-5.63679	-4.3709	0.42221
H	-6.03127	-3.96618	1.37239

H	-6.24386	-3.97716	-0.41388
H	-5.76437	-5.46608	0.44378
C	-3.34917	-4.58767	1.42632
H	-3.42189	-5.68904	1.42962
H	-2.28242	-4.32017	1.35836
H	-3.74576	-4.21415	2.38468
Cu	0.08006	0.09014	-0.34734
P	2.33563	0.2603	-0.38001
C	2.89372	0.10594	1.35851
C	3.95271	-0.70633	1.77565
C	2.2017	0.88857	2.30473
C	4.33517	-0.71937	3.12251
H	4.52787	-1.31114	1.07779
C	2.57451	0.86113	3.64792
H	1.37554	1.53066	1.97927
C	3.64748	0.0552	4.05794
H	5.20415	-1.3201	3.40089
H	2.03588	1.4772	4.37572
H	3.95378	0.04727	5.10906
C	3.21705	-0.97458	-1.39865
C	2.45213	-1.90443	-2.1254
C	4.61927	-1.00985	-1.48357
C	3.08217	-2.86766	-2.91759
H	1.3589	-1.86714	-2.07384
C	5.24625	-1.98736	-2.26189
H	5.24646	-0.3089	-0.92937
C	4.48031	-2.91176	-2.98036
H	2.48036	-3.58765	-3.48188
H	6.33815	-2.01119	-2.26757
H	4.97483	-3.67495	-3.59032
C	2.95743	1.90085	-0.92093

C	2.15165	2.66609	-1.7803
C	4.20904	2.39253	-0.51231
C	2.58954	3.91315	-2.23516
H	1.17675	2.2784	-2.09656
C	4.64064	3.6409	-0.9721
H	4.85837	1.80669	0.14474
C	3.83624	4.40184	-1.82854
H	1.95643	4.50382	-2.90522
H	5.62019	4.01367	-0.65788
H	4.18266	5.3785	-2.18186
B	7.32274	-0.55926	0.73138
F	6.73811	-1.66069	1.39277
F	8.48079	-0.15534	1.36779
F	7.56828	-0.90062	-0.61217
F	6.37014	0.51514	0.73983

5a

P	-2.64743	0.74399	-0.40712
P	-2.56363	-1.72907	-0.05413
N	-2.98295	-0.68168	-1.31347
N	-2.64377	-0.33496	0.91881
C	-2.49032	-0.12747	2.39261
C	-1.16327	-0.73623	2.87422
H	-0.30693	-0.30767	2.33093
H	-1.03192	-0.53676	3.95207
H	-1.13869	-1.82863	2.72148
C	-2.52771	1.382	2.68045
H	-3.51645	1.79967	2.439
H	-2.3487	1.54176	3.75771
H	-1.77326	1.95952	2.12236

C	-3.67682	-0.80061	3.1021
H	-3.61703	-0.60446	4.18733
H	-4.6273	-0.41002	2.711
H	-3.6721	-1.89167	2.94892
C	-3.16478	-0.89792	-2.77639
C	-3.99961	0.27229	-3.31944
H	-3.45159	1.22705	-3.23973
H	-4.21487	0.10189	-4.38861
H	-4.94721	0.35494	-2.76613
C	-1.81362	-0.97502	-3.51089
H	-1.23786	-0.04454	-3.38042
H	-1.20303	-1.81039	-3.13039
H	-1.99018	-1.13273	-4.59005
C	-3.94605	-2.20838	-2.95937
H	-4.88427	-2.17633	-2.3835
H	-4.18062	-2.34919	-4.02886
H	-3.34795	-3.07622	-2.63309
Se	-0.66463	1.5231	-0.92529
Se	-0.52981	-2.51966	-0.29546
N	-3.86363	1.80416	-0.30664
H	-4.695	1.34028	0.10356
N	-3.66722	-2.85618	0.36002
H	-4.58817	-2.41504	0.55293
C	-4.12036	3.25198	-0.61847
C	-4.22867	4.00965	0.71454
H	-4.51279	5.05994	0.52754
H	-5.00087	3.54918	1.35708
H	-3.25962	4.01348	1.23667
C	-3.01654	3.86335	-1.48281
H	-2.06922	3.95077	-0.93251
H	-2.86631	3.29356	-2.41755

H	-3.30911	4.89142	-1.75467
C	-5.46642	3.27456	-1.36427
H	-6.25868	2.79145	-0.76495
H	-5.76753	4.31825	-1.56042
H	-5.39276	2.74286	-2.32824
C	-3.60538	-4.32088	0.6572
C	-3.14433	-5.11318	-0.57673
H	-2.12859	-4.82106	-0.89395
H	-3.12732	-6.1927	-0.34438
H	-3.83568	-4.95237	-1.42045
C	-5.04814	-4.71917	1.01452
H	-5.4128	-4.15391	1.88838
H	-5.73324	-4.51128	0.17479
H	-5.09071	-5.79753	1.24521
C	-2.68126	-4.60278	1.856
H	-2.7016	-5.67944	2.10174
H	-1.63674	-4.32373	1.63688
H	-3.01584	-4.04103	2.74459
Pd	0.97973	-0.39137	-0.30765
P	2.71153	-1.96384	0.11038
C	3.48935	-1.76901	1.75932
C	4.56368	-2.57783	2.17459
C	2.93714	-0.85042	2.66491
C	5.11544	-2.4131	3.44669
H	4.9581	-3.35564	1.51599
C	3.4856	-0.69086	3.94103
H	2.083	-0.23749	2.3758
C	4.58492	-1.46178	4.32848
H	5.95828	-3.03848	3.75621
H	3.04948	0.04539	4.6222
H	5.02125	-1.33547	5.32398

C	2.27203	-3.75638	0.12396
C	1.79449	-4.33395	1.3159
C	2.2971	-4.52947	-1.04854
C	1.35824	-5.65939	1.33299
H	1.74854	-3.74168	2.23339
C	1.85743	-5.8569	-1.02645
H	2.65831	-4.10217	-1.98683
C	1.38601	-6.42387	0.16104
H	0.98537	-6.09339	2.26544
H	1.88365	-6.44854	-1.94634
H	1.03876	-7.46144	0.17409
C	3.93916	-1.85399	-1.2554
C	3.41426	-1.62359	-2.54154
C	5.31887	-2.04798	-1.1055
C	4.25375	-1.60993	-3.65794
H	2.34	-1.45337	-2.67132
C	6.15619	-2.02541	-2.22432
H	5.75924	-2.18291	-0.11755
C	5.62832	-1.81505	-3.50129
H	3.83089	-1.43192	-4.65114
H	7.23339	-2.1604	-2.09057
H	6.28937	-1.79797	-4.37302
P	2.50672	1.49936	-0.20491
C	2.3514	2.41829	1.36811
C	3.34188	3.34093	1.75814
C	1.21102	2.26122	2.16624
C	3.19308	4.06479	2.93963
H	4.2237	3.50644	1.13456
C	1.0681	2.98596	3.34916
H	0.40734	1.60203	1.84503
C	2.06001	3.88441	3.74028

H	3.95741	4.79347	3.22535
H	0.1511	2.87852	3.93373
H	1.93574	4.47486	4.65264
C	4.33088	1.23536	-0.37277
C	5.09923	0.9067	0.75946
C	4.98757	1.40678	-1.60331
C	6.48374	0.7516	0.66252
H	4.62559	0.80298	1.73504
C	6.37291	1.25286	-1.69649
H	4.42867	1.6827	-2.49767
C	7.12699	0.92516	-0.56624
H	7.0591	0.50483	1.5599
H	6.8634	1.39552	-2.66377
H	8.2128	0.81128	-0.64204
C	2.0703	2.65546	-1.55672
C	2.00202	2.1688	-2.87908
C	1.65899	3.96604	-1.26885
C	1.57259	3.0063	-3.90734
H	2.25122	1.12544	-3.09784
C	1.19847	4.78865	-2.30436
H	1.63137	4.34616	-0.24469
C	1.16838	4.31788	-3.61825
H	1.5229	2.62679	-4.93261
H	0.82228	5.78028	-2.04609
H	0.80114	4.96331	-4.42236
B	-6.48518	-0.57129	0.41297
F	-7.84964	-0.53813	0.35878
F	-5.96682	0.59603	1.05653
F	-6.031	-1.7093	1.15466
F	-5.89867	-0.64411	-0.86352
B	-0.55571	5.28604	1.13116

F	-0.96767	3.92187	1.25224
F	0.82456	5.35657	1.42278
F	-0.755	5.68991	-0.20346
F	-1.29281	6.06214	2.0067

5b

P	-0.54088	-3.12523	-0.49523
P	1.85859	-2.46335	-0.26359
N	0.91535	-3.29332	-1.42931
N	0.56623	-2.8854	0.7873
C	0.41427	-2.74116	2.26943
C	0.78771	-1.31666	2.70852
H	0.18563	-0.56681	2.1751
H	0.61177	-1.2021	3.79184
H	1.84851	-1.0941	2.50904
C	-1.03361	-3.07704	2.65561
H	-1.25971	-4.13601	2.45716
H	-1.1653	-2.91229	3.73806
H	-1.79087	-2.4746	2.13032
C	1.36145	-3.75921	2.93109
H	1.26458	-3.70519	4.02932
H	1.10704	-4.78581	2.613
H	2.41387	-3.56224	2.67069
C	1.09779	-3.41004	-2.90958
C	0.05194	-4.41482	-3.41978
H	-0.97456	-4.02864	-3.29497
H	0.21249	-4.59694	-4.4961
H	0.12852	-5.37753	-2.88711
C	0.9323	-2.07025	-3.64971
H	-0.05867	-1.63	-3.45673

H	1.69683	-1.34176	-3.3383
H	1.038	-2.24053	-4.73572
C	2.51063	-3.96812	-3.14924
H	2.65242	-4.92617	-2.61884
H	2.66372	-4.14186	-4.22826
H	3.28794	-3.26359	-2.8084
Se	-1.7271	-1.38808	-1.04827
Se	2.06407	-0.31765	-0.61911
N	-1.33696	-4.55366	-0.378
H	-0.69476	-5.28786	-0.07605
N	3.29093	-3.17645	0.07182
H	3.23412	-4.19339	0.10672
C	-2.75238	-5.07147	-0.50969
C	-3.29775	-5.35641	0.89637
H	-4.31271	-5.78186	0.82763
H	-2.6514	-6.08145	1.42667
H	-3.37513	-4.43539	1.48885
C	-3.66431	-4.08985	-1.24945
H	-3.84245	-3.18367	-0.65629
H	-3.25794	-3.82782	-2.24286
H	-4.64504	-4.5727	-1.39262
C	-2.63121	-6.37624	-1.31668
H	-1.95851	-7.10032	-0.8181
H	-3.62214	-6.85303	-1.4053
H	-2.24464	-6.18178	-2.33217
C	4.67195	-2.60434	0.39793
C	5.2623	-1.90852	-0.83439
H	4.65923	-1.03876	-1.14368
H	6.26794	-1.53412	-0.58989
H	5.33012	-2.6136	-1.68276
C	5.53611	-3.81841	0.76449

H	5.13248	-4.34717	1.64847
H	5.60927	-4.52983	-0.07987
H	6.54724	-3.45304	1.00525
C	4.59361	-1.65642	1.60074
H	5.60362	-1.29791	1.84484
H	3.97865	-0.76873	1.38373
H	4.17513	-2.17545	2.48118
Pd	-0.2911	0.67485	-0.42786
P	0.90544	2.72108	-0.22817
C	0.82244	3.45815	1.4439
C	1.4944	4.65865	1.74011
C	0.16158	2.77036	2.47311
C	1.44475	5.18888	3.03101
H	2.0825	5.16684	0.97151
C	0.11879	3.29914	3.76633
H	-0.3346	1.82015	2.27138
C	0.74956	4.51534	4.04381
H	1.96596	6.1251	3.25175
H	-0.41042	2.75273	4.55226
H	0.71819	4.9319	5.0551
C	2.70615	2.6414	-0.5585
C	3.5795	2.26579	0.48629
C	3.21318	2.77095	-1.86491
C	4.92493	1.99958	0.22617
H	3.19676	2.14095	1.50332
C	4.56572	2.52123	-2.11473
H	2.55903	3.06115	-2.69057
C	5.41715	2.11985	-1.08017
H	5.59493	1.65068	1.01828
H	4.95095	2.62575	-3.13382
H	6.46293	1.86601	-1.2644

C	0.26768	3.85835	-1.52388
C	-0.07075	3.27958	-2.76141
C	0.18308	5.24884	-1.37289
C	-0.46474	4.08167	-3.83481
H	-0.02223	2.19263	-2.88774
C	-0.2207	6.04704	-2.44686
H	0.40458	5.71933	-0.41415
C	-0.5368	5.46975	-3.67992
H	-0.7187	3.61873	-4.79307
H	-0.29623	7.12983	-2.31174
H	-0.84954	6.10063	-4.51738
P	-2.45113	1.7318	-0.02568
C	-3.06247	1.40188	1.66646
C	-4.11369	2.16115	2.21589
C	-2.57393	0.29697	2.37448
C	-4.64321	1.81823	3.4599
H	-4.53363	3.00817	1.66847
C	-3.10759	-0.04446	3.61693
H	-1.80749	-0.3321	1.92819
C	-4.14284	0.71577	4.16089
H	-5.47063	2.40274	3.87302
H	-2.75768	-0.94505	4.12514
H	-4.58525	0.42898	5.11897
C	-2.66749	3.55505	-0.2168
C	-2.32842	4.40768	0.85028
C	-3.2024	4.11883	-1.38679
C	-2.52243	5.78662	0.74982
H	-1.93677	3.99746	1.78087
C	-3.39378	5.49947	-1.48413
H	-3.49342	3.48712	-2.22642
C	-3.05706	6.33819	-0.41805

H	-2.25853	6.42803	1.59599
H	-3.81392	5.91853	-2.40302
H	-3.21351	7.41839	-0.49665
C	-3.68446	0.95625	-1.1428
C	-3.46581	0.96229	-2.53597
C	-4.74719	0.21073	-0.60669
C	-4.32616	0.25881	-3.38049
H	-2.60256	1.48678	-2.95871
C	-5.58301	-0.51911	-1.45833
H	-4.90481	0.1303	0.46927
C	-5.38255	-0.48775	-2.84077
H	-4.15468	0.27003	-4.46122
H	-6.36713	-1.13794	-1.01326
H	-6.03653	-1.0636	-3.50305
B	-4.93148	-2.31162	1.89301
F	-3.72801	-1.99454	1.17866
F	-5.62677	-1.11709	2.12819
F	-5.68874	-3.17053	1.09164
F	-4.55042	-2.92343	3.08903
B	7.93068	-0.12285	1.14085
F	9.22005	0.2454	1.46244
F	6.99989	0.46064	2.04205
F	7.59578	0.29936	-0.17108
F	7.77736	-1.53182	1.19968

5c

P	3.35044	-0.71583	0.08577
P	2.67519	1.69572	-0.04772
N	3.30499	0.51139	-1.1038
N	3.0895	0.57333	1.16983

C	2.98703	0.62878	2.65379
C	1.57856	0.22317	3.12387
H	1.34146	-0.80349	2.80045
H	1.52293	0.26479	4.2261
H	0.8116	0.897	2.70837
C	4.03827	-0.32485	3.23874
H	5.03658	-0.08567	2.83931
H	4.05218	-0.22553	4.33795
H	3.79611	-1.37335	3.00229
C	3.30036	2.0638	3.098
H	3.32576	2.10864	4.20046
H	4.276	2.38453	2.69939
H	2.52036	2.7617	2.75494
C	3.31178	0.43599	-2.59797
C	4.36507	-0.60271	-3.0089
H	4.05752	-1.61719	-2.70809
H	4.46957	-0.5989	-4.10759
H	5.34101	-0.36918	-2.55383
C	1.93014	0.03518	-3.1439
H	1.63196	-0.95801	-2.77424
H	1.15672	0.76159	-2.84425
H	1.96657	0.00039	-4.24749
C	3.71953	1.81539	-3.13469
H	4.66972	2.14441	-2.68443
H	3.83945	1.75794	-4.23026
H	2.94192	2.56742	-2.9257
Se	1.66238	-2.08011	-0.02602
Se	0.51277	1.98519	-0.15062
N	4.81371	-1.43164	0.17183
H	5.56224	-0.74188	-0.01485
N	3.53537	3.07972	-0.08393

H	4.54019	2.87758	-0.22467
C	5.29766	-2.8455	0.27869
C	4.72194	-3.54415	1.52036
H	5.09309	-4.58291	1.56489
H	5.0414	-3.02879	2.44044
H	3.61974	-3.57912	1.49881
C	4.95523	-3.64086	-0.99289
H	3.86544	-3.68572	-1.16083
H	5.42837	-3.18125	-1.87604
H	5.33037	-4.67563	-0.90302
C	6.82582	-2.73151	0.42035
H	7.09372	-2.16082	1.32656
H	7.27034	-3.73877	0.49558
H	7.26846	-2.21234	-0.44631
C	3.19215	4.54126	-0.1231
C	2.48536	4.90226	-1.4404
H	1.53748	4.34953	-1.5574
H	2.25084	5.98089	-1.45861
H	3.13343	4.67882	-2.30369
C	4.54827	5.26491	-0.04954
H	5.07486	5.01729	0.8886
H	5.20197	4.97415	-0.88907
H	4.39018	6.35634	-0.08527
C	2.32898	4.95458	1.0793
H	2.10425	6.03328	1.01476
H	1.36658	4.41626	1.10909
H	2.86598	4.77499	2.0245
Pd	-0.45533	-0.40931	0.07777
P	-2.48495	0.79449	0.35136
C	-3.37278	0.16817	1.82826
C	-4.69454	0.56594	2.1008

C	-2.6896	-0.64789	2.74423
C	-5.34079	0.0632	3.23381
H	-5.21188	1.29299	1.46746
C	-3.33923	-1.13694	3.88048
H	-1.64516	-0.90976	2.57036
C	-4.67591	-0.7986	4.11482
H	-6.37358	0.36573	3.43074
H	-2.79777	-1.7862	4.57495
H	-5.19315	-1.18696	4.99783
C	-2.41576	2.58826	0.69151
C	-1.83947	3.02319	1.90246
C	-2.9953	3.51603	-0.1847
C	-1.82424	4.37871	2.21766
H	-1.40239	2.2982	2.59632
C	-2.99078	4.87455	0.14933
H	-3.51211	3.20111	-1.09089
C	-2.40019	5.30764	1.33664
H	-1.37509	4.7143	3.15735
H	-3.48949	5.58087	-0.51944
H	-2.40421	6.37146	1.59394
C	-3.38507	0.64095	-1.22908
C	-2.59806	0.65197	-2.40077
C	-4.77822	0.65889	-1.33311
C	-3.20838	0.65771	-3.65403
H	-1.50599	0.67948	-2.33236
C	-5.38345	0.69191	-2.59314
H	-5.42332	0.69208	-0.46032
C	-4.60663	0.67724	-3.7503
H	-2.5905	0.66859	-4.55738
H	-6.47083	0.77049	-2.63476
H	-5.08622	0.70868	-4.73355

P	-1.65875	-2.49185	-0.15506
C	-1.53211	-3.63773	1.27934
C	-2.33658	-4.79202	1.33061
C	-0.63218	-3.38862	2.32726
C	-2.23792	-5.67463	2.40883
H	-3.0492	-5.001	0.52871
C	-0.53689	-4.27182	3.40628
H	0.00491	-2.50324	2.30389
C	-1.33955	-5.41568	3.45026
H	-2.87029	-6.56706	2.4364
H	0.16815	-4.06025	4.21563
H	-1.26779	-6.10533	4.29681
C	-3.45085	-2.53394	-0.57752
C	-4.41453	-2.48987	0.44707
C	-3.87955	-2.60129	-1.91459
C	-5.7756	-2.49615	0.13653
H	-4.11178	-2.45827	1.49425
C	-5.24206	-2.61359	-2.21719
H	-3.15991	-2.63776	-2.7327
C	-6.19405	-2.55502	-1.19551
H	-6.50933	-2.44465	0.94568
H	-5.55801	-2.65144	-3.26313
H	-7.26076	-2.54482	-1.43721
C	-0.84813	-3.35587	-1.56743
C	-0.62407	-2.62614	-2.74954
C	-0.39005	-4.67906	-1.48028
C	0.03096	-3.21609	-3.83037
H	-0.94776	-1.58458	-2.82015
C	0.27716	-5.26284	-2.563
H	-0.53294	-5.25662	-0.56455
C	0.48793	-4.53615	-3.73779

H	0.20018	-2.63561	-4.74192
H	0.63856	-6.29231	-2.48119
H	1.01411	-4.99499	-4.58031
B	6.74394	1.54926	-0.05772
F	8.00497	1.9137	0.31598
F	5.89093	1.37498	1.05612
F	6.14353	2.53683	-0.89605
F	6.7538	0.31333	-0.7764
B	-6.53176	3.24131	-0.50514
F	-5.66779	2.96367	0.60289
F	-7.29168	2.07554	-0.74769
F	-7.34392	4.31655	-0.21073
F	-5.71603	3.51225	-1.62463

5d

P	2.62134	-1.70422	-0.06602
P	3.34263	0.67221	-0.39031
N	3.35044	-0.76486	-1.29802
N	3.02381	-0.37007	0.92673
C	2.90017	-0.10617	2.39173
C	1.75103	0.87554	2.66987
H	0.79642	0.48883	2.2784
H	1.64558	1.03322	3.75761
H	1.93047	1.85346	2.19379
C	2.63583	-1.44291	3.09818
H	3.48197	-2.13031	2.94747
H	2.52075	-1.26206	4.18041
H	1.7129	-1.92466	2.73352
C	4.23237	0.46886	2.90079
H	4.19262	0.57288	3.99936

H	5.06685	-0.19168	2.62468
H	4.42563	1.46468	2.4731
C	3.51231	-1.00807	-2.76205
C	3.79031	-2.50513	-2.9574
H	2.90663	-3.10835	-2.69264
H	4.01523	-2.69746	-4.02058
H	4.64791	-2.82219	-2.34368
C	2.25361	-0.59782	-3.54773
H	1.36991	-1.15902	-3.20232
H	2.04306	0.47775	-3.43216
H	2.40608	-0.80963	-4.62105
C	4.73033	-0.19843	-3.23244
H	5.6125	-0.44842	-2.62161
H	4.94134	-0.43359	-4.29009
H	4.53836	0.88517	-3.16498
Se	0.49203	-1.97711	-0.46623
Se	1.66172	1.97834	-0.86715
N	3.4214	-3.05778	0.35484
H	4.39248	-2.82936	0.62514
N	4.78388	1.42534	-0.26426
H	5.51627	0.76776	0.06556
C	3.04254	-4.4962	0.5494
C	2.0313	-4.65483	1.69758
H	1.77878	-5.72172	1.827
H	2.45558	-4.28706	2.64591
H	1.09478	-4.10864	1.49464
C	2.48399	-5.1022	-0.74686
H	1.5638	-4.59067	-1.07704
H	3.22972	-5.04487	-1.55612
H	2.2341	-6.16471	-0.58234
C	4.36085	-5.19923	0.91762

H	4.79833	-4.77107	1.83569
H	4.17719	-6.27454	1.08314
H	5.10353	-5.09056	0.10798
C	5.23517	2.84736	-0.39575
C	4.96837	3.37936	-1.81299
H	3.89262	3.36832	-2.05768
H	5.32188	4.42222	-1.89415
H	5.50612	2.77562	-2.56248
C	6.75134	2.81085	-0.13663
H	6.97429	2.41192	0.86719
H	7.26164	2.16618	-0.87277
H	7.1672	3.83005	-0.2139
C	4.55341	3.74592	0.65172
H	4.9238	4.78178	0.55476
H	3.45854	3.76472	0.52257
H	4.78261	3.39756	1.6729
Pd	-0.43127	0.49544	-0.2109
P	-1.52192	2.55822	0.15299
C	-2.20993	2.74165	1.84218
C	-2.86102	3.9301	2.22273
C	-2.00588	1.73818	2.79938
C	-3.35113	4.07633	3.52174
H	-2.9721	4.75194	1.51062
C	-2.48736	1.8901	4.1029
H	-1.48783	0.81848	2.53039
C	-3.17169	3.05399	4.46267
H	-3.86923	4.99769	3.80398
H	-2.33141	1.0873	4.82918
H	-3.55748	3.1726	5.47965
C	-0.47495	4.07325	0.04342
C	0.31694	4.42485	1.15326

C	-0.37662	4.82784	-1.13561
C	1.18844	5.51054	1.08205
H	0.25974	3.84034	2.0755
C	0.50274	5.91514	-1.20298
H	-0.98325	4.57518	-2.0082
C	1.28697	6.25711	-0.09905
H	1.80068	5.77114	1.95039
H	0.56972	6.49676	-2.12721
H	1.97538	7.10569	-0.15565
C	-2.80585	2.81214	-1.12937
C	-2.46053	2.43842	-2.44172
C	-4.0674	3.36888	-0.88075
C	-3.35799	2.64053	-3.49197
H	-1.48575	1.98233	-2.64415
C	-4.9646	3.56059	-1.93444
H	-4.38234	3.60861	0.13509
C	-4.61194	3.20632	-3.23953
H	-3.08085	2.34129	-4.50695
H	-5.95701	3.96876	-1.72471
H	-5.32321	3.35071	-4.0581
P	-2.48308	-0.73592	0.05915
C	-2.53953	-1.67596	1.63709
C	-3.74834	-2.28503	2.02125
C	-1.4078	-1.80588	2.46232
C	-3.8014	-3.04172	3.19676
H	-4.6596	-2.18505	1.42638
C	-1.47535	-2.54316	3.64524
H	-0.46385	-1.34123	2.17893
C	-2.67291	-3.17186	4.01043
H	-4.74372	-3.53144	3.45742
H	-0.58497	-2.6337	4.27551

H	-2.72301	-3.76211	4.93097
C	-4.12038	0.08276	-0.0217
C	-4.69544	0.64823	1.13176
C	-4.86727	0.03612	-1.20896
C	-5.98901	1.16212	1.09126
H	-4.15697	0.64475	2.07912
C	-6.16711	0.54072	-1.23739
H	-4.47043	-0.44562	-2.10145
C	-6.72997	1.10498	-0.09365
H	-6.4331	1.57397	2.00243
H	-6.75286	0.4463	-2.15495
H	-7.76059	1.47205	-0.11336
C	-2.53388	-1.90173	-1.35756
C	-2.0095	-1.49628	-2.60179
C	-3.20732	-3.12477	-1.25065
C	-2.145	-2.31917	-3.719
H	-1.48781	-0.53946	-2.69659
C	-3.34929	-3.93848	-2.37854
H	-3.67887	-3.44677	-0.3231
C	-2.81568	-3.54492	-3.60648
H	-1.72983	-2.00142	-4.68034
H	-3.91535	-4.86822	-2.28208
H	-2.93348	-4.18492	-4.48653
B	6.65139	-1.62588	0.59914
F	7.90268	-2.16555	0.6793
F	5.77167	-2.22451	1.55918
F	6.67957	-0.22062	0.86492
F	6.06612	-1.81001	-0.66739
B	-6.52989	-3.01245	-0.25971
F	-6.48674	-1.90532	0.63154
F	-7.818	-3.50016	-0.36085

F	-6.04641	-2.59317	-1.51776
F	-5.65575	-4.00661	0.2552

5e

P	2.24805	-1.30406	0.11057
P	2.34377	1.12691	-0.44754
N	2.79167	-0.35558	-1.1836
N	2.25566	0.18831	0.974
C	1.94666	0.5403	2.39859
C	0.59116	1.25456	2.50898
H	-0.22127	0.64252	2.08317
H	0.36449	1.45689	3.57046
H	0.5989	2.21616	1.97041
C	1.91576	-0.76313	3.20576
H	2.89463	-1.2663	3.17435
H	1.68425	-0.52764	4.25852
H	1.14957	-1.46269	2.83315
C	3.06161	1.43929	2.93476
H	2.89463	1.64271	4.00718
H	4.04859	0.96983	2.81992
H	3.09869	2.40808	2.41762
C	3.14051	-0.68507	-2.60779
C	3.21242	-2.20989	-2.75815
H	2.23263	-2.68319	-2.57069
H	3.51084	-2.44646	-3.7934
H	3.97147	-2.64588	-2.09649
C	2.06417	-0.13064	-3.55516
H	1.06719	-0.52552	-3.29288
H	2.01375	0.96986	-3.52861
H	2.30589	-0.43057	-4.58969

C	4.51919	-0.07075	-2.89603
H	5.27724	-0.50067	-2.22496
H	4.81296	-0.28828	-3.93769
H	4.50462	1.02325	-2.75957
Se	0.20721	-2.05652	-0.2972
Se	0.31015	1.79218	-1.05474
N	3.26666	-2.45514	0.62178
H	4.2546	-2.20579	0.35457
N	3.41637	2.33544	-0.47084
H	4.24763	2.17422	0.15942
C	3.11082	-3.89726	1.04061
C	2.02728	-4.07401	2.11607
H	1.95541	-5.146	2.3688
H	2.28738	-3.52983	3.03755
H	1.03155	-3.74537	1.77595
C	2.80389	-4.77139	-0.1865
H	1.83624	-4.49586	-0.64282
H	3.60471	-4.66411	-0.93268
H	2.74704	-5.83233	0.11644
C	4.47225	-4.29007	1.64221
H	4.72466	-3.63501	2.49447
H	4.42318	-5.33183	2.0042
H	5.27759	-4.22075	0.89631
C	3.42465	3.68902	-1.14209
C	2.8865	3.6131	-2.58006
H	1.82107	3.33239	-2.62621
H	2.98041	4.60814	-3.04781
H	3.46748	2.89871	-3.18641
C	4.90086	4.12131	-1.20092
H	5.32937	4.25778	-0.1991
H	5.50607	3.37121	-1.73897

H	4.97137	5.08141	-1.74139
C	2.60498	4.68141	-0.30258
H	2.64522	5.68556	-0.76287
H	1.54634	4.37374	-0.24811
H	3.0264	4.73965	0.71226
Pd	-1.31262	0.0073	-0.26267
P	-2.86847	1.79877	-0.15222
C	-3.64864	1.98994	1.49835
C	-4.58266	3.01546	1.7386
C	-3.23752	1.18045	2.56704
C	-5.13848	3.17738	3.0093
H	-4.85928	3.70781	0.93924
C	-3.78491	1.35083	3.84228
H	-2.48661	0.40662	2.41112
C	-4.74639	2.34082	4.06248
H	-5.87016	3.9721	3.18277
H	-3.45227	0.70597	4.66087
H	-5.17769	2.47645	5.05885
C	-2.24669	3.50339	-0.4526
C	-1.58293	4.16499	0.5985
C	-2.31581	4.1127	-1.71486
C	-1.00445	5.41548	0.38875
H	-1.50219	3.6939	1.58187
C	-1.731	5.36782	-1.91991
H	-2.82111	3.61593	-2.54626
C	-1.07407	6.01876	-0.87325
H	-0.47964	5.91372	1.20863
H	-1.78921	5.83417	-2.90781
H	-0.60739	6.99411	-1.03916
C	-4.14283	1.55689	-1.45382
C	-3.67748	1.10217	-2.70264

C	-5.50469	1.84692	-1.29492
C	-4.55786	0.96267	-3.77815
H	-2.61644	0.86512	-2.83705
C	-6.38287	1.70099	-2.37265
H	-5.89916	2.15732	-0.32673
C	-5.91381	1.26657	-3.61558
H	-4.18174	0.61465	-4.74476
H	-7.44559	1.91847	-2.23205
H	-6.6059	1.15558	-4.45574
P	-2.97041	-1.6829	0.19785
C	-2.8591	-2.41729	1.88081
C	-3.8681	-3.27526	2.35784
C	-1.75559	-2.14115	2.70323
C	-3.76478	-3.84648	3.62892
H	-4.74055	-3.4984	1.73799
C	-1.656	-2.70933	3.9758
H	-0.95924	-1.48973	2.3446
C	-2.65959	-3.56484	4.44077
H	-4.55336	-4.51526	3.98667
H	-0.78449	-2.48387	4.59735
H	-2.58182	-4.01351	5.43569
C	-4.77778	-1.33774	0.01835
C	-5.50098	-0.79553	1.09623
C	-5.45839	-1.62607	-1.17663
C	-6.87128	-0.5511	0.98179
H	-5.00443	-0.58098	2.04295
C	-6.83008	-1.38462	-1.28532
H	-4.9283	-2.05159	-2.02996
C	-7.54186	-0.84836	-0.20856
H	-7.41489	-0.13369	1.83462
H	-7.34252	-1.61821	-2.22288

H	-8.61681	-0.6636	-0.29643
C	-2.67633	-3.05262	-0.99754
C	-2.46545	-2.71383	-2.34778
C	-2.59442	-4.39707	-0.60523
C	-2.20217	-3.70709	-3.29205
H	-2.48417	-1.665	-2.65851
C	-2.31852	-5.38767	-1.55339
H	-2.72099	-4.67774	0.44252
C	-2.12588	-5.04703	-2.89537
H	-2.03471	-3.43126	-4.33719
H	-2.24237	-6.43161	-1.23538
H	-1.90101	-5.82441	-3.63157
B	6.49497	-2.74032	-0.97643
F	7.03342	-2.13204	-2.09043
F	7.43272	-3.20919	-0.08456
F	5.65251	-1.76084	-0.29003
F	5.62036	-3.79078	-1.36059
B	5.75578	3.13622	2.07987
F	4.61066	3.97669	2.02342
F	5.89313	2.6036	3.34533
F	5.49643	2.0459	1.14585
F	6.86533	3.83018	1.64596

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P	4.52806	1.70754	-0.25263
P	5.0302	-0.7993	-0.20495
N	4.18165	0.37001	-1.196
N	5.23548	0.62935	0.81684
C	6.07832	0.83949	2.02959
C	7.54193	1.09383	1.62948

H	7.6319	2.00664	1.01391
H	8.16496	1.23224	2.53047
H	7.94181	0.24671	1.04922
C	5.52317	2.04275	2.80807
H	4.45807	1.90245	3.05456
H	6.08846	2.16404	3.74767
H	5.63119	2.98164	2.23841
C	5.97362	-0.41996	2.90209
H	6.55688	-0.27653	3.82771
H	4.92517	-0.62156	3.17624
H	6.3816	-1.30075	2.38105
C	3.23879	0.17629	-2.34117
C	1.81143	0.04272	-1.79127
H	1.49639	0.95855	-1.26272
H	1.0998	-0.13618	-2.60993
H	1.75064	-0.80751	-1.09351
C	3.34942	1.38747	-3.2777
H	3.05283	2.32228	-2.77448
H	4.37792	1.49155	-3.66612
H	2.66209	1.26166	-4.12957
C	3.64358	-1.09357	-3.10251
H	3.56853	-1.98746	-2.46469
H	2.95479	-1.24032	-3.94994
H	4.67696	-1.01929	-3.47946
Se	6.77485	-1.67183	-0.95754
N	3.25826	2.54054	0.36513
H	2.65701	1.91378	0.89966
N	3.88462	-1.78658	0.4676
H	3.11285	-1.26199	0.876
C	2.77205	3.96886	0.3681
C	3.81378	4.91443	0.9837

H	3.3969	5.93483	1.03103
H	4.07233	4.60422	2.0093
H	4.73717	4.96966	0.38391
C	2.39506	4.42023	-1.04825
H	3.27647	4.49062	-1.70892
H	1.66965	3.73148	-1.50542
H	1.92904	5.41944	-1.00941
C	1.52078	3.95456	1.25912
H	1.76192	3.61707	2.28103
H	1.08943	4.96451	1.32018
H	0.74338	3.29162	0.84259
C	3.81021	-3.26776	0.72891
C	3.95734	-4.07404	-0.57023
H	4.93496	-3.90184	-1.046
H	3.87182	-5.15059	-0.34095
H	3.15928	-3.81674	-1.28295
C	2.40761	-3.4969	1.3144
H	2.26865	-2.9256	2.24832
H	1.61789	-3.20313	0.60081
H	2.26093	-4.56275	1.55338
C	4.87553	-3.69068	1.7524
H	4.78181	-4.76937	1.96767
H	5.89166	-3.50583	1.36604
H	4.74901	-3.13937	2.6998
C	5.70008	2.82013	-1.05534
H	5.20713	3.4017	-1.84934
H	6.1628	3.50143	-0.3256
H	6.4725	2.17035	-1.49794
B	-2.55473	-0.10889	0.1036
C	-1.55245	-0.63599	1.30296
C	-1.77793	-1.91775	1.8575

C	-0.44581	0.06193	1.80329
C	-0.97102	-2.45476	2.85956
H	-2.61281	-2.51577	1.48304
C	0.37668	-0.47594	2.81091
H	-0.20582	1.05071	1.39912
C	0.1152	-1.72837	3.3594
H	0.74828	-2.14437	4.14422
C	-1.99343	1.28911	-0.57631
C	-2.07465	2.50053	0.13891
C	-1.43858	1.37123	-1.86639
C	-1.63281	3.71584	-0.39836
H	-2.49994	2.49626	1.14687
C	-0.98078	2.57833	-2.40739
H	-1.35688	0.47013	-2.47579
C	-1.08425	3.76678	-1.68147
H	-0.73059	4.71116	-2.09858
C	-2.57906	-1.31043	-1.0261
C	-3.72911	-1.86385	-1.61099
C	-1.35017	-1.83185	-1.47211
C	-3.65496	-2.86449	-2.59226
H	-4.71849	-1.52156	-1.29618
C	-1.2623	-2.81242	-2.46219
H	-0.42651	-1.4545	-1.02808
C	-2.42183	-3.34472	-3.03447
H	-2.36535	-4.12216	-3.79736
C	-4.05889	0.2038	0.68618
C	-4.47824	-0.0526	2.00161
C	-5.01977	0.77794	-0.16965
C	-5.77949	0.23409	2.43744
H	-3.78162	-0.48947	2.72141
C	-6.32596	1.04738	0.24802

H	-4.74059	1.02566	-1.19843
C	-6.71933	0.77887	1.56197
H	-7.73556	0.99314	1.89465
C	1.59558	0.27978	3.22665
C	-1.17917	-3.86469	3.34969
C	0.09455	-3.23607	-2.94486
C	-4.93437	-3.38354	-3.20052
C	-7.31581	1.58132	-0.75474
C	-6.13701	-0.0006	3.88232
C	-1.7632	4.98381	0.40442
C	-0.37577	2.62799	-3.7852
F	-2.41771	-4.31476	3.11355
F	-0.94403	-3.97383	4.67085
F	-0.32151	-4.71463	2.7353
F	2.29245	-0.2975	4.21102
F	2.48422	0.37302	2.15838
F	1.35888	1.55279	3.57892
F	0.98802	-3.31713	-1.92398
F	0.6195	-2.33734	-3.81676
F	0.09047	-4.42204	-3.5652
F	-5.87556	-3.60167	-2.26501
F	-5.4533	-2.50226	-4.07804
F	-4.74907	-4.53964	-3.86558
F	-7.46575	-0.09217	4.07187
F	-5.6966	1.00365	4.67015
F	-5.58209	-1.13239	4.35773
F	-8.41562	2.08911	-0.16954
F	-6.77771	2.55425	-1.51566
F	-7.72762	0.61404	-1.59989
F	-2.96403	5.56272	0.25894
F	-1.58647	4.76214	1.7224

F	-0.83742	5.90539	0.03591
F	0.76937	3.363	-3.79011
F	-1.19051	3.19319	-4.68795
F	-0.04626	1.40627	-4.251

6b

P	3.98151	0.8915	1.4124
P	5.10889	-0.78409	-0.16076
N	5.43084	0.78363	0.56187
N	3.59282	-0.57639	0.70433
C	2.55459	-1.605	1.04887
C	3.05222	-2.52078	2.17989
H	3.22958	-1.94477	3.10555
H	2.28575	-3.28154	2.39905
H	3.98726	-3.03091	1.90054
C	1.28539	-0.87609	1.49574
H	0.86821	-0.24662	0.69468
H	0.53017	-1.62687	1.77122
H	1.45087	-0.24691	2.38496
C	2.26664	-2.41871	-0.22117
H	1.48035	-3.16353	-0.01666
H	1.92028	-1.76701	-1.0398
H	3.16084	-2.96731	-0.56118
C	6.46018	1.80386	0.22619
C	6.02219	2.58883	-1.02441
H	5.04297	3.06933	-0.86736
H	6.75958	3.3729	-1.26996
H	5.93224	1.91206	-1.88973
C	6.61693	2.74423	1.43202
H	5.67631	3.27327	1.66386

H	6.94252	2.18541	2.32663
H	7.37671	3.51324	1.21261
C	7.79966	1.09572	-0.0303
H	7.74336	0.42381	-0.90156
H	8.5793	1.85037	-0.2333
H	8.10219	0.49202	0.84095
Se	6.38651	-2.35523	0.35124
N	2.93425	2.07891	0.98624
H	2.65421	1.93914	0.01363
N	4.75539	-0.55597	-1.76551
H	3.99549	0.10837	-1.903
C	2.44176	3.41118	1.48964
C	2.76355	3.63067	2.96928
H	2.34193	4.60228	3.27556
H	2.30735	2.85755	3.60485
H	3.84982	3.67719	3.15802
C	3.08045	4.52042	0.63567
H	4.17085	4.57931	0.7889
H	2.88631	4.3488	-0.43718
H	2.64289	5.49752	0.90416
C	0.92201	3.40953	1.27794
H	0.46006	2.55153	1.7858
H	0.46771	4.33312	1.67068
H	0.67635	3.35805	0.20514
C	5.22082	-1.21483	-3.02847
C	6.75059	-1.13974	-3.15717
H	7.25297	-1.68327	-2.34208
H	7.06536	-1.59059	-4.11436
H	7.09026	-0.08908	-3.14536
C	4.58495	-0.39989	-4.16718
H	3.48427	-0.44718	-4.11948

H	4.89088	0.66093	-4.124
H	4.89541	-0.80964	-5.14271
C	4.7304	-2.6706	-3.09667
H	5.05013	-3.13383	-4.04683
H	5.14774	-3.26467	-2.26738
H	3.62924	-2.7192	-3.04524
C	4.22966	0.804	3.19657
H	4.7395	1.70136	3.5742
H	3.26605	0.67683	3.71475
H	4.87117	-0.07668	3.36104
B	-2.5628	-0.13709	-0.12091
C	-1.29536	-0.21515	-1.17462
C	-1.15181	-1.32609	-2.0332
C	-0.39669	0.84622	-1.38203
C	-0.15528	-1.39215	-3.00842
H	-1.84653	-2.16449	-1.94499
C	0.56595	0.81507	-2.4052
H	-0.47051	1.73123	-0.74564
C	0.69976	-0.30907	-3.22103
H	1.43267	-0.33791	-4.02805
C	-2.29435	0.99427	1.07157
C	-1.60552	0.61062	2.23989
C	-2.72359	2.33519	1.03757
C	-1.36705	1.4865	3.30398
H	-1.2672	-0.41988	2.34501
C	-2.48916	3.22265	2.09773
H	-3.28122	2.71081	0.17758
C	-1.81862	2.80648	3.24898
H	-1.64877	3.49535	4.07832
C	-3.83477	0.2682	-1.09383
C	-5.0065	-0.49572	-1.23995

C	-3.75517	1.42055	-1.89877
C	-6.04753	-0.10954	-2.09487
H	-5.12088	-1.43273	-0.6905
C	-4.79372	1.82583	-2.74155
H	-2.84251	2.02375	-1.89047
C	-5.95868	1.06384	-2.84593
H	-6.76931	1.36851	-3.50843
C	-2.79827	-1.55013	0.68948
C	-1.85295	-2.58527	0.75537
C	-3.9267	-1.70192	1.52094
C	-2.01255	-3.69949	1.58957
H	-0.93892	-2.52275	0.16242
C	-4.11765	-2.8275	2.32788
H	-4.67339	-0.90357	1.5608
C	-3.1558	-3.84117	2.37566
H	-3.29073	-4.71023	3.02066
C	1.49903	1.96449	-2.62743
C	0.07856	-2.65659	-3.79328
C	-4.61929	3.10135	-3.5219
C	-7.29367	-0.95635	-2.15518
C	-5.39091	-2.94696	3.12734
C	-0.88391	-4.68572	1.699
C	-0.54306	1.02079	4.47072
C	-2.88185	4.6722	1.97504
F	-0.99616	-3.45188	-3.82886
F	1.08798	-3.37596	-3.2365
F	0.45004	-2.40223	-5.06167
F	2.70047	1.77302	-1.93376
F	1.86512	2.11899	-3.90002
F	1.03176	3.13548	-2.17621
F	-3.5113	3.06372	-4.29235

F	-4.4721	4.16199	-2.6992
F	-5.66019	3.36312	-4.32953
F	-7.00254	-2.27101	-2.1559
F	-8.09212	-0.73693	-1.09121
F	-8.02746	-0.70514	-3.25551
F	-1.26624	-5.87089	2.1915
F	0.09234	-4.21485	2.52497
F	-0.28255	-4.90927	0.5113
F	-5.29116	-3.86238	4.10914
F	-5.72884	-1.77632	3.69958
F	-6.42679	-3.3131	2.34798
F	-0.71143	-0.27775	4.74673
F	0.80501	1.17016	4.20827
F	-0.77312	1.72062	5.58878
F	-3.27018	5.19269	3.1533
F	-3.87	4.86858	1.09306
F	-1.82751	5.42141	1.55645

6c

P	3.72917	0.00871	0.40346
P	6.1278	0.11271	-0.48551
N	4.80167	-1.01741	-0.37971
N	5.01324	1.10576	0.44182
C	5.06454	2.57842	0.71061
C	4.55392	3.37223	-0.50432
H	3.49337	3.15499	-0.70829
H	4.63301	4.45504	-0.30436
H	5.1457	3.13726	-1.40361
C	4.19934	2.87426	1.94289
H	4.52525	2.27784	2.81239

H	4.28235	3.94301	2.20366
H	3.13366	2.67699	1.75443
C	6.52526	2.94776	1.01201
H	6.58674	4.02031	1.26271
H	6.91245	2.36768	1.8671
H	7.17614	2.76832	0.14064
C	4.69815	-2.46372	-0.73676
C	5.05083	-3.31009	0.49889
H	4.34594	-3.11005	1.32473
H	4.99698	-4.3864	0.26077
H	6.07561	-3.0815	0.84157
C	3.26479	-2.74373	-1.20188
H	2.5295	-2.57741	-0.39797
H	3.00542	-2.10268	-2.06009
H	3.15917	-3.7962	-1.51071
C	5.66653	-2.76623	-1.88923
H	6.71484	-2.58401	-1.60338
H	5.57077	-3.82959	-2.16783
H	5.43887	-2.1471	-2.7718
Se	6.75194	0.77032	-2.36586
N	3.24129	-0.56654	1.86543
H	4.04172	-0.83275	2.43684
N	7.29982	-0.41167	0.57683
H	6.91807	-0.63675	1.49277
C	1.93798	-0.6187	2.63914
C	1.52379	0.78991	3.07439
H	0.61563	0.74865	3.69312
H	2.31821	1.27492	3.66583
H	1.29985	1.43052	2.20922
C	0.82863	-1.28321	1.81923
H	0.50884	-0.67343	0.9627

H	1.12604	-2.27776	1.45123
H	-0.06442	-1.40652	2.45283
C	2.24195	-1.48587	3.87086
H	3.04848	-1.0427	4.4855
H	1.34157	-1.55195	4.50157
H	2.53608	-2.50849	3.5729
C	8.78981	-0.5499	0.49123
C	9.18244	-1.545	-0.61278
H	8.8464	-1.19597	-1.60194
H	10.28014	-1.65927	-0.64355
H	8.73903	-2.53706	-0.4179
C	9.22342	-1.10963	1.85715
H	8.95834	-0.41546	2.67626
H	8.7535	-2.09093	2.05469
H	10.31712	-1.24973	1.87759
C	9.46254	0.81334	0.26126
H	10.55998	0.69309	0.2472
H	9.15268	1.25214	-0.70034
H	9.20222	1.51813	1.06921
C	2.33728	0.51855	-0.5999
H	1.67061	-0.33184	-0.7979
H	1.77359	1.33207	-0.12338
H	2.75635	0.86619	-1.55632
B	-2.89235	0.09409	-0.0576
C	-2.60913	1.71712	0.01184
C	-1.34692	2.21903	0.37782
C	-3.60002	2.68483	-0.24254
C	-1.08823	3.59129	0.50069
H	-0.53746	1.51	0.57783
C	-3.35072	4.05763	-0.13677
H	-4.60434	2.36486	-0.52875

C	-2.09128	4.52681	0.24184
H	-1.89869	5.59622	0.33474
C	-4.31227	-0.1865	-0.84601
C	-5.54082	-0.03199	-0.17558
C	-4.38977	-0.51942	-2.20887
C	-6.77027	-0.18489	-0.82497
H	-5.54259	0.21706	0.8897
C	-5.61517	-0.68982	-2.86566
H	-3.47387	-0.64906	-2.7906
C	-6.81921	-0.51995	-2.1801
H	-7.77542	-0.64583	-2.68939
C	-1.68359	-0.6687	-0.89821
C	-1.33812	-2.01372	-0.68052
C	-1.02115	-0.03145	-1.97086
C	-0.41816	-2.69463	-1.48956
H	-1.79526	-2.56642	0.14369
C	-0.10509	-0.7037	-2.78679
H	-1.23619	1.01824	-2.18373
C	0.19407	-2.05218	-2.56338
H	0.89263	-2.58537	-3.20947
C	-2.97506	-0.53867	1.46611
C	-2.43674	0.07409	2.61422
C	-3.5533	-1.80651	1.66413
C	-2.44333	-0.55493	3.86476
H	-1.99871	1.07163	2.54229
C	-3.543	-2.4549	2.90502
H	-4.03077	-2.31386	0.82081
C	-2.98606	-1.83482	4.02169
H	-2.98675	-2.33085	4.99392
C	-4.436	5.04469	-0.49123
C	0.26497	4.04806	0.95839

C	0.62347	-0.00073	-3.90073
C	-0.0776	-4.1222	-1.15158
C	-4.09579	-3.85423	2.98961
C	-1.81694	0.09695	5.06571
C	-8.04002	0.07666	-0.0568
C	-5.62326	-1.1166	-4.31086
F	0.50304	3.73678	2.25284
F	0.46055	5.36343	0.82589
F	1.26728	3.43115	0.25557
F	-4.27543	6.21763	0.15282
F	-4.43561	5.32114	-1.81064
F	-5.65773	4.57881	-0.18714
F	1.97168	-0.00473	-3.66807
F	0.2622	1.28078	-4.03666
F	0.45297	-0.60905	-5.08397
F	0.59779	-4.19704	0.02841
F	-1.16574	-4.88819	-1.01353
F	0.71657	-4.69675	-2.07691
F	-2.60892	0.05576	6.14737
F	-1.4848	1.38282	4.85082
F	-0.66181	-0.5391	5.42006
F	-4.18311	-4.29727	4.2567
F	-5.31934	-3.94262	2.4421
F	-3.30619	-4.7223	2.31915
F	-7.98921	-0.44579	1.1833
F	-8.26118	1.3995	0.09002
F	-9.12292	-0.43793	-0.66769
F	-6.77683	-0.80224	-4.92864
F	-5.46349	-2.45084	-4.43512
F	-4.62304	-0.54303	-5.00817

6d

P	5.72931	1.25701	-0.06346
P	4.92159	-1.16328	-0.19655
N	5.15652	0.22818	-1.24559
N	5.33195	0.04861	1.02992
C	5.64373	-0.14099	2.47905
C	7.10675	-0.57734	2.66849
H	7.80644	0.20665	2.32798
H	7.31082	-0.76402	3.73719
H	7.31536	-1.5009	2.10409
C	5.38241	1.18717	3.20349
H	4.3487	1.53352	3.04174
H	5.54047	1.05492	4.28735
H	6.07462	1.97717	2.86626
C	4.69366	-1.2162	3.02793
H	4.86367	-1.336	4.11141
H	3.64123	-0.93194	2.86861
H	4.87419	-2.19234	2.5498
C	4.76889	0.47181	-2.6692
C	3.39535	1.16049	-2.70355
H	3.43398	2.14541	-2.20818
H	3.05712	1.30744	-3.74094
H	2.64019	0.54414	-2.19278
C	5.83663	1.36119	-3.32463
H	5.89037	2.35382	-2.84364
H	6.83104	0.88365	-3.27901
H	5.58215	1.52691	-4.38512
C	4.71561	-0.87575	-3.40249
H	3.95905	-1.54254	-2.96412
H	4.42975	-0.70405	-4.45352

H	5.69218	-1.38597	-3.37137
Se	6.23695	-2.76968	-0.44673
N	4.91361	2.67539	0.06041
H	3.9181	2.48659	0.17819
N	3.30689	-1.47152	-0.07933
H	2.76106	-0.63003	0.09902
C	5.23219	4.14057	0.17887
C	6.33788	4.5734	-0.79398
H	6.421	5.67311	-0.77711
H	7.32646	4.17617	-0.51571
H	6.1044	4.26866	-1.82801
C	3.925	4.86179	-0.19834
H	3.62684	4.61916	-1.23359
H	3.10279	4.57781	0.48065
H	4.06095	5.95362	-0.12431
C	5.62506	4.48247	1.62374
H	6.57193	3.98942	1.9066
H	5.76858	5.57142	1.73423
H	4.841	4.16029	2.3287
C	2.4877	-2.73873	-0.10449
C	2.58932	-3.42465	-1.47452
H	3.62152	-3.74472	-1.69145
H	1.93422	-4.31214	-1.48917
H	2.24645	-2.74356	-2.27186
C	1.04579	-2.27766	0.12769
H	0.95409	-1.76024	1.09708
H	0.70025	-1.61186	-0.68105
H	0.37651	-3.15025	0.14491
C	2.88884	-3.69171	1.0317
H	2.24797	-4.58928	0.9945
H	3.9394	-4.01182	0.94599

H	2.73194	-3.21328	2.01292
C	7.50729	1.54193	-0.18895
H	7.7486	2.06837	-1.12415
H	7.88669	2.11237	0.67382
H	7.96513	0.53928	-0.20623
B	-2.93184	0.04128	-0.05493
C	-2.12819	-0.85105	-1.18464
C	-2.26278	-2.2483	-1.26201
C	-1.29417	-0.25344	-2.15068
C	-1.56274	-3.01427	-2.20191
H	-2.91007	-2.76559	-0.54941
C	-0.60736	-1.00924	-3.10733
H	-1.16134	0.83141	-2.14557
C	-0.72713	-2.40248	-3.13524
H	-0.17528	-2.99926	-3.86419
C	-2.01993	1.31806	0.45406
C	-0.64155	1.14941	0.65676
C	-2.5587	2.5421	0.8955
C	0.14845	2.1194	1.28213
H	-0.17063	0.21594	0.34438
C	-1.77074	3.53155	1.49799
H	-3.63046	2.72678	0.78463
C	-0.40396	3.32883	1.70968
H	0.20267	4.08777	2.20552
C	-4.33366	0.47555	-0.77236
C	-5.48211	-0.33449	-0.70946
C	-4.41895	1.61303	-1.59393
C	-6.65488	-0.01468	-1.40253
H	-5.46471	-1.24812	-0.1088
C	-5.58498	1.93915	-2.29648
H	-3.55083	2.27122	-1.69568

C	-6.7183	1.12926	-2.20258
H	-7.63075	1.38132	-2.74432
C	-3.11646	-0.78795	1.35845
C	-2.09496	-1.64108	1.80462
C	-4.16965	-0.56797	2.26435
C	-2.10112	-2.24085	3.06596
H	-1.2509	-1.84284	1.14727
C	-4.19657	-1.17182	3.5289
H	-4.99348	0.09475	1.98447
C	-3.16125	-2.01547	3.94566
H	-3.18517	-2.48585	4.92941
C	0.28824	-0.36179	-4.12562
C	-1.60578	-4.51723	-2.12544
C	-5.58179	3.14796	-3.19512
C	-7.87482	-0.88395	-1.23496
C	-5.32456	-0.85107	4.47694
C	-0.92474	-3.10087	3.44024
C	1.58467	1.79416	1.50528
C	-2.388	4.85245	1.88659
F	-2.77288	-4.97676	-1.65509
F	-0.63823	-4.9816	-1.28706
F	-1.38311	-5.09789	-3.31738
F	-0.17206	-0.49771	-5.37892
F	0.46837	0.95414	-3.90391
F	1.52954	-0.92897	-4.11817
F	-4.9269	2.9064	-4.35057
F	-4.9616	4.19625	-2.61669
F	-6.8236	3.54689	-3.52427
F	-7.55082	-2.18589	-1.12284
F	-8.56554	-0.55865	-0.12323
F	-8.72681	-0.76842	-2.2716

F	-1.06945	-3.70047	4.631
F	0.22265	-2.37267	3.50043
F	-0.69387	-4.06674	2.52429
F	-5.49838	-1.81465	5.40203
F	-5.09254	0.29641	5.14883
F	-6.4935	-0.69369	3.83202
F	2.3071	2.80635	2.03143
F	1.78427	0.7206	2.29075
F	2.2206	1.47519	0.31481
F	-1.73523	5.42454	2.91933
F	-3.67506	4.72426	2.24097
F	-2.3431	5.73259	0.86572

6e

P	4.87222	1.13923	0.02832
P	3.53486	-1.03927	0.03275
N	4.55951	-0.08578	1.11461
N	4.09075	0.19059	-1.10959
C	3.5766	0.49052	-2.48481
C	2.23144	1.22432	-2.40943
H	2.33999	2.18754	-1.88963
H	1.84052	1.42419	-3.41914
H	1.48267	0.62889	-1.86728
C	4.61122	1.3689	-3.20234
H	5.60883	0.89581	-3.21342
H	4.28982	1.53155	-4.24476
H	4.69554	2.36296	-2.7308
C	3.43458	-0.84603	-3.22397
H	3.08672	-0.66323	-4.25246
H	4.39941	-1.38196	-3.25969

H	2.68466	-1.49288	-2.74513
C	5.04696	-0.37349	2.4946
C	6.31255	-1.24396	2.38992
H	7.10905	-0.70779	1.84135
H	6.69872	-1.49639	3.39276
H	6.09049	-2.18355	1.85593
C	5.36582	0.95233	3.20217
H	6.15607	1.51297	2.67645
H	4.46483	1.57966	3.28848
H	5.73495	0.7455	4.22105
C	3.94581	-1.10677	3.27623
H	3.69607	-2.07756	2.81917
H	4.29805	-1.29713	4.30478
H	3.02805	-0.50012	3.32015
Se	1.51256	-1.18584	0.48567
N	6.47948	1.39368	-0.27294
H	6.95221	0.51136	-0.46154
N	4.36225	-2.42393	-0.36779
H	5.27996	-2.24248	-0.76752
C	7.39816	2.58419	-0.33878
C	6.8688	3.65537	-1.30415
H	7.59348	4.4849	-1.36766
H	6.73111	3.24206	-2.31597
H	5.91296	4.08587	-0.9662
C	7.62335	3.18072	1.05965
H	6.68957	3.57602	1.49236
H	8.03351	2.42441	1.74972
H	8.34018	4.01799	1.00214
C	8.73003	2.03582	-0.87987
H	8.59954	1.59981	-1.88663
H	9.47089	2.84894	-0.95543

H	9.14703	1.26395	-0.2069
C	3.95122	-3.86957	-0.39403
C	3.51259	-4.32788	1.00544
H	2.61643	-3.7882	1.34469
H	3.25891	-5.40094	0.9858
H	4.32675	-4.17275	1.73568
C	5.21855	-4.63876	-0.80365
H	5.56942	-4.32788	-1.80575
H	6.03552	-4.48375	-0.07454
H	5.00269	-5.71931	-0.84675
C	2.84456	-4.11376	-1.43288
H	2.55795	-5.17908	-1.43492
H	1.93917	-3.53101	-1.21041
H	3.19288	-3.84438	-2.44488
C	4.02858	2.68077	0.40724
H	4.53902	3.22854	1.21358
H	3.91463	3.31977	-0.48086
H	3.02985	2.37579	0.75658
B	-2.4556	0.11731	-0.02991
C	-3.88175	0.74735	0.4996
C	-4.96479	-0.09377	0.81972
C	-4.123	2.12858	0.5903
C	-6.21132	0.41	1.20669
H	-4.83695	-1.17831	0.75715
C	-5.3661	2.64397	0.97975
H	-3.32636	2.83545	0.34364
C	-6.42373	1.78836	1.29195
H	-7.39586	2.18563	1.58624
C	-1.26867	1.24363	0.24726
C	-0.89328	2.17945	-0.73717
C	-0.64618	1.39318	1.50136

C	0.02344	3.20815	-0.48282
H	-1.32557	2.10519	-1.7377
C	0.26477	2.41938	1.76686
H	-0.86308	0.68921	2.30582
C	0.59918	3.34973	0.78073
H	1.29489	4.16463	0.99117
C	-2.11195	-1.26504	0.81479
C	-1.59381	-2.44116	0.23632
C	-2.27032	-1.29654	2.21322
C	-1.20057	-3.54229	1.0042
H	-1.47293	-2.50752	-0.84524
C	-1.85462	-2.38195	2.99454
H	-2.73173	-0.44378	2.71971
C	-1.30824	-3.5174	2.39772
H	-0.97973	-4.36352	3.00378
C	-2.55164	-0.22199	-1.63674
C	-3.75621	-0.22635	-2.36251
C	-1.40089	-0.60279	-2.35289
C	-3.81398	-0.60346	-3.7105
H	-4.68597	0.05863	-1.86438
C	-1.45172	-1.01026	-3.69077
H	-0.43458	-0.61402	-1.83998
C	-2.66263	-1.01191	-4.3866
H	-2.71097	-1.3358	-5.42693
C	-5.53369	4.13547	1.10787
C	-7.31088	-0.5512	1.57808
C	-1.94656	-2.2631	4.4927
C	-0.64789	-4.7792	0.34949
C	-0.18381	-1.44543	-4.36592
C	-5.12556	-0.52635	-4.45054
C	0.39409	4.19807	-1.55353

C	0.9834	2.47009	3.08346
F	-7.33573	-1.62192	0.76196
F	-8.52821	0.02225	1.52754
F	-7.15275	-1.02439	2.83167
F	-6.82662	4.50941	1.08907
F	-5.00993	4.59654	2.26393
F	-4.90883	4.79755	0.11423
F	-3.16228	-1.85108	4.89107
F	-1.05909	-1.35476	4.95976
F	-1.68533	-3.42459	5.12057
F	-0.39134	-4.60644	-0.96045
F	0.51898	-5.1673	0.92658
F	-1.48369	-5.82843	0.45581
F	-5.1643	-1.37327	-5.49856
F	-5.34169	0.71107	-4.94324
F	-6.1704	-0.81774	-3.65729
F	-0.39538	-2.09027	-5.52236
F	0.62721	-0.39143	-4.65387
F	0.54839	-2.26735	-3.57643
F	1.7278	4.49966	-1.49922
F	0.15656	3.73482	-2.79052
F	-0.2536	5.36625	-1.42851
F	1.25331	3.72681	3.47965
F	2.20889	1.85012	2.98152
F	0.33471	1.85217	4.07122

6f

P	3.5474	1.55353	0.08103
P	3.98955	-0.9486	-0.07984
N	3.49434	0.24157	1.11535

N	4.34117	0.51894	-0.98838
C	4.73164	0.67818	-2.42155
C	3.50391	0.63653	-3.34101
H	2.8218	1.47999	-3.14907
H	3.81885	0.70022	-4.39736
H	2.94459	-0.30026	-3.20931
C	5.4634	2.02158	-2.56668
H	6.33056	2.08072	-1.88627
H	5.82172	2.13914	-3.6035
H	4.79418	2.87349	-2.35422
C	5.69186	-0.4691	-2.77366
H	6.04492	-0.34562	-3.81151
H	6.56807	-0.47721	-2.1032
H	5.18711	-1.44684	-2.70437
C	3.1055	0.08696	2.5511
C	4.38462	-0.0893	3.38756
H	5.05048	0.78621	3.27093
H	4.13087	-0.18553	4.45729
H	4.9369	-0.99291	3.08193
C	2.36176	1.35023	2.99663
H	3.00026	2.24705	2.94413
H	1.46176	1.51067	2.38541
H	2.02484	1.23092	4.03789
C	2.18426	-1.12958	2.70066
H	2.67739	-2.06396	2.39125
H	1.87197	-1.23746	3.75262
H	1.27594	-1.00807	2.09119
Se	2.57665	-2.25007	-0.88201
N	4.45137	2.80104	0.65891
H	5.29281	2.4501	1.11678
N	5.42852	-1.58558	0.45156

H	6.07887	-0.87971	0.78857
C	4.41903	4.30552	0.64539
C	3.40204	4.86845	-0.35564
H	3.52702	5.96327	-0.39685
H	3.56117	4.47984	-1.37586
H	2.36399	4.67739	-0.04911
C	4.08174	4.79257	2.06432
H	3.05639	4.50442	2.34442
H	4.7845	4.36861	2.8041
H	4.15362	5.89303	2.11821
C	5.8352	4.75612	0.245
H	6.08835	4.40734	-0.77058
H	5.90538	5.85691	0.26427
H	6.59329	4.36341	0.94861
C	5.9158	-2.99775	0.58928
C	4.98212	-3.81966	1.49584
H	3.97155	-3.912	1.06772
H	5.39047	-4.83705	1.62673
H	4.89628	-3.35432	2.49337
C	7.29858	-2.88438	1.25366
H	7.99469	-2.29373	0.6294
H	7.22603	-2.41265	2.25126
H	7.73593	-3.88787	1.38729
C	6.06223	-3.65977	-0.79037
H	6.46762	-4.68051	-0.67729
H	5.08866	-3.73231	-1.30034
H	6.75144	-3.08047	-1.429
C	1.92079	2.07042	-0.46768
H	1.39292	2.59788	0.33993
H	1.94794	2.69504	-1.36923
H	1.38459	1.13484	-0.70041

B	-2.12647	-0.11173	-0.05353
C	-3.62785	0.49892	-0.36178
C	-4.20793	0.40661	-1.64052
C	-4.43147	1.06335	0.64434
C	-5.50479	0.86137	-1.90464
H	-3.63791	-0.04135	-2.45912
C	-5.73008	1.52222	0.39085
H	-4.04462	1.14383	1.66386
C	-6.27927	1.42729	-0.88904
H	-7.29273	1.77706	-1.08915
C	-1.51865	0.72533	1.25008
C	-1.28824	2.11362	1.19942
C	-1.34943	0.13731	2.52092
C	-0.92826	2.86295	2.32646
H	-1.42194	2.65302	0.26126
C	-0.99897	0.87756	3.65653
H	-1.50254	-0.93621	2.64019
C	-0.79641	2.25603	3.57601
H	-0.51103	2.83632	4.45494
C	-2.24352	-1.70665	0.33383
C	-1.09266	-2.45807	0.64622
C	-3.4645	-2.39934	0.39203
C	-1.15019	-3.81331	0.9893
H	-0.11272	-1.97225	0.61468
C	-3.53627	-3.75435	0.74236
H	-4.39321	-1.8744	0.15533
C	-2.3797	-4.47568	1.04193
H	-2.43431	-5.53163	1.30879
C	-1.21708	0.07659	-1.43162
C	-0.66498	-1.00785	-2.14089
C	-1.05061	1.33817	-2.04015

C	0.01505	-0.85091	-3.35431
H	-0.77733	-2.02018	-1.75259
C	-0.34115	1.51396	-3.23429
H	-1.51705	2.21963	-1.59749
C	0.19408	0.41523	-3.91089
H	0.73252	0.54441	-4.85167
C	-6.50879	2.1683	1.50726
C	-6.03918	0.78468	-3.31159
C	-4.88557	-4.41913	0.84996
C	0.1275	-4.56533	1.25085
C	-0.08777	2.89521	-3.77048
C	0.51769	-2.05552	-4.10896
C	-0.5659	4.30929	2.15632
C	-0.82408	0.1931	4.98799
F	-5.57267	1.7981	-4.07251
F	-7.38265	0.8529	-3.35204
F	-5.67368	-0.35638	-3.9252
F	-7.8283	2.21899	1.24926
F	-6.34984	1.51282	2.67289
F	-6.10194	3.43814	1.7222
F	-5.73428	-3.98616	-0.09903
F	-5.46771	-4.164	2.03956
F	-4.80097	-5.75884	0.73623
F	0.80253	-4.82127	0.10853
F	0.9745	-3.8641	2.04057
F	-0.08239	-5.7484	1.85241
F	1.74624	-1.83486	-4.63557
F	-0.2864	-2.36827	-5.14083
F	0.61069	-3.14848	-3.33195
F	-0.05562	2.93485	-5.10961
F	-0.98337	3.79526	-3.34755

F	1.14012	3.36199	-3.35675
F	0.74006	4.41827	1.71856
F	-1.30764	4.93519	1.23636
F	-0.62853	5.00972	3.29462
F	-1.9005	0.32129	5.77861
F	0.22381	0.71995	5.67345
F	-0.5761	-1.12258	4.8548