Electronic Supplementary Information for Dalton Transactions

Alkali Metal Complexes of a Naphthylamine-Substituted Phosphanide.

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SUPPORTING INFORMATION

Atomic coordinates (Å) for **2a-hh**$_{anti}$:

	x	y	z
P	-0.927100	-0.301500	1.872200
P	0.928700	-0.303600	-1.874300
N	-1.996600	-2.240000	-0.267900
N	1.996400	-2.241000	0.267000
Li	-0.000100	-1.510000	-0.000700
C	-0.475400	0.743000	3.362300
H	-0.576700	1.823200	3.203500
C	-2.607800	0.266400	1.415700
C	-3.255700	1.200000	2.239800
H	-2.815600	1.447500	3.198300
C	-4.433300	1.869800	1.870400
H	-4.879500	2.584100	2.558000
C	-4.985700	1.654500	0.630900
H	-5.858400	2.207700	0.296400
C	-4.426800	0.677800	-0.233800
C	-5.014200	0.499900	-1.515900
H	-5.846100	1.141100	-1.794200
C	-4.540300	-0.451200	-2.377700
H	-4.974900	-0.578400	-3.364900
C	-3.519100	-1.323900	-1.951900
H	-3.237400	-2.128900	-2.616200
C	-2.921000	-1.204600	-0.705900
C	-3.286200	-0.111900	0.175300
C	-1.585700	-3.194000	-1.314700
H	-2.420300	-3.806100	-1.689100
H	-0.852100	-3.881000	-0.880000
H	-1.112200	-2.669100	-2.147000
C	-2.574000	-3.014200	0.859500
H	-3.443100	-3.597500	0.519700
H	-2.871100	-2.346700	1.664100
H	-1.815800	-3.698200	1.250900
C	0.476900	0.742700	-3.363100
H	-0.576100	0.530400	-3.574700
C	2.608300	0.266000	-1.415400
C	3.256000	1.200700	-2.238400
H	2.816600	1.448400	-3.197200
C	4.432700	1.871200	-1.867500
H	4.878900	2.586300	-2.554300
C	4.984500	1.655500	-0.627800
H	5.856500	2.209000	-0.292300
C	4.425600	0.677700	0.235700
C	5.012400	0.499400	1.518200
H	5.843700	1.140900	1.797300

C	4.538500	-0.452500	2.379100
H	4.972500	-0.580100	3.366400
C	3.517900	-1.325400	1.952200
H	3.236100	-2.130900	2.615800
C	2.920500	-1.205700	0.705800
C	3.285900	-0.112400	-0.174600
C	2.574600	-3.015200	-0.860000
H	3.443300	-3.598700	-0.519500
H	2.872600	-2.347600	-1.664200
H	1.816600	-3.698900	-1.252200
C	1.584500	-3.195100	1.313300
H	2.418600	-3.807400	1.688300
H	0.851000	-3.881800	0.878000
H	1.110500	-2.670100	2.145400
H	0.577200	1.822700	-3.202800
H	1.050700	0.476700	-4.257800
H	0.577800	0.531300	3.573200
H	-1.048600	0.475300	4.256900
O	0.002000	3.071100	-0.000700
C	1.020600	3.859900	-0.618100
H	1.513200	4.498100	0.126500
H	0.590600	4.490500	-1.406700
Li	0.003200	1.159900	-0.000800
H	1.749700	3.174200	-1.052200
C	-1.020300	3.856300	0.615200
H	-1.515800	4.490900	-0.130600
H	-1.746300	3.168100	1.050500
H	-0.593300	4.490400	1.402700

Final energy: -1966.09426 a.u.
NIMAG = 0

Atomic coordinates (Å) for **2a-hh**$_{syn}$:

	x	y	z
P	1.31640	-0.90840	0.72290
P	-2.43730	-2.11920	0.61120
N	4.14660	-1.79560	-0.45380
N	-1.53940	-0.76420	-2.04930
Li	-0.46510	-1.82530	-0.62270
C	2.27050	-1.85850	2.02540
H	2.78980	-1.17820	2.70790
C	2.35320	0.53700	0.21420
C	1.63230	1.72600	0.06450
H	0.55140	1.69080	0.18320
C	2.23890	2.97900	-0.13560
H	1.62010	3.86570	-0.24630
C	3.60940	3.08150	-0.08400

H	4.10220	4.04890	-0.12820
C	4.40830	1.91550	0.02560
C	5.82150	2.04660	0.11700
H	6.24850	3.04510	0.15480
C	6.62230	0.93480	0.15710
H	7.70110	1.03170	0.24300
C	6.05190	-0.34480	-0.00640
H	6.71440	-1.19580	-0.11100
C	4.68020	-0.52390	-0.11970
C	3.79150	0.60860	0.04120
C	4.98200	-2.95770	-0.19890
H	5.82560	-3.06520	-0.90520
H	4.36510	-3.85830	-0.28800
H	5.38510	-2.91710	0.81590
C	3.53930	-1.86560	-1.78250
H	2.91600	-2.76360	-1.85010
H	4.30360	-1.90690	-2.57990
H	2.90510	-0.99690	-1.95190
C	-3.24630	-3.27250	1.83840
H	-2.45320	-3.92640	2.21480
C	-3.76720	-0.98310	0.07860
C	-5.03720	-1.10470	0.65800
H	-5.25610	-1.97210	1.26890
C	-6.03340	-0.12130	0.54080
H	-6.99510	-0.27550	1.02360
C	-5.76800	1.04800	-0.12970
H	-6.49530	1.85340	-0.17140
C	-4.52890	1.21390	-0.80190
C	-4.27860	2.44630	-1.46410
H	-5.03240	3.22660	-1.40360
C	-3.11440	2.64540	-2.15560
H	-2.90910	3.59260	-2.64560
C	-2.20390	1.57900	-2.29950
H	-1.35080	1.73160	-2.94590
C	-2.40970	0.34940	-1.69120
C	-3.54200	0.15730	-0.80680
C	-2.29740	-1.78130	-2.82350
H	-2.61620	-1.37270	-3.79370
H	-3.16630	-2.10980	-2.25760
H	-1.65710	-2.65160	-3.00150
C	-0.33470	-0.39180	-2.81790
H	-0.56990	-0.00330	-3.82000
H	0.28040	-1.28790	-2.95260
H	0.25560	0.34650	-2.27150
O	-1.51520	1.07190	2.79000
C	-2.89380	1.33650	3.06230
H	-3.19560	2.29010	2.61260
H	-3.07050	1.37160	4.14480
Li	-0.91380	-0.38670	1.72820
H	-3.47300	0.52830	2.61450

H	-3.69790	-2.76170	2.69610
H	-4.00710	-3.91260	1.37850
H	2.99740	-2.55230	1.60310
H	1.54180	-2.42900	2.61320
C	-0.63410	2.08320	3.28110
H	-0.68100	2.13680	4.37610
H	0.37370	1.81180	2.96370
H	-0.90010	3.06040	2.85900

Final Energy: -1966.06744 a.u.
NIMAG = 0

Atomic coordinates (Å) for **2a-ht**:

	x	y	z
C	5.580400	-1.476700	-0.900600
C	4.235900	-1.688600	-1.270600
C	5.953100	-0.256300	-0.411900
C	3.249500	-0.730800	-1.093300
C	4.986400	0.765300	-0.200900
C	3.573700	0.536300	-0.442300
C	3.193200	2.792300	0.417800
C	2.652700	1.580100	-0.011500
C	4.570700	3.042300	0.519500
C	5.451700	2.021900	0.259300
P	0.802700	1.451500	0.161000
N	1.925400	-1.005300	-1.608200
C	1.551300	-0.079900	-2.701600
C	1.676800	-2.380400	-2.067600
C	0.207200	2.901600	-0.876800
Li	-0.951600	0.693400	1.701500
C	-3.855300	-2.435600	-0.296800
C	-4.848300	-2.416200	-1.288100
C	-3.205800	-1.285300	0.164400
C	-5.182000	-1.228600	-1.893800
C	-3.719000	0.001600	-0.297600
C	-4.628400	-0.011500	-1.423500
C	-4.564700	2.404700	-1.614100
C	-5.001200	1.194600	-2.077700
C	-3.826400	2.457300	-0.413500
C	-3.438000	1.311900	0.264800
N	-2.850400	1.454400	1.591400
P	-1.664100	-1.496600	1.139300
C	-2.538000	2.835500	2.005000
C	-3.726200	0.848600	2.625600
C	-1.826600	-3.204500	1.894100
Li	0.572000	-0.974500	0.029500
H	0.564100	2.846800	-1.911400

H	0.498600	3.876800	-0.472200
H	-0.886400	2.860300	-0.910500
H	-1.733900	-4.025300	1.173800
H	-2.772800	-3.328400	2.431500
H	-1.017100	-3.309200	2.622700
H	6.310100	-2.265400	-1.058800
H	3.994500	-2.625100	-1.755000
H	6.991700	-0.040000	-0.177300
H	2.505100	3.566100	0.744300
H	4.924300	4.011000	0.861700
H	6.520600	2.154300	0.402800
H	1.764700	0.945200	-2.415600
H	2.110700	-0.323600	-3.618500
H	0.479600	-0.165400	-2.898200
H	0.615100	-2.465000	-2.318400
H	1.903900	-3.100300	-1.278600
H	2.255400	-2.651200	-2.965200
H	-3.528300	-3.403200	0.066900
H	-5.299600	-3.350000	-1.613800
H	-5.881500	-1.195300	-2.724100
H	-4.832900	3.328700	-2.117700
H	-5.643600	1.129300	-2.951600
H	-3.611100	3.433400	-0.001400
H	-3.434200	3.465700	2.108900
H	-2.048700	2.794500	2.983900
H	-1.846900	3.302900	1.301500
H	-4.661900	1.419400	2.720500
H	-3.205200	0.856500	3.587900
H	-3.950600	-0.183300	2.368600
O	1.691300	-1.829900	1.562500
C	1.902000	-3.233100	1.641900
C	2.544600	-1.103300	2.447100
H	1.151200	-3.711400	1.010200
H	1.773900	-3.589100	2.673000
H	2.909200	-3.499600	1.293900
H	2.295300	-0.046900	2.342100
H	3.598900	-1.255000	2.185400
H	2.375000	-1.422800	3.484200

Final Energy: -1966.07035 a.u.
NIMAG = 0