

Supplementary Material (ESI) for Dalton Transactions  
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**Complexes of a Gallium Heterocycle with Transition Metal Dicyclopentadienyl and  
Cyclopentadienylcarbonyl Fragments, and with a Dialkylmanganese Compound**

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**Supporting information**

Cartesian coordinate files and MO compositions for **6'-8'**

Cartesian coordinate files for **9-11**

**Cartesian coordinate file for [CpV(CO)<sub>3</sub>[Ga{[N(Ph)C(H)]<sub>2</sub>}]<sup>-</sup> (6')**

V	23.913332000	1.655566000	19.048949000
Ga	24.979960000	3.975786000	19.038868000
O	25.307211000	1.847820000	16.257416000
O	21.643616000	0.766814000	17.107576000
O	21.646625000	3.711767000	19.731457000
N	25.601640000	5.487579000	17.907183000
N	25.766242000	5.053864000	20.501882000
C	26.305752000	6.427820000	18.671104000
C	26.398578000	6.202226000	20.019322000
C	25.816292000	5.499004000	16.517181000
C	24.743099000	5.375951000	15.613606000
C	24.958394000	5.414193000	14.234670000
C	26.247418000	5.568316000	13.713461000
C	27.327600000	5.677899000	14.598708000
C	27.116381000	5.650260000	15.978420000
C	26.024403000	4.685120000	21.836512000
C	27.333999000	4.347439000	22.261496000
C	27.583497000	3.963798000	23.579554000
C	26.542352000	3.922050000	24.519019000
C	25.247156000	4.267277000	24.115750000
C	24.989851000	4.643601000	22.791880000
C	25.143102000	1.199377000	21.043703000
C	23.813677000	0.723002000	21.244979000
C	23.569113000	-0.310288000	20.296814000
C	24.747537000	-0.481175000	19.510137000
C	25.718396000	0.456128000	19.970510000
C	24.790506000	1.851198000	17.316098000
C	22.500169000	1.112918000	17.841636000
C	22.541566000	2.988965000	19.451156000
H	26.674350000	7.334331000	18.190439000
H	26.840013000	6.913367000	20.720494000
H	23.733899000	5.279269000	16.009814000
H	24.105835000	5.337029000	13.559185000
H	26.412074000	5.595755000	12.635051000
H	28.346655000	5.767328000	14.215366000
H	27.959488000	5.709802000	16.668049000
H	28.137239000	4.362138000	21.522179000
H	28.595444000	3.676870000	23.874782000
H	26.741682000	3.625207000	25.550216000
H	24.429920000	4.262446000	24.840017000
H	23.985880000	4.932075000	22.477094000
H	25.638774000	1.965328000	21.629670000
H	23.111081000	1.100506000	21.984300000
H	22.642504000	-0.869592000	20.193107000
H	24.875399000	-1.192538000	18.700940000
H	26.724744000	0.576857000	19.582760000

**Molecular orbital compositions for [CpV(CO)<sub>3</sub>[Ga{[N(Ph)C(H)<sub>2</sub>]}]<sup>-</sup> (6'):  
 HOMO-9 to LUMO+5**

-3.932	1.00	67 A	19.98%	1 P:y	-7.416	1.00	7 N
			18.73%	1 P:y	-7.416	1.00	6 N
			7.99%	1 P:z	-5.615	0.67	10 C
			5.96%	1 P:z	-5.615	0.67	13 C
			5.56%	1 P:y	-5.615	0.67	9 C
			2.44%	1 P:z	-7.416	1.00	6 N
			2.22%	1 P:x	-2.768	0.33	2 Ga
			2.14%	1 P:y	-5.615	0.67	15 C
			1.79%	1 P:y	-5.615	0.67	13 C
			1.63%	1 P:y	-5.615	0.67	17 C
			1.53%	1 P:z	-5.615	0.67	16 C
			1.44%	1 P:z	-7.416	1.00	7 N
			1.44%	1 P:z	-5.615	0.67	14 C
			1.39%	1 P:y	-5.615	0.67	11 C
			1.31%	1 P:z	-5.615	0.67	19 C
			1.25%	1 P:z	-5.615	0.67	12 C
			1.20%	1 P:y	-5.615	0.67	14 C
1.11%	1 S	-18.578	2.00	6 N			
-3.789	1.00	68 A	17.06%	1 P:z	-5.615	0.67	16 C
			16.50%	1 P:z	-5.615	0.67	19 C
			6.90%	1 P:z	-5.615	0.67	21 C
			5.10%	1 S	-8.924	2.00	2 Ga
			5.04%	1 P:z	-5.615	0.67	10 C
			4.78%	1 P:z	-5.615	0.67	13 C
			4.63%	1 P:z	-5.615	0.67	17 C
			4.18%	1 P:z	-5.615	0.67	18 C
			2.51%	1 P:y	-5.615	0.67	8 C
			2.33%	1 P:y	-5.615	0.67	10 C
			2.26%	1 P:z	-5.615	0.67	20 C
			2.16%	1 P:z	-5.615	0.67	14 C
			1.87%	1 P:y	-5.615	0.67	13 C
			1.79%	1 P:z	-5.615	0.67	11 C
			1.76%	1 P:y	-5.615	0.67	9 C
			1.20%	1 P:z	-7.416	1.00	7 N
			1.11%	1 P:y	-5.615	0.67	16 C
1.10%	1 D:z2	-5.531	0.60	1 V			
1.09%	1 P:y	-5.615	0.67	19 C			
1.04%	1 P:x	-5.615	0.67	19 C			
-3.661	1.00	69 A	19.44%	1 P:z	-5.615	0.67	12 C
			18.31%	1 P:z	-5.615	0.67	15 C
			16.72%	1 P:z	-5.615	0.67	14 C
			15.71%	1 P:z	-5.615	0.67	11 C
			7.10%	1 P:y	-5.615	0.67	12 C
			6.28%	1 P:y	-5.615	0.67	15 C
			5.62%	1 P:y	-5.615	0.67	11 C
-3.446	1.00	70 A	5.61%	1 P:y	-5.615	0.67	14 C
			13.15%	1 P:x	-5.615	0.67	24 C
			13.03%	1 P:x	-5.615	0.67	26 C
			10.78%	1 P:y	-5.615	0.67	24 C
			7.58%	1 P:y	-5.615	0.67	26 C
			6.06%	1 P:z	-5.615	0.67	26 C
			5.55%	1 P:y	-5.615	0.67	22 C
			5.39%	1 P:z	-5.615	0.67	24 C
			4.32%	1 D:z2	-5.531	0.60	1 V
			4.25%	1 P:x	-5.615	0.67	22 C
			3.48%	1 P:z	-5.615	0.67	22 C
			2.94%	1 D:xz	-5.531	0.60	1 V
			2.70%	1 P:x	-5.615	0.67	23 C
			2.69%	1 P:z	-5.615	0.67	23 C
2.68%	1 P:y	-5.615	0.67	23 C			
2.16%	1 D:x2-y2	-5.531	0.60	1 V			
1.95%	1 D:xy	-5.531	0.60	1 V			
1.61%	1 P:z	-0.906	0.00	1 V			
1.01%	1 P:y	-0.906	0.00	1 V			
-3.407	1.00	71 A	14.84%	1 P:x	-5.615	0.67	25 C
			10.08%	1 P:y	-5.615	0.67	25 C
			9.42%	1 P:x	-5.615	0.67	23 C
			9.33%	1 P:y	-5.615	0.67	23 C
			7.49%	1 P:x	-5.615	0.67	22 C
			6.29%	1 D:x2-y2	-5.531	0.60	1 V
			5.82%	1 P:z	-5.615	0.67	25 C
			5.25%	1 P:z	-5.615	0.67	22 C

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			5.02%	1 P:y	-5.615	0.67	22 C
			4.42%	1 P:z	-5.615	0.67	23 C
			2.41%	1 D:yz	-5.531	0.60	1 V
			1.95%	1 P:z	-5.615	0.67	26 C
			1.67%	1 D:z2	-5.531	0.60	1 V
			1.58%	1 P:y	-5.615	0.67	26 C
			1.40%	1 P:x	-5.615	0.67	26 C
			1.26%	1 P:x	-0.906	0.00	1 V
-2.779	1.00	72 A	13.00%	1 P:y	-7.416	1.00	6 N
			12.25%	1 P:y	-7.416	1.00	7 N
			7.05%	1 P:z	-5.615	0.67	13 C
			6.14%	1 P:y	-5.615	0.67	8 C
			5.31%	1 P:z	-5.615	0.67	11 C
			4.42%	1 P:z	-5.615	0.67	15 C
			4.40%	1 P:z	-5.615	0.67	19 C
			4.31%	1 P:z	-5.615	0.67	10 C
			4.03%	1 P:z	-5.615	0.67	21 C
			3.35%	1 P:x	-7.416	1.00	7 N
			3.09%	1 P:z	-5.615	0.67	17 C
			2.88%	1 P:z	-7.416	1.00	7 N
			2.67%	1 P:y	-5.615	0.67	13 C
			2.44%	1 P:y	-5.615	0.67	9 C
			1.99%	1 P:y	-5.615	0.67	10 C
			1.78%	1 P:z	-7.416	1.00	6 N
			1.65%	1 P:z	-5.615	0.67	16 C
			1.45%	1 S	-8.924	2.00	2 Ga
			1.19%	1 P:z	-5.615	0.67	14 C
			1.06%	1 D:z2	-5.531	0.60	1 V
			1.02%	1 P:x	-2.768	0.33	2 Ga
-2.606	1.00	73 A	22.04%	1 D:z2	-5.531	0.60	1 V
			14.95%	1 S	-8.924	2.00	2 Ga
			13.21%	1 P:z	-2.768	0.33	2 Ga
			4.77%	1 P:z	-9.505	1.33	5 O
			4.25%	1 P:z	-9.505	1.33	3 O
			3.46%	1 P:z	-7.416	1.00	6 N
			2.50%	1 P:z	-0.906	0.00	1 V
			2.03%	1 P:z	-5.615	0.67	29 C
			1.79%	2 P:z	1.226	0.00	2 Ga
			1.71%	1 D:xy	-5.531	0.60	1 V
			1.68%	1 P:y	-5.615	0.67	8 C
			1.65%	1 P:z	-5.615	0.67	13 C
			1.56%	1 P:z	-5.615	0.67	27 C
			1.51%	1 P:y	-7.416	1.00	7 N
			1.32%	1 P:z	-7.416	1.00	7 N
			1.15%	1 P:z	-5.615	0.67	11 C
			1.13%	1 S	-18.578	2.00	7 N
			1.06%	1 P:z	-5.615	0.67	10 C
			1.00%	1 S	-18.578	2.00	6 N
-1.478	1.00	74 A	21.91%	1 D:yz	-5.531	0.60	1 V
			14.29%	1 D:x2-y2	-5.531	0.60	1 V
			8.26%	1 D:xz	-5.531	0.60	1 V
			5.80%	1 P:z	-9.505	1.33	5 O
			5.04%	1 P:y	-2.768	0.33	2 Ga
			4.37%	1 P:z	-5.615	0.67	29 C
			3.82%	1 P:z	-9.505	1.33	3 O
			3.46%	1 P:x	-9.505	1.33	4 O
			3.31%	1 P:y	-9.505	1.33	4 O
			2.86%	1 P:x	-5.615	0.67	28 C
			2.74%	1 P:z	-5.615	0.67	27 C
			2.62%	1 P:y	-5.615	0.67	28 C
			1.99%	1 P:y	-5.615	0.67	8 C
			1.97%	1 P:y	-5.615	0.67	9 C
			1.75%	1 P:y	-9.505	1.33	3 O
			1.41%	1 P:y	-5.615	0.67	27 C
			1.10%	1 P:y	-7.416	1.00	6 N
			1.08%	1 P:y	-7.416	1.00	7 N
-1.275	1.00	75 A	25.89%	1 D:xy	-5.531	0.60	1 V
			21.43%	1 D:xz	-5.531	0.60	1 V
			6.77%	1 P:x	-9.505	1.33	5 O
			6.44%	1 P:x	-5.615	0.67	29 C
			3.75%	1 P:z	-9.505	1.33	4 O
			3.56%	1 P:y	-9.505	1.33	3 O
			3.50%	1 P:z	-5.615	0.67	28 C
			3.29%	1 P:y	-5.615	0.67	27 C
			2.62%	1 D:yz	-5.531	0.60	1 V
			1.96%	1 P:y	-9.505	1.33	4 O
			1.96%	1 P:y	-5.615	0.67	28 C

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			1.78%	1 P:z	-9.505	1.33	3 O
			1.63%	1 P:z	-5.615	0.67	27 C
			1.58%	1 D:z2	-5.531	0.60	1 V
			1.33%	1 P:x	-0.906	0.00	1 V
-0.882	1.00	76 A	15.98%	1 P:y	-5.615	0.67	8 C
			15.77%	1 P:y	-5.615	0.67	9 C
			15.40%	1 P:y	-7.416	1.00	7 N
			15.15%	1 P:y	-7.416	1.00	6 N
			5.62%	1 P:y	-2.768	0.33	2 Ga
			5.32%	1 D:yz	-5.531	0.60	1 V
			2.09%	1 P:z	-5.615	0.67	15 C
			1.71%	1 P:z	-5.615	0.67	11 C
			1.61%	1 P:z	-5.615	0.67	13 C
			1.57%	1 D:x2-y2	-5.531	0.60	1 V
			1.10%	1 P:z	-5.615	0.67	21 C
			1.05%	1 D:xy	-5.531	0.60	1 V
1.015	0.00	77 A	16.19%	1 P:z	-5.615	0.67	17 C
			15.91%	1 P:z	-5.615	0.67	20 C
			9.82%	1 P:z	-5.615	0.67	16 C
			9.23%	1 P:z	-5.615	0.67	19 C
			7.24%	1 D:z2	-5.531	0.60	1 V
			6.67%	1 S	-8.924	2.00	2 Ga
			5.10%	1 P:y	-2.768	0.33	2 Ga
			1.69%	1 P:z	-5.615	0.67	28 C
			1.30%	1 P:z	-5.615	0.67	13 C
			1.23%	1 P:z	-5.615	0.67	10 C
			1.21%	1 D:xz	-5.531	0.60	1 V
			1.10%	1 P:z	-5.615	0.67	15 C
			1.00%	1 P:y	-5.615	0.67	17 C
1.118	0.00	78 A	23.81%	1 P:z	-5.615	0.67	21 C
			23.14%	1 P:z	-5.615	0.67	18 C
			7.72%	1 P:z	-5.615	0.67	17 C
			6.55%	1 P:z	-5.615	0.67	20 C
			4.73%	1 P:z	-5.615	0.67	16 C
			4.71%	1 P:z	-5.615	0.67	19 C
			4.12%	1 D:z2	-5.531	0.60	1 V
			2.99%	1 S	-8.924	2.00	2 Ga
			1.79%	1 P:x	-5.615	0.67	18 C
			1.65%	1 P:x	-5.615	0.67	21 C
			1.34%	1 P:y	-5.615	0.67	21 C
			1.33%	1 P:z	10.942	0.00	38 H
			1.29%	1 P:z	10.942	0.00	41 H
			1.26%	1 P:y	-5.615	0.67	18 C
			-1.25%	2 P:z	11.745	0.00	18 C
			1.13%	1 P:z	-5.615	0.67	28 C
			1.11%	1 P:y	-5.615	0.67	8 C
			-1.11%	2 P:z	11.745	0.00	21 C
1.444	0.00	79 A	10.70%	1 P:z	-5.615	0.67	14 C
			10.57%	1 P:z	-5.615	0.67	11 C
			7.36%	1 D:z2	-5.531	0.60	1 V
			6.28%	1 P:z	-5.615	0.67	19 C
			5.99%	1 P:z	-5.615	0.67	16 C
			5.14%	1 S	-8.924	2.00	2 Ga
			3.85%	1 P:y	-5.615	0.67	11 C
			3.46%	1 D:xz	-5.531	0.60	1 V
			3.45%	1 P:y	-5.615	0.67	14 C
			2.99%	1 P:z	-5.615	0.67	20 C
			2.73%	1 P:z	-5.615	0.67	13 C
			2.57%	1 P:z	-5.615	0.67	15 C
			2.43%	1 P:z	-5.615	0.67	10 C
			2.32%	1 P:z	-5.615	0.67	12 C
			2.24%	1 P:z	-5.615	0.67	28 C
			1.59%	1 P:z	-5.615	0.67	17 C
			1.31%	1 P:z	-5.615	0.67	18 C
			1.02%	1 P:y	-5.615	0.67	13 C
1.464	0.00	80 A	8.81%	1 P:z	-5.615	0.67	15 C
			7.93%	1 P:z	-5.615	0.67	12 C
			7.69%	1 P:x	-5.615	0.67	29 C
			7.54%	1 P:y	-5.615	0.67	27 C
			6.47%	1 D:x2-y2	-5.531	0.60	1 V
			4.37%	1 P:z	-5.615	0.67	11 C
			3.91%	1 P:z	-5.615	0.67	14 C
			3.41%	1 P:x	-9.505	1.33	5 O
			3.28%	1 P:y	-9.505	1.33	3 O
			2.98%	1 P:y	-5.615	0.67	12 C
			2.61%	1 P:y	-5.615	0.67	15 C
			2.53%	1 D:xz	-5.531	0.60	1 V

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			2.16%	1 P:z	-5.615	0.67	16 C
			2.11%	1 P:z	-5.615	0.67	19 C
			1.95%	1 P:y	-0.906	0.00	1 V
			1.94%	1 D:yz	-5.531	0.60	1 V
			1.78%	1 P:z	-5.615	0.67	27 C
			1.56%	1 P:z	-5.615	0.67	20 C
			1.47%	1 P:y	-5.615	0.67	14 C
			1.42%	1 P:y	-5.615	0.67	11 C
			1.39%	1 P:y	-2.768	0.33	2 Ga
			1.20%	1 P:z	-5.615	0.67	29 C
			1.13%	1 P:x	-0.906	0.00	1 V
			1.02%	1 P:x	-5.615	0.67	26 C
1.495	0.00	81 A	10.05%	1 P:x	-5.615	0.67	29 C
			7.52%	1 P:z	-5.615	0.67	15 C
			6.86%	1 P:z	-5.615	0.67	12 C
			6.79%	1 D:x <sup>2</sup> -y <sup>2</sup>	-5.531	0.60	1 V
			5.33%	1 P:y	-5.615	0.67	27 C
			4.27%	1 P:x	-9.505	1.33	5 O
			3.64%	1 P:z	-5.615	0.67	19 C
			3.60%	1 P:z	-5.615	0.67	16 C
			3.37%	1 P:z	-5.615	0.67	11 C
			3.20%	1 P:z	-5.615	0.67	14 C
			2.42%	1 P:y	-5.615	0.67	12 C
			2.42%	1 P:z	-5.615	0.67	29 C
			2.37%	1 D:yz	-5.531	0.60	1 V
			2.22%	1 P:y	-9.505	1.33	3 O
			2.22%	1 P:y	-5.615	0.67	15 C
			2.00%	1 P:x	-0.906	0.00	1 V
			1.98%	1 P:z	-5.615	0.67	27 C
			1.46%	1 P:y	-0.906	0.00	1 V
			1.41%	1 D:z <sup>2</sup>	-5.531	0.60	1 V
			1.39%	1 P:z	-5.615	0.67	18 C
			1.29%	1 P:z	-9.505	1.33	5 O
			1.10%	1 P:y	-5.615	0.67	14 C
			1.10%	1 P:z	-5.615	0.67	20 C
			1.09%	1 P:y	-5.615	0.67	11 C
1.693	0.00	82 A	11.61%	1 P:z	-5.615	0.67	10 C
			11.00%	1 P:z	-5.615	0.67	13 C
			7.12%	1 P:y	-2.768	0.33	2 Ga
			7.12%	1 D:z <sup>2</sup>	-5.531	0.60	1 V
			6.83%	1 D:yz	-5.531	0.60	1 V
			4.33%	1 P:z	-5.615	0.67	14 C
			4.18%	1 P:y	-5.615	0.67	13 C
			3.75%	1 P:y	-5.615	0.67	10 C
			2.95%	1 P:z	-5.615	0.67	11 C
			2.67%	1 P:z	-5.615	0.67	12 C
			2.58%	1 P:z	-5.615	0.67	29 C
			2.56%	1 P:z	-5.615	0.67	28 C
			2.09%	1 S	-8.924	2.00	2 Ga
			1.51%	1 P:x	-2.768	0.33	2 Ga
			1.49%	1 P:z	-5.615	0.67	15 C
			1.32%	1 P:y	-5.615	0.67	14 C
			1.18%	1 P:z	-9.505	1.33	5 O
			1.16%	1 P:y	-5.615	0.67	27 C
			1.12%	1 P:x	-5.615	0.67	22 C
			1.07%	1 P:y	-5.615	0.67	9 C
			1.06%	1 P:y	-5.615	0.67	28 C
			1.00%	1 P:z	-5.615	0.67	18 C

**Cartesian coordinate file for [Cp'Mn(CO)<sub>2</sub>[Ga{[N(Ph)C(H)]<sub>2</sub>}]<sup>-</sup> (7')**

Mn	27.886672000	7.944369000	6.825158000
Ga	29.416581000	6.189067000	7.389952000
O	26.158250000	7.504964000	9.202918000
O	29.561961000	10.012403000	8.164790000
N	30.602874000	4.948671000	6.315679000
N	29.936444000	4.978565000	8.893298000
C	30.981330000	3.847540000	7.095179000
C	30.645965000	3.870216000	8.410760000
C	30.734682000	4.885281000	4.933819000
C	31.102216000	6.056706000	4.192067000
C	31.234636000	6.011239000	2.808757000
C	31.021699000	4.819751000	2.097892000
C	30.668103000	3.666295000	2.807699000
C	30.530561000	3.692016000	4.196402000
C	29.409860000	4.875053000	10.194800000
C	29.817456000	5.775312000	11.226361000
C	29.335983000	5.630255000	12.529134000
C	28.439772000	4.599829000	12.850869000
C	28.022995000	3.716440000	11.846042000
C	28.502089000	3.856412000	10.533507000
C	26.906140000	7.652352000	8.299284000
C	28.923921000	9.162568000	7.644097000
C	26.340974000	7.174293000	5.368129000
C	26.156856000	8.580125000	5.615714000
C	27.330807000	9.271524000	5.164668000
C	28.246582000	8.291285000	4.645502000
C	27.628779000	7.012182000	4.780635000
C	25.324448000	6.081649000	5.581214000
H	31.628577000	3.083389000	6.667106000
H	30.987521000	3.116109000	9.118638000
H	31.304501000	6.972814000	4.746974000
H	31.532123000	6.914565000	2.270849000
H	31.130062000	4.793015000	1.012513000
H	30.476772000	2.733614000	2.271327000
H	30.222205000	2.793639000	4.733019000
H	30.537834000	6.554811000	10.975269000
H	29.677225000	6.316060000	13.307611000
H	28.067400000	4.491205000	13.870992000
H	27.304922000	2.926503000	12.075784000
H	28.166390000	3.177586000	9.748217000
H	25.273261000	9.037333000	6.051012000
H	27.497757000	10.344571000	5.210799000
H	29.225596000	8.484000000	4.219248000
H	28.055732000	6.068830000	4.455263000
H	24.896153000	6.109821000	6.592077000
H	24.494736000	6.175829000	4.859637000
H	25.783760000	5.094773000	5.436023000

**Molecular orbital compositions for [Cp'Mn(CO)<sub>2</sub>[Ga{[N(Ph)C(H)<sub>2</sub>]}]<sup>-</sup> (7<sup>-</sup>):  
 HOMO-5 to LUMO+5**

-2.584	1.00	70 A	10.13%	1 D:z2	-7.240	1.00	1 Mn			
			9.39%	1 S	-8.924	2.00	2 Ga			
			8.59%	1 P:y	-7.416	1.00	5 N			
			7.67%	1 P:z	-2.768	0.33	2 Ga			
			7.00%	1 P:z	-7.416	1.00	6 N			
			5.86%	1 P:y	-7.416	1.00	6 N			
			5.41%	1 P:z	-5.615	0.67	18 C			
			4.14%	1 P:z	-5.615	0.67	16 C			
			3.69%	1 P:z	-5.615	0.67	20 C			
			3.38%	1 P:y	-5.615	0.67	8 C			
			2.79%	1 P:z	-5.615	0.67	15 C			
			2.75%	1 P:z	-0.721	0.00	1 Mn			
			2.38%	1 P:z	-5.615	0.67	12 C			
			2.26%	1 P:z	-5.615	0.67	10 C			
			1.76%	1 P:z	-5.615	0.67	14 C			
			1.72%	1 S	-5.227	2.00	1 Mn			
			1.58%	1 P:y	-5.615	0.67	7 C			
			1.27%	1 P:z	-5.615	0.67	9 C			
			1.19%	1 P:y	-5.615	0.67	12 C			
			-2.552	1.00	71 A	10.26%	1 D:z2	-7.240	1.00	1 Mn
9.37%	1 S	-8.924				2.00	2 Ga			
8.60%	1 P:y	-7.416				1.00	6 N			
8.17%	1 P:z	-2.768				0.33	2 Ga			
6.27%	1 P:y	-5.615				0.67	7 C			
5.88%	1 P:z	-7.416				1.00	5 N			
5.52%	1 P:z	-5.615				0.67	12 C			
3.94%	1 P:z	-5.615				0.67	10 C			
3.28%	1 P:z	-0.721				0.00	1 Mn			
3.25%	1 P:z	-5.615				0.67	14 C			
2.99%	1 P:x	-7.416				1.00	5 N			
2.93%	1 P:y	-7.416				1.00	5 N			
2.66%	1 P:z	-5.615				0.67	9 C			
2.24%	1 P:y	-5.615				0.67	12 C			
1.83%	1 P:y	-5.615				0.67	14 C			
1.66%	1 S	-5.227				2.00	1 Mn			
1.34%	1 P:y	-5.615				0.67	10 C			
1.03%	2 P:z	1.226				0.00	2 Ga			
-1.874	1.00	72 A				1.00%	1 P:x	-5.615	0.67	9 C
						40.74%	1 D:xy	-7.240	1.00	1 Mn
			12.44%	1 D:x2-y2	-7.240	1.00	1 Mn			
			6.99%	1 D:xz	-7.240	1.00	1 Mn			
			6.84%	1 P:x	-9.505	1.33	4 O			
			6.43%	1 P:y	-9.505	1.33	3 O			
			5.37%	1 D:yz	-7.240	1.00	1 Mn			
			4.15%	1 P:x	-5.615	0.67	22 C			
			3.77%	1 P:y	-5.615	0.67	21 C			
			1.22%	1 P:x	-0.721	0.00	1 Mn			
			-1.427	1.00	73 A	49.17%	1 D:yz	-7.240	1.00	1 Mn
						7.46%	1 P:y	-2.768	0.33	2 Ga
7.42%	1 P:z	-9.505				1.33	4 O			
5.60%	1 P:z	-5.615				0.67	22 C			
5.24%	1 D:xy	-7.240				1.00	1 Mn			
2.55%	1 P:x	-5.615				0.67	26 C			
1.82%	1 D:z2	-7.240				1.00	1 Mn			
1.80%	1 P:y	-5.615				0.67	8 C			
1.78%	1 P:y	-5.615				0.67	7 C			
1.18%	1 P:z	-5.615				0.67	26 C			
1.01%	1 P:y	-7.416				1.00	6 N			
-1.333	1.00	74 A				56.93%	1 D:xz	-7.240	1.00	1 Mn
			8.56%	1 P:z	-9.505	1.33	3 O			
			6.67%	1 P:z	-5.615	0.67	21 C			
			4.80%	1 D:z2	-7.240	1.00	1 Mn			
			3.13%	1 D:x2-y2	-7.240	1.00	1 Mn			
			1.65%	1 D:xy	-7.240	1.00	1 Mn			
			1.57%	1 P:z	-0.721	0.00	1 Mn			
			1.28%	1 P:x	-5.615	0.67	23 C			
			1.12%	1 P:y	-9.505	1.33	3 O			
			-0.733	1.00	75 A	15.99%	1 P:y	-7.416	1.00	6 N
15.44%	1 P:y	-5.615				0.67	7 C			
14.22%	1 P:y	-7.416				1.00	5 N			
14.00%	1 P:y	-5.615				0.67	8 C			



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			8.24%	1 D:yz	-7.240	1.00	1 Mn
			4.38%	1 P:y	-2.768	0.33	2 Ga
			2.65%	1 P:z	-5.615	0.67	14 C
			2.16%	1 P:z	-5.615	0.67	10 C
			2.06%	1 P:z	-5.615	0.67	12 C
			1.17%	1 P:z	-5.615	0.67	16 C
			1.15%	1 P:z	-5.615	0.67	18 C
			1.12%	1 P:z	-7.416	1.00	6 N
			1.00%	1 P:y	-5.615	0.67	12 C
1.301	0.00	76 A	14.29%	1 D:z2	-7.240	1.00	1 Mn
			12.54%	1 P:z	-5.615	0.67	20 C
			11.84%	1 P:z	-5.615	0.67	17 C
			6.94%	1 S	-8.924	2.00	2 Ga
			6.17%	1 P:y	-2.768	0.33	2 Ga
			5.78%	1 P:z	-5.615	0.67	15 C
			5.28%	1 P:z	-5.615	0.67	18 C
			3.34%	1 P:z	-5.615	0.67	9 C
			2.86%	1 P:z	-5.615	0.67	12 C
			2.17%	1 D:xy	-7.240	1.00	1 Mn
			1.73%	1 P:z	-5.615	0.67	14 C
			1.58%	1 P:z	-5.615	0.67	11 C
			1.34%	1 P:x	-5.615	0.67	27 C
			1.26%	1 P:y	-5.615	0.67	12 C
			1.25%	1 P:y	-5.615	0.67	9 C
			1.23%	1 P:z	-5.615	0.67	19 C
			1.22%	1 P:z	-5.615	0.67	16 C
			1.03%	1 D:xz	-7.240	1.00	1 Mn
1.367	0.00	77 A	23.54%	1 P:z	-5.615	0.67	16 C
			23.20%	1 P:z	-5.615	0.67	19 C
			8.86%	1 D:z2	-7.240	1.00	1 Mn
			6.60%	1 P:z	-5.615	0.67	20 C
			5.82%	1 P:z	-5.615	0.67	17 C
			5.48%	1 P:z	-5.615	0.67	18 C
			5.12%	1 P:z	-5.615	0.67	15 C
			4.58%	1 S	-8.924	2.00	2 Ga
			1.48%	1 P:y	-5.615	0.67	7 C
			1.35%	1 P:z	10.942	0.00	39 H
			1.35%	1 P:z	10.942	0.00	36 H
			-1.25%	2 P:z	11.745	0.00	19 C
			-1.04%	2 P:z	11.745	0.00	16 C
1.472	0.00	78 A	17.60%	1 P:z	-5.615	0.67	10 C
			16.86%	1 P:z	-5.615	0.67	13 C
			13.07%	1 P:z	-5.615	0.67	14 C
			11.80%	1 P:z	-5.615	0.67	11 C
			6.91%	1 P:y	-5.615	0.67	13 C
			6.75%	1 P:y	-5.615	0.67	10 C
			4.83%	1 P:y	-5.615	0.67	11 C
			4.65%	1 P:y	-5.615	0.67	14 C
			1.75%	1 P:x	-5.615	0.67	10 C
			1.58%	1 P:x	-5.615	0.67	13 C
			1.52%	1 D:z2	-7.240	1.00	1 Mn
			1.01%	1 P:z	10.942	0.00	34 H
			1.01%	1 P:z	10.942	0.00	31 H
1.547	0.00	79 A	19.05%	1 D:x2-y2	-7.240	1.00	1 Mn
			12.46%	1 P:y	-2.768	0.33	2 Ga
			6.05%	1 D:yz	-7.240	1.00	1 Mn
			5.44%	1 D:z2	-7.240	1.00	1 Mn
			3.45%	1 P:z	-5.615	0.67	19 C
			3.38%	1 P:z	-5.615	0.67	16 C
			3.33%	1 P:y	-0.721	0.00	1 Mn
			2.94%	1 S	-13.830	2.00	21 C
			2.86%	1 P:x	-5.615	0.67	23 C
			2.80%	1 P:x	-5.615	0.67	22 C
			2.40%	1 S	-8.924	2.00	2 Ga
			2.27%	1 D:xy	-7.240	1.00	1 Mn
			2.04%	1 P:x	-5.615	0.67	26 C
			1.98%	1 P:x	-0.721	0.00	1 Mn
			1.69%	1 P:y	-5.615	0.67	21 C
			1.46%	1 P:x	-9.505	1.33	4 O
			1.35%	1 P:y	-5.615	0.67	23 C
			1.32%	1 S	-6.383	1.00	45 H
			1.32%	1 P:x	-2.768	0.33	2 Ga
			1.31%	1 P:z	-5.615	0.67	23 C
			1.29%	1 P:z	-5.615	0.67	26 C
			1.12%	1 P:x	-5.615	0.67	24 C
1.645	0.00	80 A	15.91%	1 P:z	-5.615	0.67	15 C
			15.26%	1 P:z	-5.615	0.67	18 C

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			11.71%	1 P:z	-5.615	0.67	17 C
			8.87%	1 P:z	-5.615	0.67	20 C
			4.56%	1 D:z2	-7.240	1.00	1 Mn
			4.53%	1 P:z	-5.615	0.67	9 C
			4.10%	1 P:z	-5.615	0.67	12 C
			2.90%	1 P:z	-5.615	0.67	11 C
			2.70%	1 P:z	-5.615	0.67	14 C
			1.92%	1 P:y	-5.615	0.67	8 C
			1.83%	1 P:y	-5.615	0.67	12 C
			1.79%	1 P:y	-5.615	0.67	9 C
			1.40%	1 P:y	-5.615	0.67	7 C
			1.33%	1 D:xy	-7.240	1.00	1 Mn
			1.26%	1 P:y	-5.615	0.67	11 C
			1.23%	1 S	-8.924	2.00	2 Ga
1.809	0.00	81 A	9.81%	1 P:z	-5.615	0.67	9 C
			8.91%	1 P:z	-5.615	0.67	12 C
			7.18%	1 D:z2	-7.240	1.00	1 Mn
			5.33%	1 D:x2-y2	-7.240	1.00	1 Mn
			4.06%	1 P:y	-5.615	0.67	12 C
			3.74%	1 D:xy	-7.240	1.00	1 Mn
			3.65%	1 P:y	-5.615	0.67	9 C
			3.48%	1 P:z	-5.615	0.67	11 C
			2.78%	1 D:xz	-7.240	1.00	1 Mn
			2.56%	1 P:y	-2.768	0.33	2 Ga
			2.44%	1 P:z	-5.615	0.67	13 C
			2.38%	1 S	-13.830	2.00	22 C
			1.90%	1 P:y	-0.721	0.00	1 Mn
			1.83%	1 S	-8.924	2.00	2 Ga
			1.79%	1 P:z	-5.615	0.67	14 C
			1.62%	1 P:x	-5.615	0.67	25 C
			1.50%	1 P:y	-5.615	0.67	21 C
			1.49%	1 P:z	-5.615	0.67	19 C
			1.49%	1 P:y	-5.615	0.67	8 C
			1.44%	1 P:y	-5.615	0.67	11 C
			1.39%	1 P:x	-5.615	0.67	22 C
			1.24%	1 P:z	-5.615	0.67	15 C
			1.14%	1 P:z	-5.615	0.67	18 C
			1.12%	1 P:y	-7.416	1.00	5 N
			1.09%	1 P:z	-5.615	0.67	16 C
			1.06%	1 P:x	-5.615	0.67	9 C
			1.05%	2 P:z	1.226	0.00	2 Ga

**Cartesian coordinate file for [CpCo(CO)[Ga{[N(Ph)C(H)]<sub>2</sub>}]<sup>-</sup> (8')**

Co	3.101145000	2.402361000	11.212092000
Ga	3.934909000	3.789402000	9.572717000
O	5.764432000	1.228441000	11.382055000
N	3.657028000	5.718456000	9.042941000
N	5.085997000	3.751022000	7.955532000
C	4.260232000	5.962801000	7.800051000
C	5.003112000	4.965362000	7.257113000
C	2.601524000	6.538078000	9.443549000
C	2.465255000	6.909577000	10.805854000
C	1.404762000	7.729647000	11.234947000
C	0.438711000	8.207078000	10.312760000
C	0.568298000	7.841748000	8.950777000
C	1.636886000	7.024175000	8.526656000
C	5.554853000	2.636300000	7.216417000
C	4.718842000	1.989498000	6.286023000
C	5.169272000	0.899941000	5.539019000
C	6.483068000	0.433162000	5.692868000
C	7.331821000	1.065450000	6.606000000
C	6.867252000	2.163500000	7.370838000
C	1.714524000	3.085533000	12.773154000
C	1.171328000	3.389377000	11.489614000
C	0.948099000	2.150990000	10.777157000
C	1.399755000	1.091724000	11.600697000
C	1.898911000	1.668579000	12.828312000
C	4.682431000	1.706927000	11.304886000
H	4.204228000	6.961056000	7.366722000
H	5.584753000	5.090456000	6.344124000
H	3.216756000	6.561791000	11.512614000
H	1.335968000	8.015132000	12.286919000
H	-0.386682000	8.840227000	10.642473000
H	-0.174969000	8.170143000	8.220375000
H	1.710194000	6.718511000	7.481281000
H	3.698984000	2.355490000	6.171527000
H	4.491393000	0.404086000	4.840583000
H	6.836727000	-0.418659000	5.108501000
H	8.358901000	0.717298000	6.733381000
H	7.523712000	2.663757000	8.084714000
H	1.962520000	3.801549000	13.550858000
H	0.919321000	4.379662000	11.124710000
H	0.516429000	2.060548000	9.785589000
H	1.385807000	0.034443000	11.354950000
H	2.312000000	1.111071000	13.663610000

**Molecular orbital compositions for [CpCo(CO)[Ga{N(Ph)C(H)<sub>2</sub>}]<sup>-</sup> (8'):  
 HOMO-9 to LUMO+5**

-3.457	1.00	59 A	13.37%	1 P:z	-5.615	0.67	17 C			
			12.98%	1 P:z	-5.615	0.67	14 C			
			7.45%	1 P:x	-7.416	1.00	5 N			
			7.00%	1 P:x	-7.416	1.00	4 N			
			6.58%	1 P:z	-5.615	0.67	15 C			
			4.91%	1 P:z	-5.615	0.67	19 C			
			4.87%	1 D:z <sup>2</sup>	-8.771	1.40	1 Co			
			3.14%	1 P:z	-5.615	0.67	18 C			
			2.30%	1 P:z	-7.416	1.00	4 N			
			2.15%	1 S	-8.924	2.00	2 Ga			
			1.92%	1 P:y	-2.768	0.33	2 Ga			
			1.71%	1 P:z	-5.615	0.67	21 C			
			1.55%	1 P:z	-7.416	1.00	5 N			
			1.39%	1 P:z	-5.615	0.67	16 C			
			1.21%	1 P:x	-5.615	0.67	24 C			
			1.18%	1 S	-6.383	1.00	26 H			
			1.18%	1 S	-18.578	2.00	4 N			
			1.10%	1 P:x	-5.615	0.67	21 C			
			-3.257	1.00	60 A	16.77%	1 D:z <sup>2</sup>	-8.771	1.40	1 Co
						9.19%	1 P:z	-5.615	0.67	21 C
7.77%	1 P:x	-5.615				0.67	24 C			
6.98%	1 P:x	-5.615				0.67	21 C			
5.34%	1 P:z	-5.615				0.67	24 C			
4.85%	1 P:z	-5.615				0.67	17 C			
4.27%	1 P:z	-5.615				0.67	14 C			
3.32%	1 P:z	-5.615				0.67	22 C			
2.91%	1 P:y	-5.615				0.67	22 C			
2.76%	1 D:xy	-8.771				1.40	1 Co			
2.49%	1 P:z	-5.615				0.67	19 C			
2.45%	1 P:z	-5.615				0.67	15 C			
2.37%	1 P:x	-5.615				0.67	22 C			
2.30%	1 P:z	-7.416				1.00	5 N			
1.93%	1 P:z	-5.615				0.67	23 C			
1.81%	1 P:y	-5.615				0.67	24 C			
1.67%	1 P:x	-0.498				0.00	1 Co			
1.65%	1 P:z	-2.768				0.33	2 Ga			
1.46%	1 P:y	-5.615				0.67	21 C			
1.25%	1 P:y	-5.615				0.67	23 C			
1.18%	1 S	-13.830	2.00	25 C						
-3.117	1.00	61 A	13.30%	1 P:x	-5.615	0.67	20 C			
			11.90%	1 D:x <sup>2</sup> -y <sup>2</sup>	-8.771	1.40	1 Co			
			10.94%	1 P:z	-5.615	0.67	20 C			
			9.18%	1 P:z	-5.615	0.67	22 C			
			8.12%	1 P:x	-5.615	0.67	23 C			
			6.59%	1 P:z	-5.615	0.67	23 C			
			5.37%	1 D:yz	-8.771	1.40	1 Co			
			4.97%	1 P:x	-5.615	0.67	22 C			
			4.32%	1 P:y	-5.615	0.67	23 C			
			3.20%	1 D:xy	-8.771	1.40	1 Co			
			2.74%	1 P:y	-5.615	0.67	22 C			
			2.49%	1 D:xz	-8.771	1.40	1 Co			
			2.24%	1 P:z	-5.615	0.67	21 C			
			2.02%	1 P:y	-5.615	0.67	20 C			
			1.52%	1 P:y	-0.498	0.00	1 Co			
			1.25%	1 P:y	-5.615	0.67	24 C			
			1.19%	1 P:y	-5.615	0.67	21 C			
			-2.615	1.00	62 A	13.44%	1 P:x	-7.416	1.00	5 N
						9.32%	1 P:x	-7.416	1.00	4 N
						6.08%	1 S	-8.924	2.00	2 Ga
5.05%	1 P:z	-7.416				1.00	5 N			
4.46%	1 P:z	-5.615				0.67	11 C			
4.05%	1 P:z	-2.768				0.33	2 Ga			
3.81%	1 P:z	-5.615				0.67	9 C			
3.60%	1 P:x	-5.615				0.67	6 C			
2.87%	1 P:z	-5.615				0.67	13 C			
2.51%	1 P:x	-5.615				0.67	7 C			
2.48%	1 P:z	-5.615				0.67	8 C			
2.24%	1 D:z <sup>2</sup>	-8.771				1.40	1 Co			
2.09%	1 P:y	-7.416				1.00	4 N			
2.08%	1 P:z	-0.498				0.00	1 Co			
2.04%	1 P:z	-5.615				0.67	17 C			
1.98%	1 D:xz	-8.771				1.40	1 Co			

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			1.59%	1 P:z	-5.615	0.67	19 C
			1.40%	1 S	-5.593	2.00	1 Co
			1.37%	1 P:x	-5.615	0.67	11 C
			1.26%	1 P:z	-5.615	0.67	15 C
			1.14%	1 P:x	-5.615	0.67	8 C
			1.11%	1 P:y	-5.615	0.67	11 C
			1.10%	1 D:yz	-8.771	1.40	1 Co
-2.501	1.00	63 A	10.15%	1 S	-8.924	2.00	2 Ga
			10.00%	1 P:z	-2.768	0.33	2 Ga
			5.51%	1 D:z2	-8.771	1.40	1 Co
			5.35%	1 P:z	-7.416	1.00	4 N
			5.12%	1 P:z	-0.498	0.00	1 Co
			5.05%	1 P:x	-7.416	1.00	5 N
			4.55%	1 P:y	-7.416	1.00	4 N
			4.35%	1 P:x	-5.615	0.67	6 C
			3.86%	1 P:z	-5.615	0.67	11 C
			2.96%	1 S	-5.593	2.00	1 Co
			2.75%	1 P:z	-5.615	0.67	9 C
			2.29%	1 P:z	-5.615	0.67	24 C
			2.26%	1 P:z	-5.615	0.67	13 C
			2.11%	1 P:x	-5.615	0.67	24 C
			1.91%	1 P:x	-5.615	0.67	21 C
			1.66%	1 P:z	-5.615	0.67	8 C
			1.33%	1 P:y	-5.615	0.67	8 C
			1.32%	1 D:xz	-8.771	1.40	1 Co
			1.31%	2 P:z	1.226	0.00	2 Ga
			1.18%	1 P:z	-9.505	1.33	3 O
			1.09%	1 S	-18.578	2.00	4 N
			1.05%	1 P:z	-5.615	0.67	21 C
			1.00%	1 S	-6.383	1.00	26 H
-2.067	1.00	64 A	54.01%	1 D:xz	-8.771	1.40	1 Co
			19.70%	1 D:yz	-8.771	1.40	1 Co
			9.88%	1 P:z	-9.505	1.33	3 O
			4.33%	1 P:z	-5.615	0.67	25 C
			1.78%	1 P:z	-5.615	0.67	24 C
			1.19%	1 P:z	-0.498	0.00	1 Co
-1.190	1.00	65 A	46.82%	1 D:x2-y2	-8.771	1.40	1 Co
			16.87%	1 D:yz	-8.771	1.40	1 Co
			7.11%	1 D:xy	-8.771	1.40	1 Co
			6.15%	1 D:xz	-8.771	1.40	1 Co
			4.62%	1 P:y	-9.505	1.33	3 O
			3.62%	1 P:y	-5.615	0.67	25 C
			2.45%	1 P:z	-5.615	0.67	23 C
			1.92%	1 P:x	-9.505	1.33	3 O
			1.54%	1 P:x	-5.615	0.67	25 C
			1.41%	1 P:x	-5.615	0.67	23 C
			1.19%	1 P:z	-5.615	0.67	20 C
-0.870	1.00	66 A	11.84%	1 P:x	-5.615	0.67	6 C
			11.79%	1 P:x	-7.416	1.00	5 N
			11.75%	1 P:x	-5.615	0.67	7 C
			10.71%	1 P:x	-2.768	0.33	2 Ga
			9.72%	1 D:yz	-8.771	1.40	1 Co
			8.37%	1 P:x	-7.416	1.00	4 N
			2.92%	1 P:y	-7.416	1.00	4 N
			2.67%	1 P:y	-2.768	0.33	2 Ga
			2.05%	1 D:xy	-8.771	1.40	1 Co
			1.78%	1 D:x2-y2	-8.771	1.40	1 Co
			1.74%	1 P:z	-5.615	0.67	13 C
			1.56%	1 P:z	-5.615	0.67	9 C
			1.41%	1 P:z	-5.615	0.67	11 C
			1.20%	1 P:y	-9.505	1.33	3 O
			1.16%	1 P:y	-5.615	0.67	25 C
			1.15%	1 P:y	-5.615	0.67	6 C
			1.11%	1 P:y	-5.615	0.67	7 C
			1.10%	1 P:y	-0.498	0.00	1 Co
-0.599	1.00	67 A	48.79%	1 D:xy	-8.771	1.40	1 Co
			24.35%	1 D:z2	-8.771	1.40	1 Co
			11.11%	1 D:x2-y2	-8.771	1.40	1 Co
			6.52%	1 S	-5.593	2.00	1 Co
			1.23%	1 D:yz	-8.771	1.40	1 Co
-0.421	1.00	68 A	30.24%	1 D:yz	-8.771	1.40	1 Co
			13.53%	1 D:xz	-8.771	1.40	1 Co
			6.51%	1 P:x	-7.416	1.00	5 N
			4.74%	1 P:x	-7.416	1.00	4 N
			4.54%	1 P:x	-5.615	0.67	6 C
			3.88%	1 P:x	-5.615	0.67	7 C
			2.43%	1 P:x	-5.615	0.67	22 C

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			2.37%	1 D:xy	-8.771	1.40	1 Co
			2.33%	1 P:y	-5.615	0.67	25 C
			2.26%	1 D:x2-y2	-8.771	1.40	1 Co
			1.95%	1 P:x	-5.615	0.67	20 C
			1.89%	1 P:y	-9.505	1.33	3 O
			1.87%	1 P:y	-0.498	0.00	1 Co
			1.63%	1 P:z	-5.615	0.67	22 C
			1.42%	1 P:z	-5.615	0.67	20 C
			1.13%	1 P:y	-5.615	0.67	22 C
			1.06%	1 P:y	-2.768	0.33	2 Ga
1.136	0.00	69 A	17.95%	1 D:z2	-8.771	1.40	1 Co
			12.66%	1 S	-8.924	2.00	2 Ga
			8.70%	1 P:z	-5.615	0.67	15 C
			8.12%	1 P:z	-5.615	0.67	18 C
			5.81%	1 P:z	-5.615	0.67	17 C
			5.34%	1 P:z	-5.615	0.67	14 C
			5.23%	1 D:xy	-8.771	1.40	1 Co
			3.21%	1 S	-13.830	2.00	25 C
			2.01%	1 P:z	-5.615	0.67	8 C
			1.98%	1 P:z	-5.615	0.67	11 C
			1.74%	1 P:z	-5.615	0.67	24 C
			1.54%	1 P:x	-5.615	0.67	21 C
			1.54%	1 P:x	-5.615	0.67	24 C
			1.52%	1 P:z	-5.615	0.67	21 C
			1.51%	1 P:x	-2.768	0.33	2 Ga
			1.15%	1 D:x2-y2	-8.771	1.40	1 Co
1.291	0.00	70 A	26.95%	1 P:z	-5.615	0.67	19 C
			24.86%	1 P:z	-5.615	0.67	16 C
			14.74%	1 P:z	-5.615	0.67	15 C
			13.27%	1 P:z	-5.615	0.67	18 C
			2.92%	1 D:z2	-8.771	1.40	1 Co
			2.17%	1 S	-8.924	2.00	2 Ga
			1.79%	1 P:z	-5.615	0.67	14 C
			1.56%	1 P:z	-5.615	0.67	17 C
			1.44%	1 P:z	10.942	0.00	34 H
			1.43%	1 P:z	10.942	0.00	37 H
			-1.37%	2 P:z	11.745	0.00	16 C
			-1.27%	2 P:z	11.745	0.00	19 C
			1.08%	1 P:x	-5.615	0.67	6 C
			1.04%	1 D:xz	33.369	0.00	14 C
1.450	0.00	71 A	15.51%	1 P:z	-5.615	0.67	9 C
			14.80%	1 P:z	-5.615	0.67	12 C
			13.83%	1 P:z	-5.615	0.67	13 C
			12.57%	1 P:z	-5.615	0.67	10 C
			4.00%	1 P:y	-5.615	0.67	9 C
			3.85%	1 P:x	-5.615	0.67	9 C
			3.81%	1 P:y	-5.615	0.67	12 C
			3.70%	1 P:x	-5.615	0.67	12 C
			3.36%	1 P:x	-5.615	0.67	13 C
			3.36%	1 P:x	-5.615	0.67	10 C
			2.98%	1 P:y	-5.615	0.67	13 C
			2.89%	1 P:y	-5.615	0.67	10 C
			1.49%	1 P:z	-5.615	0.67	17 C
			1.46%	1 P:z	-5.615	0.67	14 C
			1.09%	1 D:z2	-8.771	1.40	1 Co
1.542	0.00	72 A	21.78%	1 P:z	-5.615	0.67	17 C
			21.50%	1 P:z	-5.615	0.67	14 C
			9.49%	1 P:z	-5.615	0.67	18 C
			5.57%	1 P:z	-5.615	0.67	15 C
			4.57%	1 P:z	-5.615	0.67	16 C
			4.54%	1 D:z2	-8.771	1.40	1 Co
			2.65%	1 P:z	-5.615	0.67	13 C
			2.37%	1 P:z	-5.615	0.67	10 C
			2.15%	1 P:z	-5.615	0.67	19 C
			1.44%	1 S	-8.924	2.00	2 Ga
			-1.39%	2 P:z	11.745	0.00	14 C
			-1.35%	2 P:z	11.745	0.00	17 C
			1.32%	1 P:z	10.942	0.00	35 H
			1.19%	1 D:xy	-8.771	1.40	1 Co
			1.12%	2 P:z	1.226	0.00	2 Ga
1.763	0.00	73 A	13.88%	1 P:z	-5.615	0.67	8 C
			13.79%	1 P:z	-5.615	0.67	11 C
			8.42%	1 P:x	-2.768	0.33	2 Ga
			5.32%	1 P:z	-5.615	0.67	12 C
			4.04%	1 P:x	-5.615	0.67	11 C
			4.00%	1 P:z	-5.615	0.67	10 C
			3.72%	1 P:y	-5.615	0.67	8 C

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3.60%	1 P:y	-5.615	0.67	11 C
3.12%	1 P:x	-5.615	0.67	8 C
2.93%	1 D:z2	-8.771	1.40	1 Co
2.77%	1 P:z	-5.615	0.67	25 C
2.61%	1 P:z	-5.615	0.67	9 C
2.06%	1 D:xxz	-8.771	1.40	1 Co
1.74%	1 P:z	-5.615	0.67	13 C
1.60%	1 D:xy	-8.771	1.40	1 Co
1.57%	1 P:x	-5.615	0.67	7 C
1.41%	1 P:y	-5.615	0.67	12 C
1.34%	1 P:z	-9.505	1.33	3 O
1.15%	1 P:x	-5.615	0.67	12 C
1.12%	1 P:x	-5.615	0.67	10 C
1.11%	1 P:z	-5.615	0.67	19 C
1.02%	1 P:z	-5.615	0.67	16 C

**Cartesian coordinate file for [CpV(CO)<sub>3</sub>[C{[N(Ph)C(H)]<sub>2</sub>}] (9)**

V	23.8887	1.4652	19.1091
C	23.8887	1.4652	21.4241
O	26.4396	3.2909	19.2069
O	23.1456	3.9731	17.4052
O	20.9187	2.1472	19.8718
N	24.1612	2.5166	22.2982
N	23.4335	0.4791	22.3012
C	23.8906	2.1835	23.6328
C	23.4374	0.9090	23.6369
C	24.8053	3.7884	22.0236
C	24.1389	4.8131	21.3429
C	24.7798	6.0474	21.1701
C	26.0658	6.2604	21.6863
C	26.7186	5.2339	22.3797
C	26.0891	3.9957	22.5488
C	23.0980	-0.9034	22.0238
C	24.0108	-1.8939	22.4124
C	23.6921	-3.2451	22.2303
C	22.4591	-3.6017	21.6643
C	21.5460	-2.6038	21.2908
C	21.8589	-1.2489	21.4745
C	24.3728	-0.9208	18.9656
C	23.2396	-0.6520	18.1467
C	23.6478	0.2367	17.1084
C	25.0336	0.5261	17.2944
C	25.4802	-0.1886	18.4529
C	25.4544	2.6686	19.3227
C	23.4225	3.0329	18.0573
C	22.0450	1.9018	19.6270
H	24.0324	2.8906	24.4368
H	23.1066	0.2734	24.4454
H	23.1417	4.6413	20.9480
H	24.2701	6.8439	20.6314
H	26.5576	7.2218	21.5488
H	27.7184	5.3889	22.7821
H	26.5918	3.1842	23.0727
H	24.9674	-1.5997	22.8409
H	24.4055	-4.0145	22.5260
H	22.2078	-4.6532	21.5242
H	20.5820	-2.8806	20.8636
H	21.1555	-0.4686	21.1954
H	24.3934	-1.5784	19.8238
H	22.2475	-1.0710	18.2719
H	23.0207	0.6122	16.3080
H	25.6454	1.1580	16.6611
H	26.4894	-0.1949	18.8502



**Cartesian coordinate file for [Cp'Mn(CO)<sub>2</sub>[C{[N(Ph)C(H)]<sub>2</sub>}] (10)**

Mn	28.1596	7.3596	6.9622
C	28.1596	7.3596	9.0236
O	25.3963	8.2507	6.3381
O	29.3082	10.1100	6.9550
N	29.0159	6.7360	9.9487
N	27.3549	8.1285	9.8727
C	28.7425	7.1234	11.2721
C	27.7126	7.9926	11.2208
C	30.0367	5.7363	9.7404
C	31.2653	6.0608	9.1526
C	32.2735	5.0905	9.0811
C	32.0674	3.8089	9.6122
C	30.8414	3.4941	10.2140
C	29.8261	4.4552	10.2755
C	26.1871	8.9348	9.5682
C	26.3283	10.2834	9.2195
C	25.1862	11.0887	9.1154
C	23.9153	10.5510	9.3655
C	23.7829	9.1962	9.7052
C	24.9197	8.3869	9.8072
C	26.4682	7.9452	6.7202
C	28.8483	9.0232	6.9855
C	27.7073	5.3434	5.9282
C	27.9190	6.3890	4.9556
C	29.2550	6.8633	5.0800
C	29.8909	6.1249	6.1317
C	28.9312	5.2014	6.6479
C	26.4825	4.4661	6.0488
H	29.3288	6.7609	12.1047
H	27.2054	8.5415	12.0020
H	31.4226	7.0641	8.7654
H	33.2292	5.3411	8.6235
H	32.8607	3.0645	9.5679
H	30.6759	2.5063	10.6414
H	28.8703	4.2249	10.7436
H	27.3194	10.6927	9.0365
H	25.2913	12.1410	8.8508
H	23.0313	11.1860	9.3050
H	22.7979	8.7715	9.9004
H	24.8337	7.3358	10.0783
H	27.1856	6.7388	4.2367
H	29.7139	7.6366	4.4747
H	30.9218	6.2237	6.4457
H	29.1019	4.4860	7.4448
H	25.5628	5.0215	5.8303
H	26.5382	3.6257	5.3386
H	26.3925	4.0397	7.0554

**Cartesian coordinate file for [CpCo(CO)[C{[N(Ph)C(H)]<sub>2</sub>}] (11)**

H	0.3515	-4.2784	0.9615
C	-0.4450	-3.6888	1.4121
H	-1.8301	-5.3471	1.5178
C	-1.6706	-4.2907	1.7296
C	-0.2378	-2.3286	1.6717
H	1.6313	0.0702	-1.2209
C	0.8837	0.8448	-1.3373
C	-2.6917	-3.5308	2.3132
C	-1.2640	-1.5752	2.2536
H	-0.4646	0.0454	-2.9401
H	-3.6509	-3.9888	2.5500
H	1.4787	2.3693	0.1970
C	-0.2197	0.8361	-2.2409
H	-0.8727	-0.4627	4.7369
C	0.7945	2.0618	-0.5865
C	-2.4891	-2.1710	2.5789
N	-1.0589	-0.1817	2.5846
C	-0.9067	0.2387	3.9154
O	-3.3026	-0.9197	-0.6133
Co	-1.0446	0.8938	-0.2210
C	-2.3976	-0.1999	-0.4090
C	-1.0446	0.8938	1.6967
C	-0.7972	1.5909	3.8975
C	-0.9407	2.0880	-2.1002
C	-0.3039	2.8511	-1.0960
H	-0.6737	2.3022	4.7017
N	-0.8944	1.9904	2.5531
H	-1.8187	2.3753	-2.6668
H	-0.5977	3.8338	-0.7506
C	-0.0911	4.3084	2.2933
C	-1.1207	3.3680	2.1858
H	0.4636	6.3840	2.0458
C	-0.3414	5.6518	1.9762
C	-2.4039	3.7564	1.7804
C	-1.6206	6.0515	1.5628
C	-2.6552	5.1022	1.4686
H	-1.8148	7.0957	1.3175
H	-3.6560	5.4061	1.1596
H	-3.1874	3.0067	1.7047
H	0.7057	-1.8473	1.4264
H	-3.2809	-1.5655	3.0148
H	0.9007	3.9869	2.6033