Supporting information

Neutral binuclear rare-earth metal complexes with four μ_2-bridging hydrides

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Contents

1. Experimental section

General Methods. All manipulations were performed under a nitrogen atmosphere using standard Schlenk techniques or an MBraun glovebox. All solvents were purified from an MBraun SPS system. Samples of yttrium complexes for NMR spectroscopic measurements were prepared in the glovebox

by use of NMR tubes sealed by paraffin film. ^{1}H, and ^{13}C NMR spectra were recorded on a Bruker AV400 (FT, 400 MHz for ^{1}H; 100 MHz for ^{13}C) spectrometer. Elemental analysis was performed at National Analytical Research Centre of Changchun Institute of Applied Chemistry (CIAC). Phenylsilane was dried over CaH_2 under stirring for 24 h and distilled under reduced pressure before use.

Synthesis of [2,6-^{i}Pr$_2$C$_6$H$_3$N=PPh$_2$HNPh$_2$P=NC$_6$H$_3$^{i}Pr$_2$-2,6] (HL). 2,6-diisopropylphenyl azide (4.87 g, 24 mmol) in 10 mL of toluene was added dropwise to a toluene solution (50 mL) of bis(diphenylphosphine)amine ($Ph_2PNHPPh_2$) (3.85 g, 10 mmol) at room temperature. The reaction mixture was stirred at 60 ^{o}C, till the evolution of nitrogen gas ended up (about 4 h). Finally, the solution was concentrated to approximately 20 ml, which stayed under –30 ^{o}C for 2 h. Filtration, washing with hexane and drying up the residual solvents afforded the product as a pale yellow solid (6.47 g, 88%). ^{1}H NMR (300 MHz, $CDCl_3$, 7.26 ppm, 25 ^{o}C): δ 0.76 (d, $^{3}J_{HH}$ = 6.9 Hz, 24H, CH(C*H*$_3$)$_2$), 3.55 (sept, $^{3}J_{HH}$ = 6.9 Hz, 4H, C*H*(CH$_3$)$_2$), 6.91 (s, 6H, *p*-C$_6$H$_3$ and *m*-NC$_6$H$_3$), 7.20–7.30 (m, 8H, *m*-PC$_6$H$_5$), 7.38 (t, $^{3}J_{HH}$ = 7.2 Hz, 4H, *p*-PC$_6$H$_5$), 7.49 (quart, $^{3}J_{HH}$ = 7.2 Hz, 8H, *o*-PC$_6$H$_5$) (the N*H* signal doesn't appear). Anal. Calcd (%) for $C_{36}H_{55}N_3P_2$: C, 73.10; H, 9.31; N, 7.11. Found: C, 73.48; H, 9.38; N, 6.95.

Synthesis of (NPNPN)Y(CH$_2$SiMe$_3$)$_2$ (1-Y). To a hexane solution (2.0 mL) of Y(CH$_2$SiMe$_3$)$_3$(THF)$_2$ (0.247 g, 0.50 mmol) was added dropwise 1 equiv of the ligand HL (0.368 g, 0.50 mmol in 2 mL of THF) at room temperature. The mixture was stirred for 3 h at room temperature and then concentrated to about 0.5 mL. Addition of 1 mL of hexane and cooling to –30 ^{o}C for 2 days afforded crystalline solids, which were washed with a small amount of hexane to remove impurities and dried in vacuo to give white solids of **1-Y** (0.335 g, 67%). ^{1}H NMR (400

MHz, C_6D_6, 7.16 ppm, 25 °C): δ 0.10 (d, J_{YH} = 2.8 Hz, 4H, CH_2SiMe$_3$), 0.34 (s, 18H, CH$_2$SiMe_3), 0.63 (d, $^3J_{HH}$ = 5.6 Hz, 12H, C$_6$H$_3$CH(CH_3)$_2$), 1.55 (d, $^3J_{HH}$ = 5.6 Hz, 12H, C$_6$H$_3$CH(CH_3)$_2$), 3.81 (sept, $^3J_{HH}$ = 6.8 Hz, 4H, C$_6$H$_3$CH(CH$_3$)$_2$), 6.78–6.88 (m, 12H, *m*-PC$_6H_5$ and *p*-PC$_6H_5$), 7.15 (s, 6H, *m*-NC$_6H_3$ and *p*-NC$_6H_3$), 7.38 (m, 8H, *o*-PC$_6H_5$). ^{13}C NMR (100 MHz, C_6D_6, 128.06 ppm, 25 °C) δ 4.48 (s, 6C, CH$_2$SiMe_3), 23.30 (s, 4C, C$_6$H$_3$CH(*C*H$_3$)$_2$), 27.75 (s, 4C, C$_6$H$_3$CH(*C*H$_3$)$_2$), 29.20 (s, 4C, C$_6$H$_3$*C*H(CH$_3$)$_2$), 46.95 (d, J_{YC} = 27.7 Hz, 2C, *C*H$_2$SiMe$_3$), 124.66 (s, aromatic *C*H), 124.90 (s, aromatic *C*H), 125.70 (s, aromatic *C*H), 129.33 (s, aromatic *C*H), 131.48 (s, aromatic *C*H), 132.12 (m, aromatic *C*H), 132.78 (d, J_{PC} = 5.4 Hz, 2C, aromatic *ipso*-*C*), 133.51 (d, J_{PC} = 5.4 Hz, 2C, aromatic *ipso*-*C*), 139.16 (s, aromatic *ipso*-*C*), 145.67 (s, aromatic *ipso*-*C*). Anal. Calcd (%) for $C_{44}H_{76}N_3P_2Si_2Y$: C, 52.80; H, 7.60; N, 4.20. Found: C, 53.05; H, 7.49; N, 4.08.

Synthesis of (NPNPN)Lu(CH$_2$SiMe$_3$)$_2$ (1-Lu). Following a procedure similar to that described for the preparation of **1-Y**, treatment of Lu(CH$_2$SiMe$_3$)$_3$(THF)$_2$ (0.290 g, 0.50 mmol) with HL (0.368 g, 0.50 mmol) gave white solids of **1-Lu** (0.348 g, 64%). Single crystals suitable for X-ray analysis were obtained from a mixture of THF/toluene at –30 °C overnight. ^{1}H NMR (400 MHz, C_6D_6, 7.16 ppm, 25 °C): δ –0.10 (s, 4H, CH_2SiMe$_3$), 0.35 (s, 18H, CH$_2$SiMe_3), 0.66 (d, $^3J_{HH}$ = 6.8 Hz, 12H, C$_6$H$_3$CH(CH_3)$_2$), 1.56 (d, $^3J_{HH}$ = 6.8 Hz, 12H, C$_6$H$_3$CH(CH_3)$_2$), 3.87 (sept, $^3J_{HH}$ = 6.8 Hz, 4H, C$_6$H$_3$CH(CH$_3$)$_2$), 6.75–6.84 (m, 12H, *m*-PC$_6H_5$ and *p*-PC$_6H_5$), 7.16 (s, 6H, *m*-NC$_6H_3$ and *p*-NC$_6H_3$), 7.40 (m, 8H, *o*-PC$_6H_5$). ^{13}C NMR (150 MHz, C_6D_6, 128.06 ppm, 25 °C) δ 4.62 (s, 6C, CH$_2$SiMe_3), 23.50 (s, 4C, C$_6$H$_3$CH(*C*H$_3$)$_2$), 27.80 (s, 4C, C$_6$H$_3$CH(*C*H$_3$)$_2$), 29.11 (s, 4C, C$_6$H$_3$*C*H(CH$_3$)$_2$), 47.31 (s, 2C, *C*H$_2$SiMe$_3$), 124.69 (s, aromatic *C*H), 125.07 (s, aromatic *C*H), 130.73 (s, aromatic *C*H), 131.51 (s, aromatic *C*H), 132.22 (m, aromatic *C*H), 132.77 (d, J_{PC} = 5.4 Hz, 2C, aromatic *ipso*-*C*), 133.50 (d, J_{PC} = 5.4 Hz, 2C, aromatic *ipso*-*C*), 139.04 (s, aromatic *ipso*-*C*), 145.89 (s, aromatic *ipso*-*C*). Anal.

Calcd (%) for $C_{44}H_{76}N_3P_2Si_2Lu$: C, 48.57; H, 6.99; N, 3.86. Found: C, 48.95; H, 6.74; N, 3.75.

Synthesis of the Hydride [(NPNPN)YH_2]$_2$ (NPNPN: N[$Ph_2PNC_6H_3(^iPr)_2$]$_2$) (2-Y).

Method A: a solution of $PhSiH_3$ (27 mg, 0.25 mmol in 2 mL of toluene) was added dropwise to **1-Y** (100 mg, 0.1 mmol) in 10 mL of toluene at room temperature, and the reaction solution was stirred for 8 h, then concentrated to approximately 5 mL. **2-Y** precipitated from the solution, which was isolated as white crystalline solids (59 mg, 71%). Method B: In an ampoule bottle, a solution of **1-Y** (100 mg, 0.1 mmol) in toluene (5 mL) was degassed by two freeze-pump-thaw cycles and then pressurized with H_2 (1 bar). The reaction solution stood at room temperature for 24 h. The filtration gave **2-Y** as white crystalline solids (57 mg, 69%). The filtrate (containing several drops of benzene) stood at room temperature for 24 h and single crystals, suitable for X-ray analysis, were grown on the walls of a round-bottomed flask. Although the quality of crystals prevented us from obtaining the precise bond lengths, the structure data showed that complex **2-Y** is isostructural to complex **2-Lu** (Table S1)**.** ^{1}H NMR (400 MHz, C_6D_6, 7.16 ppm, 25 ^{o}C): δ 0.34 (d, $^3J_{HH}$ = 6.4 Hz, CH(CH_3)$_2$), 0.51 (d, $^3J_{HH}$ = 6.4 Hz, CH(CH_3)$_2$), 1.26–1.40 (br, CH(CH$_3$)$_2$), 3.62 (s, CH(CH$_3$)$_2$), 6.61 (br, aromatic *H*), 6.73–7.06 (m, aromatic *H*), 7.57–7.80 (m, aromatic *H* and Y-H_4-Y). As a result of the extremely poor solubility of **2-Y** in C_6D_6, the ^{13}C NMR spectrum is unreliable, so they are not provided. Anal. Calcd (%) for $C_{96}H_{112}Y_2N_6P_4$: C, 69.81; H, 6.83; N, 5.09. Found: C, 69.33; H, 6.91; N, 5.18.

Synthesis of the Hydride [(NPNPN)LuH_2]$_2$ (NPNPN: N[$Ph_2PNC_6H_3(^iPr)_2$]$_2$) (2-Lu). By a procedure similar to that described for the preparation of **2-Y**, treatment of $PhSiH_3$ (27 mg, 0.25 mmol) or H_2 (1 bar) with **1-Lu** (109 mg, 0.1 mmol) at 60 ^{o}C for 12 h or 48 h gave white solids of **2-Lu** (71 mg, 78%; 66 mg, 72%). ^{1}H NMR (400 MHz, C_6D_6, 7.16 ppm, 25 ^{o}C): δ 0.16 (d, $^3J_{HH}$ = 4.8 Hz, CH(CH_3)$_2$), 0.41 (d, $^3J_{HH}$ = 4.8 Hz, CH(CH_3)$_2$), 1.26–1.55 (br, CH(CH$_3$)$_2$), 3.36 (sept, $^3J_{HH}$ = 4.8

Hz, C*H*$(CH_3)_2$), 3.81 (sept, $^3J_{HH}$ = 4.8 Hz, C*H*$(CH_3)_2$), 6.25–6.58 (m, aromatic *H*), 6.71–7.13 (m, aromatic *H*), 7.75 (m, aromatic *H*), 10.26 (s, 4H, Lu-*H*$_4$-Lu). As a result of the extremely poor solubility of **2-Lu** in C_6D_6, the ^{13}C NMR spectrum is unreliable, so they are not provided. Anal. Calcd (%) for $C_{96}H_{112}Lu_2N_6P_4$: C, 63.22; H, 6.19; N, 4.61. Found: C, 63.63; H, 6.31; N, 4.49.

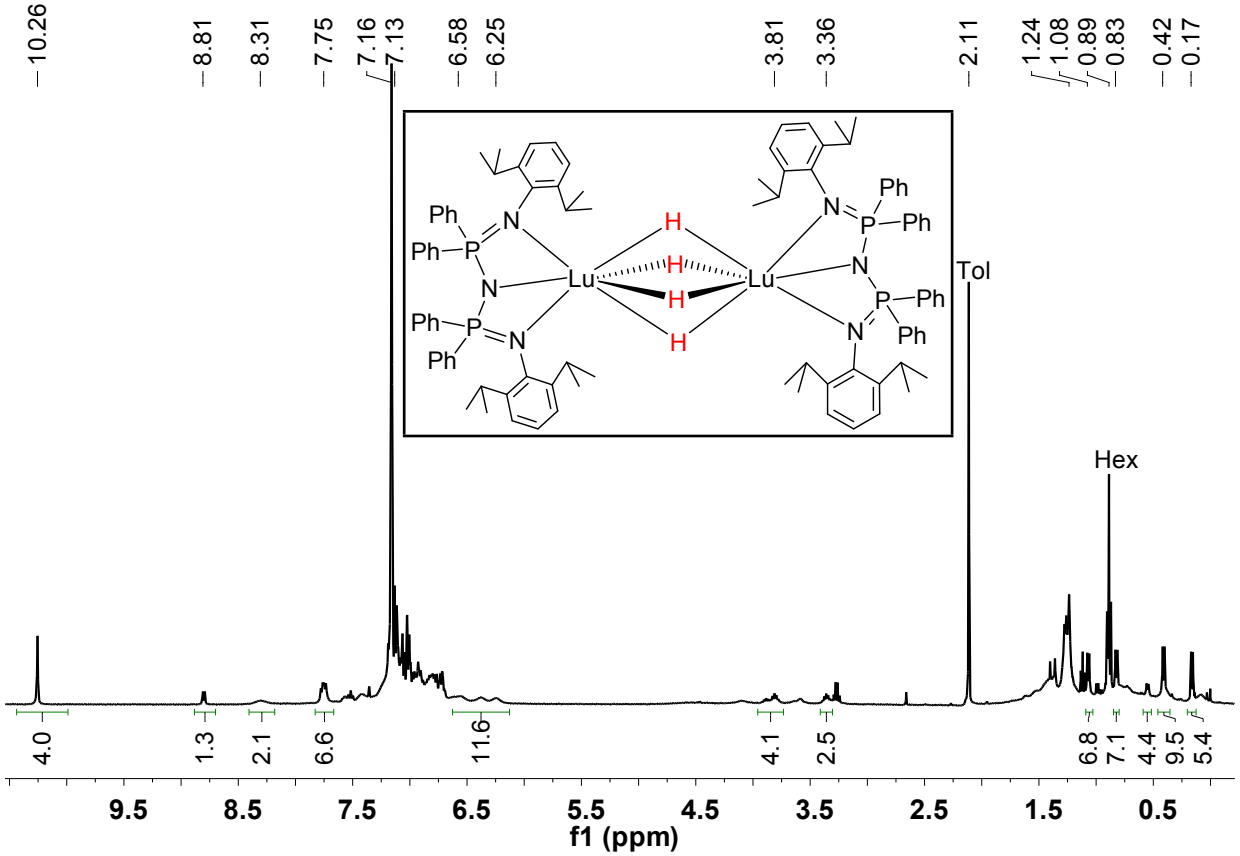


Fig. S1. ^1H NMR spectrum of **2-Lu** (C_6D_6) (the bridging hydride appear at downfield as a distinct singlet).

Synthesis of the Hydride {[(^{i}Pr)$_2$C$_6$H$_3$]N=P(Ph)$_2$N(Ph)(C$_6$H$_4$)P=N[C$_6$H$_3$(^{i}Pr)$_2$]}{N[Ph$_2$PNC$_6$H$_3$(^{i}Pr)$_2$]$_2$}Y$_2$H$_3$ (3-Y). Several drops of THF were added to **2-Y** (100 mg, 0.06 mmol) in 10 mL of toluene at room temperature, then the yellow clear solution was carefully concentrated to approximately 1 mL, after filtration, layered with hexane (2 mL) and kept at −30 °C for 2 d to give 3-Y as colorless crystals (74 mg, 68%), which were suitable for X-ray analysis. ^1H NMR (400 MHz, C_6D_6, 7.16 ppm, 25 °C): δ 0.26 (d, $^3J_{HH}$

= 6.4 Hz, CH(CH_3)$_2$), 0.47 (d, $^3J_{HH}$ = 6.4 Hz, CH(CH_3)$_2$), 0.60 (br, CH(CH_3)$_2$), 1.35 (m, 8H, THF), 3.62 (m, 8H, THF), 3.48+3.89+4.27 (s, CH(CH$_3$)$_2$), 6.69–7.13 (m, aromatic *H*), 7.26–7.55 (m, aromatic *H* and Y-H_3-Y), 7.75 (s, aromatic *H*). As a result of the extremely poor solubility of **3-Y** in C_6D_6, the ^{13}C NMR spectrum is unreliable, so they are not provided. Anal. Calcd (%) for $C_{96}H_{112}Lu_2N_6P_4$: C, 69.63; H, 7.08; N, 4.68. Found: C, 69.27; H, 6.91; N, 4.59.

2. Single crystal X-ray diffraction studies

Crystals for X-ray analysis were obtained as described in the preparations. The crystals were manipulated in a glove box. Data collections were performed at –88.5 °C on a Bruker SMART APEX diffractometer with a CCD area detector, using graphite-monochromated Mo *K*α radiation (λ = 0.71073 Å). The determination of crystal class and unit cell parameters was carried out by the SMART program package. The raw frame data were processed using SAINT and SADABS to yield the reflection data file. The structures were solved by using the SHELXTL program. Refinement was performed on F^2 anisotropically for all non hydrogen atoms by the full-matrix least-squares method. All non-hydrogen atoms and bridging H atoms fragments were found from Fourier syntheses of electron density and were refined anisotropically and isotropically for hydrogens. All other hydrogen atoms were placed in calculated positions and were included in the structure calculation without further refinement of the parameters. As a result of highly structural symmetry, the structure of **2-Ln** were found as only one quarter (two nitrogen atoms; one phosphorus atom, one metal atom, one hydride ligand). After 222 symmetry operator, the whole molecule with two metal centers and four bridging hydrides eventually came into sight. The diffraction intensity of collected data was still weak because of the heavy Ln atom and light bridging hydride ligands, although we attemted many

times in the recrystallization of **2-Ln** and the measurement of single crystals. The relatively high R_{int} values (0.130 for **2-Y** and 0.119 for **2-Lu**) also indicated that the quality of obtained crystals is not very satisfactory (The checkcif report of **2-Y** has a mistake in level A, but the data can undoubtedly prove its geometry; **2-Lu** and **3-Y** are good without any mistakes in level A).

Table S1. Crystallographic data and structure refinement details for complexes **2-Y, 2-Lu** and **3-Y.**

	2-Y·solvents	**2-Lu**	**3-Y**·$3C_7H_8$·C_6H_{14}
formula	$C_{108}H_{112}Y_2N_6P_4$	$C_{48}H_{56}LuN_3P_2$	$C_{121}H_{149}Y_2N_6P_4O_2$
M_w	1794.82	911.87	2021.15
cryst. system	orthorhombic	orthorhombic	monoclinic
space group	I222	I222	P21/c
a [Å]	13.1802(19)	13.164(2)	18.5724(9)
b [Å]	18.730(3)	18.573(3)	19.0815(10)
c [Å]	19.619(2)	19.615(3)	33.6472(16)
α [°]	90	90	90
β [°]	90	90	101.101(1)
γ [°]	90	90	90
V [Å^3]	4843.2(12)	4795.8(13)	11701.1(10)
Z	2	4	4
Dcalcd [g cm^{-3}]	1.231	1.263	1.147
radiation [λ, Å]	$Mo_{K\alpha}$(0.71073)	$Mo_{K\alpha}$(0.71073)	$Mo_{K\alpha}$(0.71073)
$2\theta_{max}$ [°]	50.2	50.2	50.0
μ [mm^{-1}]	1.31	2.16	1.09
F [000]	1880	1864	4284
independent reflns	4294	4256	20646
reflns [I>2σ(I)]	2339	2862	11463
GOF	1.04	1.05	1.01
R_1 [I>2σ(I)]	0.135	0.118	0.077
wR_2 [I>2σ(I)]	0.345	0.289	0.251

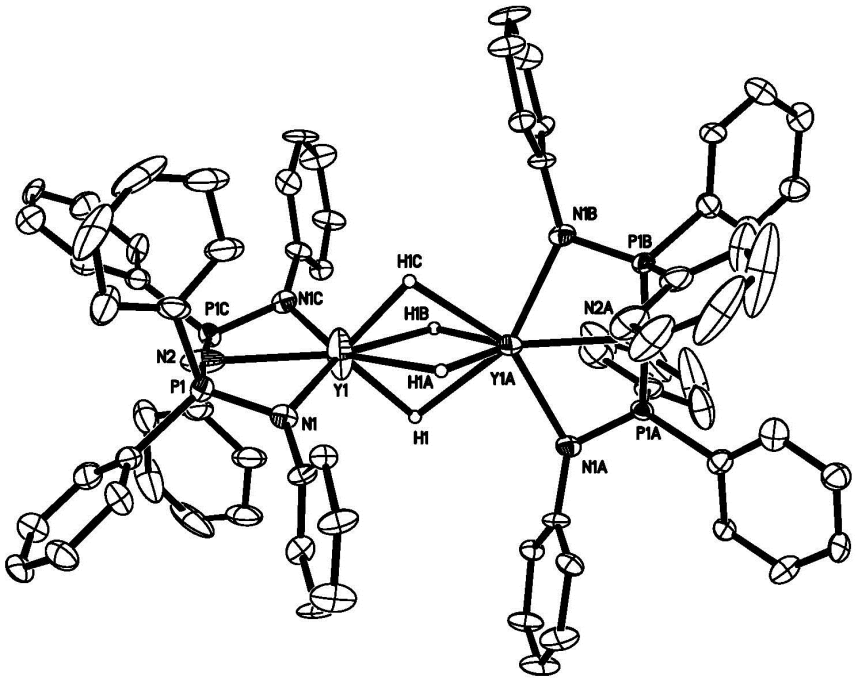


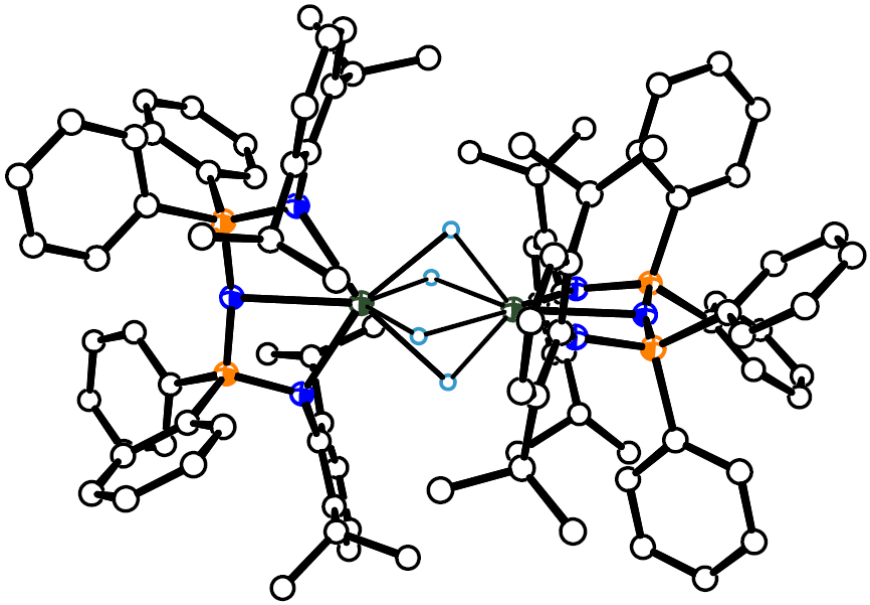
Fig. S2. Molecular structure of **2-Y** with thermal ellipsoids at 35% probability level. Isopropyl groups of DIPP and hydrogen atoms except bridging hydrides have been removed for clarity.

3. Computational studies

Molecular geometries of the model complexes were optimized without constraints via DFT calculations using the B3PW91 functional.[1] Yttrium was represented with Stuttgart–Dresden pseudo-potential in combination with its adapted basis set.[2] The 6-31G(d,p) basis set was used for the H, N and P atoms bonding with Yttrium as well as one phenyl ring involved in C-H activation. For all other main group atoms, the 3-21G basis set was used. Frequency calculations were carried out at the same level of theory to identify all of the stationary points as minima (zero imaginary frequencies) or transition states (one imaginary frequency), and to provide free energies at 298.15 K. Intrinsic reaction coordinates[3] (IRC) were calculated for the transition states to confirm that the structures

indeed connect two relevant minima. All calculations were performed with the Gaussian 09 software package.[4]

1. Cartesian coordinates of optimized structures of complex **2-Y**

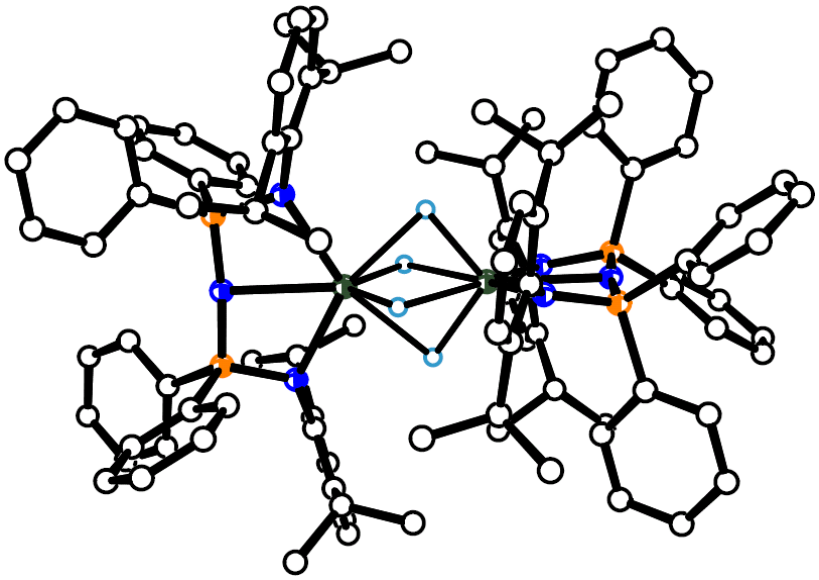


Y	0.032725	1.511802	-0.033659	H	-5.230033	0.241937	-1.064193
Y	0.006470	-1.510788	-0.010309	H	-3.717701	-0.285502	-1.842485
P	1.199781	4.249974	1.046403	H	-5.138284	0.137001	-2.838586
N	1.286474	2.750847	1.654594	C	-2.617319	4.737386	-0.122369
N	0.077661	4.105969	-0.079817	C	-3.069838	3.874278	0.892827
P	-1.151177	4.228093	-1.088967	H	-2.581450	2.917171	1.063099
N	-1.279129	2.732439	-1.689120	C	-4.152628	4.231009	1.692160
P	-1.183521	-4.227229	1.059152	H	-4.490285	3.554655	2.471000
N	-1.282654	-2.732818	1.669058	C	-4.802330	5.452177	1.487360
N	-0.001427	-4.103076	-0.002579	H	-5.647845	5.727490	2.109428
P	1.181231	-4.238561	-1.062529	C	-4.364800	6.312241	0.481439
N	1.285574	-2.748353	-1.680692	H	-4.869292	7.259071	0.316793
C	2.722941	4.799435	0.187620	C	-3.276503	5.959645	-0.321326
H	2.684513	3.088521	-1.141853	H	-2.939859	6.632736	-1.102511
C	3.200248	4.005735	-0.866747	C	-0.931103	5.549755	-2.310285
C	4.334137	4.380768	-1.578762	C	-1.864812	5.716814	-3.348882
H	4.690653	3.754038	-2.391117	H	-2.711602	5.043636	-3.437063
C	5.010365	5.557063	-1.247617	C	-1.692048	6.742201	-4.278091
H	5.897150	5.849642	-1.803233	H	-2.409974	6.864509	-5.082291
C	4.544942	6.352300	-0.204088	C	-0.595809	7.602393	-4.179372
H	5.066049	7.268966	0.058689	H	-0.465881	8.398610	-4.905122
C	3.406258	5.977221	0.511319	C	0.336528	7.434466	-3.154224

H	3.048483	6.602762	1.322975	H	1.192939	8.096833	-3.081488
H	-1.127407	0.258450	1.083120	C	0.173036	6.409137	-2.221862
H	1.166859	-0.244665	1.091565	H	0.902485	6.267370	-1.431096
H	-1.134453	-0.244030	-1.129186	C	-1.775165	-2.447967	2.972414
H	1.164956	0.219564	-1.129994	C	-0.907442	-2.551376	4.095438
C	1.778102	2.460418	2.957276	C	0.570954	-2.891386	3.947963
C	0.909619	2.558809	4.080730	H	0.730906	-3.262733	2.930602
C	-0.571394	2.888105	3.933767	C	1.026146	-3.990615	4.928704
H	-0.732835	3.267813	2.919828	H	0.390852	-4.877771	4.846915
C	-1.041246	3.972408	4.924020	H	0.996838	-3.628169	5.963616
H	-0.416886	4.867875	4.851946	H	2.061021	-4.277497	4.702250
H	-1.010563	3.600407	5.955522	C	1.423418	-1.619556	4.139116
H	-2.078861	4.248827	4.697477	H	1.163614	-0.851423	3.403552
C	-1.411773	1.606157	4.111190	H	2.490018	-1.856708	4.027644
H	-1.144298	0.848443	3.367710	H	1.265963	-1.202433	5.140626
H	-2.480511	1.834434	4.001137	C	-1.407886	-2.285132	5.373159
H	-1.251529	1.180274	5.108541	H	-0.741092	-2.360372	6.226605
C	1.411276	2.292298	5.357990	C	-2.738457	-1.928100	5.571232
H	0.744440	2.364213	6.211634	H	-3.111652	-1.736019	6.572617
C	2.742600	1.937634	5.555368	C	-3.580243	-1.804662	4.471161
H	3.116560	1.745630	6.556480	H	-4.614628	-1.506790	4.617352
C	3.583399	1.813298	4.454634	C	-3.120236	-2.048037	3.172462
H	4.617073	1.512540	4.599900	C	-4.077621	-1.840927	2.008385
C	3.122827	2.057163	3.156194	H	-3.527936	-2.044386	1.085467
C	4.076771	1.836267	1.991421	C	-5.279942	-2.803535	2.087227
H	3.529513	2.050132	1.069096	H	-5.942106	-2.652493	1.225502
C	5.298933	2.773314	2.070736	H	-5.857112	-2.627814	3.003410
H	5.956919	2.609475	1.208070	H	-4.942472	-3.846130	2.080189
H	5.874553	2.582407	2.984918	C	-4.553666	-0.374315	1.965369
H	4.984852	3.823294	2.069288	H	-5.225485	-0.219871	1.112555
C	4.523851	0.360277	1.945297	H	-3.689298	0.289182	1.855701
H	5.190300	0.193617	1.090373	H	-5.092622	-0.112577	2.884392
H	3.645899	-0.285363	1.837064	C	-2.678038	-4.728115	0.131384
H	5.059648	0.087898	2.863175	C	-3.132902	-3.874187	-0.890759
C	0.882752	5.560050	2.261488	H	-2.625095	-2.933302	-1.091147
C	1.754024	5.721294	3.355239	C	-4.240149	-4.220661	-1.660292
H	2.588345	5.041516	3.496966	H	-4.579492	-3.551273	-2.444436
C	1.536205	6.749717	4.271410	C	-4.912213	-5.423141	-1.419077
H	2.207688	6.867522	5.115468	H	-5.776573	-5.690874	-2.018126
C	0.453679	7.617227	4.109106	C	-4.471679	-6.274449	-0.407334
H	0.287586	8.415606	4.825046	H	-4.992126	-7.207388	-0.215414
C	-0.418994	7.452856	3.032591	C	-3.359006	-5.931692	0.366040
H	-1.266831	8.118905	2.910344	H	-3.019748	-6.598807	1.151099
C	-0.207683	6.427873	2.109096	C	-0.937171	-5.553840	2.269891

H	-0.892405	6.298399	1.278088	C	-1.850486	-5.719011	3.327191
C	-1.791518	2.443237	-2.983812	H	-2.691892	-5.041862	3.434575
C	-0.940492	2.538122	-4.120187	C	-1.664648	-6.747605	4.250136
C	0.541480	2.873038	-3.996637	H	-2.367251	-6.868548	5.067965
H	0.716107	3.255629	-2.985648	C	-0.574247	-7.612105	4.127968
C	0.987268	3.958145	-4.997235	H	-0.433369	-8.410578	4.849195
H	0.362490	4.852463	-4.911442	C	0.338711	-7.445006	3.085534
H	0.932923	3.585747	-6.027502	H	1.191789	-8.109437	2.995163
H	2.029951	4.236456	-4.797099	C	0.161395	-6.417549	2.157915
C	1.385471	1.594938	-4.184228	H	0.877461	-6.278898	1.354964
H	1.134132	0.837259	-3.434917	C	1.778884	-2.467318	-2.984319
H	2.454912	1.827914	-4.092611	C	0.912580	-2.575815	-4.107898
H	1.210152	1.165517	-5.177534	C	-0.565434	-2.918472	-3.961153
C	-1.460824	2.265924	-5.388691	H	-0.725805	-3.287664	-2.943083
H	-0.806836	2.333330	-6.252551	C	-1.017022	-4.021294	-4.939550
C	-2.795126	1.911588	-5.564854	H	-0.380288	-4.907050	-4.853995
H	-3.183726	1.714855	-6.559438	H	-0.986520	-3.661819	-5.975460
C	-3.620605	1.796696	-4.451596	H	-2.051776	-4.309430	-4.714119
H	-4.658019	1.501571	-4.580552	C	-1.420986	-1.649182	-4.156366
C	-3.140238	2.045753	-3.161400	H	-1.165436	-0.879207	-3.421148
C	-4.080602	1.849546	-1.981734	H	-2.487274	-1.889386	-4.047432
H	-3.512708	2.045191	-1.068169	H	-1.262197	-1.233318	-5.158195
C	-5.270982	2.828492	-2.041253	C	1.414019	-2.311706	-5.385723
H	-5.923397	2.684589	-1.170876	H	0.748509	-2.390869	-6.239826
H	-5.862359	2.662420	-2.950110	C	2.743802	-1.951242	-5.582972
H	-4.919469	3.866557	-2.036890	H	3.117681	-1.760554	-6.584367
C	-4.575447	0.389539	-1.931415	C	3.583868	-1.822243	-4.482146
C	4.458606	-6.290524	0.421217	H	4.617441	-1.521307	-4.627766
H	4.973595	-7.228184	0.237754	C	3.122974	-2.063745	-3.183461
C	3.347587	-5.948564	-0.354853	C	4.077757	-1.850984	-2.018256
H	3.004320	-6.620922	-1.133666	H	3.525782	-2.050530	-1.095875
C	0.931576	-5.571594	-2.265240	C	5.280292	-2.813875	-2.090373
C	1.847231	-5.745874	-3.319051	H	5.940873	-2.658915	-1.228113
H	2.691538	-5.072494	-3.427567	H	5.859013	-2.642109	-3.006324
C	1.660190	-6.778643	-4.237033	H	4.942925	-3.856513	-2.079430
H	2.364621	-6.906588	-5.052216	C	4.553107	-0.383948	-1.979930
C	0.566256	-7.638420	-4.113231	H	5.218649	-0.224592	-1.122857
H	0.424382	-8.440234	-4.830542	H	3.687287	0.279337	-1.880357
C	-0.348946	-7.462368	-3.074235	H	5.098613	-0.126641	-2.896331
H	-1.204679	-8.123229	-2.982722	C	2.673699	-4.738877	-0.131168
C	-0.170520	-6.430586	-2.151594	C	3.134136	-3.878028	0.882606
H	-0.888407	-6.284988	-1.351447	H	2.632426	-2.931993	1.073838
C	4.904599	-5.432324	1.424729	C	4.239755	-4.223702	1.654837
H	5.767752	-5.699411	2.025804	H	4.583581	-3.548757	2.432225

2. Cartesian coordinates of optimized structures of complex **2-Lu**



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P	-4.140145	-1.039167	1.194315	C	-7.524842	4.116717	-0.717893
N	-2.632619	-1.630681	1.277798	H	-8.329383	4.836045	-0.605196
N	-4.039864	0.003492	-0.005179	C	-7.380983	3.081079	0.206455
P	-4.123172	1.044498	-1.205508	H	-8.069853	2.993975	1.039865
N	-2.619203	1.639893	-1.275937	C	-6.345095	2.157023	0.06453
P	4.13353	-1.035199	-1.200053	H	-6.223641	1.357597	0.787207
N	2.63183	-1.635002	-1.277908	C	2.360825	-2.935902	-1.791625
N	4.043948	-0.001703	0.006049	C	2.513623	-4.073101	-0.950225
P	4.128914	1.031869	1.212419	C	2.868784	-3.949051	0.52688
N	2.627293	1.632504	1.283452	H	3.209993	-2.924964	0.707769
C	-4.649285	-0.10868	2.686786	C	3.999303	-4.909456	0.947018
H	-2.877568	1.13851	2.620935	H	4.879699	-4.784635	0.309484
C	-3.813333	0.925472	3.134207	H	3.667132	-5.95349	0.890383
C	-4.165971	1.689114	4.241466	H	4.286191	-4.70492	1.986195
H	-3.506343	2.484061	4.576598	C	1.609561	-4.19341	1.384271
C	-5.359024	1.429997	4.919212	H	0.831379	-3.458789	1.154434
H	-5.632733	2.0261	5.785516	H	1.85553	-4.115931	2.451676
C	-6.194949	0.40546	4.483491	H	1.207448	-5.195467	1.195051
H	-7.124104	0.197991	5.007388	C	2.28038	-5.347604	-1.474886
C	-5.84349	-0.361321	3.37147	H	2.392155	-6.211583	-0.827865
H	-6.498151	-1.159466	3.0364	C	1.912704	-5.529154	-2.804429
H	-0.29279	-1.093752	-1.145529	H	1.748623	-6.527818	-3.196908
H	0.291549	-1.101737	1.13175	C	1.741515	-4.416034	-3.61963

H	0.304518	1.096469	-1.146175	H	1.434072	-4.549848	-4.652502
H	-0.279641	1.090999	1.128616	C	1.947317	-3.11963	-3.134771
C	-2.360897	-2.931125	1.792661	C	1.681251	-1.945148	-4.065213
C	-2.508697	-4.069348	0.951227	H	1.860422	-1.02572	-3.501602
C	-2.849733	-3.946569	-0.529412	C	2.618589	-1.970639	-5.289743
H	-3.19765	-2.925235	-0.713284	H	2.424863	-1.102301	-5.931641
C	-3.96648	-4.916121	-0.964984	H	2.455978	-2.880693	-5.880537
H	-4.856348	-4.800118	-0.339115	H	3.66859	-1.938324	-4.978584
H	-3.625833	-5.957303	-0.906065	C	0.204087	-1.950285	-4.510611
H	-4.24126	-4.712555	-2.007597	H	0.004817	-1.095991	-5.168557
C	-1.57844	-4.179727	-1.37217	H	-0.44342	-1.876009	-3.630647
H	-0.808955	-3.438994	-1.13302	H	-0.034372	-2.871464	-5.056694
H	-1.812305	-4.102862	-2.442263	C	4.602822	-0.0872	-2.688833
H	-1.170475	-5.178645	-1.179122	C	3.725307	0.919605	-3.132343
C	-2.279698	-5.343336	1.478988	H	2.782059	1.095197	-2.619184
H	-2.387511	-6.208051	0.83237	C	4.050311	1.700519	-4.238218
C	-1.920196	-5.523668	2.810962	H	3.362841	2.4711	-4.570008
H	-1.759934	-6.522049	3.205713	C	5.252612	1.486696	-4.919134
C	-1.750246	-4.409678	3.625149	H	5.502436	2.094938	-5.782178
H	-1.446322	-4.542579	4.659187	C	6.126924	0.489927	-4.489606
C	-1.951511	-3.113638	3.137256	H	7.059659	0.31886	-5.017098
C	-1.678767	-1.938041	4.064683	C	5.806447	-0.295304	-3.37881
H	-1.854351	-1.019045	3.498418	H	6.489248	-1.070436	-3.049713
C	-2.611016	-1.957213	5.293217	C	5.464534	-2.250405	-1.0054
H	-2.409415	-1.090167	5.934685	C	5.616732	-3.292439	-1.938034
H	-2.450637	-2.867667	5.883937	H	4.919661	-3.393688	-2.763213
H	-3.662662	-1.921667	4.987199	C	6.656996	-4.209058	-1.789258
C	-0.199893	-1.949598	4.504915	H	6.768141	-5.015642	-2.506069
H	0.00638	-1.095664	5.161033	C	7.545254	-4.096105	-0.716989
H	0.4447	-1.879908	3.622498	H	8.352204	-4.81288	-0.605171
H	0.035563	-2.871501	5.051024	C	7.390194	-3.069661	0.215716
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C	-5.611981	-3.318693	1.891278	C	6.351205	-2.148829	0.075304
H	-4.918727	-3.428154	2.718849	H	6.219772	-1.358335	0.805778
C	-6.651227	-4.234329	1.729571	C	2.353876	2.933964	1.794438
H	-6.765259	-5.047418	2.43858	C	2.512135	4.070467	0.953032
C	-7.534841	-4.111968	0.654539	C	2.875298	3.945224	-0.521986
H	-8.341273	-4.827719	0.532855	H	3.217456	2.921001	-0.700257
C	-7.375786	-3.077136	-0.268128	C	4.008069	4.905248	-0.936853
H	-8.053906	-2.987806	-1.11008	H	4.885152	4.780825	-0.294682
C	-6.338522	-2.156372	-0.114094	H	3.675681	5.94934	-0.882663
H	-6.205511	-1.358414	-0.836195	H	4.300322	4.699997	-1.974393
C	-2.342075	2.942557	-1.782042	C	1.620643	4.188825	-1.386193
C	-2.491608	4.075777	-0.93474	H	0.840885	3.455018	-1.159169

C	-2.847771	3.944917	0.541541	H	1.872106	4.109265	-2.452155
H	-3.191551	2.920308	0.715908	H	1.217845	5.191317	-1.200921
C	-3.975793	4.906295	0.966141	C	2.276441	5.345483	1.475287
H	-4.858488	4.783714	0.331354	H	2.392398	6.208863	0.828211
H	-3.642081	5.949791	0.909557	C	1.900868	5.528263	2.802441
H	-4.259536	4.702251	2.006385	H	1.735002	6.527308	3.193203
C	-1.588125	4.181191	1.400468	C	1.724053	4.415874	3.61738
H	-0.811464	3.446432	1.166176	H	1.410281	4.550668	4.648205
H	-1.833633	4.097651	2.467579	C	1.932192	3.118959	3.134853
H	-1.183488	5.183379	1.217619	C	1.659864	1.945596	4.064867
C	-2.253257	5.352266	-1.452219	H	1.839749	1.025428	3.502606
H	-2.362184	6.213177	-0.800672	C	2.592275	1.970395	5.293244
C	-1.883447	5.539654	-2.780325	H	2.394436	1.102965	5.935139
H	-1.715394	6.539817	-3.167246	H	2.428732	2.88126	5.882524
C	-1.714808	4.430289	-3.601139	H	3.643499	1.936063	4.986464
H	-1.405292	4.56853	-4.632801	C	0.1809	1.954229	4.504363
C	-1.925774	3.132034	-3.123554	H	-0.022444	1.101412	5.162966
C	-1.662163	1.961791	-4.059937	H	-0.463759	1.880281	3.622216
H	-1.843811	1.039981	-3.501081	H	-0.058236	2.876428	5.048308
C	-2.598999	1.996034	-5.284708	C	4.590658	0.083501	2.703391
H	-2.407142	1.130654	-5.931138	C	3.711044	-0.923485	3.142229
H	-2.433766	2.908831	-5.870535	H	2.770618	-1.099167	2.624059
H	-3.649253	1.964682	-4.974285	C	4.030326	-1.704527	4.249669
C	-0.18491	1.965271	-4.504905	H	3.341285	-2.4753	4.577735
H	0.012287	1.113392	-5.166595	C	5.228986	-1.490602	4.936928
H	0.462222	1.885405	-3.625178	H	5.474381	-2.098923	5.801185
H	0.056046	2.888167	-5.046963	C	6.105381	-0.493652	4.512091
C	-4.590957	0.10676	-2.7012	H	7.035311	-0.322514	5.044486
C	-3.71401	-0.898488	-3.149254	C	5.790636	0.291635	3.3997
H	-2.771561	-1.077658	-2.635954	H	6.475089	1.066832	3.074221
C	-4.038186	-1.67253	-4.260157	C	5.461579	2.246168	1.02408
H	-3.351115	-2.441892	-4.595617	C	5.60971	3.288102	1.957467
C	-5.239145	-1.453132	-4.941671	H	4.908559	3.389772	2.779133
H	-5.488358	-2.05592	-5.808706	C	6.651246	4.204103	1.813925
C	-6.112879	-0.457735	-4.507723	H	6.759276	5.010624	2.531282
H	-7.044475	-0.282326	-5.035796	C	7.544786	4.09061	0.746119
C	-5.793175	0.3206	-3.391844	H	8.352708	4.806908	0.63834
H	-6.475458	1.094712	-3.059232	C	7.393755	3.064296	-0.187398
C	-5.450113	2.264294	-1.008776	H	8.07987	2.981892	-1.023535
C	-5.591711	3.315077	-1.933244	C	6.35351	2.144093	-0.052237
H	-4.88902	3.420321	-2.75312	H	6.225158	1.353765	-0.78344

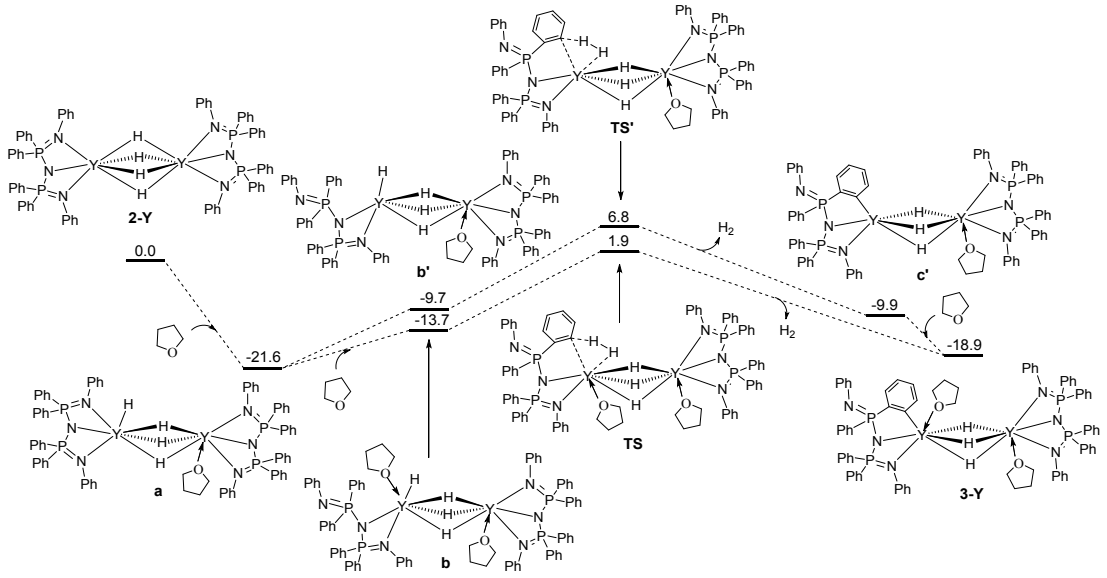
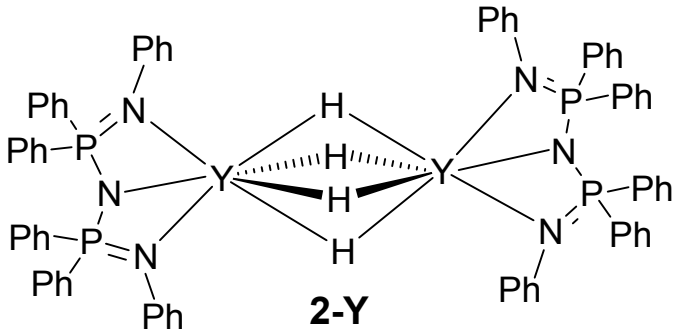


Fig. S3. Calculated energy profile from **2-Y** to **3-Y**. (Due to the great amount of calculation time required with the ligand as used in experiments, the 2,6-diisopropylphenyl substituents on N atoms were modeled by phenyl groups)

3. Cartesian Coordinates of Optimized Structures



Y	-1.522411	0.23466	-0.342764	C	-7.36938	-0.7765	-3.129724
Y	1.458018	0.133595	-0.165552	H	-8.01903	0.057428	-3.374262
P	-4.291895	1.480847	0.559969	C	-6.36364	-0.610756	-2.176722
N	-2.783468	2.069655	0.577704	H	-6.22916	0.348332	-1.691121
N	-4.101569	0.027434	-0.071692	C	1.951559	-2.86573	1.702529
P	-4.165278	-1.453816	-0.662604	C	2.452568	-3.39936	2.904898
N	-2.687649	-1.649248	-1.29586	C	1.89917	-4.554746	3.456812
P	4.034645	-1.326436	0.941208	H	2.303072	-4.946073	4.386174
N	2.473531	-1.713076	1.090307	C	0.833295	-5.201837	2.831761
N	3.92473	0.014777	0.069365	H	0.410853	-6.105063	3.259976
P	4.32842	1.280467	-0.828623	C	0.31668	-4.668862	1.646926
N	2.868435	1.81361	-1.268413	H	-0.51516	-5.154351	1.145133
C	-5.432158	2.474334	-0.465352	C	0.862332	-3.515958	1.087756

H	-3.924152	2.778753	-1.978881	C	4.990838	-2.626011	0.103251
C	-4.959074	2.955017	-1.695876	C	4.296828	-3.664846	-0.537867
C	-5.802282	3.668147	-2.542679	H	3.217018	-3.724777	-0.449271
H	-5.426524	4.038517	-3.492426	C	4.998984	-4.623293	-1.270291
C	-7.125357	3.911385	-2.168044	H	4.458037	-5.428678	-1.756305
H	-7.781624	4.473273	-2.827182	C	6.388975	-4.549661	-1.370356
C	-7.60186	3.438773	-0.946666	H	6.932311	-5.297067	-1.93952
H	-8.62954	3.631005	-0.650668	C	7.084219	-3.517825	-0.734603
C	-6.759908	2.720657	-0.097052	H	8.164931	-3.460498	-0.813908
H	-7.13094	2.3576	0.856881	C	6.390527	-2.558676	0.001075
H	-0.374203	-0.717896	1.051135	H	6.933767	-1.759089	0.495955
H	0.159964	1.456751	0.706808	C	4.945946	-0.968709	2.47699
H	0.186064	-1.101804	-1.183379	C	5.673484	-1.961651	3.154963
H	-0.122834	1.096513	-1.584492	H	5.767173	-2.953639	2.724251
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C	-1.652833	5.629186	2.573227	C	5.430217	0.587611	4.274131
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C	-1.219795	4.381489	3.029685	C	4.830899	0.309669	3.046215
H	-0.580388	4.315159	3.904926	H	4.282275	1.085427	2.522675
C	-1.602022	3.214795	2.37147	C	2.595291	2.991991	-1.986423
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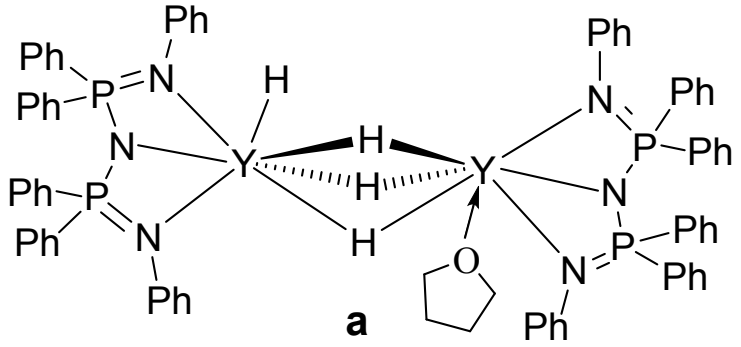

a

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N	3.759654	-0.274182	0.429332	C	-2.965897	5.07604	-2.654238
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P	3.852717	-1.493342	-0.613665	H	-1.545597	6.306762	0.172844
C	-6.122335	-1.119438	2.365424	H	-2.162434	7.010892	-2.131522
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C	-0.344124	1.728034	-3.964225	H	4.627797	-4.174003	3.45478
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C	-1.772141	-2.791028	1.901699	H	6.499716	-2.834571	-1.017274
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C	-3.163313	-2.911577	-1.623071	H	5.09779	3.383162	-0.584821
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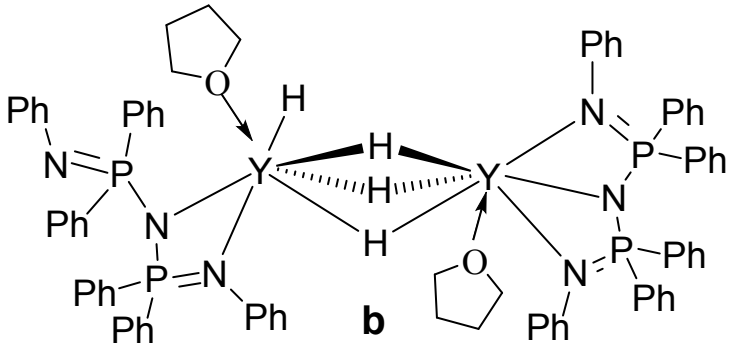

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O	-1.707358	-0.835593	-2.865317	H	3.880419	2.750849	-5.379842
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P	3.841724	-0.89108	-0.988515	C	1.567454	-3.991123	-1.920911
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H	1.448628	-1.058278	2.704431	C	-0.373664	5.076333	-3.02462
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H	-0.917605	-4.10794	1.603976	H	-2.148348	5.23681	-4.237636
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H	-0.288075	-4.752756	4.209391	C	-3.561763	3.005385	2.470413
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H	1.771917	-3.410757	4.207205	H	-3.369803	4.971686	-0.316703
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H	-2.429841	-2.73394	-3.299593	H	-3.075214	6.089419	3.820634
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C	-1.039219	-1.970884	-4.850403	C	-6.124502	3.410092	-0.72014
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C	6.719381	2.988841	1.789386	C	-7.229201	0.172631	0.758232
C	7.9649	4.060134	-0.459902	C	-6.649551	-1.597611	-0.800542
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C	5.463322	-1.719809	-0.913655	H	-4.573618	-1.559116	6.492856
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C	5.489173	-3.12532	-0.913083	C	-4.854769	-3.893126	0.860225
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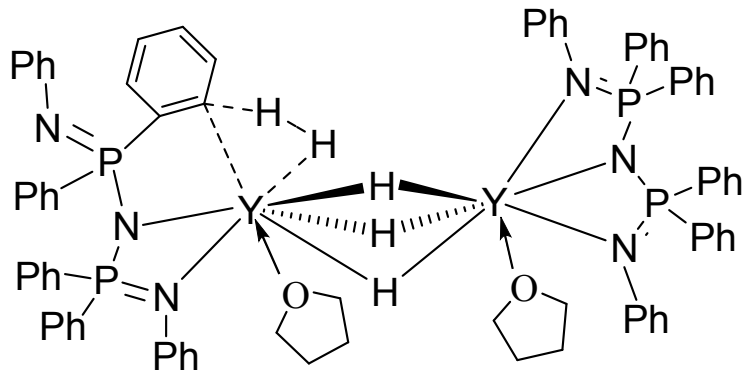

TS

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C	4.853088	9.260085	10.665692	H	-1.341011	13.496821	6.954359
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C	7.977113	10.584812	14.726748	H	2.988373	11.945233	3.413878
H	7.40966	11.279584	12.764705	C	6.169352	11.187611	5.474922
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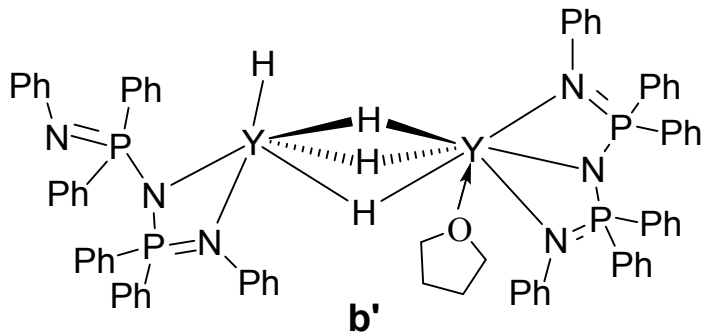

b'

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P	-4.232653	-1.131783	1.099244	H	-3.773065	3.235506	-2.6679
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H	-0.323979	-0.012611	-0.538609	H	-0.118496	-4.454713	-5.018021
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H	0.678302	3.51921	-1.758181	C	3.008285	-4.539014	2.512253
C	0.951578	3.45717	-3.921258	H	3.500852	-2.44169	2.332449
H	0.345359	4.363977	-3.990544	C	2.71696	-5.718344	1.823613
H	1.79615	3.513951	-4.618384	H	2.478123	-6.645451	-0.108799
C	0.124871	2.179242	-4.171746	H	3.009015	-4.5272	3.59729

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H	-8.877765	1.392521	0.0657	C	4.844066	3.676425	1.870495
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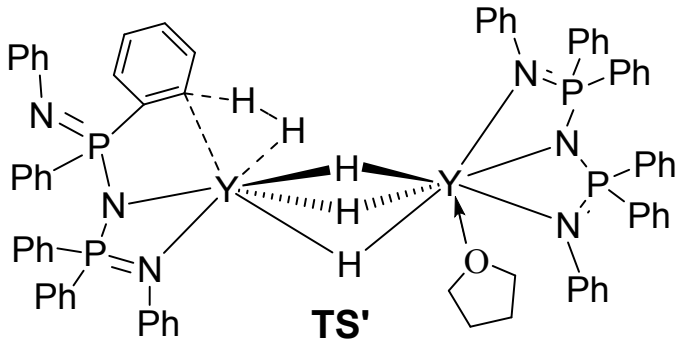
C	-4.038054	-0.366506	-4.706076				



TS'

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N	3.537829	12.626989	13.087811	H	5.45432	18.615598	14.488206
N	5.528817	12.788388	11.621856	C	6.78395	13.005407	11.052454
N	2.153296	13.485639	15.396304	C	7.120706	12.277346	9.887598
N	3.124053	13.324997	5.793807	C	7.751511	13.900617	11.559276
N	0.963848	14.497356	6.392309	C	8.354618	12.439622	9.265211
N	1.372029	16.177757	8.217658	H	6.390823	11.581217	9.486597
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P	5.091287	13.07217	13.173057	C	9.302157	13.330879	9.7796
P	1.645626	13.653769	5.201762	H	8.583756	11.858135	8.376566
P	0.365432	15.869242	6.985173	H	9.710815	14.747202	11.350319
C	0.910369	12.44822	11.719526	H	10.268678	13.445895	9.300767
C	-0.245674	12.666261	10.950355	C	1.108116	17.130281	9.230876
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C	-1.383951	13.282165	11.47423	C	1.17923	18.514007	8.982926
H	-2.24932	13.454694	10.83853	C	0.599911	17.615342	11.558563
C	-1.402653	13.695089	12.807461	H	0.754815	15.627753	10.727567
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C	0.843698	12.851021	13.070554	H	0.368983	17.254113	12.556131
H	4.322422	13.028194	8.882488	H	1.021021	20.494972	9.803268
H	2.945062	14.522867	10.151947	H	0.505385	19.702372	12.103918
H	2.022262	12.630073	8.938513	C	-1.348198	15.593625	7.49473
H	1.697841	11.219041	11.200362	C	-2.067058	16.614172	8.143392
H	2.287592	10.596654	10.801495	C	-1.933674	14.330883	7.319798
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H	6.191866	15.16039	6.609308	H	-1.614569	17.588297	8.300051
H	6.214174	14.400617	8.242355	C	-3.231305	14.095741	7.77602
C	6.986326	16.439462	8.239672	H	-1.365896	13.541173	6.838326
H	7.952849	16.037092	8.553422	C	-3.943872	15.112106	8.414994

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H	6.443117	17.952407	9.760972	H	-4.951385	14.925754	8.772244
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C	4.72568	16.92971	8.869371	C	-0.875849	17.672509	5.185977
H	4.486311	17.84194	8.312335	C	1.533285	17.835108	5.419134
H	3.963687	16.739131	9.629357	C	-0.850956	18.719786	4.263249
C	2.803701	13.441628	16.619927	H	-1.819567	17.214105	5.462411
C	3.472477	14.602098	17.075392	C	1.552523	18.873243	4.491266
C	2.797145	12.318403	17.480459	H	2.456664	17.500986	5.883967
C	4.111602	14.630365	18.31214	C	0.359412	19.318735	3.915193
H	3.475907	15.471516	16.426969	H	-1.778146	19.07057	3.821798
C	3.440762	12.355539	18.714942	H	2.494802	19.338821	4.220566
H	2.280043	11.419875	17.164497	H	0.375274	20.134528	3.199882
C	4.107394	13.506841	19.143257	C	1.669364	14.562469	3.633068
H	4.618586	15.537198	18.629795	C	0.476395	14.975402	3.015796
H	3.415282	11.476273	19.352934	C	2.903736	14.898162	3.056188
H	4.600903	13.532183	20.109289	C	0.522363	15.697602	1.824958
C	2.136269	10.726554	14.521725	H	-0.481393	14.740857	3.470808
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C	0.831545	8.90717	15.467179	C	1.753518	16.015295	1.246224
H	0.176926	10.956728	15.404418	H	-0.399807	16.01893	1.352631
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H	4.04976	10.166687	13.710377	H	1.785352	16.574626	0.316931
C	1.853504	8.00657	15.152476	C	0.665031	12.14858	4.944426
H	-0.073329	8.554886	15.952335	C	0.478893	11.322708	6.070109
H	3.809305	7.767336	14.279739	C	0.131985	11.763555	3.70619
H	1.743911	6.954436	15.395487	C	-0.243871	10.137755	5.950891
C	6.114439	12.133786	14.33874	H	0.908645	11.601774	7.030181
C	5.941275	12.282393	15.726135	C	-0.591662	10.574386	3.597197
C	7.035453	11.195074	13.84427	H	0.284726	12.38508	2.829943
C	6.685868	11.495093	16.603949	C	-0.781538	9.76408	4.716175
H	5.220856	12.992287	16.122602	H	-0.378378	9.503235	6.820909
C	7.780401	10.419163	14.732071	H	-1.000873	10.28015	2.636295
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H	6.531988	11.607731	17.671096	C	3.880443	11.813831	3.967914
H	8.497101	9.700516	14.347678	C	5.121345	11.980958	6.029511
H	8.183233	9.958977	16.797237	C	4.81723	10.901006	3.484409
C	5.215741	14.820081	13.676984	H	3.038755	12.081654	3.338737
C	6.249171	15.306959	14.492783	C	6.055916	11.076894	5.535127
C	4.266666	15.718526	13.1598	H	5.212624	12.367274	7.041428
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H	6.977634	14.620843	14.9131	H	4.682295	10.479453	2.492685
C	4.354847	17.079236	13.449784	H	6.896069	10.787888	6.160029
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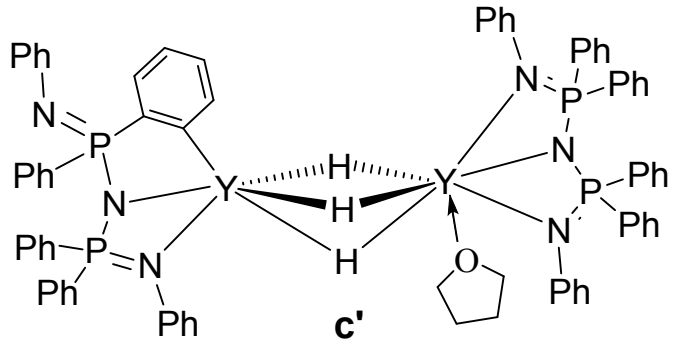

c'

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N	-5.448269	1.255034	-1.318445	H	1.338563	-5.635499	-2.417689
N	2.760201	-2.045095	0.117515	C	2.032078	-3.922135	-1.32481
N	4.113481	0.041451	0.197423	C	3.875276	-1.131183	-2.381756
N	3.115523	1.967107	1.442667	C	2.605802	-0.780565	-2.875745
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P	-3.869342	1.191913	-1.187739	C	2.425988	-0.558047	-4.239166
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P	4.044379	-1.360126	-0.591145	C	3.505904	-0.683242	-5.1166
P	4.248187	1.640096	0.323134	H	3.363064	-0.513925	-6.178924
C	-1.846745	2.409961	0.24576	C	4.76851	-1.027153	-4.631313
C	-1.172187	3.569262	0.684132	H	5.605422	-1.126432	-5.31483
H	-0.297266	3.471591	1.324927	C	4.957434	-1.251625	-3.266955
C	-1.583979	4.859851	0.337849	H	5.93681	-1.533547	-2.893336
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H	-4.294881	4.07204	-1.557056	H	7.001556	-5.285957	-1.144053
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H	0.209463	-1.411074	1.402718	H	8.663702	-4.490722	0.518316
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H	0.640793	0.31918	-0.190618	H	8.337758	-2.305136	1.653199
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C	-1.621875	1.23213	-4.666938	C	2.635953	2.587469	-1.704772
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H	-1.250391	-0.394344	-6.033487	H	1.321843	3.320328	-3.231931
C	-2.410554	-1.029521	-4.329842	C	3.368469	3.903653	-3.5971
H	-2.480556	-2.061085	-4.661448	H	3.138369	4.442465	-4.510452
C	-3.026942	-0.640277	-3.141411	C	4.682322	3.853862	-3.130217
H	-3.572554	-1.365128	-2.543806	H	5.474453	4.353702	-3.678022
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C	-6.759421	3.541482	-3.973104	C	5.946114	2.028373	0.842608
H	-6.427358	4.026826	-4.887004	C	7.0362	1.539472	0.100577
C	-8.069061	3.722724	-3.526406	H	6.862401	0.942755	-0.790422
H	-8.759506	4.351557	-4.078307	C	8.340505	1.801506	0.517209
C	-8.474347	3.07534	-2.355167	H	9.177913	1.423222	-0.059903
H	-9.489948	3.203459	-1.990878	C	8.567337	2.541678	1.680289
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C	-5.423753	0.367754	1.913537	C	7.489662	3.015996	2.428674
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H	-4.020003	2.016197	2.016027	C	6.180408	2.761949	2.015126
C	-5.878974	2.49906	2.977795	H	5.342299	3.143555	2.588649
H	-5.555964	3.499582	3.247077	C	2.768108	3.24515	1.910511
C	-7.16361	2.060886	3.309938	C	1.782063	3.337964	2.915443
H	-7.8396	2.718981	3.846202	C	1.410711	4.568779	3.448213
C	-7.579308	0.780716	2.943964	H	0.638337	4.605152	4.21097
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C	-6.715361	-0.065649	2.246223	H	1.713466	6.7085	3.413739
H	-7.046262	-1.056919	1.955427	C	2.973676	5.676387	1.997742
C	-5.156627	-2.163167	0.517834	H	3.438761	6.583548	1.62348
C	-6.110756	-1.986334	-0.501855	C	3.353262	4.447532	1.45869
H	-6.287537	-0.988	-0.900946	C	3.349803	-0.082973	4.485569
C	-6.794426	-3.092788	-1.004023	H	3.659923	0.813168	3.940494
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C	-6.53079	-4.369927	-0.500612	C	2.581925	0.208373	5.77784
H	-7.065072	-5.228186	-0.895721	H	3.251536	0.38956	6.623186
C	-5.578878	-4.545537	0.504536	H	1.928408	1.075471	5.633694
H	-5.370682	-5.538036	0.890908	C	1.744164	-1.077699	5.941459
C	-4.886604	-3.445872	1.015792	H	0.864585	-0.932362	6.573955
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C	-2.976684	-1.842227	3.228533	C	1.341539	-1.406904	4.493076
C	-1.97059	-2.807569	3.447645	H	0.391787	-0.950412	4.207085
C	-1.939994	-3.554117	4.623674	H	1.320498	-2.477406	4.278189
H	-1.164648	-4.303499	4.759947	H	-4.863653	2.583323	-3.652979
C	-2.906336	-3.362832	5.614469	H	-7.899093	1.781393	-0.725907
H	-2.885967	-3.951148	6.525792	H	-4.714068	-0.903112	4.105068
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H	-4.65977	-2.242285	6.172196	H	1.279029	2.428633	3.231795
C	-3.941711	-1.652292	4.239113	H	4.096254	4.428978	0.66815
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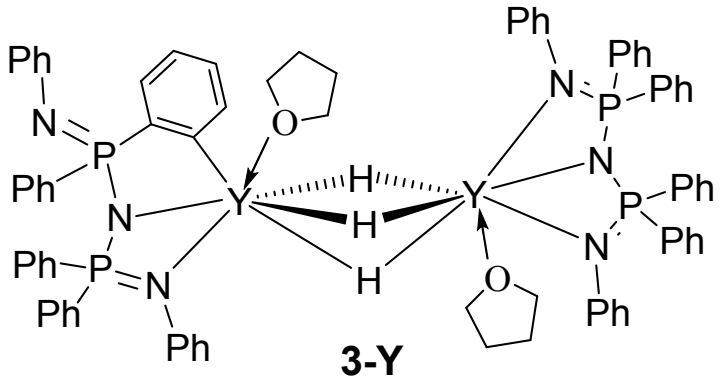

3-Y

Y	-1.324713	-0.501761	-0.429834	H	-3.078743	-4.688381	-3.601438
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N	-3.629427	0.001764	-0.146665	H	-3.590417	-2.442467	-2.081521
N	-2.608334	-1.667392	1.342721	H	-2.659624	-3.80509	-1.367857
N	-5.64738	1.721107	-0.207051	C	2.953361	-3.210174	-1.026582
N	3.18545	-1.906575	-0.564824	C	2.040613	-4.020961	-0.319061
N	4.316948	0.16723	0.256329	C	1.766044	-5.321575	-0.730919
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O	-1.525712	-2.199796	-2.060176	C	2.390824	-5.860573	-1.860216
O	1.897356	-0.533224	2.828704	H	2.18232	-6.878052	-2.173153
P	-4.46648	1.0919	-1.06293	C	3.288909	-5.069186	-2.574501
P	-3.950685	-0.741815	1.249046	H	3.778789	-5.466637	-3.458701
P	4.583009	-1.093998	-0.707967	C	3.566819	-3.762836	-2.170332
P	4.328502	1.764476	0.482793	C	4.935056	-0.584416	-2.415127
C	-1.823648	1.590462	-1.696341	C	3.843634	-0.465554	-3.294023
C	-0.853109	2.418052	-2.303606	H	2.845325	-0.725227	-2.949185
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C	-1.147033	3.668232	-2.854052	H	3.198479	0.074346	-5.272202
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H	0.705132	-0.080544	-1.292946	H	6.538701	-2.935747	-2.009849
C	-5.042569	0.131688	-2.530182	C	7.787806	-3.659437	-0.417061
C	-4.358107	0.152884	-3.756498	H	8.355944	-4.317365	-1.06614

H	-3.467633	0.764645	-3.861385	C	8.081506	-3.596324	0.945359
C	-4.822	-0.602795	-4.837273	H	8.88014	-4.205267	1.356056
H	-4.294807	-0.564511	-5.786472	C	7.346907	-2.751903	1.781065
C	-5.966692	-1.390358	-4.703519	H	7.573944	-2.702555	2.841196
H	-6.330446	-1.970957	-5.545758	C	6.318422	-1.971092	1.256726
C	-6.653826	-1.416387	-3.486659	H	5.746798	-1.30868	1.899134
H	-7.5514	-2.018049	-3.381664	C	5.101383	2.709875	-0.862962
C	-6.20043	-0.656552	-2.408653	C	4.331382	2.934424	-2.017835
H	-6.744854	-0.66629	-1.469822	H	3.311501	2.566054	-2.067606
C	-6.691843	2.53945	-0.583772	C	4.865934	3.656287	-3.082137
C	-7.054867	2.866054	-1.91477	H	4.264764	3.829335	-3.968267
C	-8.144962	3.690387	-2.184743	C	6.163552	4.166466	-3.00248
H	-8.391896	3.918751	-3.21815	H	6.573141	4.736725	-3.829839
C	-8.919655	4.219848	-1.151886	C	6.927359	3.958896	-1.853664
H	-9.765507	4.863554	-1.368536	H	7.929179	4.37016	-1.783992
C	-8.580145	3.907041	0.168166	C	6.400157	3.235912	-0.783244
H	-9.166627	4.313551	0.987714	H	6.987719	3.102944	0.11897
C	-7.49424	3.087235	0.448466	C	5.333305	2.05236	1.971566
C	-4.11677	0.467556	2.602693	C	6.620804	1.497579	2.077613
C	-3.259482	1.580465	2.595191	H	7.025272	0.90408	1.262848
H	-2.579826	1.735786	1.762623	C	7.369228	1.680318	3.239615
C	-3.296703	2.50252	3.639329	H	8.363464	1.251793	3.314748
H	-2.638726	3.365474	3.61667	C	6.835193	2.403773	4.309002
C	-4.189426	2.326047	4.699549	H	7.41848	2.543602	5.213267
H	-4.222614	3.049681	5.507596	C	5.550463	2.939724	4.217289
C	-5.046902	1.225776	4.711832	H	5.131478	3.495255	5.050111
H	-5.749524	1.092095	5.528115	C	4.797468	2.765568	3.054384
C	-5.013418	0.298585	3.668527	H	3.799921	3.185523	2.98132
H	-5.694446	-0.546763	3.675519	C	2.227114	3.417387	0.79004
C	-5.481876	-1.719529	1.278304	C	0.826476	3.571259	0.774764
C	-6.732368	-1.075551	1.221578	C	0.241776	4.826571	0.909469
H	-6.772667	0.009823	1.173955	H	-0.840278	4.909903	0.873526
C	-7.901404	-1.83554	1.184701	C	1.02966	5.970397	1.061373
H	-8.863668	-1.336176	1.134868	H	0.569812	6.947626	1.16157
C	-7.833815	-3.23113	1.206061	C	2.416764	5.836462	1.063647
H	-8.746577	-3.817943	1.180265	H	3.048946	6.71375	1.165776
C	-6.595163	-3.871698	1.261369	C	3.012053	4.582221	0.929423
H	-6.54274	-4.955553	1.283031	C	1.436421	0.570384	3.680792
C	-5.418565	-3.120918	1.295122	H	1.054059	1.360202	3.028025
H	-4.455163	-3.616324	1.348107	H	2.29779	0.927841	4.257322
C	-2.290243	-2.585851	2.338396	C	0.363811	-0.054018	4.575502
C	-1.389327	-3.629685	2.017188	H	0.222759	0.509676	5.502343
C	-1.041997	-4.600549	2.951945	H	-0.585156	-0.115589	4.033062
H	-0.354912	-5.393136	2.667153	C	0.929306	-1.469424	4.813279

C	-1.575045	-4.571129	4.245125	H	0.15567	-2.184235	5.103786
H	-1.313342	-5.33576	4.968701	H	1.72152	-1.441448	5.571007
C	-2.459173	-3.54468	4.581459	C	1.506126	-1.821318	3.433333
H	-2.885746	-3.502903	5.579911	H	0.743854	-2.270444	2.791392
C	-2.81193	-2.565856	3.652371	H	2.402274	-2.447379	3.478314
C	-0.526023	-2.550171	-3.074649	H	-6.481588	2.455003	-2.740106
H	0.438818	-2.636149	-2.57262	H	-7.218047	2.858635	1.473104
H	-0.50675	-1.740122	-3.812022	H	-3.48428	-1.768957	3.949806
C	-1.025695	-3.868028	-3.68419	H	-0.968958	-3.647898	1.017049
H	-0.664345	-4.713219	-3.088669	H	0.208211	2.689774	0.632344
H	-0.695127	-3.985899	-4.719959	H	4.095299	4.517578	0.920775
C	-2.556811	-3.728401	-3.554591	H	1.540656	-3.595861	0.544116
H	-2.950486	-3.057976	-4.325577	H	4.242789	-3.157331	-2.764214

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