

Supporting information

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Can P–H σ -Bond complexes be prepared? A computational study using DFT and AIM methods

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S7	–	[CpMn(CO) ₂ (η^2 -HPFCl·BCl ₃)] 1
S7-S8	–	[CpMn(CO) ₂ (η^2 -HPClCl·BCl ₃)] 2
S 8	–	[CpMn(CO) ₂ (η^2 -HPBrCl·BCl ₃)] 3
S8-S 9	–	[CpMn(CO) ₂ (η^2 -HPPhCl·BCl ₃)] 4
S9	–	[CpMn(CO) ₂ (η^2 -HPMeCl·BCl ₃)] 5
S9-S 10	–	[CpMn(CO) ₂ (η^2 -HP(OMe)Cl·BCl ₃)] 6
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S11	–	[CpMn(CO) ₂ (η^2 -HPFPh·BCl ₃)] 8
S11-S12	–	[CpMn(CO) ₂ (η^2 -HPClPh·BCl ₃)] 9
S12-S13	–	[CpMn(CO) ₂ (η^2 -HPBrPh·BCl ₃)] 10
S13-S14	–	[CpMn(CO) ₂ (η^2 -HPPhPh·BCl ₃)] 11
S14	–	[CpMn(CO) ₂ (η^2 -HPMePh·BCl ₃)] 12
S15	–	[CpMn(CO) ₂ (η^2 -HP(OMe)Ph·BCl ₃)] 13
S15-S16	–	[CpMn(CO) ₂ (η^2 -HP(NH ₂)Ph·BCl ₃)] 14
S16-S17	–	[CpMn(CO) ₂ (η^2 -HPFH·BCl ₃)] 15

S17	–	[CpMn(CO) ₂ (η ² -HPClH·BCl ₃)] 16
S17-S18	–	[CpMn(CO) ₂ (η ² -HPBrH·BCl ₃)] 17
S18	–	[CpMn(CO) ₂ (η ² -HPPhH·BCl ₃)] 18
S18-S19	–	[CpMn(CO) ₂ (η ² -HPMeH·BCl ₃)] 19
S19	–	[CpMn(CO) ₂ (η ² -HP(OMe)H·BCl ₃)] 20
S20	–	[CpMn(CO) ₂ (η ² -HP(NH ₂)H·BCl ₃)] 21

- S21 – S28 Cartesian Coordinates for complexes 1a-21a as determined by DFT calculations at the [B3LYP/6-311G(d,p)] level of approximation.

S21	–	HPFCl·BCl ₃ 1a
S21	–	HPClCl·BCl ₃ 2a
S21	–	HPBrCl·BCl ₃ 3a
S21-S22	–	HPPhCl·BCl ₃ 4a
S22	–	HPMeCl·BCl ₃ 5a
S22	–	HPF(OMe)Cl·BCl ₃ 6a
S22	–	HP(NH ₂)Cl·BCl ₃ 7a
S23	–	HPFPh·BCl ₃ 8a
S23	–	HPClPh·BCl ₃ 9a
S23-S24	–	HPBrPh·BCl ₃ 10a
S24	–	HPPhPh·BCl ₃ 11a
S24-S25	–	HPMePh·BCl ₃ 12a
S25	–	HP(OMe)Ph·BCl ₃ 13a
S25-S26	–	HP(NH ₂)Ph·BCl ₃ 14a
S26	–	HPFH·BCl ₃ 15a
S26	–	HPClH·BCl ₃ 16a
S26	–	HPBrH·BCl ₃ 17a
S27	–	HPPhH·BCl ₃ 18a
S27	–	HPMeH·BCl ₃ 19a
S27	–	HP(OMe)H·BCl ₃ 20a
S28	–	HP(NH ₂)H·BCl ₃ 21a

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Computational Details

DFT calculations were performed with the GAUSSIAN 03 program suite¹ using the B3LYP density functional,² along with the implemented 6-311G(d,p) basis set.³ The geometry optimisations of complexes **1-21** and ligands **1a-21a** were performed with no imposed symmetry constraints. The reported structures were found to be true minima on the respective potential energy surface by calculating analytical frequencies.

Complex	Interatomic Distances (Å)			
	$r_{\text{PH (free)}}$	r_{PH}	r_{MnH}	r_{MnP}
[CpMn(CO) ₂ (η ² -HPFCl·BCl ₃)] 1	1.407 (1a)	1.996	1.535	2.262
[CpMn(CO) ₂ (η ² -HPClCl·BCl ₃)] 2	1.408 (2a)	2.031	1.533	2.291
[CpMn(CO) ₂ (η ² -HPBrCl·BCl ₃)] 3	1.409 (3a)	2.027	1.533	2.297
[CpMn(CO) ₂ (η ² -HPPhCl·BCl ₃)] 4	1.406 (4a)	2.121	1.531	2.341
[CpMn(CO) ₂ (η ² -HPMeCl·BCl ₃)] 5	1.407 (5a)	2.089	1.527	2.331
[CpMn(CO) ₂ (η ² -HP(OMe)Cl·BCl ₃)] 6	1.403 (6a)	2.071	1.529	2.286
[CpMn(CO) ₂ (η ² -HP(NH ₂)Cl·BCl ₃)] 7	1.404 (7a)	2.083	1.529	2.310
[CpMn(CO) ₂ (η ² -HPFPh·BCl ₃)] 8	1.405 (8a)	1.948	1.538	2.282
[CpMn(CO) ₂ (η ² -HPClPh·BCl ₃)] 9	1.406 (9a)	1.994	1.533	2.314
[CpMn(CO) ₂ (η ² -HPBrPh·BCl ₃)] 10	1.407 (10a)	1.983	1.533	2.323
[CpMn(CO) ₂ (η ² -HPPh ₂ ·BCl ₃)] 11	1.408 (11a)	2.090	1.529	2.376
[CpMn(CO) ₂ (η ² -HPMePh·BCl ₃)] 12	1.407 (12a)	2.080	1.526	2.366
[CpMn(CO) ₂ (η ² -HP(OMe)Ph·BCl ₃)] 13	1.414 (13a)	1.997	1.533	2.329
[CpMn(CO) ₂ (η ² -HP(NH ₂)Ph·BCl ₃)] 14	1.415 (14a)	2.057	1.528	2.341
[CpMn(CO) ₂ (η ² -HPFH·BCl ₃)] 15	1.405 (15a)	1.953	1.540	2.265
[CpMn(CO) ₂ (η ² -HPClH·BCl ₃)] 16	1.407 (16a)	1.997	1.536	2.294
[CpMn(CO) ₂ (η ² -HPBrH·BCl ₃)] 17	1.408 (17a)	1.992	1.536	2.301
[CpMn(CO) ₂ (η ² -HPPhH·BCl ₃)] 18	1.407 (18a)	2.085	1.530	2.351
[CpMn(CO) ₂ (η ² -HPMeH·BCl ₃)] 19	1.407 (19a)	2.067	1.528	2.341
[CpMn(CO) ₂ (η ² -HP(MeO)H·BCl ₃)] 20	1.413 (20a)	2.039	1.531	2.291
[CpMn(CO) ₂ (η ² -HP(NH ₂)H·BCl ₃)] 21	1.407 (21a)	2.040	1.530	2.314

Table 1. Bond lengths (Å) for the P–H bond in the free phosphines **1a-21a** and the P–H, Mn–H and Mn–P bonds in the coordinated Mn–P–H moiety of complexes **1-21**.

Complex	Atom	Net Charge	Bond	δ
1	Mn	0.879	Mn–P	0.73
	P	1.026	Mn–H	0.63
	H	–0.123	P–H	0.23
2	Mn	0.887	Mn–P	0.71
	P	0.678	Mn–H	0.63
	H	–0.113	P–H	0.22
3	Mn	0.892	Mn–P	0.71
	P	0.551	Mn–H	0.63
	H	–0.112	P–H	0.22
4	Mn	0.880	Mn–P	0.68
	P	0.824	Mn–H	0.62
	H	–0.089	P–H	0.18
5	Mn	0.880	Mn–P	0.68
	P	0.826	Mn–H	0.64
	H	–0.096	P–H	0.19
6	Mn	0.886	Mn–P	0.70
	P	1.059	Mn–H	0.64
	H	–0.108	P–H	0.20
7	Mn	0.881	Mn–P	0.68
	P	1.032	Mn–H	0.64
	H	–0.105	P–H	0.19

Table 2. AIM charges of the Mn, P and H atoms and delocalisation indices (δ) between atom pairs Mn–P, Mn–H and P–H for complexes **1-7**.

Complex	Atom	Net Charge	Bond	δ
8	Mn	0.889	Mn-P	0.71
	P	1.180	Mn-H	0.62
	H	-0.155	P-H	0.26
9	Mn	0.896	Mn-P	0.69
	P	0.823	Mn-H	0.63
	H	-0.146	P-H	0.24
10	Mn	0.899	Mn-P	0.69
	P	0.690	Mn-H	0.63
	H	-0.145	P-H	0.25
11	Mn	0.89	Mn-P	0.65
	P	0.98	Mn-H	0.64
	H	-0.12	P-H	0.21
12	Mn	0.874	Mn-P	0.66
	P	0.990	Mn-H	0.65
	H	-0.123	P-H	0.21
13	Mn	0.885	Mn-P	0.67
	P	1.231	Mn-H	0.63
	H	-0.145	P-H	0.24
14	Mn	0.881	Mn-P	0.67
	P	1.192	Mn-H	0.65
	H	-0.132	P-H	0.21

Table 3. AIM charges of the Mn, P and H atoms and delocalisation indices (δ) between atom pairs Mn-P, Mn-H and P-H for complexes **8-14**.

Complex	Atom	Net Charge	Bond	δ
15	Mn	0.877	Mn–P	0.71
	P	1.230	Mn–H	0.62
	H	-0.136	P–H	0.26
16	Mn	0.885	Mn–P	0.70
	P	0.890	Mn–H	0.62
	H	-0.120	P–H	0.23
17	Mn	0.887	Mn–P	0.69
	P	0.763	Mn–H	0.62
	H	-0.119	P–H	0.24
18	Mn	0.879	Mn–P	0.66
	P	1.048	Mn–H	0.63
	H	-0.101	P–H	0.19
19	Mn	0.885	Mn–P	0.66
	P	1.025	Mn–H	0.64
	H	-0.103	P–H	0.20
20	Mn	0.876	Mn–P	0.69
	P	1.268	Mn–H	0.64
	H	-0.118	P–H	0.22
21	Mn	0.871	Mn–P	0.67
	P	1.246	Mn–H	0.64
	H	-0.116	P–H	0.21

Table 4. AIM charges of the Mn, P and H atoms and delocalisation indices (δ) between atom pairs Mn–P, Mn–H and P–H for complexes **15-21**.

Cartesian Coordinates for complexes 1-21 as determined by DFT calculations at the [B3LYP/6-311G(d,p)] level of approximation.

[CpMn(CO)₂(η²-HPFCl·BCl₃)] 1

6	2.520534000	-1.390735000	-1.315923000
6	1.231844000	-1.917513000	-1.042403000
6	1.158496000	-2.191068000	0.350970000
6	2.405046000	-1.837468000	0.934293000
6	3.251513000	-1.335746000	-0.096261000
1	2.883151000	-1.086976000	-2.286734000
1	0.447402000	-2.091726000	-1.761465000
1	0.299237000	-2.589200000	0.867539000
1	2.663733000	-1.935060000	1.977761000
1	4.268787000	-0.995429000	0.021399000
25	1.527731000	-0.072690000	0.095663000
6	2.012127000	1.305697000	-0.999415000
8	2.366390000	2.137099000	-1.692654000
6	2.127357000	0.916608000	1.485355000
8	2.504812000	1.493311000	2.393883000
15	-0.577859000	0.577198000	-0.413759000
9	-0.713982000	0.743340000	-2.022898000
1	0.466712000	0.038220000	1.199593000
17	-0.854871000	2.544675000	0.175378000
5	-2.255552000	-0.429361000	0.164970000
17	-2.193400000	-2.072333000	-0.707041000
17	-2.060478000	-0.612246000	2.004401000
17	-3.718422000	0.547802000	-0.315772000

[CpMn(CO)₂(η²-HPClCl·BCl₃)] 2

6	2.497403000	-1.025749000	-1.600026000
6	1.274892000	-1.698677000	-1.352896000
6	1.339879000	-2.266422000	-0.051487000
6	2.613290000	-1.955749000	0.498549000
6	3.332650000	-1.180389000	-0.453852000
1	2.751952000	-0.495582000	-2.505544000
1	0.437960000	-1.769710000	-2.028943000
1	0.554339000	-2.830706000	0.426451000
1	2.969758000	-2.254469000	1.472857000
1	4.336377000	-0.800835000	-0.340164000
25	1.573305000	-0.116257000	0.132905000
6	2.058843000	1.514371000	-0.544408000
8	2.415114000	2.507619000	-0.971775000
6	2.103253000	0.485723000	1.751269000
8	2.441128000	0.808049000	2.791892000
15	-0.576690000	0.591278000	-0.218660000
17	-0.854036000	1.197130000	-2.209976000
1	0.516074000	-0.335886000	1.220780000
17	-0.861697000	2.379575000	0.812336000

5	-2.217170000	-0.570631000	0.258494000
17	-2.133692000	-2.053612000	-0.854529000
17	-1.916125000	-1.019341000	2.034872000
17	-3.724691000	0.414695000	0.004093000

[CpMn(CO)₂(η²-HPBrCl·BCl₃)] **3**

6	2.486773000	0.425732000	-1.853801000
6	1.343553000	-0.370434000	-2.112383000
6	1.578597000	-1.666379000	-1.578237000
6	2.878310000	-1.673512000	-1.003052000
6	3.443467000	-0.377469000	-1.163430000
1	2.610944000	1.459639000	-2.138739000
1	0.447815000	-0.052843000	-2.621185000
1	0.885221000	-2.492374000	-1.607995000
1	3.351126000	-2.516940000	-0.522728000
1	4.426371000	-0.066724000	-0.844359000
25	1.686744000	-0.227645000	0.045307000
6	2.027486000	1.446470000	0.704833000
8	2.296477000	2.481487000	1.095681000
6	2.308472000	-0.884575000	1.608775000
8	2.709683000	-1.352798000	2.568429000
15	-0.527446000	0.310561000	0.337002000
35	-1.070469000	2.233041000	-0.750124000
1	0.729545000	-1.241227000	0.683080000
17	-0.814193000	0.836001000	2.336283000
5	-2.046034000	-1.039704000	-0.073868000
17	-1.979096000	-1.348663000	-1.901729000
17	-1.545305000	-2.540565000	0.899117000
17	-3.629677000	-0.325788000	0.463906000

[CpMn(CO)₂(η²-HPPhCl·BCl₃)] **4**

6	-1.694757000	-1.867634000	-1.724309000
6	-1.115842000	-0.654020000	-2.171823000
6	-2.095853000	0.369912000	-2.071817000
6	-3.291316000	-0.219049000	-1.578042000
6	-3.048017000	-1.600996000	-1.351730000
1	-1.199797000	-2.826095000	-1.684050000
1	-0.108287000	-0.522881000	-2.530279000
1	-1.947749000	1.407012000	-2.328003000
1	-4.222159000	0.297628000	-1.398074000
1	-3.763536000	-2.322207000	-0.987815000
25	-1.753708000	-0.458774000	-0.090444000
6	-1.481848000	-1.820256000	1.084940000
8	-1.384960000	-2.707595000	1.797637000
6	-2.874376000	0.261271000	1.117499000
8	-3.611964000	0.750506000	1.840266000
15	0.424211000	0.208776000	0.449588000
1	-1.527796000	1.015878000	0.254252000

17	0.524238000	0.361677000	2.538397000
5	1.048081000	2.063380000	-0.170776000
17	0.996692000	2.089810000	-2.049098000
17	-0.198662000	3.252924000	0.516059000
17	2.742470000	2.353626000	0.462348000
6	1.688088000	-1.087328000	0.102368000
6	2.469661000	-0.992518000	-1.057300000
1	2.380799000	-0.136894000	-1.713049000
6	1.860705000	-2.185778000	0.955382000
1	1.290592000	-2.264469000	1.871142000
6	2.792403000	-3.172154000	0.648636000
6	3.397480000	-1.987103000	-1.358693000
6	3.559731000	-3.078587000	-0.510706000
1	4.003901000	-1.894645000	-2.252283000
1	2.923629000	-4.010362000	1.323271000
1	4.288034000	-3.846636000	-0.744613000

[CpMn(CO)₂(η²-HPMeCl·BCl₃)] **5**

6	2.528031000	-1.316711000	-1.386387000
6	1.281696000	-1.912498000	-1.068078000
6	1.275481000	-2.205288000	0.322251000
6	2.528983000	-1.802205000	0.858815000
6	3.305767000	-1.242218000	-0.193920000
1	2.838920000	-0.986742000	-2.366479000
1	0.476024000	-2.123327000	-1.752002000
1	0.457625000	-2.651439000	0.866165000
1	2.834356000	-1.900244000	1.889624000
1	4.309367000	-0.854784000	-0.110708000
25	1.538601000	-0.067203000	0.084950000
6	2.028300000	1.380727000	-0.901788000
8	2.380252000	2.265317000	-1.532841000
6	2.018219000	0.850736000	1.559756000
8	2.328496000	1.379525000	2.522945000
15	-0.619976000	0.610370000	-0.478304000
6	-0.892073000	0.929978000	-2.270624000
1	0.467896000	-0.060371000	1.173883000
17	-0.883655000	2.539054000	0.299468000
5	-2.210353000	-0.462961000	0.188804000
17	-2.154536000	-2.069181000	-0.782547000
17	-1.963712000	-0.756276000	2.002478000
17	-3.747565000	0.475114000	-0.176193000
1	-0.819265000	-0.016047000	-2.809994000
1	-0.157507000	1.635576000	-2.657841000
1	-1.896488000	1.334754000	-2.401339000

[CpMn(CO)₂(η²-HP(OMe)Cl·BCl₃)] **6**

6	2.536478000	-0.874440000	-1.716325000
6	1.318081000	-1.565288000	-1.497814000

6	1.400086000	-2.210283000	-0.234369000
6	2.677166000	-1.924612000	0.321770000
6	3.383586000	-1.091202000	-0.591370000
1	2.777957000	-0.286252000	-2.588981000
1	0.472039000	-1.592556000	-2.164907000
1	0.622159000	-2.803578000	0.220141000
1	3.044280000	-2.278376000	1.273272000
1	4.385800000	-0.711561000	-0.465897000
25	1.620583000	-0.077915000	0.080937000
6	1.977789000	1.587232000	-0.578410000
8	2.256825000	2.606186000	-1.005754000
6	2.219265000	0.497536000	1.680477000
8	2.603264000	0.804676000	2.710995000
15	-0.553472000	0.585089000	-0.168041000
8	-0.685712000	1.138306000	-1.691331000
1	0.646130000	-0.374469000	1.221590000
17	-0.880881000	2.294034000	1.020690000
5	-2.101209000	-0.661436000	0.296586000
17	-2.120182000	-1.944301000	-1.065267000
17	-1.676206000	-1.413250000	1.939615000
17	-3.679425000	0.277972000	0.354413000
6	-1.911931000	1.622637000	-2.295429000
1	-1.616186000	2.038165000	-3.256869000
1	-2.613131000	0.800839000	-2.434277000
1	-2.359810000	2.397947000	-1.672954000

[CpMn(CO)₂(η²-HP(NH₂)Cl·BCl₃)] 7

6	2.506134000	-1.382477000	-1.341325000
6	1.265037000	-1.959798000	-0.973975000
6	1.285976000	-2.190259000	0.427374000
6	2.550175000	-1.765725000	0.922895000
6	3.307904000	-1.257121000	-0.168135000
1	2.797885000	-1.097799000	-2.341253000
1	0.439148000	-2.172515000	-1.633163000
1	0.477387000	-2.610035000	1.004813000
1	2.874587000	-1.817848000	1.951252000
1	4.314004000	-0.869985000	-0.121295000
25	1.548552000	-0.065195000	0.086481000
6	2.015542000	1.327218000	-0.981733000
8	2.341889000	2.172625000	-1.678555000
6	2.050839000	0.927050000	1.506204000
8	2.376861000	1.503269000	2.435719000
15	-0.597295000	0.560798000	-0.498084000
7	-0.798402000	0.615664000	-2.160125000
1	0.487615000	-0.010468000	1.186174000
17	-0.868525000	2.542643000	0.227711000
5	-2.226567000	-0.444127000	0.187093000
17	-2.134538000	-2.181028000	-0.490838000
17	-2.113858000	-0.430257000	2.032214000

17	-3.715892000	0.436438000	-0.460510000
1	-0.148410000	1.150012000	-2.720526000
1	-1.756770000	0.704522000	-2.482302000

[CpMn(CO)₂(η²-HPFPh·BCl₃)] **8**

6	3.343099000	-1.846837000	-0.165904000
6	2.420197000	-2.062220000	-1.232126000
6	1.194029000	-2.504029000	-0.676316000
6	1.349848000	-2.564019000	0.735020000
6	2.675377000	-2.165573000	1.049557000
1	4.367641000	-1.523209000	-0.264927000
1	2.618981000	-1.915782000	-2.283151000
1	0.299830000	-2.752696000	-1.225547000
1	0.589769000	-2.862411000	1.439403000
1	3.101618000	-2.111819000	2.039952000
25	1.683302000	-0.515478000	0.088289000
6	2.223549000	0.689365000	-1.182422000
8	2.666549000	1.353892000	-1.993597000
6	2.374508000	0.610198000	1.330957000
8	2.826853000	1.263201000	2.147802000
15	-0.410694000	0.208320000	-0.460290000
1	0.605734000	-0.219883000	1.145967000
5	-1.031403000	2.034422000	0.132820000
17	-1.118368000	1.917499000	1.998065000
17	-2.677105000	2.341896000	-0.630116000
17	0.243651000	3.267526000	-0.403760000
6	-1.718588000	-1.027570000	-0.126849000
6	-2.487695000	-1.523418000	-1.186944000
1	-2.292500000	-1.189040000	-2.197036000
6	-2.003455000	-1.440643000	1.181543000
1	-1.443716000	-1.041245000	2.018072000
6	-3.034921000	-2.343751000	1.420384000
6	-3.513317000	-2.432995000	-0.939743000
6	-3.788307000	-2.845930000	0.360919000
1	-4.104244000	-2.808679000	-1.767151000
1	-3.255135000	-2.647042000	2.437426000
1	-4.591685000	-3.548429000	0.550690000
9	-0.492624000	0.228933000	-2.099329000

[CpMn(CO)₂(η²-HPClPh·BCl₃)] **9**

6	3.444504000	-1.701715000	-0.226328000
6	2.529760000	-1.842562000	-1.313369000
6	1.327348000	-2.395719000	-0.808970000
6	1.486287000	-2.596943000	0.588751000
6	2.794385000	-2.177707000	0.945986000
1	4.454181000	-1.325800000	-0.286736000
1	2.716726000	-1.575666000	-2.342422000
1	0.441420000	-2.615668000	-1.383268000

1	0.740665000	-2.999845000	1.255524000
1	3.220115000	-2.209555000	1.937669000
25	1.731721000	-0.476687000	0.158461000
6	2.311014000	0.898728000	-0.911105000
8	2.791196000	1.670659000	-1.595454000
6	2.312581000	0.500664000	1.568320000
8	2.693406000	1.056932000	2.487509000
15	-0.407988000	0.195062000	-0.411262000
1	0.629544000	-0.319340000	1.212085000
5	-1.118185000	1.979635000	0.296222000
17	-1.089858000	1.783799000	2.154099000
17	-2.819114000	2.208717000	-0.354828000
17	0.051794000	3.298133000	-0.256911000
6	-1.667627000	-1.111787000	-0.075294000
6	-2.504974000	-1.628399000	-1.070178000
1	-2.408611000	-1.294309000	-2.093639000
6	-1.842657000	-1.542676000	1.249043000
1	-1.232553000	-1.136882000	2.045612000
6	-2.825681000	-2.475727000	1.563037000
6	-3.481767000	-2.568762000	-0.749483000
6	-3.645108000	-2.996439000	0.564067000
1	-4.122026000	-2.957270000	-1.533055000
1	-2.954592000	-2.787415000	2.593147000
1	-4.410254000	-3.723452000	0.810706000
17	-0.493535000	0.359457000	-2.517220000

[CpMn(CO)₂(η²-HPBrPh·BCl₃)] **10**

6	3.526774000	1.619260000	0.313489000
6	2.577662000	1.685861000	1.377347000
6	1.407934000	2.315249000	0.885576000
6	1.622358000	2.640619000	-0.480999000
6	2.931077000	2.219097000	-0.831386000
1	4.523856000	1.210895000	0.372383000
1	2.720357000	1.320090000	2.382788000
1	0.507792000	2.504946000	1.448241000
1	0.911322000	3.122903000	-1.132587000
1	3.393223000	2.329681000	-1.800874000
25	1.800150000	0.482745000	-0.241261000
6	2.304905000	-1.006105000	0.706529000
8	2.746146000	-1.856989000	1.320149000
6	2.413584000	-0.369192000	-1.716542000
8	2.817774000	-0.843709000	-2.671142000
15	-0.389009000	-0.171310000	0.180211000
1	0.731236000	0.435240000	-1.339822000
5	-1.111898000	-1.869209000	-0.724061000
17	-0.981252000	-1.504246000	-2.552217000
17	-2.850321000	-2.105587000	-0.187311000
17	-0.005967000	-3.267349000	-0.241788000
6	-1.589105000	1.204105000	-0.119115000

6	-2.478299000	1.666025000	0.857047000
1	-2.459119000	1.246565000	1.853088000
6	-1.662340000	1.749793000	-1.411084000
1	-1.012554000	1.391370000	-2.198669000
6	-2.593752000	2.739611000	-1.708165000
6	-3.403534000	2.663028000	0.554840000
6	-3.463996000	3.204515000	-0.724897000
1	-4.083559000	3.006997000	1.325637000
1	-2.642291000	3.139577000	-2.714473000
1	-4.188090000	3.976552000	-0.958329000
35	-0.595545000	-0.551751000	2.428164000

[CpMn(CO)₂(η²-HPPPh₂·BCl₃)] **11**

6	3.556320000	0.202066000	-1.623519000
6	2.319126000	0.506627000	-2.273217000
6	1.581223000	-0.697268000	-2.387680000
6	2.346289000	-1.743940000	-1.807223000
6	3.569227000	-1.188773000	-1.347724000
1	4.347733000	0.900708000	-1.399532000
1	2.005132000	1.478626000	-2.621565000
1	0.605506000	-0.812413000	-2.830700000
1	2.059682000	-2.781474000	-1.746174000
1	4.366168000	-1.730019000	-0.860150000
25	1.935703000	-0.233858000	-0.283660000
6	2.012210000	1.461839000	0.388215000
8	2.167302000	2.537357000	0.734882000
6	2.697545000	-0.797371000	1.252369000
8	3.220097000	-1.209818000	2.179121000
15	-0.398153000	-0.002024000	0.098772000
1	1.158586000	-1.366629000	0.388536000
5	-0.936563000	-0.190905000	2.060943000
17	-0.576357000	-1.961257000	2.516890000
17	-2.738240000	0.199406000	2.224226000
17	0.114135000	0.963518000	3.089060000
6	-1.429334000	-1.241188000	-0.802633000
6	-2.714350000	-0.895484000	-1.244387000
1	-3.078593000	0.114983000	-1.118881000
6	-1.011980000	-2.571660000	-0.935383000
1	-0.046476000	-2.878145000	-0.556054000
6	-1.842554000	-3.524099000	-1.518627000
6	-3.542080000	-1.849607000	-1.830004000
6	-3.107935000	-3.164259000	-1.974950000
1	-4.533471000	-1.562925000	-2.161714000
1	-1.503075000	-4.550008000	-1.605133000
1	-3.755456000	-3.906140000	-2.428244000
6	-0.954410000	1.620302000	-0.597211000
6	-1.070674000	1.797641000	-1.984514000
6	-1.203793000	2.711664000	0.243586000
1	-0.907862000	0.964138000	-2.656822000

1	-1.124375000	2.605090000	1.316410000
6	-1.430498000	3.031771000	-2.516298000
6	-1.562317000	3.947013000	-0.293764000
1	-1.525826000	3.146873000	-3.590313000
1	-1.757181000	4.778623000	0.373492000
6	-1.675669000	4.112550000	-1.670304000
1	-1.957360000	5.074448000	-2.083353000

[CpMn(CO)₂(η²-HPMePh·BCl₃)] **12**

6	3.384223000	-1.784527000	-0.153405000
6	2.471423000	-2.017034000	-1.226292000
6	1.251926000	-2.481247000	-0.675457000
6	1.397095000	-2.534875000	0.736694000
6	2.715752000	-2.115243000	1.056980000
1	4.403653000	-1.443324000	-0.245562000
1	2.679596000	-1.874497000	-2.275993000
1	0.362123000	-2.746445000	-1.223748000
1	0.637290000	-2.845130000	1.436184000
1	3.135720000	-2.052972000	2.049601000
25	1.703998000	-0.480011000	0.092647000
6	2.300280000	0.771145000	-1.090776000
8	2.778171000	1.480893000	-1.846758000
6	2.288527000	0.608011000	1.408046000
8	2.678793000	1.237004000	2.276603000
15	-0.451174000	0.222901000	-0.583920000
1	0.632388000	-0.197092000	1.141584000
5	-1.097556000	1.993486000	0.154338000
17	-1.060570000	1.924629000	2.017321000
17	-2.815399000	2.268451000	-0.487776000
17	0.088455000	3.288394000	-0.478152000
6	-1.701866000	-1.074708000	-0.191172000
6	-2.398291000	-1.754341000	-1.198568000
1	-2.214438000	-1.534435000	-2.242027000
6	-1.996182000	-1.375590000	1.146913000
1	-1.495035000	-0.844408000	1.945955000
6	-2.955805000	-2.331866000	1.463742000
6	-3.354701000	-2.716438000	-0.877459000
6	-3.635409000	-3.009450000	0.453178000
1	-3.885441000	-3.228256000	-1.672292000
1	-3.179285000	-2.539341000	2.504059000
1	-4.383587000	-3.753172000	0.702241000
6	-0.540101000	0.394976000	-2.420247000
1	-0.211415000	-0.513881000	-2.926119000
1	-1.561729000	0.640581000	-2.713178000
1	0.106418000	1.220594000	-2.715269000

[CpMn(CO)₂(η²-HP(OMe)Ph·BCl₃)] **13**

6	3.455019000	-1.686473000	-0.323931000
6	2.557434000	-1.731798000	-1.431550000
6	1.342143000	-2.313760000	-0.993548000
6	1.479229000	-2.632211000	0.385027000
6	2.782903000	-2.253024000	0.795479000
1	4.467178000	-1.312810000	-0.337908000
1	2.764089000	-1.384253000	-2.432345000
1	0.464924000	-2.474492000	-1.599380000
1	0.719922000	-3.080090000	1.005799000
1	3.192678000	-2.368175000	1.787697000
25	1.739668000	-0.483025000	0.133131000
6	2.290126000	0.963119000	-0.823308000
8	2.773400000	1.793499000	-1.441873000
6	2.323018000	0.380897000	1.608651000
8	2.703758000	0.869694000	2.567114000
15	-0.421146000	0.184457000	-0.422736000
1	0.631572000	-0.360253000	1.184837000
5	-1.138308000	1.884555000	0.418515000
17	-1.146511000	1.593536000	2.258565000
17	-2.846740000	2.159239000	-0.244438000
17	0.009883000	3.284920000	-0.014903000
6	-1.637699000	-1.158679000	-0.103297000
6	-2.446762000	-1.632194000	-1.142718000
1	-2.329622000	-1.222780000	-2.136410000
6	-1.809101000	-1.682501000	1.185418000
1	-1.213812000	-1.314699000	2.011496000
6	-2.768111000	-2.662138000	1.424738000
6	-3.398831000	-2.619760000	-0.898609000
6	-3.562366000	-3.137359000	0.382802000
1	-4.018772000	-2.976522000	-1.713331000
1	-2.898692000	-3.047855000	2.429385000
1	-4.307991000	-3.901206000	0.571971000
8	-0.538917000	0.227117000	-2.070682000
6	-0.489872000	1.412960000	-2.888535000
1	0.497994000	1.874354000	-2.856247000
1	-0.700691000	1.074118000	-3.902737000
1	-1.243187000	2.134904000	-2.575624000

[CpMn(CO)₂(η²-HP(NH₂)Ph·BCl₃)] **14**

6	3.365376000	-1.815237000	-0.068563000
6	2.503977000	-2.012659000	-1.188508000
6	1.248862000	-2.461883000	-0.709610000
6	1.322298000	-2.543463000	0.706614000
6	2.629777000	-2.152168000	1.101652000
1	4.393759000	-1.490518000	-0.103665000
1	2.761884000	-1.852847000	-2.224580000
1	0.385190000	-2.688144000	-1.313132000

1	0.521606000	-2.846662000	1.362538000
1	2.999119000	-2.113057000	2.115328000
25	1.695650000	-0.486957000	0.116229000
6	2.293621000	0.743883000	-1.082038000
8	2.763348000	1.431600000	-1.864552000
6	2.297847000	0.605219000	1.423126000
8	2.695590000	1.238792000	2.284396000
15	-0.434487000	0.215364000	-0.553564000
1	0.619198000	-0.203725000	1.162908000
5	-1.073944000	2.004190000	0.121429000
17	-1.054319000	2.028700000	1.982555000
17	-2.786028000	2.243801000	-0.566556000
17	0.112788000	3.267863000	-0.572301000
6	-1.699120000	-1.064323000	-0.163981000
6	-2.264783000	-1.846464000	-1.178106000
1	-1.941810000	-1.710289000	-2.202462000
6	-2.127527000	-1.251728000	1.157557000
1	-1.723101000	-0.641298000	1.954863000
6	-3.099803000	-2.202528000	1.452998000
6	-3.238393000	-2.797046000	-0.876155000
6	-3.657313000	-2.978905000	0.438494000
1	-3.670991000	-3.391401000	-1.673142000
1	-3.429379000	-2.328023000	2.478082000
1	-4.417503000	-3.715688000	0.671773000
7	-0.512634000	0.229620000	-2.277683000
1	0.231570000	0.785997000	-2.683681000
1	-1.397245000	0.625308000	-2.592960000

[CpMn(CO)₂(η²-HPFH·BCl₃)] **15**

6	2.283575000	-0.934637000	-1.643697000
6	1.003633000	-1.493261000	-1.389444000
6	1.031694000	-2.084709000	-0.096754000
6	2.331170000	-1.898360000	0.441869000
6	3.111117000	-1.180148000	-0.511462000
1	2.576927000	-0.417834000	-2.545208000
1	0.157483000	-1.484176000	-2.058562000
1	0.200424000	-2.576189000	0.383951000
1	2.669767000	-2.242743000	1.407425000
1	4.147202000	-0.897807000	-0.406226000
25	1.463353000	0.036733000	0.105985000
6	1.983168000	1.635809000	-0.577568000
8	2.353551000	2.621287000	-1.019088000
6	2.111968000	0.593299000	1.695701000
8	2.514397000	0.900858000	2.718957000
15	-0.609795000	0.883508000	-0.234975000
9	-0.712795000	1.440592000	-1.765037000
1	0.368871000	-0.028492000	1.187458000
1	-0.757623000	2.095880000	0.470008000
5	-2.319458000	-0.091513000	0.166108000

17	-2.430177000	-1.663793000	-0.810804000
17	-2.168767000	-0.415727000	2.002238000
17	-3.687470000	1.071728000	-0.227896000

[CpMn(CO)₂(η²-HPClH·BCl₃)] **16**

6	-2.290869000	0.542286000	1.788132000
6	-1.056799000	-0.113358000	2.030682000
6	-1.171512000	-1.454647000	1.575632000
6	-2.485075000	-1.631828000	1.066450000
6	-3.182375000	-0.395522000	1.188782000
1	-2.514201000	1.571423000	2.025812000
1	-0.178377000	0.324619000	2.478460000
1	-0.389167000	-2.196798000	1.609910000
1	-2.884777000	-2.546530000	0.654982000
1	-4.207209000	-0.211040000	0.905868000
25	-1.511339000	-0.123507000	-0.113382000
6	-2.033688000	1.446899000	-0.870535000
8	-2.406315000	2.421456000	-1.332066000
6	-2.119024000	-0.945669000	-1.598190000
8	-2.497623000	-1.513994000	-2.513496000
15	0.610794000	0.668483000	-0.475685000
17	0.874374000	2.581041000	0.364564000
1	-0.439677000	-1.003529000	-0.774227000
1	0.770157000	1.006665000	-1.835912000
5	2.283588000	-0.421482000	-0.084776000
17	2.387741000	-0.784333000	1.727201000
17	1.980357000	-1.965481000	-1.095350000
17	3.717200000	0.537853000	-0.701852000

[CpMn(CO)₂(η²-HPBrH·BCl₃)] **17**

6	-2.300707000	0.770257000	1.700562000
6	-1.154298000	-0.000417000	2.021742000
6	-1.439978000	-1.361698000	1.730942000
6	-2.772669000	-1.433274000	1.245915000
6	-3.309626000	-0.114448000	1.217085000
1	-2.391354000	1.840251000	1.811226000
1	-0.220777000	0.375315000	2.410427000
1	-0.755293000	-2.186026000	1.855685000
1	-3.288267000	-2.333577000	0.946903000
1	-4.307418000	0.160840000	0.912137000
25	-1.635196000	-0.208768000	-0.105480000
6	-1.994392000	1.298896000	-1.059545000
8	-2.267596000	2.239284000	-1.645113000
6	-2.336633000	-1.145568000	-1.476632000
8	-2.779768000	-1.783687000	-2.313749000
15	0.563959000	0.291736000	-0.559216000
35	1.119966000	2.399155000	0.097496000
1	-0.666341000	-1.272207000	-0.644419000

1	0.737315000	0.450304000	-1.950766000
5	2.098209000	-0.955882000	-0.056579000
17	2.180644000	-1.136984000	1.783450000
17	1.587477000	-2.547553000	-0.895758000
17	3.634911000	-0.263112000	-0.773276000

[CpMn(CO)₂(η²-HPPPhH·BCl₃)] **18**

6	1.654427000	-1.757306000	1.713157000
6	1.131294000	-0.484454000	2.053921000
6	2.141247000	0.487804000	1.827187000
6	3.300661000	-0.190543000	1.364662000
6	3.003750000	-1.579729000	1.283064000
1	1.125017000	-2.695730000	1.778745000
1	0.139291000	-0.278349000	2.420419000
1	2.034461000	1.550104000	1.980808000
1	4.243510000	0.271050000	1.112136000
1	3.683914000	-2.359306000	0.976667000
25	1.721327000	-0.519757000	-0.056531000
6	1.276991000	-1.938444000	-1.091553000
8	1.046295000	-2.858336000	-1.731706000
6	2.853077000	-0.015476000	-1.354381000
8	3.597207000	0.341793000	-2.146610000
15	-0.440990000	0.223184000	-0.605610000
1	1.525786000	0.912944000	-0.556813000
1	-0.522650000	0.247769000	-2.012722000
5	-0.990067000	2.113117000	-0.123538000
17	-0.991817000	2.328305000	1.736151000
17	0.305526000	3.200870000	-0.912285000
17	-2.662496000	2.397713000	-0.844401000
6	-1.768410000	-0.991425000	-0.232974000
6	-2.425418000	-0.981413000	1.004115000
1	-2.184661000	-0.229296000	1.744925000
6	-2.144925000	-1.934882000	-1.197790000
1	-1.662181000	-1.946996000	-2.167974000
6	-3.150875000	-2.857652000	-0.925639000
6	-3.430883000	-1.906862000	1.270935000
6	-3.792818000	-2.848614000	0.310580000
1	-3.941455000	-1.880310000	2.226779000
1	-3.437047000	-3.577520000	-1.683860000
1	-4.579327000	-3.564559000	0.519913000

[CpMn(CO)₂(η²-HPMeH·BCl₃)] **19**

6	2.310666000	-0.316710000	-1.855592000
6	1.046310000	-0.956882000	-1.803225000
6	1.087986000	-1.934909000	-0.773902000
6	2.388095000	-1.909848000	-0.201658000
6	3.147987000	-0.902374000	-0.861475000
1	2.594313000	0.468820000	-2.539893000

1	0.192379000	-0.750634000	-2.428579000
1	0.268321000	-2.572263000	-0.480570000
1	2.737011000	-2.543347000	0.599898000
1	4.177984000	-0.648466000	-0.664695000
25	1.481472000	0.007460000	0.118745000
6	2.013312000	1.734798000	0.057900000
8	2.379407000	2.818353000	0.003553000
6	2.043509000	-0.042276000	1.823875000
8	2.396407000	-0.125707000	2.908586000
15	-0.644478000	0.984839000	0.054486000
1	0.404933000	-0.457353000	1.098574000
1	-0.768299000	1.822599000	1.183093000
5	-2.285222000	-0.179181000	0.160451000
17	-2.455871000	-1.105995000	-1.455299000
17	-2.044810000	-1.344057000	1.593928000
17	-3.722712000	0.958252000	0.437698000
6	-0.888795000	2.189081000	-1.326076000
1	-0.115631000	2.957496000	-1.322614000
1	-0.869979000	1.658265000	-2.278181000
1	-1.867812000	2.655862000	-1.208931000

[CpMn(CO)₂(η²-HP(OMe)H·BCl₃)] **20**

6	-2.318862000	0.426122000	1.848851000
6	-1.083652000	-0.252462000	2.009913000
6	-1.210160000	-1.541776000	1.426327000
6	-2.529750000	-1.663198000	0.915863000
6	-3.220524000	-0.442368000	1.169686000
1	-2.533753000	1.429099000	2.185373000
1	-0.197716000	0.140691000	2.482283000
1	-0.430378000	-2.285382000	1.372213000
1	-2.937199000	-2.530815000	0.419154000
1	-4.246643000	-0.225268000	0.916337000
25	-1.558701000	-0.055959000	-0.120044000
6	-1.951145000	1.634559000	-0.652868000
8	-2.242532000	2.691515000	-0.973477000
6	-2.259462000	-0.632832000	-1.672295000
8	-2.700631000	-1.049053000	-2.641651000
15	0.589167000	0.679478000	-0.429227000
8	0.707149000	2.074692000	0.434265000
1	-0.575622000	-0.923458000	-0.911170000
1	0.762059000	1.098611000	-1.773358000
5	2.170960000	-0.532645000	-0.128549000
17	2.412226000	-0.765949000	1.703146000
17	1.761825000	-2.134939000	-0.991385000
17	3.648378000	0.276426000	-0.910884000
6	1.882312000	2.912711000	0.436221000
1	2.189034000	3.154608000	-0.584692000
1	1.594717000	3.823013000	0.960620000
1	2.705000000	2.423026000	0.957296000

[CpMn(CO)₂(η²-HP(NH₂)H·BCl₃)] **21**

6	2.290144000	-0.544436000	-1.801889000
6	1.039572000	-1.194117000	-1.642058000
6	1.122040000	-2.031117000	-0.497449000
6	2.429983000	-1.905575000	0.043817000
6	3.157316000	-0.979804000	-0.756521000
1	2.542346000	0.152386000	-2.586911000
1	0.168960000	-1.060265000	-2.264018000
1	0.321569000	-2.641632000	-0.110060000
1	2.804518000	-2.420272000	0.915871000
1	4.184481000	-0.682238000	-0.612988000
25	1.483987000	0.022565000	0.117782000
6	1.976126000	1.730544000	-0.192789000
8	2.306423000	2.804922000	-0.418254000
6	2.056277000	0.219439000	1.812203000
8	2.416534000	0.293846000	2.894447000
15	-0.627344000	0.944065000	-0.098805000
1	0.393584000	-0.319959000	1.135655000
1	-0.767528000	1.933781000	0.907478000
5	-2.288546000	-0.149644000	0.170847000
17	-2.394016000	-1.523652000	-1.076192000
17	-2.170530000	-0.799948000	1.910336000
17	-3.706625000	1.043616000	-0.027503000
7	-0.796534000	1.696554000	-1.617795000
1	-0.166399000	2.457603000	-1.834091000
1	-1.755071000	1.927827000	-1.857425000

Cartesian Coordinates for complexes 1a-21a as determined by DFT calculations at the [B3LYP/6-311G(d,p)] level of approximation.

HPFCl·BCl₃ 1a

15	0.950652000	0.537673000	-0.432524000
9	1.329490000	1.957042000	0.164775000
1	1.131386000	0.751209000	-1.811508000
17	2.536008000	-0.623605000	0.049599000
5	-0.894359000	-0.152160000	0.063967000
17	-1.953843000	1.228139000	-0.527921000
17	-0.984063000	-1.657224000	-0.991787000
17	-0.944266000	-0.457244000	1.852259000

HPCl₂·BCl₃ 2a

15	0.904454000	0.000107000	-0.485172000
17	2.002287000	1.631813000	0.062991000
1	1.068579000	-0.000028000	-1.883671000
17	2.002316000	-1.631413000	0.063366000
5	-1.103136000	0.000005000	0.071121000
17	-1.679533000	1.536315000	-0.743750000
17	-1.678682000	-1.536085000	-0.745156000
17	-1.182843000	-0.000724000	1.880528000

HPBrCl·BCl₃ 3a

15	-0.432065000	0.485861000	-0.499494000
35	-2.240169000	-0.677483000	0.028178000
1	-0.548968000	0.579686000	-1.900775000
17	-0.788093000	2.419703000	0.067011000
5	1.421037000	-0.307377000	0.072526000
17	1.373875000	-1.929989000	-0.773904000
17	2.556533000	0.903337000	-0.701425000
17	1.465370000	-0.370628000	1.881515000

HPPhCl·BCl₃ 4a

15	0.148024000	0.750329000	-0.439171000
1	0.170636000	1.115202000	-1.796625000
17	0.352614000	2.581556000	0.490757000
5	1.673858000	-0.538458000	-0.049945000
17	1.181224000	-1.978215000	-1.104452000
17	1.693654000	-0.908932000	1.749311000
17	3.187650000	0.309966000	-0.644262000
6	-1.552747000	0.207407000	-0.181915000
6	-2.522207000	0.498060000	-1.151501000
6	-1.898006000	-0.512132000	0.970151000
1	-2.258495000	1.052836000	-2.044729000

1	-1.148486000	-0.747909000	1.715059000
6	-3.832026000	0.070151000	-0.966238000
6	-3.211477000	-0.932879000	1.144718000
1	-4.581340000	0.291447000	-1.716798000
1	-3.480046000	-1.492653000	2.032497000
6	-4.175593000	-0.643650000	0.180364000
1	-5.196998000	-0.977689000	0.321394000

HPMeCl·BCl₃ **5a**

15	0.979063000	0.430875000	-0.503664000
1	1.098088000	0.493622000	-1.904047000
17	2.497179000	-0.852192000	0.007336000
5	-0.877441000	-0.140643000	0.053054000
17	-1.867317000	1.194056000	-0.787861000
17	-1.173228000	-1.806146000	-0.638849000
17	-0.942292000	-0.051988000	1.884635000
6	1.509423000	2.062031000	0.101598000
1	2.498693000	2.308478000	-0.283485000
1	1.524786000	2.041659000	1.191759000
1	0.779333000	2.800743000	-0.233565000

HP(OMe)Cl·BCl₃ **6a**

15	0.855490000	-0.126853000	-0.704479000
1	0.876570000	-0.441952000	-2.071689000
17	1.964795000	-1.647731000	0.115760000
5	-1.004689000	-0.006217000	0.077236000
17	-1.694665000	1.474845000	-0.787507000
17	-1.794277000	-1.582433000	-0.436007000
17	-0.848879000	0.202926000	1.893906000
8	1.766534000	1.182141000	-0.715590000
6	1.929850000	2.072030000	0.426529000
1	2.604992000	2.850665000	0.082085000
1	0.967226000	2.495944000	0.708518000
1	2.372382000	1.530599000	1.263042000

HP(NH₂)Cl·BCl₃ **7a**

15	-0.975548000	-0.516800000	-0.517316000
1	-1.197772000	-0.612149000	-1.900026000
17	-2.546913000	0.726741000	0.020391000
5	0.864012000	0.162748000	0.038979000
17	1.984955000	-0.837343000	-1.030703000
17	0.917989000	1.952251000	-0.310769000
17	0.990117000	-0.263099000	1.833112000
7	-1.217983000	-2.053388000	0.018088000
1	-1.992904000	-2.618178000	-0.298577000
1	-0.854803000	-2.293044000	0.932295000

HPFPh·BCl₃ **8a**

15	-0.153936000	0.992068000	-0.124485000
1	-0.181438000	2.019491000	0.833540000
5	-1.699495000	-0.249571000	0.142435000
17	-1.314027000	-0.920837000	1.830474000
17	-1.702501000	-1.530701000	-1.178984000
17	-3.192688000	0.825207000	0.119422000
6	1.528295000	0.373034000	-0.045828000
6	1.858794000	-0.867600000	-0.610907000
1	1.096815000	-1.474809000	-1.082783000
6	2.516087000	1.148813000	0.579655000
1	2.264773000	2.105410000	1.023782000
6	3.825518000	0.685990000	0.635406000
6	3.172242000	-1.318656000	-0.550986000
6	4.152101000	-0.545354000	0.069595000
1	3.429144000	-2.277778000	-0.984083000
1	4.587779000	1.283074000	1.121319000
1	5.173513000	-0.905093000	0.116146000
9	-0.258402000	1.822979000	-1.493325000

HPClPh·BCl₃ **9a**

15	0.148024000	0.750329000	-0.439171000
1	0.170636000	1.115202000	-1.796625000
17	0.352614000	2.581556000	0.490757000
5	1.673858000	-0.538458000	-0.049945000
17	1.181224000	-1.978215000	-1.104452000
17	1.693654000	-0.908932000	1.749311000
17	3.187650000	0.309966000	-0.644262000
6	-1.552747000	0.207407000	-0.181915000
6	-2.522207000	0.498060000	-1.151501000
6	-1.898006000	-0.512132000	0.970151000
1	-2.258495000	1.052836000	-2.044729000
1	-1.148486000	-0.747909000	1.715059000
6	-3.832026000	0.070151000	-0.966238000
6	-3.211477000	-0.932879000	1.144718000
1	-4.581340000	0.291447000	-1.716798000
1	-3.480046000	-1.492653000	2.032497000
6	-4.175593000	-0.643650000	0.180364000
1	-5.196998000	-0.977689000	0.321394000

HPBrPh·BCl₃ **10a**

15	0.123958000	0.331257000	-0.561741000
1	0.153925000	0.491120000	-1.958995000
5	1.563772000	-1.006655000	-0.003950000
17	0.958892000	-2.526980000	-0.869683000
17	1.566836000	-1.148757000	1.826552000
17	3.131702000	-0.355527000	-0.696537000

6	-1.606185000	-0.069548000	-0.231880000
6	-1.993630000	-0.530555000	1.033771000
1	-1.261575000	-0.648478000	1.822776000
6	-2.554783000	0.069056000	-1.254047000
1	-2.259290000	0.423882000	-2.234781000
6	-3.884936000	-0.254077000	-1.008826000
6	-3.326788000	-0.847462000	1.267452000
6	-4.270220000	-0.710204000	0.250231000
1	-3.627464000	-1.207392000	2.244058000
1	-4.617745000	-0.151169000	-1.800196000
1	-5.307540000	-0.961661000	0.438590000
35	0.482412000	2.420182000	0.147673000

HPhPh₂·BCl₃ 11a

15	0.003498000	0.105875000	-0.676148000
1	-0.089165000	0.174702000	-2.079316000
5	-0.130014000	1.990586000	0.041066000
17	-1.753627000	2.609289000	-0.594425000
17	1.302401000	2.922365000	-0.673267000
17	-0.081096000	1.895219000	1.890825000
6	1.546110000	-0.812729000	-0.351623000
6	1.735648000	-2.058210000	-0.967358000
6	2.532951000	-0.295624000	0.493817000
1	0.971752000	-2.469586000	-1.617971000
1	2.399017000	0.665683000	0.971251000
6	2.903980000	-2.775687000	-0.740029000
6	3.699059000	-1.024755000	0.719809000
1	3.047912000	-3.736118000	-1.221075000
1	4.461130000	-0.620923000	1.375761000
6	3.886150000	-2.259177000	0.105126000
1	4.796477000	-2.820484000	0.282147000
6	-1.390033000	-0.974344000	-0.230650000
6	-1.416892000	-1.600767000	1.021188000
6	-2.461728000	-1.136072000	-1.115891000
1	-0.593792000	-1.473840000	1.714182000
1	-2.454584000	-0.643344000	-2.081230000
6	-2.508083000	-2.386177000	1.377596000
6	-3.548963000	-1.925412000	-0.751865000
1	-2.527490000	-2.867812000	2.348127000
1	-4.376792000	-2.048954000	-1.440157000
6	-3.572594000	-2.550086000	0.492762000
1	-4.421024000	-3.162962000	0.774612000

HPhMePh·BCl₃ 12a

15	0.185557000	0.839447000	-0.633230000
1	0.222883000	0.859851000	-2.039479000
5	1.644679000	-0.357206000	0.054133000
17	1.286055000	-2.051359000	-0.575619000

17	1.595707000	-0.243157000	1.907720000
17	3.206905000	0.356986000	-0.652481000
6	-1.524281000	0.344859000	-0.272978000
6	-1.982023000	0.298152000	1.050632000
1	-1.319403000	0.548205000	1.870316000
6	-2.382211000	-0.015123000	-1.319102000
1	-2.034291000	0.005701000	-2.345588000
6	-3.688315000	-0.409807000	-1.043538000
6	-3.289196000	-0.095982000	1.316465000
6	-4.142488000	-0.448531000	0.272312000
1	-3.638295000	-0.134603000	2.341565000
1	-4.347583000	-0.689175000	-1.856905000
1	-5.159155000	-0.758079000	0.485188000
6	0.406049000	2.581844000	-0.125431000
1	0.356684000	2.641183000	0.962444000
1	1.391217000	2.919106000	-0.449399000
1	-0.371341000	3.207675000	-0.564043000

HP(OMe)Ph·BCl₃ **13a**

15	0.145989000	0.648510000	-0.624354000
1	0.198187000	0.625050000	-2.036735000
5	1.498988000	-0.648889000	0.067176000
17	0.872081000	-2.294164000	-0.495566000
17	1.567737000	-0.480185000	1.910571000
17	3.105490000	-0.199465000	-0.753376000
6	-1.583708000	0.300270000	-0.264054000
6	-2.035012000	0.282406000	1.062152000
1	-1.349876000	0.485664000	1.875759000
6	-2.469075000	0.022893000	-1.312024000
1	-2.124494000	0.032928000	-2.339769000
6	-3.800336000	-0.271053000	-1.033619000
6	-3.368134000	-0.006896000	1.329602000
6	-4.248973000	-0.284259000	0.284980000
1	-3.717889000	-0.021795000	2.355013000
1	-4.484668000	-0.487562000	-1.845298000
1	-5.286392000	-0.513388000	0.499955000
8	0.319735000	2.188388000	-0.164730000
6	1.598489000	2.850222000	0.005616000
1	2.189663000	2.346861000	0.769794000
1	2.148596000	2.873057000	-0.936289000
1	1.354487000	3.862236000	0.321215000

HP(NH₂)Ph·BCl₃ **14a**

15	-0.192566000	-0.501841000	-0.935856000
1	-0.252048000	0.121910000	-2.204376000
5	-1.634489000	0.273659000	0.217021000
17	-1.423495000	2.104345000	0.068518000
17	-1.398203000	-0.351467000	1.934149000

17	-3.225681000	-0.326814000	-0.547601000
6	1.520655000	-0.220182000	-0.436068000
6	2.091269000	-1.001405000	0.576918000
1	1.519902000	-1.802152000	1.029730000
6	2.252515000	0.822682000	-1.016123000
1	1.812844000	1.434154000	-1.796080000
6	3.551080000	1.078621000	-0.586734000
6	3.392107000	-0.741504000	0.995127000
6	4.120450000	0.296604000	0.416040000
1	3.834597000	-1.345791000	1.778233000
1	4.116855000	1.886137000	-1.036020000
1	5.132766000	0.496945000	0.747755000
7	-0.390324000	-2.155757000	-1.049885000
1	0.206101000	-2.696323000	-1.659810000
1	-1.340818000	-2.497252000	-0.988584000

HPFH·BCl₃ 15a

15	1.414793000	0.587414000	-0.000176000
9	2.640357000	-0.434024000	0.000031000
1	1.692179000	1.406870000	-1.107840000
1	1.691812000	1.406944000	1.107536000
5	-0.455007000	-0.095564000	0.000009000
17	-1.207664000	1.622906000	-0.002006000
17	-0.751692000	-1.026235000	-1.540398000
17	-0.752060000	-1.022611000	1.542558000

HPClH·BCl₃ 16a

15	0.995289000	0.885118000	-0.000380000
17	2.777509000	-0.125983000	0.000070000
1	1.121793000	1.754975000	-1.098572000
1	1.121627000	1.755744000	1.097226000
5	-0.770694000	-0.129497000	0.000005000
17	-1.858351000	1.379697000	-0.000575000
17	-0.851307000	-1.102277000	-1.539083000
17	-0.851338000	-1.100849000	1.540001000

HPBrH·BCl₃ 17a

15	0.450863000	0.948447000	-0.001246000
35	2.430013000	-0.053419000	-0.000092000
1	0.531115000	1.827630000	-1.097671000
1	0.531014000	1.829763000	1.093454000
5	-1.284714000	-0.137005000	-0.000022000
17	-2.436656000	1.321887000	-0.000301000
17	-1.325285000	-1.113041000	-1.538271000
17	-1.323468000	-1.110575000	1.540116000

HPhH·BCl₃ 18a

15	0.194746000	-0.305987000	-1.146426000
6	-1.519548000	-0.134137000	-0.582967000
6	-2.069640000	1.140776000	-0.398863000
1	-1.488620000	2.028251000	-0.620676000
6	-2.270829000	-1.273713000	-0.272598000
1	-1.848899000	-2.263663000	-0.402587000
6	-3.568301000	-1.135654000	0.211356000
6	-3.368138000	1.267801000	0.083101000
6	-4.117042000	0.132389000	0.387269000
1	-3.792771000	2.254613000	0.223921000
1	-4.148119000	-2.019139000	0.450660000
1	-5.127854000	0.236477000	0.764099000
1	0.318311000	0.517436000	-2.281522000
1	0.264749000	-1.600764000	-1.691079000
5	1.700457000	0.025508000	0.156830000
17	3.223637000	-0.299065000	-0.841425000
17	1.543511000	1.788813000	0.684994000
17	1.461129000	-1.176554000	1.533232000

HPMeH·BCl₃ 19a

15	1.257885000	0.956852000	-0.000766000
1	1.365829000	1.830092000	-1.098928000
1	1.365857000	1.831494000	1.096277000
5	-0.467798000	-0.070780000	0.000046000
17	-1.800690000	1.203104000	-0.001086000
17	-0.429491000	-1.092274000	-1.542420000
17	-0.429527000	-1.089552000	1.544320000
6	2.785395000	-0.043414000	-0.000055000
1	3.669489000	0.594421000	-0.000641000
1	2.786126000	-0.677267000	0.887309000
1	2.786075000	-0.678873000	-0.886258000

HP(OMe)H·BCl₃ 20a

15	0.015043883	0.676151925	-0.402566880
1	0.021354883	0.980599925	-1.782332880
5	1.718473000	-0.484767000	0.006047000
17	1.351492000	-1.953096000	-1.072573000
17	1.663268000	-0.879461000	1.806795000
17	3.251743000	0.404136000	-0.500387000
1	-1.298693883	0.192636075	-0.210613120
8	0.183172883	2.078889925	0.379370120
6	-0.688480117	3.202066925	0.149487120
1	-0.339671117	3.992286925	0.810454120
1	-0.616671117	3.535030925	-0.890084880
1	-1.722902117	2.945240925	0.388965120

HP(NH₂)H·BCl₃ **21a**

15	-1.270383000	0.911629000	-0.011454000
1	-1.395592000	1.787721000	1.081907000
1	-1.400058000	1.759458000	-1.126251000
5	0.453358000	-0.073936000	0.000540000
17	1.748158000	1.240563000	-0.010263000
17	0.429482000	-1.081815000	1.555533000
17	0.436180000	-1.114384000	-1.532464000
7	-2.731679000	0.059749000	-0.000368000
1	-2.856522000	-0.514743000	0.827075000
1	-2.872065000	-0.509621000	-0.828735000

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