Insights into the stability and structures of phosphine-boranes and their α-metalated derivatives

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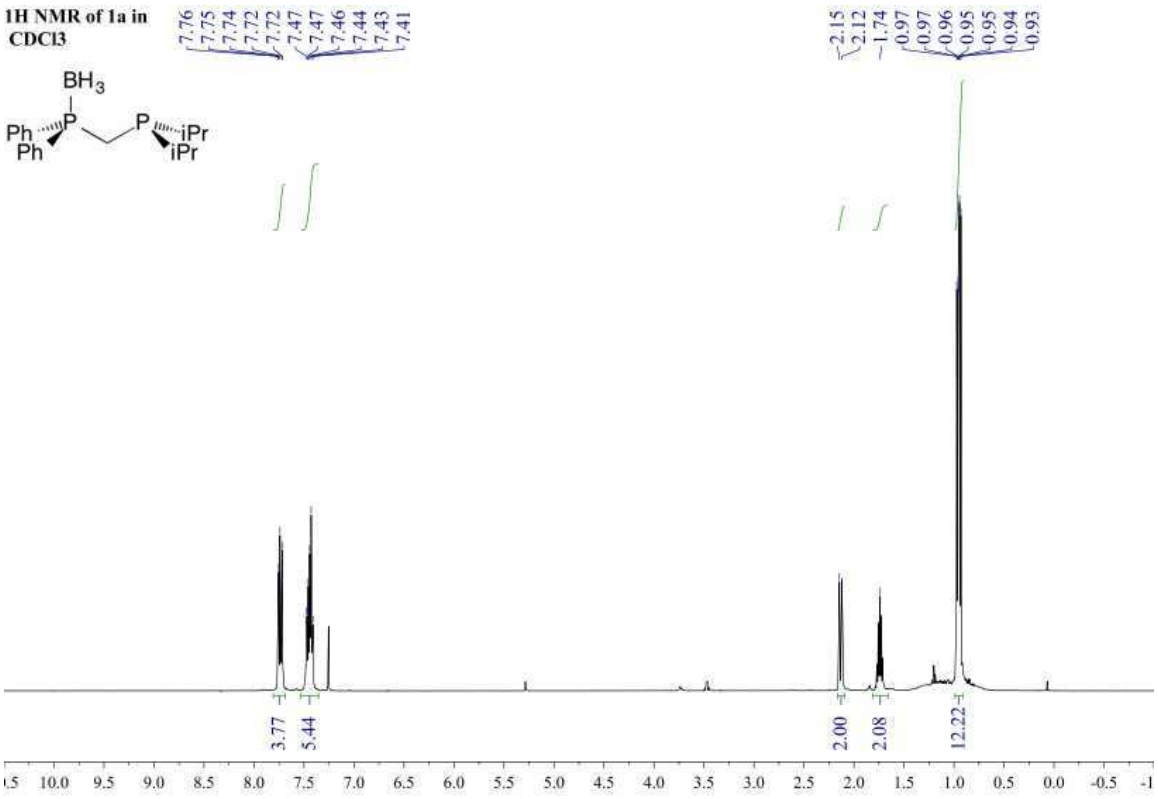
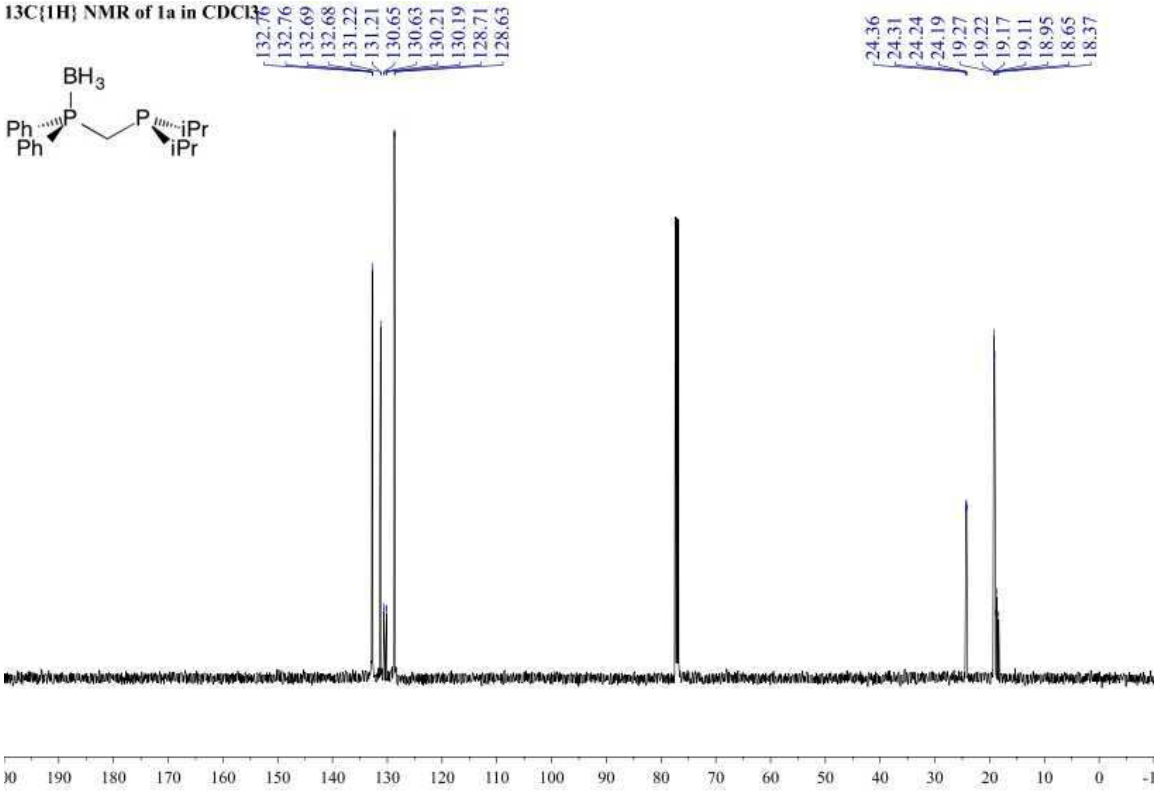
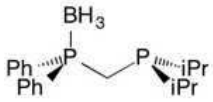
SUPPORTING INFORMATION

NMR data for 1a, 2a, 3a and 4a:

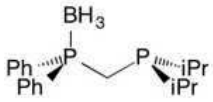




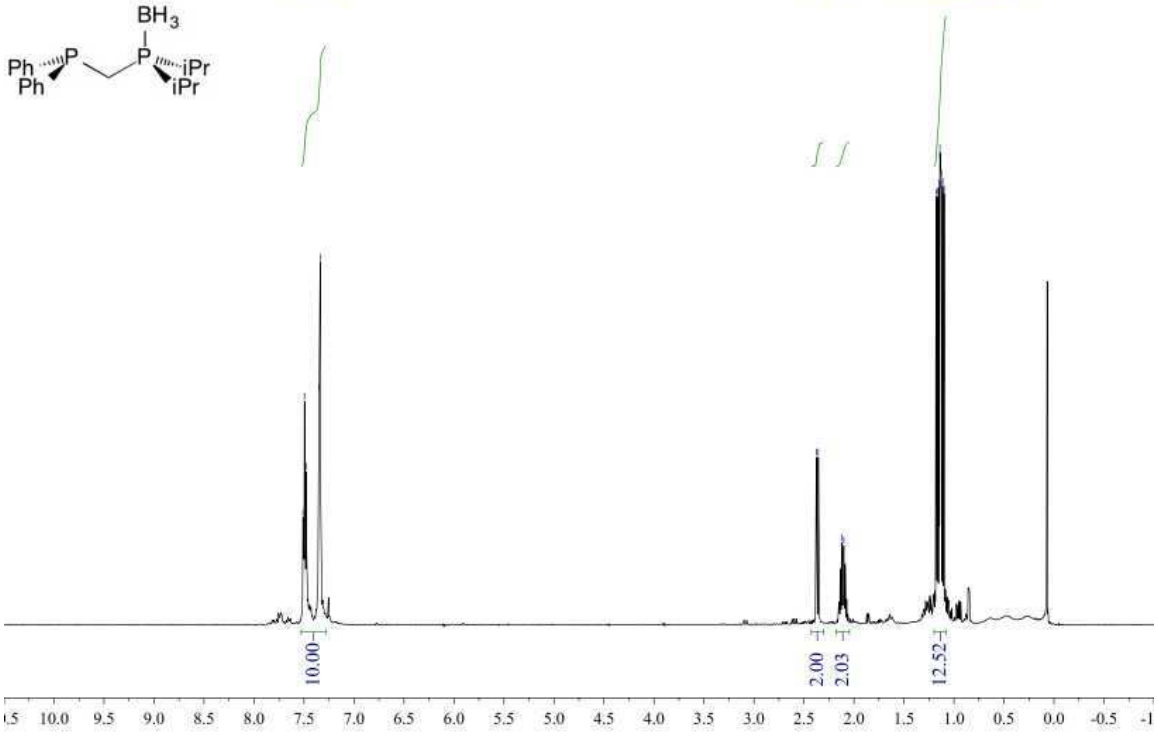
11B{1H} NMR of 1a in CDCl3



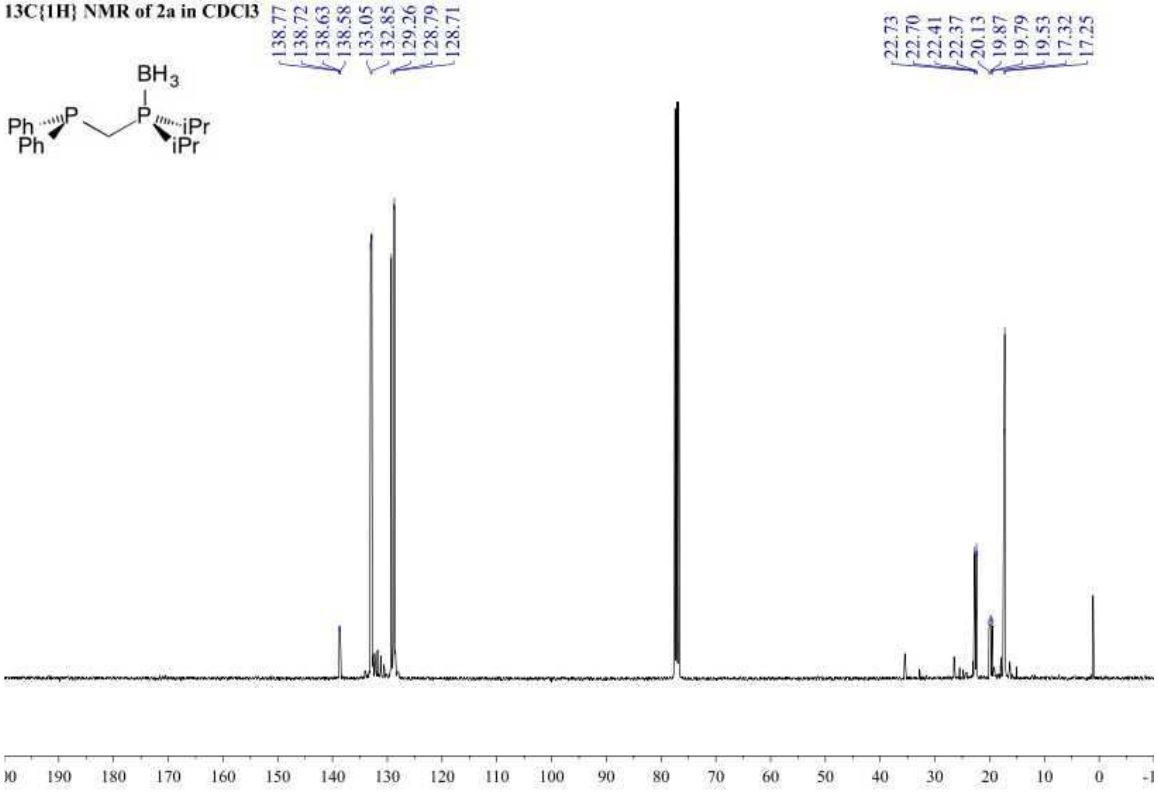
31P{1H} NMR of 1a in CDCl3



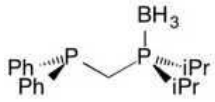
1H NMR of 2a in CDCl3



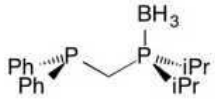
13C{1H} NMR of 2a in CDCl3



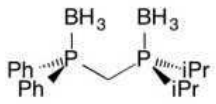
11B{1H} NMR of 2a in CDCl3



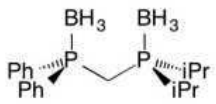
31P{1H} NMR of 2a in CDCl3



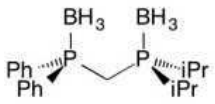
1H NMR of 3a in CDCl3



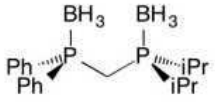
13C{1H} NMR of 3a in CDCl3



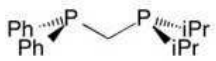
11B{1H} NMR of 3a in CDCl3



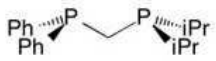
31P{1H} NMR of 3a in CDCl3



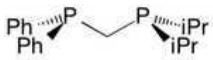
1H NMR of 4a in CDCl3



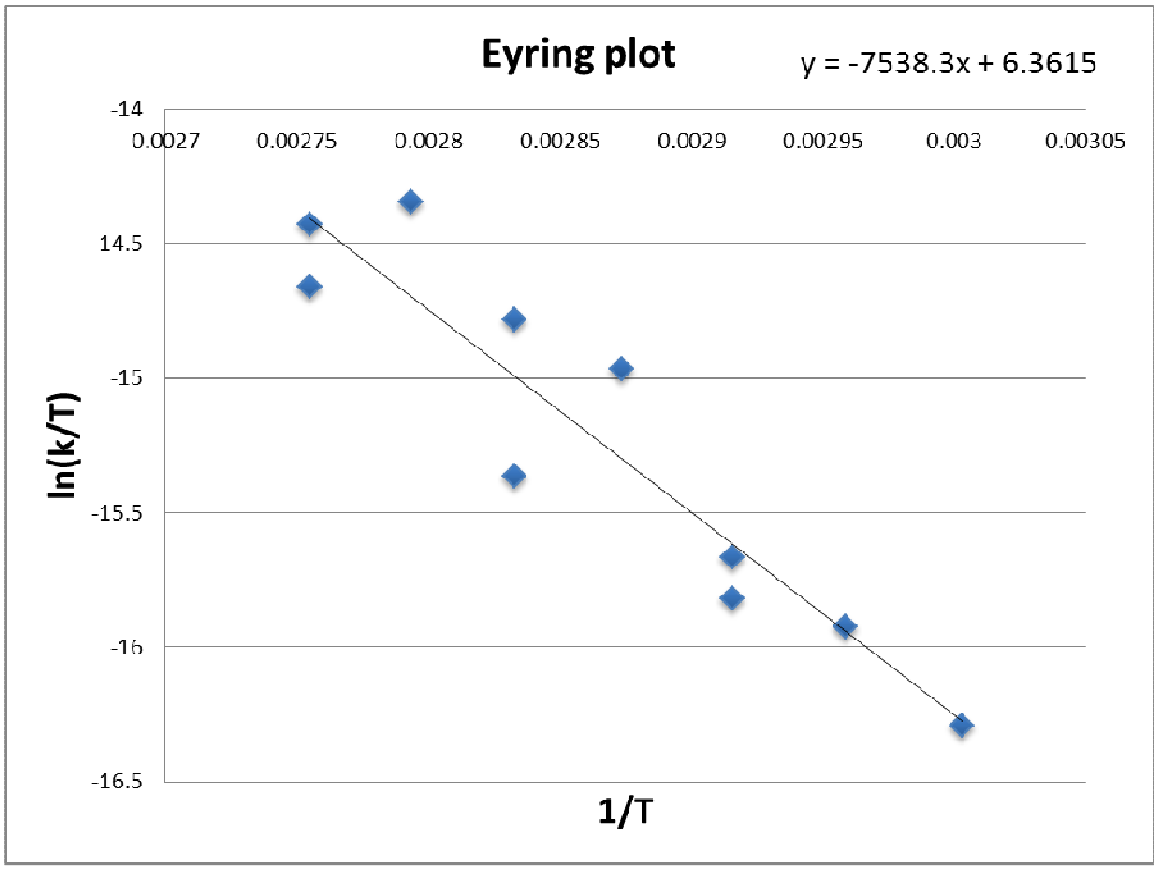
13C{1H} NMR of 4a in CDCl3



31P{1H} NMR of 4a in CDCl3

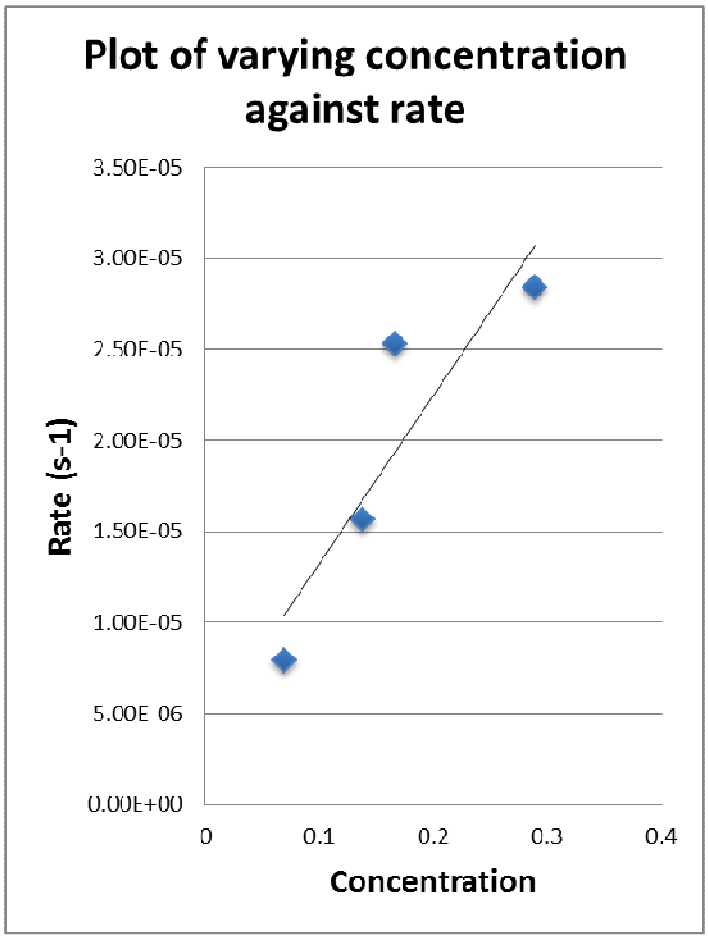


Eyring plot (data in table) for the conversion of 1a to 2a:



T (Kelvin)	k (s^{-1})	(1/T)	ln(k/T)
333	0.000028	0.003003003	-16.29144854
338	0.000041	0.00295858	-15.92498439
343	0.000054	0.002915452	-15.66425696
348	0.00011	0.002873563	-14.96723267
353	0.000075	0.002832861	-15.3644905
358	0.000211	0.002793296	-14.34418541
363	0.000197	0.002754821	-14.42670966
363	0.000156	0.002754821	-14.66005738
353	0.0001345	0.002832861	-14.78041442
343	0.00004632	0.002915452	-15.81766717

Concentration dependence of the rate of conversion of 1a into 2a:



Concentration (mol dm^{-3})	Rate (s^{-1})
0.069	7.89E-06
0.138	1.57E-05
0.167	2.53E-05
0.289	2.84E-05

Table S1. Crystallographic data for **1a**, **1b**, **1c**, **2b**, **3b** and **4b**.

Compound	**1a**	**1b**	**1c**	**2b**	**3b**	**4b**
formula	$C_{19}H_{29}BP_2$	$C_{25}H_{44}BLiN_2P_2$	$C_{27}H_{44}BLiO_2P_2$	$C_{25}H_{44}BLiN_2P_2$	$C_{25}H_{47}B_2LiN_2P_2$	$C_{25}H_{41}LiN_2P_2$
M_w	330.17	452.31	480.31	452.31	466.14	438.5
cryst. size (mm)	0.10x0.10x0.15	0.20x0.20x0.20	0.40x0.30x0.04	0.40x0.30x0.30	0.42x0.40x0.30	0.40x0.35x0.32
cryst. syst.	monoclinic	monoclinic	triclinic	monoclinic	triclinic	monoclinic
space group	$P2_1$	$P2_1/n$	$P\bar{1}$	$P2_1/c$	$P\bar{1}$	$P2_1$
a (Å)	9.9903(5)	11.7737(6)	9.3112(5)	10.2843(4)	12.4933(4)	9.2843(6)
b (Å)	9.5798(5)	16.1992(6)	11.9453(5)	12.3798(5)	14.0993(5)	17.0975(7)
c (Å)	10.6039(6)	15.1880(7)	14.0786(7)	21.8415(9)	17.8125(6)	9.3062(5)
α (deg)			74.945(4)		78.471(3)	
β (deg)	108.572(6)	103.595(4)	77.243(4)	90.176(4)	79.092(3)	113.598(7)
γ (deg)			76.944(4)		76.368(3)	
V (Å^3)	962.00(9)	2815.6(2)	1451.01(12)	2780.79(19)	2954.24(18)	1353.72(13)
Z	2	4	2	4	4	2
μ (mm^{-1})	0.221	0.168	0.170	0.170	0.161	0.174
trans. coeff. range	0.959-1.000	0.967-0.967	0.935-0.993	0.935-0.951	0.935-0.953	0.960-0.966
reflns. measd.	5004	16487	11266	12571	27195	11248
unique reflns.	3135	4941	5541	5601	12382	5295

R_{int}	0.035	0.045	0.023	0.026	0.025	0.020
reflns. with $F^2>2\sigma$	2918	3811	4603	4486	9703	5248
refined parameters	215	304	333	301	649	287
R (on F, $F^2>2\sigma$)[a]	0.036	0.042	0.046	0.039	0.041	0.029
R_w (on F^2, all data)[a]	0.083	0.102	0.123	0.100	0.106	0.070
goodness of fit[a]	1.074	1.029	1.038	1.042	1.034	1.060
Flack parameter	0.05(8)					0.08(3)
max, min electron density (e Å^{-3})	0.31, -0.29	0.24, -0.25	0.63, -0.38	0.29, -0.31	0.34,-0.31	0.21,-0.21

[a] $R = \Sigma||F_o|-|F_c||/\Sigma|F_o|$; $R_w = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$; $S = [\Sigma w(F_o^2-F_c^2)^2/(\text{no. data - no. params})]^{1/2}$ for all data

Molecular structure of 1a:

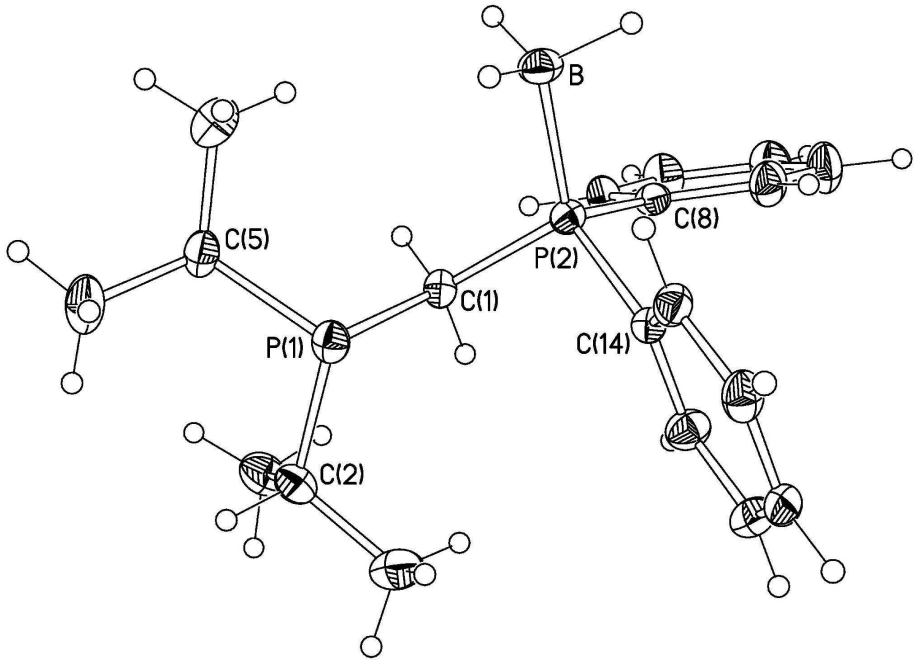


Figure S1. Molecular structure of **1a** with 40% probability ellipsoids. Selected bond lengths (Å) and angles (°): P(1)–C(1) 1.865(3), P(1)–C(2) 1.868(4), P(1)–C(5) 1.861(3), P(2)–B 1.913(3), P(2)–C(1) 1.813(3), P(2)–C(8) 1.821(3), P(2)–C(14) 1.814(3), C(1)–P(1)–C(2) 99.35(15), C(1)–P(1)–C(5) 100.30(14), C(2)–P(1)–C(5) 100.41(16), B–P(2)–C(1) 115.00(16), B–P(2)–C(8) 111.51(16), B–P(2)–C(14) 113.35(16), C(1)–P(2)–C(8) 104.57(14), C(1)–P(2)–C(14) 106.45(14), P(1)–C(1)–P(2) 114.99(17).

Molecular structure of 1c:

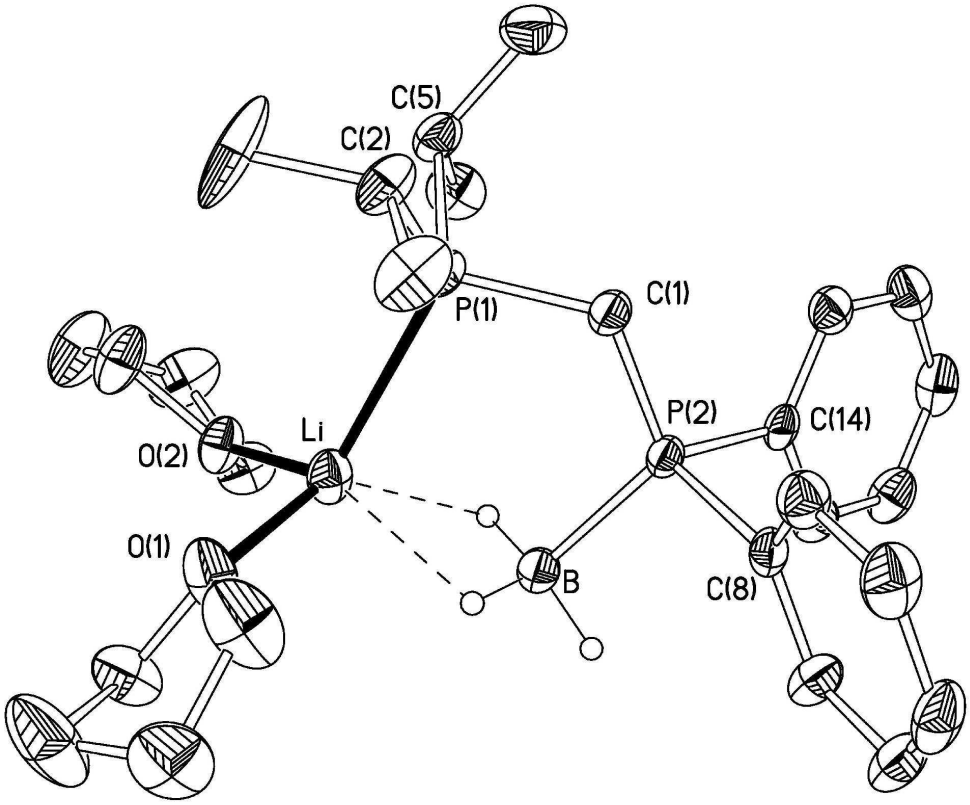


Figure S2. Molecular structure of **1c** with C-bound H atoms omitted for clarity and with 40% probability ellipsoids. Selected bond lengths (Å) and angles (°): P(1)–Li 2.555(4), P(1)–C(1) 1.7412(19), P(1)–C(2) 1.865(2), P(1)–C(5) 1.869(2), P(2)–B 1.939(2), P(2)–C(1) 1.7016(19), P(2)–C(8) 1.8391(19), P(2)–C(14) 1.840(2), Li…B 2.439(4), Li–O(1) 1.939(11), Li–O(2) 1.951(3), P(1)–Li…B 87.79(12), P(1)–C(1)–P(2) 120.28(11).

Computational details:

Geometry optimizations were performed with the Gaussian09 suite of programs (revisions B.01, C.01, or D.01).[S1] A brief benchmarking exercise showed that the GGA meta-hybrid wB97XD functional,[S2] which explicitly includes mid-to-long-range dispersive interactions, outperformed both the highly parameterized M06-2X functional[S3] and the ever-popular B3LYP hybrid functional[S4] in generating an optimized geometry for **1a′** which correlated with the data obtained by X-ray crystallography for **1a** (Table S2). In view of this, ground state optimizations were performed using the wB97XD functional, which includes a correction for dispersion effects; the 6-311+G(d,p) all-electron basis set[S5] was used on all atoms [default parameters were used throughout]. The global minimum energy conformations of **1a′**-**4a′** were located by relaxed potential energy surface scans at the HF/3-21G* level in which the P-C-P-C(*i*Pr) dihedral angle was increased in 10° steps through a full 360° rotation; the located minimum energy geometries were then re-optimized at the wB97XD/6-311+G(d,p) level. The identity of minima was confirmed by the absence of imaginary vibrational frequencies in each case. Natural Bond Orbital analyses were performed using the NBO 3.1 module of Gaussian09.[S6] For the rearrangement of **1a′** to **2a′** the transition states $\mathbf{1}_{\mathbf{intra}}$**′** and $\mathbf{1}_{\mathbf{inter}}$**′** were initially located using the QST3 method[S7] at the HF/3-21G* level;[S8] the geometries obtained were then re-optimized at the wB97XD/6-311+G(d,p) level. The nature of these transition states was confirmed by the presence of a single imaginary vibrational frequency which correlated with the expected displacement vector for migration of the BH_3 group between the two phosphine centers in each case. For the dissociation of **1a′** and **3a′** and the migration of BH_3 between two molecules of **1a′** via $\mathbf{1}_{\mathbf{inter}}$**′** the free energy was corrected for basis set superposition error (using the counterpoise method);[S9] the absence of a transition state for the dissociation of both **1a′** and **3a′** was confirmed by performing a relaxed potential energy surface scan, increasing the P-B distance in 20 increments of 0.1 Å, which showed

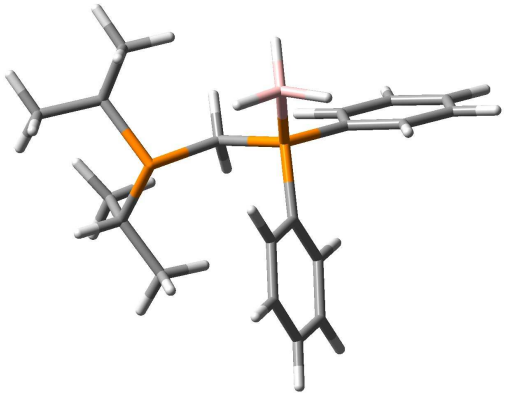
no maximum on the pathway to complete dissociation. In all calculations solvation by toluene was included implicitly using the EIF Polarizable Continuum Model.[S10] All energies were corrected to 298.15 K.

Table S2. Comparison of bond lengths (Å) and angles (°) for the calculated structures of 1a′ using different DFT methods:

	Exp[(a)]	B3LYP/ 6-311+G(d,p)	Δ[(b)]	M06-2X/ 6-311+G(d,p)	Δ	wB97xD/ 6-311+G(d,p)	Δ
C1-P1	1.867(4)	1.897	0.030	1.886	0.019	1.880	0.013
C1-P2	1.815(5)	1.844	0.029	1.830	0.015	1.827	0.012
P1-C2	1.869(5)	1.892	0.023	1.873	0.004	1.873	0.004
P1-C5	1.854(4)	1.887	0.033	1.868	0.014	1.868	0.014
P2-C8	1.814(4)	1.834	0.020	1.825	0.011	1.824	0.010
P2-C14	1.820(4)	1.831	0.011	1.825	0.005	1.822	0.002
P2-B1	1.913(6)	1.940	0.027	1.933	0.020	1.928	0.015
P1-C1-P2	115.0(3)	114.99	0.0	111.28	-3.7	112.50	-2.5
B1-P2-C1	115.3(2)	114.94	0.4	114.30	1.0	114.23	1.1
B1-P2-C1-P1	-64.73	-62.11	2.62	-62.60	2.13	-62.27	2.46

[(a)] Determined by X-ray crystallography; [(b)] Difference between calculated and experimental values.

Final atomic coordinates for 1a′:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.264974	-0.131786	-0.226027
2	15	0	0.750348	-0.392324	-0.810789
3	5	0	0.542791	-0.971188	-2.638187
4	1	0	-0.493099	-0.490526	-3.040484
5	1	0	1.525450	-0.561360	-3.219194
6	1	0	0.505839	-2.181988	-2.551594
7	6	0	-0.621235	-0.883680	0.291683
8	1	0	-0.380168	-0.571201	1.310091
9	1	0	-0.686377	-1.974734	0.279043
10	6	0	-2.828564	0.592628	1.406764
11	1	0	-3.831020	0.971960	1.176195
12	6	0	-2.938881	-0.376352	2.584365
13	1	0	-3.275636	0.156592	3.479433
14	1	0	-1.973596	-0.833406	2.824482
15	1	0	-3.651681	-1.181513	2.393146
16	6	0	-1.953803	1.800219	1.761479
17	1	0	-2.383318	2.339640	2.610832
18	1	0	-1.857108	2.496873	0.924271
19	1	0	-0.943198	1.493501	2.048379
20	6	0	-3.281888	-1.692709	-0.363335
21	1	0	-3.081453	-2.319798	0.513213
22	6	0	-4.773918	-1.353870	-0.399944
23	1	0	-5.359833	-2.262902	-0.566216
24	1	0	-4.998206	-0.660966	-1.217623
25	1	0	-5.122906	-0.900893	0.531378
26	6	0	-2.872133	-2.462077	-1.622292
27	1	0	-3.426592	-3.403689	-1.683399
28	1	0	-1.805192	-2.697632	-1.644941
29	1	0	-3.091739	-1.879673	-2.521870
30	6	0	2.274081	-1.046225	-0.051777
31	6	0	2.279914	-1.774919	1.136386
32	1	0	1.355337	-1.981957	1.661942
33	6	0	3.477035	-2.252184	1.661144
34	1	0	3.469979	-2.819147	2.585157
35	6	0	4.674582	-2.002499	1.004354
36	1	0	5.606483	-2.374948	1.414459

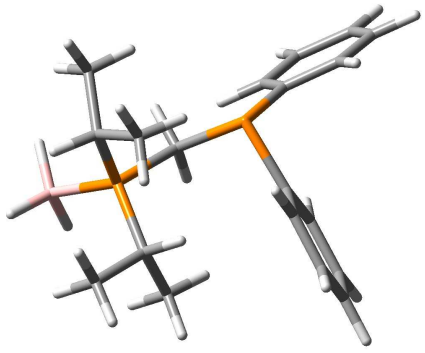
37	6	0	4.675097	-1.278224	-0.184274
38	1	0	5.606948	-1.086018	-0.703557
39	6	0	3.482156	-0.806125	-0.712339
40	1	0	3.486319	-0.251921	-1.644727
41	6	0	0.863770	1.411360	-0.580288
42	6	0	1.493221	1.961842	0.537221
43	1	0	1.995365	1.317519	1.251703
44	6	0	1.484596	3.335588	0.736673
45	1	0	1.974099	3.757689	1.606978
46	6	0	0.847999	4.167453	-0.179317
47	1	0	0.839485	5.240236	-0.021680
48	6	0	0.230218	3.624480	-1.299569
49	1	0	-0.260302	4.271136	-2.018068
50	6	0	0.238586	2.249233	-1.503383
51	1	0	-0.243455	1.823077	-2.375478

Final energy (Hartrees) for **1a′**: -1449.02808295

Final free energy (G/kJ mol^{-1}) for **1a′**: -3803423.4

NIMAG = 0

Final atomic coordinates for 2a′:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	15	0	0.742370	-0.431614	-0.784706
3	6	0	-0.282087	-1.054623	0.635662
4	1	0	-0.010129	-0.568187	1.577496
5	1	0	-0.051500	-2.118228	0.755460
6	6	0	-2.666803	-1.825156	-1.006660
7	1	0	-3.725929	-2.021438	-0.803561
8	6	0	-2.563183	-0.965280	-2.269036
9	1	0	-3.003752	-1.507912	-3.110517
10	1	0	-1.521049	-0.754494	-2.519018
11	1	0	-3.095724	-0.016435	-2.175752
12	6	0	-1.967291	-3.176390	-1.191556
13	1	0	-2.435249	-3.720486	-2.016128
14	1	0	-2.036244	-3.794301	-0.293897
15	1	0	-0.911652	-3.039768	-1.444270

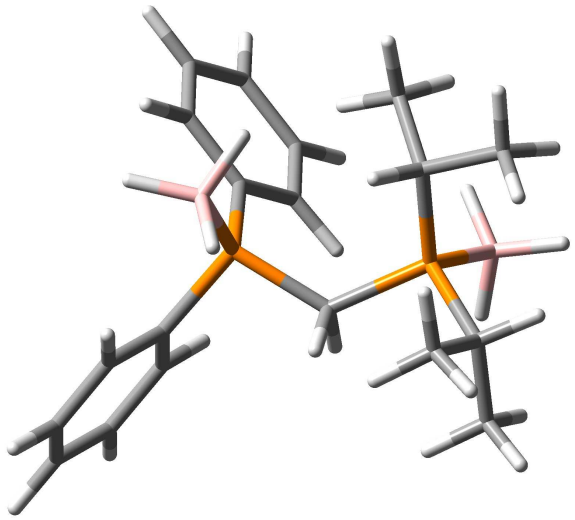
16	6	0	-2.679767	0.730054	0.492833
17	1	0	-2.260028	1.165709	-0.416981
18	6	0	-4.210242	0.781322	0.412601
19	1	0	-4.532940	1.823185	0.334460
20	1	0	-4.661614	0.351044	1.309690
21	1	0	-4.605425	0.246204	-0.454301
22	6	0	-2.171018	1.531479	1.693286
23	1	0	-2.541428	2.557966	1.622741
24	1	0	-1.081557	1.580185	1.725132
25	1	0	-2.530956	1.102673	2.631820
26	6	0	2.444272	-0.825262	-0.198934
27	6	0	3.486792	-0.475748	-1.064411
28	1	0	3.261103	0.001161	-2.013730
29	6	0	4.808575	-0.724864	-0.724624
30	1	0	5.602253	-0.440690	-1.406444
31	6	0	5.112108	-1.347046	0.482969
32	1	0	6.143979	-1.549560	0.746679
33	6	0	4.085857	-1.710433	1.344186
34	1	0	4.311837	-2.197574	2.286208
35	6	0	2.759726	-1.448983	1.008253
36	1	0	1.982123	-1.737770	1.705397
37	6	0	0.700184	1.386442	-0.474006
38	6	0	1.344092	1.987152	0.610479
39	1	0	1.941335	1.383228	1.286185
40	6	0	1.228537	3.353068	0.830248
41	1	0	1.729682	3.807117	1.677780
42	6	0	0.465921	4.136913	-0.030893
43	1	0	0.370126	5.202404	0.145297
44	6	0	-0.163777	3.552738	-1.122826
45	1	0	-0.749196	4.160738	-1.803439
46	6	0	-0.037644	2.185554	-1.347279
47	1	0	-0.522634	1.734791	-2.207885
48	5	0	-2.785352	-1.979626	2.106000
49	1	0	-2.387993	-1.374373	3.080726
50	1	0	-3.994724	-1.987990	2.004201
51	1	0	-2.299144	-3.089943	2.023599

Final energy (Hartrees) for **2a′**: -1449.03347437

Final free energy (G/kJ mol^{-1}) for **2a′**: -3803435.7

NIMAG = 0

Final atomic coordinates for 3a′:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.192463	-0.122833	0.048940
2	15	0	0.847160	-0.246411	-0.887151
3	6	0	-0.527904	-0.937806	0.118736
4	1	0	-0.202289	-0.940575	1.161641
5	1	0	-0.651923	-1.980167	-0.186852
6	6	0	-2.751993	-0.182918	1.813104
7	1	0	-3.746978	0.272469	1.762839
8	6	0	-2.871893	-1.593177	2.392852
9	1	0	-3.217352	-1.538573	3.429121
10	1	0	-1.904858	-2.106594	2.400474
11	1	0	-3.580611	-2.214372	1.841203
12	6	0	-1.876546	0.713423	2.695227
13	1	0	-2.341186	0.825664	3.678632
14	1	0	-1.742123	1.704444	2.259293
15	1	0	-0.887037	0.272928	2.854931
16	6	0	-3.228612	-1.362116	-0.849962
17	1	0	-3.034872	-2.329724	-0.372118
18	6	0	-4.718245	-1.032565	-0.719629
19	1	0	-5.302922	-1.778939	-1.264410
20	1	0	-4.935773	-0.052275	-1.148946
21	1	0	-5.062325	-1.034603	0.317756
22	6	0	-2.809564	-1.443024	-2.320144
23	1	0	-3.419215	-2.194303	-2.830245
24	1	0	-1.760569	-1.715976	-2.448618
25	1	0	-2.958447	-0.482474	-2.818458
26	6	0	2.320578	-1.082974	-0.201559
27	6	0	2.260269	-2.335878	0.406453
28	1	0	1.311523	-2.843015	0.538011
29	6	0	3.422015	-2.958290	0.850008
30	1	0	3.361941	-3.931715	1.323347
31	6	0	4.652433	-2.337016	0.684663
32	1	0	5.557538	-2.822637	1.031347
33	6	0	4.720702	-1.091102	0.070192
34	1	0	5.678891	-0.602919	-0.065881

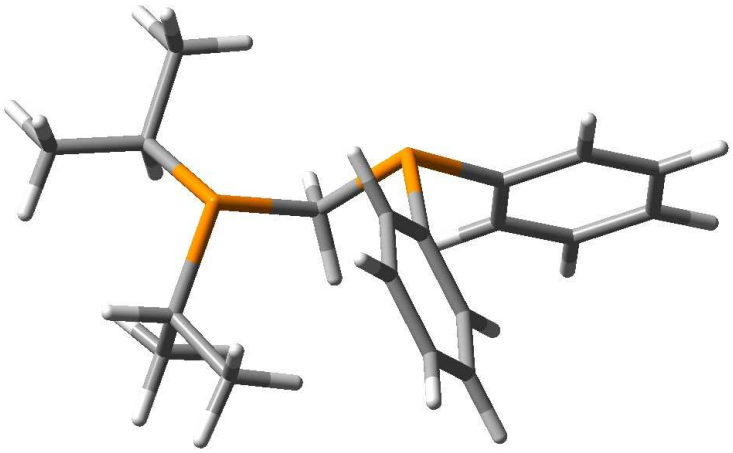
35	6	0	3.562737	-0.467934	-0.371845
36	1	0	3.623917	0.504344	-0.848928
37	6	0	1.029119	1.473796	-0.339346
38	6	0	1.234774	1.784377	1.005415
39	1	0	1.340020	0.992561	1.740683
40	6	0	1.312979	3.108413	1.408123
41	1	0	1.465365	3.347718	2.454448
42	6	0	1.199040	4.126426	0.465354
43	1	0	1.257244	5.162372	0.780470
44	6	0	1.013467	3.819154	-0.875508
45	1	0	0.921696	4.611694	-1.608808
46	6	0	0.924992	2.492855	-1.280793
47	1	0	0.750322	2.246980	-2.321578
48	5	0	-2.378832	1.663394	-0.658184
49	1	0	-1.996874	1.637055	-1.803375
50	1	0	-3.579001	1.828325	-0.549882
51	1	0	-1.742442	2.402299	0.054330
52	5	0	0.710060	-0.502527	-2.787343
53	1	0	0.602832	-1.706914	-2.901529
54	1	0	-0.256735	0.117962	-3.159067
55	1	0	1.765565	-0.078583	-3.207072

Final energy (Hartrees) for **3a′**: -1475.6877991

Final free energy (G/kJ mol^{-1}) for **3a′**: -3873335.6

NIMAG = 0

Final atomic coordinates for 4a′:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.237118	-0.153986	-0.344357
2	15	0	0.734057	-0.440564	-1.068917
3	6	0	-0.581629	-0.866527	0.167305
4	1	0	-0.304232	-0.487181	1.154262

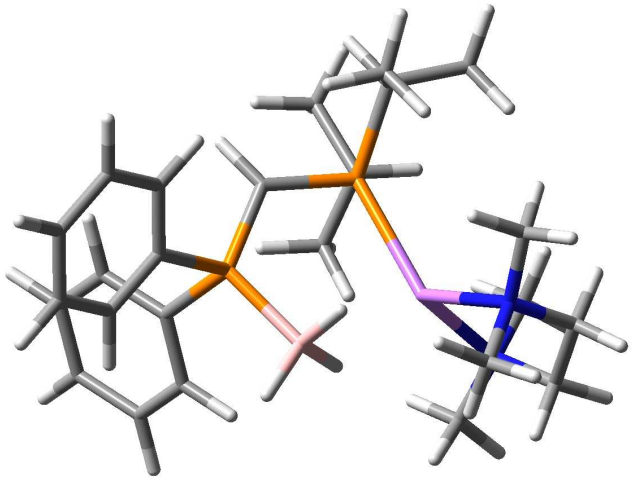
5	1	0	-0.661487	-1.954962	0.237088
6	6	0	-2.831183	0.567879	1.278316
7	1	0	-3.848669	0.906378	1.049595
8	6	0	-2.898352	-0.397276	2.462359
9	1	0	-3.250222	0.126936	3.356943
10	1	0	-1.914441	-0.815838	2.695770
11	1	0	-3.581781	-1.229698	2.278863
12	6	0	-2.000441	1.810259	1.618997
13	1	0	-2.429930	2.324219	2.484326
14	1	0	-1.961014	2.515894	0.785009
15	1	0	-0.968306	1.549011	1.871545
16	6	0	-3.227931	-1.732072	-0.486866
17	1	0	-3.025854	-2.352457	0.394069
18	6	0	-4.725832	-1.427165	-0.546004
19	1	0	-5.291972	-2.348594	-0.714059
20	1	0	-4.954346	-0.741895	-1.369062
21	1	0	-5.093916	-0.976436	0.379113
22	6	0	-2.781145	-2.498774	-1.735117
23	1	0	-3.322568	-3.446862	-1.812226
24	1	0	-1.711712	-2.727229	-1.722236
25	1	0	-2.984285	-1.919393	-2.641025
26	6	0	2.256933	-1.104163	-0.269633
27	6	0	2.266220	-1.864910	0.899898
28	1	0	1.341059	-2.080235	1.421594
29	6	0	3.461182	-2.357005	1.419216
30	1	0	3.447631	-2.946680	2.329445
31	6	0	4.664389	-2.090433	0.780310
32	1	0	5.594266	-2.471932	1.186920
33	6	0	4.668163	-1.334343	-0.388953
34	1	0	5.602627	-1.124505	-0.897555
35	6	0	3.475420	-0.855642	-0.911804
36	1	0	3.489701	-0.275519	-1.829946
37	6	0	0.901047	1.356528	-0.676092
38	6	0	1.562883	1.829462	0.459649
39	1	0	2.067788	1.132220	1.120759
40	6	0	1.583168	3.187254	0.751206
41	1	0	2.100340	3.541096	1.636422
42	6	0	0.938657	4.091435	-0.087940
43	1	0	0.952983	5.151339	0.141152
44	6	0	0.283732	3.632543	-1.223962
45	1	0	-0.216988	4.331853	-1.884365
46	6	0	0.270582	2.272930	-1.518830
47	1	0	-0.243939	1.918843	-2.405635

Final energy (Hartrees) for **4a′**: -1422.3591708

Final free energy (G/kJ mol^{-1}) for **4a′**: -3733484.7

NIMAG = 0

Final atomic coordinates for 1b′:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.904987	0.099077	1.535561
2	15	0	-1.501878	-0.233844	-0.220725
3	5	0	-0.277687	-0.482453	-1.710185
4	1	0	-0.940643	-0.640368	-2.710203
5	1	0	0.417456	0.515927	-1.815825
6	1	0	0.371964	-1.476598	-1.441932
7	3	0	1.936365	-0.255747	-0.773078
8	7	0	3.358540	-1.679746	-1.418678
9	7	0	3.299965	1.248977	-1.468403
10	6	0	-0.802879	-0.244452	1.348307
11	1	0	-1.483075	-0.101653	2.187783
12	6	0	1.058858	1.843459	2.229964
13	1	0	2.134087	2.040188	2.326859
14	6	0	0.397947	2.048696	3.592352
15	1	0	0.442646	3.102832	3.887850
16	1	0	0.880050	1.464869	4.380516
17	1	0	-0.658289	1.762529	3.551750
18	6	0	0.476129	2.819468	1.205613
19	1	0	0.686282	3.856605	1.487507
20	1	0	-0.608316	2.697153	1.134374
21	1	0	0.879420	2.648374	0.202508
22	6	0	1.466524	-0.934292	2.989037
23	1	0	0.821595	-0.686669	3.840167
24	6	0	2.917654	-0.619583	3.356989
25	1	0	3.259244	-1.260469	4.176584
26	1	0	3.049632	0.419093	3.671387
27	1	0	3.580942	-0.795827	2.501250
28	6	0	1.285225	-2.419117	2.678857
29	1	0	1.559121	-3.029909	3.545949
30	1	0	1.918765	-2.725147	1.840591
31	1	0	0.249774	-2.635715	2.409339
32	6	0	-2.501831	1.289407	-0.522140
33	6	0	-2.175986	2.171337	-1.550470
34	1	0	-1.373756	1.922150	-2.235709

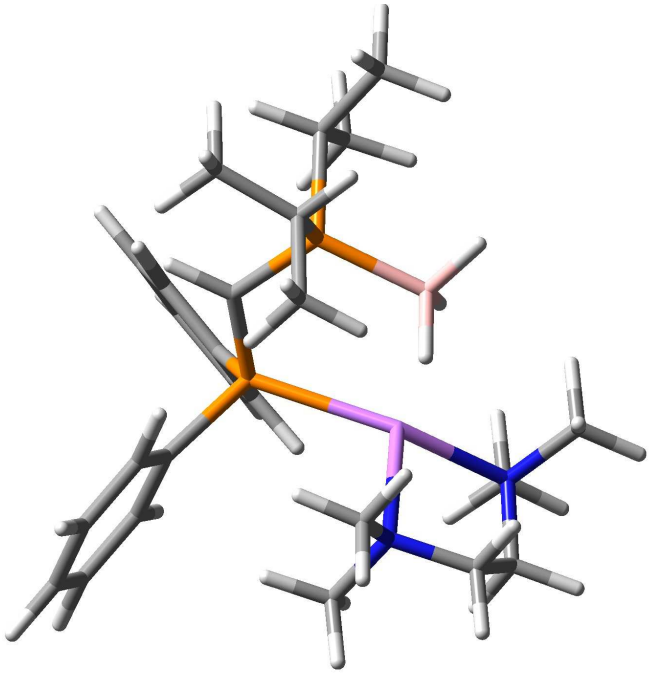
35	6	0	-2.869530	3.369279	-1.702487
36	1	0	-2.604050	4.048146	-2.505902
37	6	0	-3.898491	3.695113	-0.828505
38	1	0	-4.437135	4.629240	-0.944725
39	6	0	-4.236971	2.816014	0.197747
40	1	0	-5.041620	3.063256	0.881852
41	6	0	-3.542860	1.623531	0.347923
42	1	0	-3.811599	0.944254	1.151667
43	6	0	-2.810602	-1.522511	-0.317463
44	6	0	-3.741339	-1.510904	-1.358417
45	1	0	-3.717324	-0.714477	-2.095362
46	6	0	-4.700648	-2.509548	-1.455379
47	1	0	-5.420087	-2.491642	-2.266793
48	6	0	-4.741973	-3.531175	-0.509727
49	1	0	-5.493883	-4.309411	-0.583218
50	6	0	-3.818356	-3.549152	0.528121
51	1	0	-3.846978	-4.341692	1.268230
52	6	0	-2.854600	-2.548573	0.622153
53	1	0	-2.123462	-2.550116	1.424280
54	6	0	3.583500	-2.775557	-0.480641
55	1	0	4.354460	-3.476507	-0.838663
56	1	0	2.652081	-3.326593	-0.338351
57	1	0	3.895856	-2.375925	0.486763
58	6	0	2.877823	-2.204352	-2.697259
59	1	0	3.644357	-2.818656	-3.195986
60	1	0	2.587302	-1.391111	-3.364004
61	1	0	1.988888	-2.811539	-2.527022
62	6	0	4.572258	-0.876556	-1.584510
63	1	0	5.325545	-1.410648	-2.186652
64	1	0	5.011693	-0.725214	-0.594853
65	6	0	4.282616	0.472170	-2.230289
66	1	0	5.227694	1.026853	-2.346278
67	1	0	3.884292	0.321193	-3.236047
68	6	0	2.696098	2.283142	-2.304790
69	1	0	3.442493	3.005740	-2.671599
70	1	0	1.941938	2.825516	-1.731881
71	1	0	2.199332	1.821185	-3.159815
72	6	0	3.901597	1.845789	-0.277241
73	1	0	4.744759	2.506772	-0.535309
74	1	0	4.259404	1.070927	0.403580
75	1	0	3.151352	2.429692	0.256066

Final energy (Hartrees) for **1b′**: -1803.7769337

Final free energy (G/kJ mol^{-1}) for **1b′**: -4734294.3

NIMAG = 0

Final atomic coordinates for 2b′:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.450880	-0.660372	0.321110
2	15	0	-0.142051	0.863757	0.145380
3	7	0	-2.166726	-2.333869	0.406931
4	7	0	-1.708394	-2.322083	-2.480706
5	5	0	1.612513	-1.998254	-0.812061
6	1	0	1.146480	-1.431699	-1.785323
7	1	0	0.748982	-2.558907	-0.156299
8	1	0	2.462400	-2.796680	-1.140846
9	3	0	-0.731473	-1.413205	-0.841290
10	6	0	1.416657	0.615321	0.865597
11	1	0	1.863784	1.385197	1.492035
12	6	0	3.919100	0.062056	-0.572027
13	1	0	4.279026	0.866167	0.081111
14	6	0	5.054001	-0.936108	-0.809349
15	1	0	5.853549	-0.463869	-1.389367
16	1	0	4.699164	-1.803249	-1.373525
17	1	0	5.494506	-1.295975	0.123595
18	6	0	3.453221	0.691006	-1.887266
19	1	0	4.278324	1.235604	-2.357269
20	1	0	2.629286	1.390770	-1.727800
21	1	0	3.115189	-0.079552	-2.586078
22	6	0	3.211213	-1.508733	1.791375
23	1	0	3.905859	-2.247958	1.378666
24	6	0	2.135731	-2.248989	2.587162
25	1	0	2.581223	-2.739413	3.458483
26	1	0	1.640023	-3.009686	1.981203
27	1	0	1.374353	-1.547573	2.940802
28	6	0	3.980443	-0.535939	2.686477

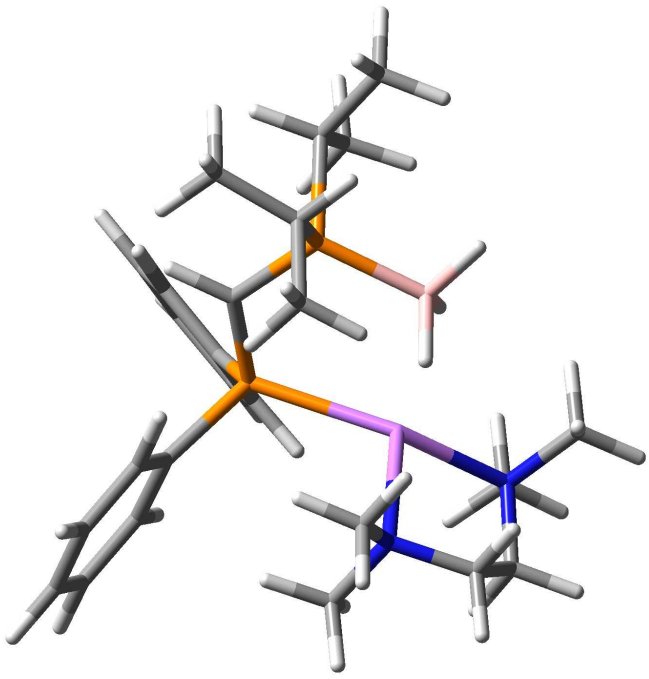
29	1	0	4.412090	-1.066594	3.540955
30	1	0	3.310005	0.235077	3.079041
31	1	0	4.798419	-0.038983	2.158330
32	6	0	-0.146054	2.399854	-0.893803
33	6	0	0.800511	3.408829	-0.716953
34	1	0	1.555788	3.296896	0.054735
35	6	0	0.798312	4.536532	-1.528925
36	1	0	1.542465	5.311766	-1.379415
37	6	0	-0.153096	4.671418	-2.536284
38	1	0	-0.152906	5.549981	-3.172248
39	6	0	-1.096026	3.668774	-2.730518
40	1	0	-1.834125	3.760891	-3.520318
41	6	0	-1.084371	2.539001	-1.917593
42	1	0	-1.813437	1.750572	-2.086518
43	6	0	-1.256872	1.401591	1.521413
44	6	0	-2.396298	2.181697	1.304227
45	1	0	-2.584086	2.606395	0.323761
46	6	0	-3.298356	2.427930	2.332742
47	1	0	-4.176326	3.036536	2.143011
48	6	0	-3.079677	1.898530	3.600994
49	1	0	-3.786463	2.088035	4.401388
50	6	0	-1.941084	1.135071	3.833748
51	1	0	-1.752839	0.727273	4.821501
52	6	0	-1.038387	0.892603	2.803573
53	1	0	-0.143982	0.303310	2.979300
54	6	0	-3.257119	-1.405767	0.703913
55	1	0	-4.127691	-1.927200	1.133603
56	1	0	-3.576610	-0.879534	-0.197927
57	1	0	-2.912150	-0.655304	1.414418
58	6	0	-2.606886	-3.430793	-0.457968
59	1	0	-3.507958	-3.921893	-0.054471
60	1	0	-1.813037	-4.182516	-0.472303
61	6	0	-2.888075	-2.954712	-1.878751
62	1	0	-3.238670	-3.803498	-2.485719
63	1	0	-3.699777	-2.224232	-1.867097
64	6	0	-2.078164	-1.366656	-3.521310
65	1	0	-2.596475	-1.848571	-4.365583
66	1	0	-1.178451	-0.878493	-3.901825
67	1	0	-2.733598	-0.598548	-3.104167
68	6	0	-1.587202	-2.841053	1.648073
69	1	0	-2.327094	-3.383038	2.258644
70	1	0	-1.195454	-2.004886	2.230531
71	1	0	-0.757966	-3.512710	1.418849
72	6	0	-0.785821	-3.323286	-3.017078
73	1	0	-1.255042	-3.908983	-3.823531
74	1	0	-0.461171	-4.003000	-2.228024
75	1	0	0.105448	-2.829205	-3.403870

Final energy (Hartrees) for **2b′**: -1803.7842971

Final free energy (G/kJ mol^{-1}) for **2b′**: -4734306.4

NIMAG = 0

Final atomic coordinates for 3b′:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.034108	2.207629	-0.645190
2	15	0	-1.251814	-0.590566	-0.065749
3	5	0	1.822835	1.832056	-0.235737
4	1	0	2.183880	0.994315	-1.040223
5	1	0	1.920997	1.460069	0.917380
6	1	0	2.429062	2.870420	-0.394758
7	5	0	0.346657	-1.393400	0.671960
8	1	0	1.086292	-1.578299	-0.278717
9	1	0	0.797855	-0.635805	1.507934
10	1	0	0.016967	-2.450832	1.161077
11	3	0	2.511934	-0.375340	0.373424
12	7	0	3.699838	-0.807635	2.058989
13	7	0	4.069437	-1.186433	-0.818461
14	6	0	-1.128465	0.889165	-0.937216
15	1	0	-2.052536	1.194426	-1.427351
16	6	0	-0.090491	3.176842	-2.229998
17	1	0	-1.155542	3.252768	-2.478985
18	6	0	0.609429	2.393579	-3.343693
19	1	0	0.459298	2.893848	-4.305485
20	1	0	0.219659	1.376091	-3.416181
21	1	0	1.685172	2.334350	-3.155595
22	6	0	0.489683	4.587022	-2.104265
23	1	0	0.481194	5.077873	-3.082359
24	1	0	1.525208	4.555105	-1.754700
25	1	0	-0.083052	5.213536	-1.417020
26	6	0	-0.701164	3.385964	0.634347
27	1	0	-0.011433	4.237472	0.642896
28	6	0	-2.111401	3.865099	0.290806

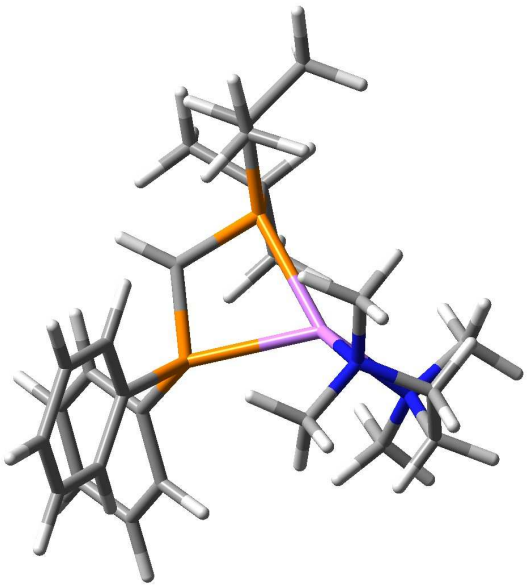
29	1	0	-2.478672	4.549030	1.062263
30	1	0	-2.798000	3.013714	0.245068
31	1	0	-2.155542	4.390286	-0.667187
32	6	0	-0.679353	2.727787	2.016180
33	1	0	-1.011470	3.442822	2.775414
34	1	0	0.320413	2.381735	2.286397
35	1	0	-1.358650	1.870904	2.048921
36	6	0	-2.528429	-0.489067	1.266617
37	6	0	-3.747695	0.138016	1.000982
38	1	0	-3.947355	0.524916	0.006294
39	6	0	-4.701488	0.284909	1.997621
40	1	0	-5.644629	0.773100	1.777497
41	6	0	-4.444972	-0.190024	3.281964
42	1	0	-5.187763	-0.072104	4.063311
43	6	0	-3.234533	-0.812343	3.557246
44	1	0	-3.028760	-1.182391	4.555871
45	6	0	-2.280777	-0.963139	2.553194
46	1	0	-1.335899	-1.446577	2.772994
47	6	0	-2.017062	-1.810470	-1.206293
48	6	0	-2.662988	-2.942945	-0.706846
49	1	0	-2.767079	-3.078881	0.364697
50	6	0	-3.182166	-3.895200	-1.574427
51	1	0	-3.683203	-4.770682	-1.176092
52	6	0	-3.061267	-3.725725	-2.950781
53	1	0	-3.467933	-4.468867	-3.628067
54	6	0	-2.419167	-2.600599	-3.453814
55	1	0	-2.322587	-2.462286	-4.525259
56	6	0	-1.897575	-1.647464	-2.584369
57	1	0	-1.394144	-0.764968	-2.964622
58	6	0	3.739988	0.306724	3.001241
59	1	0	4.406556	0.104041	3.854838
60	1	0	2.733452	0.493596	3.381129
61	1	0	4.080739	1.210167	2.491818
62	6	0	3.165885	-2.003564	2.708194
63	1	0	3.829187	-2.356179	3.514336
64	1	0	3.033519	-2.807840	1.982996
65	1	0	2.183056	-1.781907	3.124123
66	6	0	5.016709	-1.056092	1.466000
67	1	0	5.680385	-1.584489	2.169566
68	1	0	5.481458	-0.088037	1.262644
69	6	0	4.914051	-1.858356	0.173141
70	1	0	5.925691	-2.043952	-0.222033
71	1	0	4.474189	-2.836534	0.380731
72	6	0	4.776600	-0.085468	-1.469697
73	1	0	5.677090	-0.439464	-1.996949
74	1	0	5.070819	0.669061	-0.738351
75	1	0	4.112548	0.399867	-2.185268
76	6	0	3.564476	-2.124885	-1.817125
77	1	0	4.376634	-2.579956	-2.406410
78	1	0	2.890679	-1.599713	-2.497083
79	1	0	2.995932	-2.917076	-1.326541

Final energy (Hartrees) for **3b′**: -1830.4590492

Final free energy (G/kJ mol^{-1}) for **3b′**: -4804260.9

NIMAG = 0

Final atomic coordinates for 4b′:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.642564	1.270348	-0.911816
2	15	0	0.931578	0.015629	-0.189221
3	3	0	-1.335892	-0.609633	0.770531
4	7	0	-1.753240	-2.656645	0.746823
5	7	0	-1.691576	-0.594491	2.824406
6	6	0	-0.004047	0.856640	-1.384268
7	1	0	0.456772	1.306086	-2.265624
8	6	0	-1.723783	3.101811	-0.483719
9	1	0	-2.785300	3.336844	-0.340804
10	6	0	-1.146497	4.007552	-1.569086
11	1	0	-1.168209	5.058049	-1.257910
12	1	0	-1.698237	3.928232	-2.510086
13	1	0	-0.103428	3.738682	-1.766600
14	6	0	-1.006084	3.325784	0.848245
15	1	0	-1.073719	4.374925	1.155858
16	1	0	0.054131	3.065713	0.766954
17	1	0	-1.441141	2.712306	1.643905
18	6	0	-2.630432	1.213540	-2.501187
19	1	0	-2.055719	1.770965	-3.251132
20	6	0	-4.013862	1.852504	-2.364590
21	1	0	-4.594220	1.706470	-3.281891
22	1	0	-3.957256	2.927599	-2.178789
23	1	0	-4.575691	1.397507	-1.540512
24	6	0	-2.749717	-0.234707	-2.976546
25	1	0	-3.230219	-0.282131	-3.959716
26	1	0	-3.358444	-0.821565	-2.279485
27	1	0	-1.767569	-0.707228	-3.048780
28	6	0	2.289454	1.092810	0.476749
29	6	0	2.886371	0.811286	1.707513
30	1	0	2.575849	-0.067848	2.266168
31	6	0	3.867532	1.645253	2.236295
32	1	0	4.320356	1.410735	3.194041

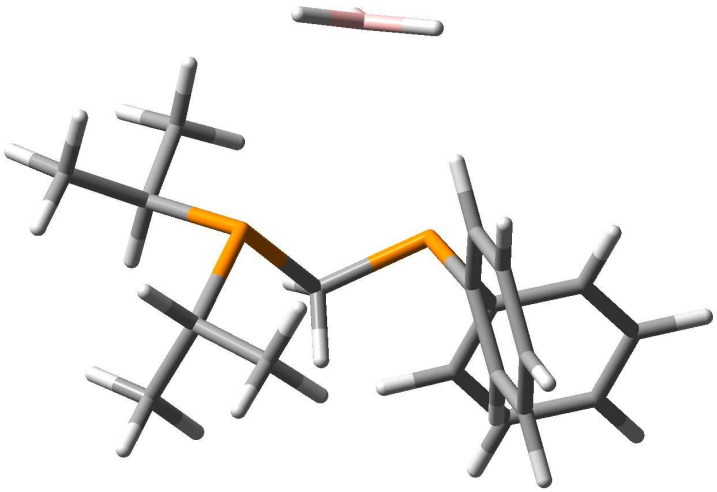
33	6	0	4.257351	2.785499	1.542775
34	1	0	5.015653	3.442366	1.954933
35	6	0	3.660069	3.085037	0.321820
36	1	0	3.953702	3.977818	-0.220424
37	6	0	2.684085	2.245999	-0.201966
38	1	0	2.201971	2.492456	-1.142882
39	6	0	1.939089	-1.264453	-1.076416
40	6	0	3.091033	-1.836982	-0.528630
41	1	0	3.501010	-1.450017	0.398471
42	6	0	3.735021	-2.893415	-1.162542
43	1	0	4.629284	-3.320856	-0.720846
44	6	0	3.239778	-3.400863	-2.360112
45	1	0	3.741502	-4.226149	-2.853603
46	6	0	2.100658	-2.833875	-2.920404
47	1	0	1.710777	-3.213464	-3.859443
48	6	0	1.458374	-1.776957	-2.283216
49	1	0	0.569743	-1.326723	-2.714807
50	6	0	-2.625112	-3.083379	-0.344198
51	1	0	-2.860738	-4.158134	-0.288476
52	1	0	-2.135457	-2.882597	-1.298819
53	1	0	-3.559709	-2.518592	-0.315330
54	6	0	-0.472986	-3.362542	0.672433
55	1	0	-0.601413	-4.445946	0.825812
56	1	0	0.222624	-2.978707	1.419966
57	1	0	-0.017103	-3.192675	-0.304024
58	6	0	-2.404023	-2.839862	2.048283
59	1	0	-2.419202	-3.902088	2.341918
60	1	0	-3.446784	-2.527598	1.945653
61	6	0	-1.729355	-2.024789	3.147605
62	1	0	-2.244176	-2.207628	4.104084
63	1	0	-0.699913	-2.366549	3.276594
64	6	0	-0.625917	0.093031	3.549147
65	1	0	-0.780198	0.062495	4.639433
66	1	0	-0.580144	1.136131	3.230128
67	1	0	0.334143	-0.367857	3.311645
68	6	0	-2.977341	0.055280	3.066673
69	1	0	-3.256253	0.024497	4.132080
70	1	0	-3.766418	-0.427069	2.486845
71	1	0	-2.922644	1.097550	2.746894

Final energy (Hartrees) for **4b′**: -1777.0905588

Final free energy (G/kJ mol^{-1}) for **4b′**: -4664309.6

NIMAG = 0

Final atomic coordinates for $1_{intra}'$:



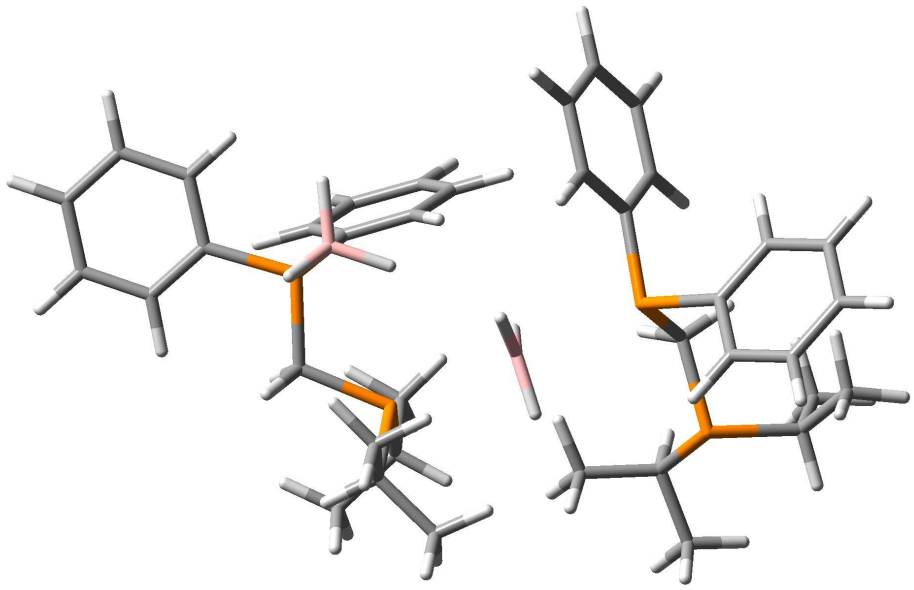
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.210875	-0.182950	0.146275
2	15	0	-0.736821	-0.456723	0.878552
3	5	0	1.432609	-0.404245	3.664400
4	1	0	2.557081	-0.038028	3.510017
5	1	0	0.588308	0.379002	3.979060
6	1	0	1.168293	-1.565962	3.609036
7	6	0	0.541844	-0.817061	-0.413800
8	1	0	0.259806	-0.377041	-1.373750
9	1	0	0.603354	-1.900520	-0.546750
10	6	0	2.759245	0.829799	-1.331097
11	1	0	3.785662	1.114424	-1.071264
12	6	0	2.788627	0.101066	-2.675127
13	1	0	3.141679	0.778909	-3.459149
14	1	0	1.791976	-0.242364	-2.968766
15	1	0	3.453777	-0.765502	-2.664721
16	6	0	1.932524	2.116197	-1.413479
17	1	0	2.337719	2.775683	-2.187086
18	1	0	1.932401	2.659282	-0.465618
19	1	0	0.889638	1.908964	-1.670444
20	6	0	3.223786	-1.745573	-0.024059
21	1	0	2.984124	-2.207865	-0.988561
22	6	0	4.720281	-1.429709	0.018548
23	1	0	5.300405	-2.357599	0.003610
24	1	0	4.979759	-0.891351	0.936233
25	1	0	5.042258	-0.823888	-0.831942
26	6	0	2.851418	-2.723575	1.093810
27	1	0	3.380731	-3.671754	0.957327
28	1	0	1.780309	-2.942936	1.121350
29	1	0	3.127443	-2.317494	2.070516
30	6	0	-2.272808	-1.157586	0.140316
31	6	0	-2.316842	-1.873535	-1.056360
32	1	0	-1.413711	-2.034510	-1.633250
33	6	0	-3.520007	-2.387623	-1.533371

34	1	0	-3.534480	-2.940799	-2.466151
35	6	0	-4.696477	-2.187493	-0.824069
36	1	0	-5.633198	-2.584936	-1.198406
37	6	0	-4.664851	-1.476854	0.372850
38	1	0	-5.578614	-1.318004	0.934707
39	6	0	-3.463325	-0.976172	0.853343
40	1	0	-3.449232	-0.430975	1.792549
41	6	0	-1.001589	1.340034	0.544553
42	6	0	-1.694612	1.803253	-0.577200
43	1	0	-2.150677	1.094408	-1.261093
44	6	0	-1.806615	3.164407	-0.825865
45	1	0	-2.345967	3.510489	-1.700812
46	6	0	-1.226362	4.083042	0.044662
47	1	0	-1.314194	5.146195	-0.150101
48	6	0	-0.543799	3.633664	1.167433
49	1	0	-0.095437	4.343992	1.853215
50	6	0	-0.436912	2.268988	1.418531
51	1	0	0.095794	1.924875	2.298120

Final energy (Hartrees) for $\mathbf{1}_{\mathbf{intra}}'$: -1448.9717743

Final free energy (G/kJ mol^{-1}) for $\mathbf{1}_{\mathbf{intra}}'$: -3803291.2; NIMAG = 1 (-106.2 cm^{-1})

Final atomic coordinates for $1_{inter}'$:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	4.133014	-1.672963	-0.551658
2	15	0	2.541539	0.750496	0.492637
3	5	0	0.342424	-0.499088	0.868129
4	1	0	0.217491	-0.235784	-0.297591
5	1	0	0.867683	-1.531443	1.179125
6	1	0	-0.036853	0.272165	1.698956
7	6	0	3.377889	-0.009394	-0.969108
8	1	0	4.152571	0.657997	-1.353509
9	1	0	2.622388	-0.132982	-1.750256
10	6	0	5.872639	-1.454106	-1.215073
11	1	0	6.320415	-2.445005	-1.074371
12	6	0	5.997394	-1.074330	-2.691044
13	1	0	7.053345	-0.984466	-2.966523
14	1	0	5.526103	-0.108651	-2.899131
15	1	0	5.545776	-1.817110	-3.352615
16	6	0	6.642816	-0.473083	-0.324998
17	1	0	7.700267	-0.457071	-0.606236
18	1	0	6.572189	-0.739558	0.732303
19	1	0	6.259890	0.546774	-0.428279
20	6	0	3.327421	-2.734412	-1.864241
21	1	0	3.375871	-2.203458	-2.821980
22	6	0	4.059986	-4.071345	-1.999255
23	1	0	3.524985	-4.724902	-2.695281
24	1	0	4.113914	-4.587095	-1.034668
25	1	0	5.079208	-3.951283	-2.374829
26	6	0	1.857259	-2.960605	-1.505342
27	1	0	1.364175	-3.555973	-2.281255
28	1	0	1.304157	-2.025116	-1.397247
29	1	0	1.770354	-3.498134	-0.555319
30	6	0	1.972313	2.375674	-0.147494
31	6	0	2.342786	2.915037	-1.380588
32	1	0	3.015526	2.374444	-2.036227

33	6	0	1.853660	4.152113	-1.789833
34	1	0	2.151232	4.557458	-2.750754
35	6	0	0.985820	4.865214	-0.971605
36	1	0	0.599568	5.825965	-1.292912
37	6	0	0.603038	4.333771	0.255954
38	1	0	-0.084817	4.876650	0.894206
39	6	0	1.089087	3.097570	0.661649
40	1	0	0.769485	2.680131	1.611167
41	6	0	4.003901	1.227038	1.504980
42	6	0	4.762032	2.372980	1.255460
43	1	0	4.462478	3.061773	0.472683
44	6	0	5.900030	2.642777	2.004694
45	1	0	6.479225	3.536903	1.801503
46	6	0	6.295331	1.768887	3.012660
47	1	0	7.186226	1.978033	3.594542
48	6	0	5.540256	0.632692	3.277345
49	1	0	5.839175	-0.048746	4.066099
50	6	0	4.396176	0.366665	2.532104
51	1	0	3.809337	-0.521329	2.741634
52	1	0	-0.703969	-4.556068	3.189977
53	6	0	-0.658966	-3.910979	2.307093
54	6	0	-1.900517	-3.016969	2.260270
55	1	0	0.253790	-3.314345	2.374598
56	1	0	-0.576954	-4.556930	1.429414
57	15	0	-1.861706	-1.858513	0.800166
58	1	0	-2.788236	-3.653621	2.163853
59	6	0	-2.020359	-2.183638	3.540126
60	6	0	-3.683078	-1.419666	0.696970
61	6	0	-1.665403	-2.982455	-0.671374
62	1	0	-2.096377	-2.841570	4.411280
63	1	0	-2.895023	-1.527724	3.534228
64	1	0	-1.139419	-1.547981	3.666272
65	15	0	-4.004462	0.378964	0.728339
66	1	0	-4.106370	-1.835093	-0.220460
67	1	0	-4.210549	-1.864454	1.545016
68	1	0	-0.635286	-3.337272	-0.560524
69	6	0	-2.593988	-4.195256	-0.732136
70	6	0	-1.734772	-2.159482	-1.961515
71	5	0	-3.443579	1.260044	2.347914
72	6	0	-5.795500	0.568679	0.438408
73	6	0	-3.236396	0.995240	-0.802078
74	1	0	-2.347237	-4.810753	-1.603299
75	1	0	-3.642099	-3.896977	-0.836009
76	1	0	-2.512313	-4.828047	0.154407
77	1	0	-1.433424	-2.773652	-2.815664
78	1	0	-1.083402	-1.283089	-1.920887
79	1	0	-2.751655	-1.804392	-2.154946
80	1	0	-2.254324	1.072428	2.458160
81	1	0	-3.742170	2.425828	2.190700
82	1	0	-4.099740	0.710993	3.210739
83	6	0	-6.672270	-0.509839	0.338052
84	6	0	-6.296982	1.869138	0.332684
85	6	0	-3.850693	0.818899	-2.044366
86	6	0	-1.979879	1.591370	-0.728940
87	1	0	-6.310000	-1.527347	0.425477
88	6	0	-8.030789	-0.292417	0.128453
89	6	0	-7.650373	2.083392	0.117540
90	1	0	-5.622864	2.714697	0.419338
91	1	0	-4.835056	0.365897	-2.107220
92	6	0	-3.205381	1.226125	-3.202902
93	6	0	-1.333936	1.994752	-1.892175
94	1	0	-1.496373	1.723587	0.231482
95	1	0	-8.705237	-1.138043	0.054949
96	6	0	-8.520553	1.001731	0.014728

97	1	0	-8.028884	3.095699	0.033610
98	1	0	-3.685159	1.088258	-4.165335
99	6	0	-1.943681	1.811079	-3.126072
100	1	0	-0.353273	2.450250	-1.826576
101	1	0	-9.578766	1.169788	-0.150269
102	1	0	-1.438880	2.128117	-4.032185

Final energy (Hartrees) for $\mathbf{1}_{\mathbf{inter}}'$: -2898.0386164

Final free energy (G/kJ mol^{-1}) for $\mathbf{1}_{\mathbf{inter}}'$: -1818055.487

NIMAG = 1 (-342.6 cm^{-1})

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