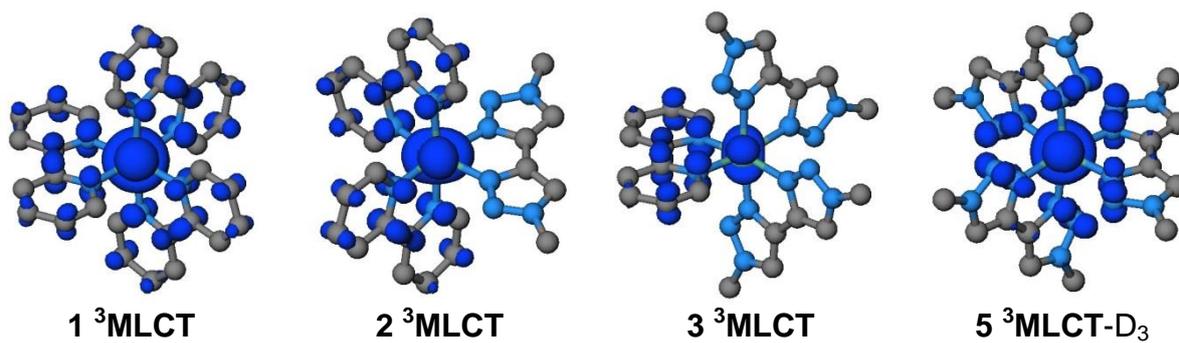


Electronic Supporting Information for

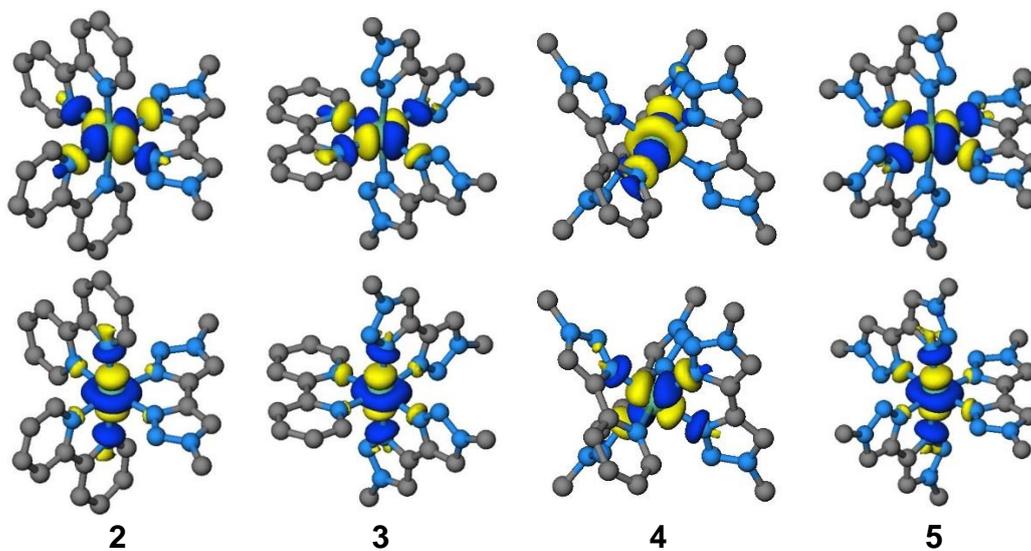
Theoretical illumination of highly original photoreactive  $^3\text{MC}$  states  
and the mechanism of the photochemistry of Ru(II) tris(bidentate)  
complexes

Isabelle M. Dixon,\* Jean-Louis Heully, Fabienne Alary and Paul I.P. Elliott\*

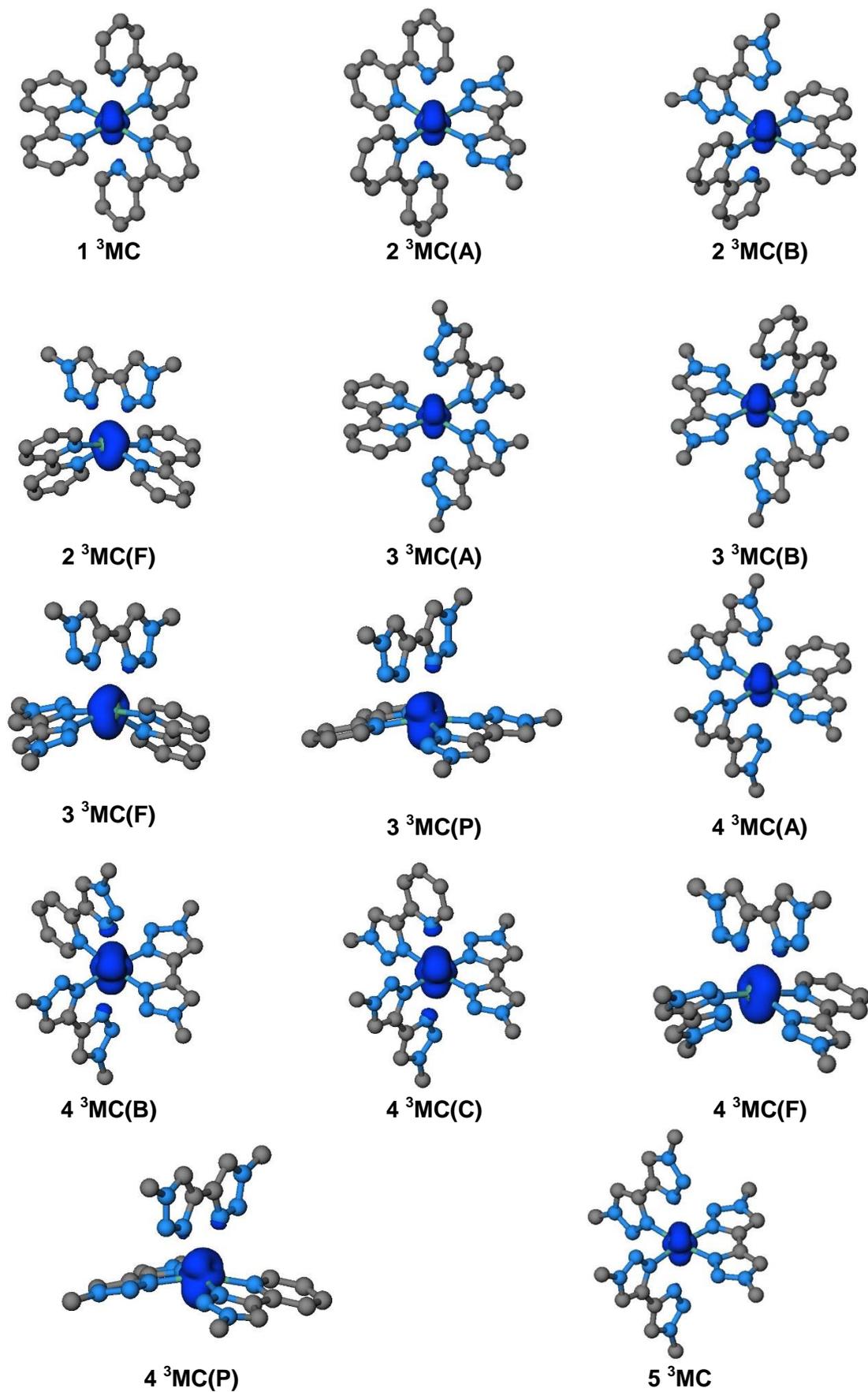
<b>Figure S1.</b> Spin density plots for $^3\text{MLCT}$ states of complexes <b>1</b> to <b>4</b> .	2
<b>Figure S2.</b> Antibonding $d\sigma^*$ orbitals for complexes <b>2</b> to <b>4</b> .	2
<b>Figure S3.</b> Spin density plots of $^3\text{MC}$ states of complexes <b>1</b> to <b>5</b> .	3
<b>Table S1.</b> Structural parameters for classical $^3\text{MC}$ states of complexes <b>1</b> to <b>5</b>	4
<b>Figure S4.</b> Relaxed $^3\text{PES}$ scans for <b>2</b>	5
<b>Figure S5.</b> Relaxed $^3\text{PES}$ scans for <b>3</b>	6
<b>Figure S6.</b> Relaxed $^3\text{PES}$ scans for <b>4</b>	7
<b>Table S2.</b> Energies and key structural parameters for $^3\text{MC}(\text{F})$ , $^3\text{MC}(\text{P})$ and $^1\text{GS}(\text{P})$ states of <b>2</b> , <b>3</b> and <b>4</b>	8
<b>Figure S7.</b> Optimised geometry of <b>3</b> $^3\text{MC}(\text{F}')$	8
<b>Figure S8.</b> Nudged elastic band calculations for <b>2</b>	9
<b>Figure S9.</b> Nudged elastic band calculations for <b>3</b>	9
<b>Figure S10.</b> Nudged elastic band calculations for <b>4</b>	10
<b>Table S3.</b> Computed energies for $^1\text{GS}$ , $^3\text{MLCT}$ and $^3\text{MC}$ states for complexes <b>1</b> to <b>5</b> .	11
Atomic coordinates of $^3\text{MLCT}$ and $^3\text{MC}$ states, $^{1,3}\text{MECP}$ for $^3\text{MC}$ states and $^1\text{GS}(\text{P})$ states	12



**Figure S1.** Spin density plots for  $^3\text{MLCT}$  states of complexes (hydrogen atoms omitted for clarity).



**Figure S2.** Antibonding  $d_{0^*}$  orbitals for the ground states of btz complexes 2 to 4 (hydrogen atoms omitted for clarity).

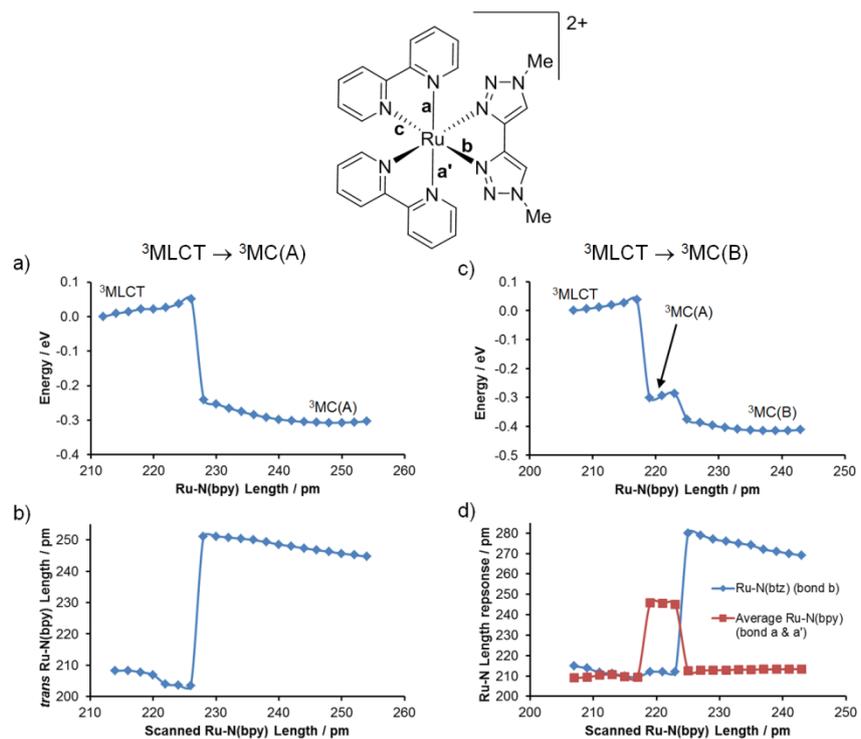


**Figure S3.** Spin density plots of <sup>3</sup>MC states of complexes **1** to **5** (hydrogen atoms omitted for clarity).

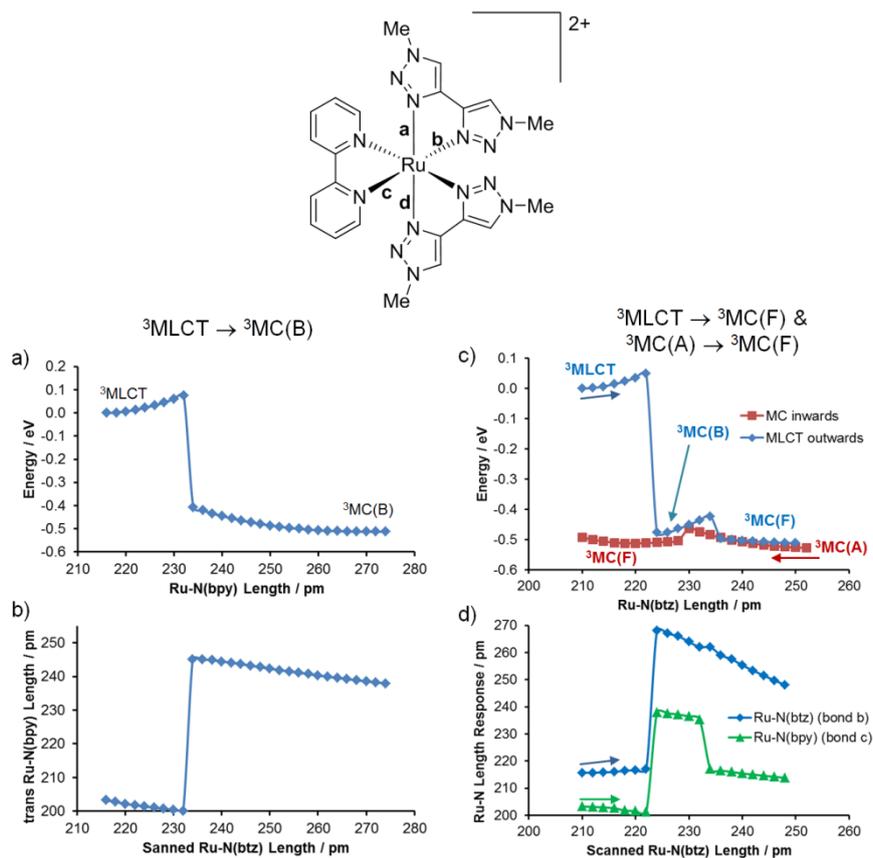
**Table S1.** Structural parameters for classical <sup>3</sup>MC states of complexes **1** to **5** (elongated bond distances in bold).

Complex	Ligand	Ru-N bond length / Å	N-C-C-N dihedral angle / °
<b>1</b>	$\kappa^2$ -bpy	2.11	2.4
	$\kappa^1$ -bpy	2.17, <b>2.46</b>	13.2
<b>2</b>	<sup>3</sup> MC(A)	$\kappa^2$ -btz	2.12
		$\kappa^1$ -bpy	2.15, <b>2.46</b>
	<sup>3</sup> MC(B)	$\kappa^2$ -bpy	2.10 <sup>a</sup> , 2.11 <sup>b</sup>
		$\kappa^1$ -bpy	2.16, <b>2.38</b>
$\kappa^1$ -btz		2.15, <b>2.71</b>	
<b>3</b>	<sup>3</sup> MC(A)	$\kappa^2$ -bpy	2.10
		$\kappa^1$ -btz	2.16, <b>2.54</b>
	<sup>3</sup> MC(B)	$\kappa^2$ -btz	2.11 <sup>a</sup> , 2.11 <sup>b</sup>
		$\kappa^1$ -bpy	2.14, <b>2.38</b>
		$\kappa^1$ -btz	2.13, <b>2.71</b>
<b>4</b>	<sup>3</sup> MC(A)	$\kappa^2$ -pytz	2.14 <sup>c</sup> , 2.08 <sup>d</sup>
		$\kappa^1$ -btz <sup>e</sup>	2.14 <sup>e</sup> , <b>2.54</b>
		$\kappa^1$ -btz <sup>f</sup>	2.15 <sup>f</sup> , <b>2.54</b>
	<sup>3</sup> MC(B)	$\kappa^1$ -pytz	2.16 <sup>c</sup> , <b>2.40<sup>d</sup></b>
		$\kappa^2$ -btz <sup>e</sup>	2.11, 2.11
		$\kappa^1$ -btz <sup>f</sup>	<b>2.66<sup>f</sup></b> , 2.14
			4.2
	<sup>3</sup> MC(C)	$\kappa^1$ -pytz	<b>2.53<sup>c</sup></b> , 2.12 <sup>d</sup>
		$\kappa^1$ -btz <sup>e</sup>	<b>2.57<sup>e</sup></b> , 2.13
$\kappa^2$ -btz <sup>f</sup>		2.11, 2.11	
<b>5</b>	$\kappa^2$ -btz	2.11	
	$\kappa^1$ -btz	2.13, <b>2.54</b>	

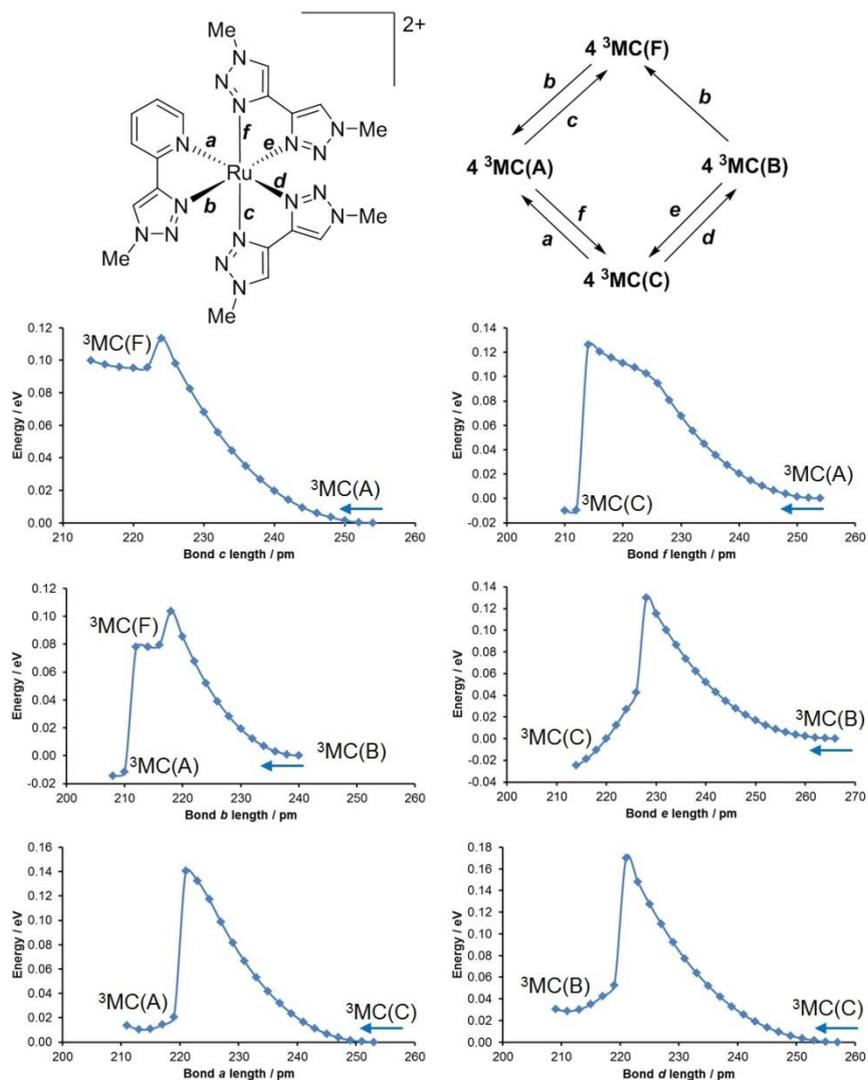
*a* trans to bpy, *b* trans to btz, *c* py, *d* tz, *e* trans to pytz py, *f* trans to pytz tz



**Figure S4.** Relaxed PES scans for **2**: a) PES scan for the elongation of Ru-N(bpy) bond **a**, b) response of the length of Ru-N(bpy) bond **a'** during elongation of bond **a**, c) PES scan for elongation of Ru-N(bpy) bond **c** and d) response of the length of Ru-N(btz) bond **b** and average length of Ru-N(bpy) bonds **a** & **a'** during elongation of bond **c** (energies measured relative to **2**  ${}^3\text{MLCT} = 0$  eV).



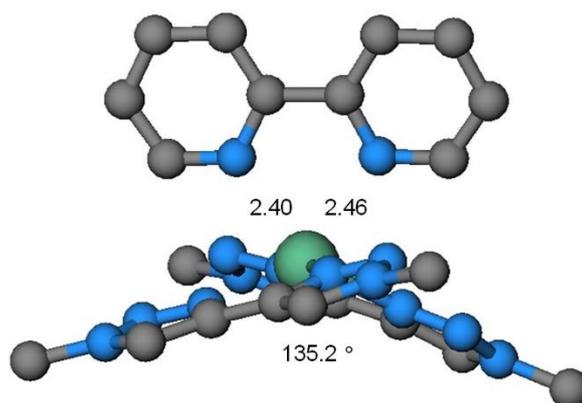
**Figure S5.** Relaxed PES scans for **3**: a) PES scan during adjustment of Ru-N(btz) bond **a** with elongation starting from the  ${}^3\text{MLCT}$  state geometry and contraction starting from the  ${}^3\text{MC(A)}$  state geometry, arrows indicate direction of scan, b) response of lengths of Ru-N(btz) and Ru-N(bpy) bonds **b** and **c** during elongation of bond **a** (arrows indicate direction of PES scan), c) PES scan for Ru-N(btz) bond **b** elongation and d) response of the length of Ru-N(bpy) bond **c** during elongation of bond **a** (energies measured relative to **3**  ${}^3\text{MLCT} = 0.0$  eV).



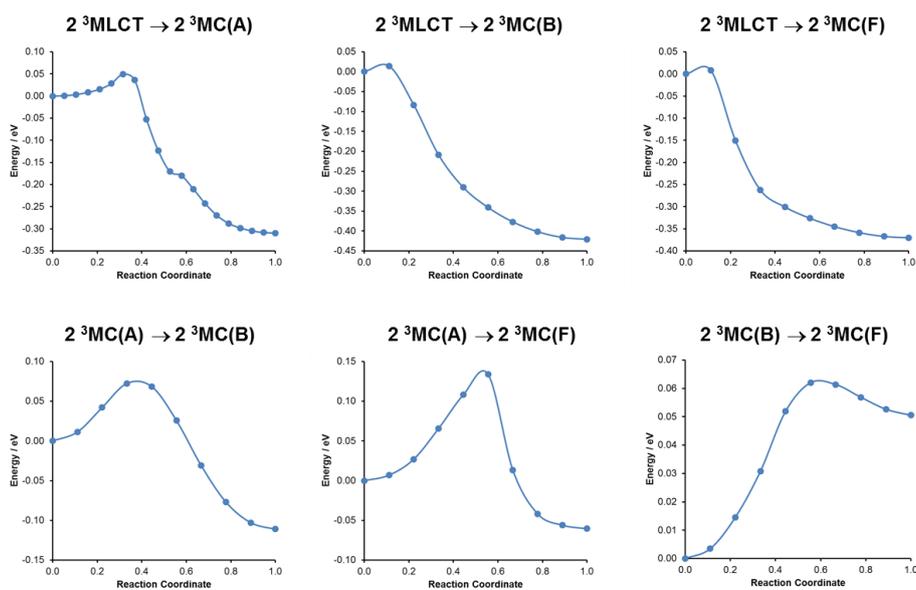
**Figure S6.** Summary of <sup>3</sup>PES scan data for Ru-N bond contractions for <sup>3</sup>MC states of **4** (the reaction scheme summarises the interconversions observed between <sup>3</sup>MC states on contractions of bonds *a* through *f*). Energies in each case measured relative to the energy of the starting geometry of each scan.

**Table S2.** Energies and key structural parameters for flattened and pseudo-pentacoordinate <sup>3</sup>MC states of complexes **2**, **3** and **4** as well as those of pentacoordinate ground states for **3** and **4** (energy quoted relative to the ground state in each case, distances in bold indicate elongated Ru-N bonds).

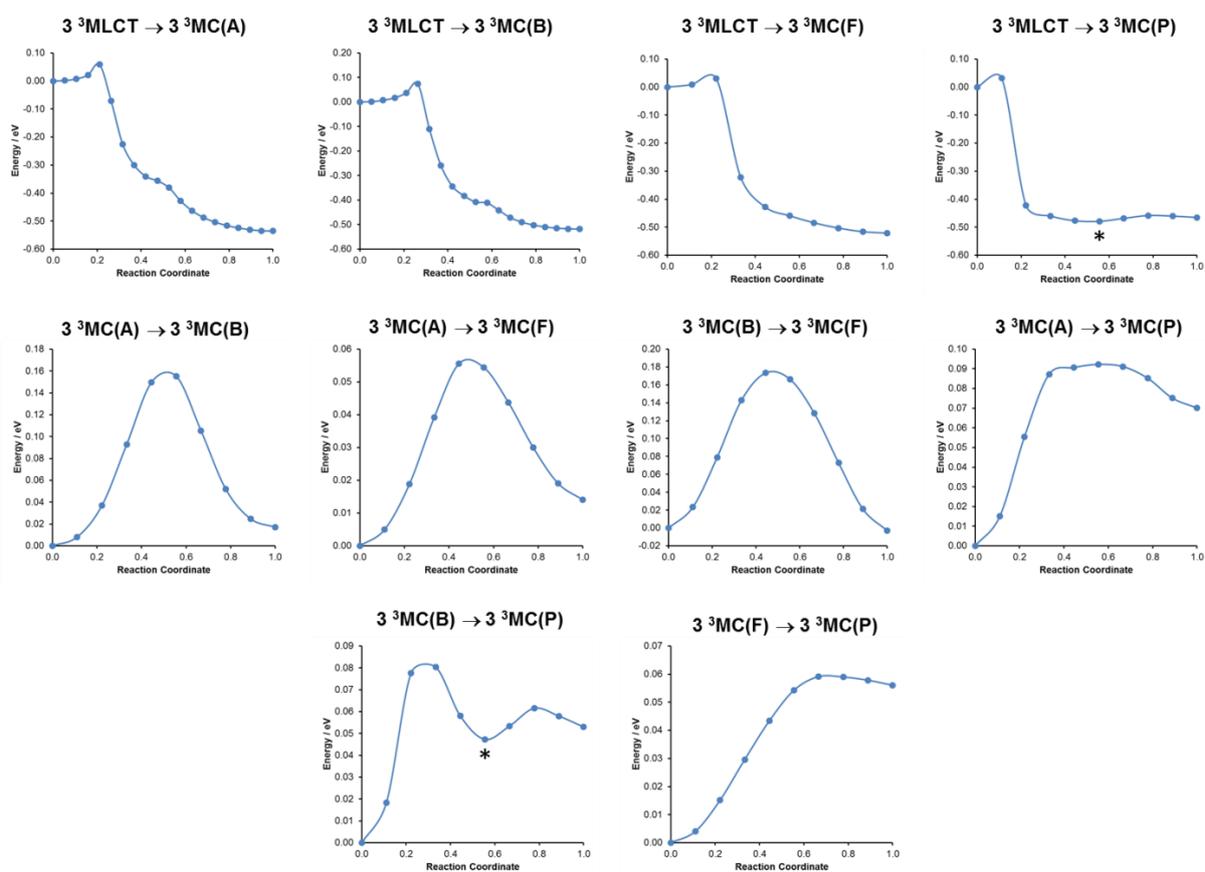
	<b>2</b> <sup>3</sup> MC(F)	<b>3</b> <sup>3</sup> MC(F)	<b>3</b> <sup>3</sup> MC(P)	<b>3</b> <sup>1</sup> GS(P)	<b>4</b> <sup>3</sup> MC(F)	<b>4</b> <sup>3</sup> MC(P)	<b>4</b> <sup>1</sup> GS(P)
Energy / eV	2.04	1.99	2.05	1.67	2.06	2.20	1.74
Ru-N / Å							
<i>distal</i> -btz	<b>2.40</b>	<b>2.46</b>	<b>2.43</b>	2.05	<b>2.39</b>	<b>2.51</b>	2.04
	<b>2.53</b>	<b>2.52</b>	<b>3.20</b>	<b>3.97</b>	<b>2.51</b>	<b>2.77</b>	<b>4.00</b>
bpy	2.19	2.13	2.11	2.09			
	2.16	2.09	2.10	2.10			
	2.11						
	2.10						
pytz					2.12	2.08	2.08
					2.12	2.15	2.13
κ <sup>2</sup> -btz		2.20	2.13	2.11	2.23	2.12	2.10
		2.12	2.15	2.12	2.11	2.15	2.11
θ N-Ru-N / °	124.5	136.1	164.4	170.7	127.9	162.5	169.6



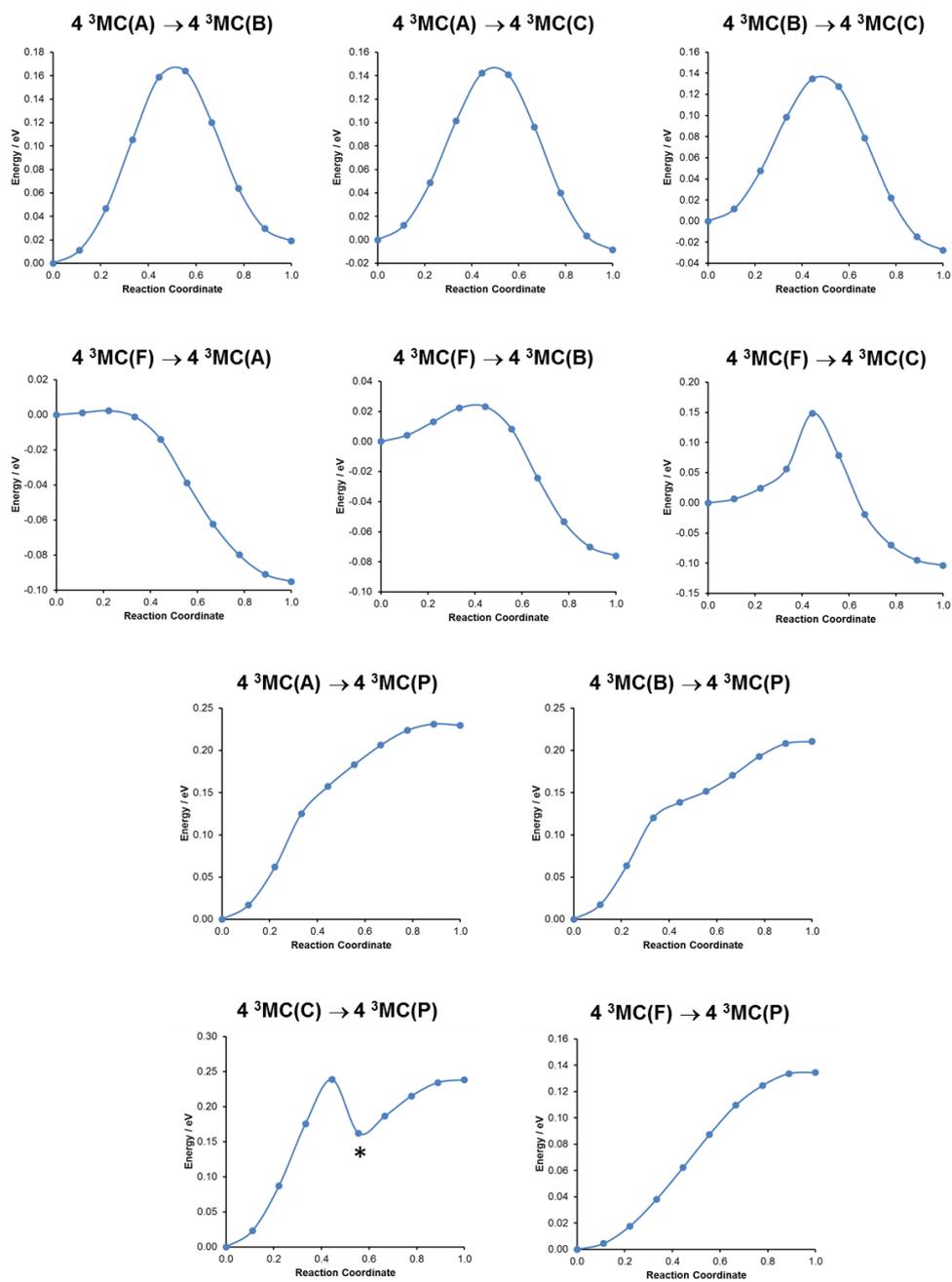
**Figure S7.** Optimised geometry of **3** <sup>3</sup>MC(F') with annotated distances for elongated Ru-N bonds and N-Ru-N angle θ.



**Figure S8.** Energy profiles for nudged elastic band triplet-triplet conversion calculations for **2**.



**Figure S9.** Energy profiles for nudged elastic band triplet-triplet conversion calculations for **3**. (\* The apparent minima in the energy profile for the transits  $3\ ^3\text{MLCT} \rightarrow 3\ ^3\text{MC(P)}$  and  $3\ ^3\text{MC(B)} \rightarrow 3\ ^3\text{MC(P)}$  corresponds to the NEB calculations passing through a transitory MC(F)-like geometry).



**Figure S10.** Energy profiles for nudged elastic band triplet-triplet conversion calculations for **4** (\* The apparent minimum in the energy profile for the transit  $4^3\text{MC}(\text{C}) \rightarrow 4^3\text{MC}(\text{P})$  corresponds to the NEB calculation passing through a transitory MC(F)-like geometry).

**Table S3.** Computed energies (Hartrees) for  $^1\text{GS}$ ,  $^3\text{MLCT}$  and  $^3\text{MC}$  states for complexes **1** to **5**.

State	Energy
<b>1</b> $^1\text{GS}$	-1581.11737278
<b>1</b> $^3\text{MLCT}$	-1581.03282062
<b>1</b> $^3\text{MC}$	-1581.04093744
<b>2</b> $^1\text{GS}$	-1647.65315617
<b>2</b> $^3\text{MLCT}$	-1647.56484803
<b>2</b> $^3\text{MC(A)}$	-1647.57604069
<b>2</b> $^3\text{MC(B)}$	-1647.58010821
<b>2</b> $^3\text{MC(F)}$	-1647.57826809
<b>3</b> $^1\text{GS}$	-1714.1877857
<b>3</b> $^3\text{MLCT}$	-1714.09587627
<b>3</b> $^3\text{MC(A)}$	-1714.11528668
<b>3</b> $^3\text{MC(B)}$	-1714.11474571
<b>3</b> $^3\text{MC(F)}$	-1714.11474225
<b>3</b> $^3\text{MC(P)}$	-1714.11250158
<b>3</b> $^1\text{GS(P)}$	-1714.12644061
<b>4</b> $^1\text{GS}$	-1747.45571466
<b>4</b> $^3\text{MC(A)}$	-1747.3833547
<b>4</b> $^3\text{MC(B)}$	-1747.38270596
<b>4</b> $^3\text{MC(C)}$	-1747.38373255
<b>4</b> $^3\text{MC(F)}$	-1747.37983788
<b>4</b> $^3\text{MC(P)}$	-1747.37469747
<b>4</b> $^1\text{GS(P)}$	-1747.39160559
<b>5</b> $^1\text{GS}$	-1780.72012722
<b>5</b> $^3\text{MLCT-D}_3$	-1780.59350880
<b>5</b> $^3\text{MC}$	-1780.64884702

## Atomic coordinates for 1 <sup>3</sup>MLCT

61

geometry

C	0.11463247	-4.12214193	1.22816229
C	0.96496327	-4.18177911	2.31677706
C	1.59106729	-3.00876564	2.76053022
C	1.32576153	-1.82619561	2.09783324
N	0.48598780	-1.75333968	1.04359106
C	-0.11747868	-2.89817422	0.58170284
C	-0.97052344	-2.73378188	-0.58317160
N	-1.10826178	-1.44622195	-1.04275780
C	-1.91595426	-1.20174719	-2.09624403
C	-2.59975059	-2.20138220	-2.76043159
C	-2.45064711	-3.52362259	-2.31948939
C	-1.63798745	-3.78433429	-1.23168410
N	1.26918673	1.30379256	1.04313163
C	0.90709701	2.07705597	2.08873008
C	1.79598918	2.90060486	2.75136097
C	3.12865012	2.93702310	2.31734536
C	3.50784939	2.16103786	1.23791624
C	2.56622365	1.34598880	0.59023896
C	2.85614785	0.51678077	-0.56664696
C	4.10525154	0.45276516	-1.20396166
C	4.29031186	-0.38761661	-2.28596843
C	3.21879105	-1.17370584	-2.73268915
C	2.00644706	-1.07174141	-2.07905910
N	1.80978488	-0.24341495	-1.03146850
Ru	-0.00077303	0.00024872	-0.00087671
N	-1.77300567	0.45555171	1.02848101
C	-2.45393266	1.55537310	0.56583383
C	-1.87327998	2.21370749	-0.59252743
C	-2.43884468	3.32267093	-1.24018150
C	-1.79691916	3.89638649	-2.32219090
C	-0.57771487	3.35928765	-2.75747800
C	-0.06365276	2.26247003	-2.09338558
N	-0.68922963	1.68506463	-1.04605538
C	-2.26752773	-0.23733509	2.07585868
C	-3.42786959	0.12703413	2.73088886
C	-4.12168141	1.26083576	2.28654361
C	-3.63296099	1.96950993	1.20443463
H	-0.37233463	-5.02257960	0.87775078
H	1.14489758	-5.12601035	2.81723738
H	2.27090362	-3.01329291	3.60303502
H	1.78136749	-0.89544309	2.40940651
H	-1.99519040	-0.16799151	-2.40644928
H	-3.23357318	-1.95277950	-3.60213553
H	-2.96646448	-4.33375893	-2.82147681
H	-1.51716964	-4.80170407	-0.88373049
H	-0.12898435	2.01167287	2.39405972
H	1.45542751	3.49922915	3.58663377
H	3.85465144	3.56650669	2.81836050
H	4.53383260	2.18349442	0.89507771
H	4.92677514	1.06210351	-0.85111104
H	5.25392148	-0.43787345	-2.77923685

H	3.32365529	-1.85134417	-3.57041983
H	1.15054230	-1.65485841	-2.39278420
H	-3.37955155	3.73167603	-0.89604453
H	-2.23281437	4.75239147	-2.82379647
H	-0.03815862	3.78381798	-3.59452153
H	0.87131860	1.81065394	-2.39784760
H	-1.69622113	-1.10147642	2.38895491
H	-3.78111494	-0.46117102	3.56829219
H	-5.03169155	1.57948808	2.78119149
H	-4.16222112	2.84531308	0.85303918

## Atomic coordinates for 1 <sup>3</sup>MC

61			
geometry			
C	2.83411625	-3.08255394	1.35016124
C	3.57995108	-2.45262919	2.33745533
C	3.26424472	-1.14242144	2.68228570
C	2.22489699	-0.51573094	2.01224998
N	1.49458785	-1.12053824	1.05563559
C	1.78220722	-2.40749688	0.72370871
C	0.94739307	-3.04756948	-0.32545566
N	0.15585099	-2.22454707	-1.04257507
C	-0.61500121	-2.73619421	-2.00930660
C	-0.63895468	-4.09043893	-2.32071068
C	0.16243297	-4.95019120	-1.57522303
C	0.96031450	-4.42614365	-0.56439014
N	0.33575107	2.19141875	1.05219894
C	-0.40562216	2.77036411	2.00402215
C	-0.32773422	4.12506810	2.30473729
C	0.54774724	4.91328863	1.56356574
C	1.31629317	4.31960814	0.56856232
C	1.19956310	2.94399956	0.34097582
C	1.99836834	2.23218710	-0.68995520
C	3.11990520	2.81242698	-1.29009258
C	3.83006996	2.12003653	-2.26173951
C	3.40835649	0.84292878	-2.61717212
C	2.30334471	0.30928226	-1.97211208
N	1.60699808	0.97519863	-1.03075803
Ru	-0.03555499	-0.00387628	-0.00380446
N	-1.72645038	-0.74918622	1.01452486
C	-2.93597066	-0.31067505	0.56193146
C	-2.88504776	0.58184604	-0.60548585
C	-4.01658154	1.09060726	-1.24544683
C	-3.87213480	1.92038009	-2.34957731
C	-2.59039023	2.23010109	-2.79642663
C	-1.50352098	1.70064300	-2.11840605
N	-1.63312898	0.89364741	-1.04781387
C	-1.69001847	-1.57200282	2.08022084
C	-2.83158119	-1.99236955	2.74467663
C	-4.07073040	-1.54977174	2.28963624
C	-4.11943984	-0.70379775	1.18940756
H	3.08359047	-4.09331889	1.05714577
H	4.39608848	-2.97502463	2.82314548
H	3.81318974	-0.60751067	3.44748102
H	1.95092786	0.50746717	2.23678263
H	-1.23224626	-2.02860031	-2.55396081
H	-1.27186559	-4.45698261	-3.11986408
H	0.16438358	-6.01615510	-1.77247943
H	1.56901705	-5.09229601	0.03268333
H	-1.08347071	2.11786433	2.54546832
H	-0.94034430	4.54700136	3.09232609
H	0.62912896	5.97772332	1.75183652
H	1.98249002	4.93080853	-0.02595835
H	3.45090033	3.79664256	-0.98741159

H	4.70019696	2.56872313	-2.72693895
H	3.92543654	0.26231391	-3.37116063
H	1.94683821	-0.68607498	-2.20559288
H	-5.00730736	0.83953650	-0.89077488
H	-4.74616767	2.31677326	-2.85306764
H	-2.42953321	2.87128582	-3.65429400
H	-0.49006261	1.91752399	-2.42935700
H	-0.70706009	-1.89359616	2.39830658
H	-2.74495418	-2.65269857	3.59874103
H	-4.98526841	-1.85726189	2.78325925
H	-5.07602041	-0.35087172	0.82779441

## Atomic coordinates for 2<sup>3</sup>MLCT

61

geometry

C	-3.61422835	2.72119337	-1.87753022
C	-2.98113129	3.05607389	-0.69915369
C	-1.94708922	2.24908313	-0.19361199
N	-1.57162820	1.11071002	-0.88368802
C	-2.21216041	0.78576755	-2.03190155
C	-3.22082848	1.55698108	-2.56327422
C	-1.44386629	3.61622229	1.86991961
C	-0.67700241	3.78863679	3.00334889
C	0.32701965	2.85056360	3.30367633
C	0.50399369	1.78004603	2.45261264
N	-0.24779133	1.59239652	1.34667237
C	-1.22354655	2.51113121	1.02666460
C	-0.39893384	-3.83610770	-2.99222791
C	-1.16086836	-3.72586328	-1.84756135
C	-1.02323216	-2.60314503	-1.01040086
N	-0.13426159	-1.60587045	-1.34644946
C	0.61420589	-1.73230054	-2.46317632
C	0.51650523	-2.81687705	-3.30952891
C	-2.70435714	-3.28936051	0.74130321
C	-3.34758777	-3.00539787	1.92777633
C	-3.04452802	-1.81015415	2.60551186
C	-2.11129955	-0.95855646	2.05898300
N	-1.46125714	-1.23200807	0.90284122
C	-1.74915816	-2.39961312	0.22022992
N	1.62835232	2.14362353	-1.60265605
N	2.91903962	2.43941113	-1.74022163
C	3.71004117	1.57751948	-1.05211531
C	2.83224331	0.69740939	-0.46014752
N	1.57259404	1.09126031	-0.83433539
N	1.82605250	-1.98939162	1.57893602
N	3.13907120	-2.16948671	1.70545808
C	3.84453207	-1.24565279	1.00491962
C	2.88702602	-0.44891226	0.41817104
N	1.67063652	-0.94959484	0.80719382
C	3.32749221	3.57933086	-2.57035571
C	3.65314697	-3.28277729	2.51274936
Ru	-0.09016301	-0.00140657	-0.00128404
H	-4.40868518	3.34672265	-2.26705207
H	-3.28199259	3.94545823	-0.16122435
H	-1.88071252	-0.12015964	-2.52053902
H	-3.69498568	1.25836732	-3.48933149
H	-2.21693783	4.33417982	1.62937720
H	-0.84792293	4.63828058	3.65383014
H	0.94861077	2.94961535	4.18443954
H	1.25195896	1.02279563	2.65256606
H	-0.50629002	-4.69949324	-3.63822179
H	-1.86600126	-4.50646713	-1.59375047
H	1.29192757	-0.91474437	-2.67567642
H	1.13104299	-2.86534532	-4.19945981
H	-2.93663666	-4.20241289	0.20901075

H	-4.08116878	-3.69447350	2.32933198
H	-3.52985163	-1.54895995	3.53710093
H	-1.85085106	-0.02652171	2.54135979
H	4.78453350	1.66113763	-1.03938022
H	4.92205095	-1.23451411	0.98198940
H	3.90148973	3.22429741	-3.42563017
H	3.92664405	4.26678491	-1.97469641
H	2.42295872	4.07557901	-2.91091490
H	4.11292380	-4.02605909	1.86223380
H	2.81011938	-3.72181762	3.03904717
H	4.38263942	-2.90655841	3.22824082

### Atomic coordinates for 2<sup>3</sup>MC(A)

61			
geometry			
C	3.61237421	-2.71986075	-2.08212490
C	2.89668268	-3.21523206	-1.00053973
C	1.87850338	-2.45322536	-0.42135061
N	1.59476000	-1.21226307	-0.89554539
C	2.29473020	-0.73654234	-1.94148136
C	3.30170151	-1.45464036	-2.56776151
C	1.12371694	-4.27312864	1.16906292
C	0.37555677	-4.65029988	2.27797623
C	-0.40138339	-3.69600877	2.92861727
C	-0.40552438	-2.40102308	2.42496452
N	0.31620157	-2.03095164	1.36097821
C	1.08651589	-2.94322297	0.73568163
C	0.42110370	4.64531826	-2.29042698
C	1.16909596	4.26154091	-1.18370398
C	1.11559302	2.93377959	-0.74556636
N	0.33048253	2.03001553	-1.36485634
C	-0.39090324	2.40647040	-2.42686461
C	-0.37181036	3.69977096	-2.93447695
C	2.93260472	3.18924043	0.98619537
C	3.64568537	2.68782594	2.06679810
C	3.32394461	1.42597885	2.55391621
C	2.30865961	0.71726766	1.93036816
N	1.61062344	1.19927883	0.88603061
C	1.90557458	2.43696689	0.41000316
N	-1.73066458	-1.94779456	-1.72114384
N	-3.03780439	-2.13264425	-1.90821978
C	-3.78006694	-1.28030862	-1.15787059
C	-2.85622144	-0.52532450	-0.47135194
N	-1.61450795	-0.97632402	-0.85477065
N	-1.70518471	1.96839802	1.72676374
N	-3.00970685	2.16594880	1.91875161
C	-3.76304549	1.31909324	1.17314148
C	-2.84916126	0.55461247	0.48389307
N	-1.60166741	0.99473266	0.86117356
C	-3.50793561	-3.17405421	-2.82697718
C	-3.46636645	3.20572522	2.84610642
Ru	0.06148249	0.00148246	-0.00135167
H	4.40262707	-3.31023236	-2.53129806
H	3.14495018	-4.18842981	-0.59968454
H	2.02410225	0.25637639	-2.27703493
H	3.82943519	-1.02225148	-3.40884838
H	1.71596147	-5.01445744	0.64945755
H	0.39858373	-5.67649320	2.62642256
H	-0.99180421	-3.94619466	3.80180773
H	-1.00261811	-1.62335076	2.89128805
H	0.45660738	5.67012299	-2.64211590
H	1.77386400	4.99650336	-0.66953079
H	-1.00028759	1.63550401	-2.88830987
H	-0.96319802	3.95547305	-3.80541844
H	3.18950245	4.15963104	0.58398881
H	4.44240947	3.27094091	2.51408277

H	3.84930771	0.98907487	3.39415151
H	2.02958497	-0.27305157	2.26667152
H	-4.85766032	-1.28174127	-1.17544226
H	-4.84049996	1.33060375	1.19522401
H	-4.20430385	-2.74125452	-3.54393193
H	-3.99555815	-3.97035426	-2.26517907
H	-2.63929096	-3.56742110	-3.34792686
H	-4.02238658	3.96772737	2.30081420
H	-2.58426860	3.64692191	3.30205238
H	-4.09669861	2.76067011	3.61506755

**Atomic coordinates for 2<sup>3</sup>MC(B)**

61

geometry

C	1.82365396	-4.61845043	-1.66895418
C	1.16372979	-4.41564472	-0.46180805
C	0.83653437	-3.11445205	-0.07002199
N	1.14707266	-2.05813959	-0.84736974
C	1.78626589	-2.25634836	-2.00420132
C	2.14587051	-3.51988982	-2.45894188
C	-0.14073134	-3.77109553	2.16854538
C	-0.77456142	-3.41587590	3.35185314
C	-1.11364524	-2.08255531	3.55865056
C	-0.80424385	-1.16141809	2.56932924
N	-0.18831724	-1.50022176	1.42111472
C	0.14690264	-2.79919599	1.20606107
C	1.74066245	3.49496083	-3.14323340
C	2.49280533	3.10477485	-2.04331913
C	2.01732592	2.10272030	-1.19606721
N	0.81435270	1.50448297	-1.43014087
C	0.09311520	1.88777137	-2.50124894
C	0.51839350	2.87128383	-3.37979692
C	3.98066575	2.11020156	0.39741718
C	4.60670727	1.56516427	1.51068787
C	3.98952666	0.51454678	2.18319295
C	2.76775825	0.05306640	1.71846790
N	2.15029144	0.57940961	0.64509978
C	2.75037035	1.60404326	-0.02373618
N	-2.20094665	-1.23052417	-1.49069643
N	-3.51324381	-1.06415870	-1.63554779
C	-3.95353525	0.02363406	-0.95909595
C	-2.82785302	0.55560309	-0.36542830
N	-1.77975025	-0.25311026	-0.72574520
N	-1.36470895	2.95654299	1.77940174
N	-2.58757838	3.49831142	1.69237007
C	-3.39561468	2.75358534	0.90220183
C	-2.60134318	1.70040558	0.49498598
N	-1.36901725	1.87104477	1.06055061
C	-4.29059630	-2.00706955	-2.44454671
C	-2.89790146	4.73839574	2.40677884
Ru	0.25243123	0.00867153	-0.06569358
H	2.08301371	-5.62249737	-1.98481657
H	0.90888943	-5.26801847	0.15367033
H	2.01665764	-1.36817623	-2.58342402
H	2.66392710	-3.63392674	-3.40344284
H	0.13647320	-4.80322870	2.00332897
H	-0.99481858	-4.16834323	4.10036708
H	-1.60497753	-1.75505094	4.46659978
H	-1.04435550	-0.11134365	2.68217755
H	2.10519979	4.27066336	-3.80660995
H	3.44751454	3.57646873	-1.85294777
H	-0.85018875	1.37743775	-2.64439201
H	-0.09865966	3.13930733	-4.22854699
H	4.45006614	2.92691490	-0.13449440
H	5.56093800	1.95439577	1.84610686

H	4.44164596	0.05658693	3.05424072
H	2.25388063	-0.76136336	2.21111363
H	-4.99054553	0.31703368	-0.94648300
H	-4.41924156	3.02578742	0.70179739
H	-4.78181100	-1.47587305	-3.25907690
H	-5.03362546	-2.50229193	-1.82020745
H	-3.59817285	-2.74114725	-2.84750273
H	-3.19586300	5.51075498	1.69826590
H	-1.99546096	5.04570888	2.92856980
H	-3.69768859	4.56292818	3.12574406

### Atomic coordinates for 2<sup>3</sup>MC(F)

61

geometry

C	1.17272543	-4.12808083	2.90337671
C	-0.10528134	-3.86904275	2.42101165
C	-0.33679287	-2.72343692	1.65884424
N	0.67208685	-1.85549739	1.38737613
C	1.90230387	-2.11051191	1.85797393
C	2.19885296	-3.23320098	2.61748524
C	-2.77843471	-3.19515165	1.19706814
C	-3.99375160	-2.78395164	0.66500490
C	-4.06906967	-1.53802427	0.05044884
C	-2.92571498	-0.75473656	-0.00714741
N	-1.74630575	-1.14273667	0.51179692
C	-1.66246071	-2.36054790	1.11474492
C	4.04157020	2.77539203	0.38799265
C	2.85898777	3.18298692	0.99162223
C	1.74499963	2.34211549	0.97995993
N	1.79755955	1.12190048	0.37777028
C	2.94626407	0.73604299	-0.20719670
C	4.08627601	1.52596486	-0.22288428
C	0.24814102	3.84789056	2.35669500
C	-0.99878415	4.09051106	2.92120609
C	-2.02118154	3.16731804	2.72549925
C	-1.75397491	2.03540741	1.96995353
N	-0.55264693	1.79521974	1.41916533
C	0.45397853	2.69163327	1.60414155
Ru	0.02723440	-0.01051453	0.38995776
N	1.14382164	-2.30419605	-1.83368317
N	1.17119518	-2.52924634	-3.14996650
C	0.60380585	-1.50778214	-3.83546724
C	0.21552874	-0.60980287	-2.86332414
N	0.56918415	-1.14476893	-1.65784644
N	-1.31206327	2.40247556	-1.84441381
N	-1.38189513	2.60416134	-3.16555164
C	-0.85067794	1.56174296	-3.84864239
C	-0.43782315	0.68255731	-2.86930232
N	-0.74290322	1.24361861	-1.66398618
C	1.71749433	-3.78322371	-3.67361406
C	-1.99086245	3.82508047	-3.69718604
H	1.36032421	-5.01385435	3.49938492
H	-0.91102347	-4.55305917	2.65148033
H	2.66680432	-1.38276960	1.61587480
H	3.20796887	-3.39449677	2.97621216
H	-2.70308477	-4.16607170	1.66790330
H	-4.86369765	-3.42733126	0.72710506
H	-4.99332354	-1.17439923	-0.38167585
H	-2.93081626	0.21560046	-0.48687902
H	4.91044702	3.42309272	0.39411633
H	2.80772192	4.15449225	1.46460185
H	2.93008692	-0.23818725	-0.67875730
H	4.98510796	1.16439036	-0.70719199
H	1.05209073	4.55428491	2.51445037
H	-1.16535338	4.98530081	3.50988284

H	-3.00667475	3.31448803	3.14985467
H	-2.51683058	1.28747193	1.79646729
H	0.52443954	-1.50534449	-4.91033233
H	-0.80850549	1.53707772	-4.92543501
H	2.25462009	-3.58354060	-4.59915496
H	0.91137294	-4.49367530	-3.85779034
H	2.40146519	-4.18660546	-2.93137524
H	-1.29555529	4.31846114	-4.37530050
H	-2.20672415	4.47623190	-2.85429704
H	-2.91471380	3.58320434	-4.22244875

## Atomic coordinates for 2<sup>3</sup>MECP(A)

61

Coordinates from ORCA-job 2Mca\_GS\_MECP\_defSD

C	3.70347692671117	2.63760085548934	1.88406414073054
C	2.90983860204549	3.12906059566783	0.85558827643778
C	1.83392372037163	2.38232208401805	0.36600952339919
N	1.58410707812693	1.14191267130480	0.86423761373570
C	2.36493053928769	0.66707921873847	1.85761401968446
C	3.42008658540892	1.37941849015491	2.40383075271182
C	0.74355377876611	4.30057632867616	-0.83815800065218
C	-0.02539922304984	4.77174778246519	-1.89919058229717
C	-0.54615856180483	3.85825129134371	-2.80950619585471
C	-0.28206290560505	2.50582536709427	-2.60793758488074
N	0.45382422522494	2.04198657841975	-1.59354970027427
C	0.97583499548565	2.92518584397080	-0.72493689467769
C	0.86613445926318	-4.81636427429813	2.63334256285303
C	1.58122744527490	-4.36891842561785	1.52785952380355
C	1.19172154241644	-3.18184048544639	0.89747416900383
N	0.15222620186871	-2.45982433848200	1.35177650380908
C	-0.53585558976173	-2.89884897045406	2.41047375056225
C	-0.22501123005364	-4.07761697111669	3.08111779517833
C	2.83555626369193	-3.38271173969183	-1.00534372828887
C	3.48367350535230	-2.83079402418967	-2.10293126968735
C	3.17312125084222	-1.52987266848071	-2.47994499572309
C	2.22418709591203	-0.83720776342690	-1.74337875055034
N	1.58761621626339	-1.36809705230687	-0.67920063451999
C	1.89364906383724	-2.63474996987486	-0.29268051954075
N	-1.63591493749899	2.03446373329198	1.66457933777536
N	-2.91541106656097	2.40086450279443	1.70919501175496
C	-3.69244515958790	1.62737780140270	0.90783023384386
C	-2.82103173076316	0.72526099308902	0.34217647953569
N	-1.57167634362523	1.02011957643437	0.84002572311318
N	-1.79977874766786	-2.00758464421373	-1.61885800983311
N	-3.08033706642045	-2.01284730938602	-1.98315440527355
C	-3.78771253238026	-1.03368149007915	-1.36280891034752
C	-2.86558043116956	-0.39099387059659	-0.56836095170730
N	-1.66289972630172	-1.02878329247348	-0.76379041940390
C	-3.34040587174480	3.50051914243152	2.58082949675877
C	-3.57541987686120	-3.02773992443162	-2.92008064193892
Ru	0.02999036801341	-0.15908451308167	0.21519983036571
H	4.53552995065073	3.22070960966528	2.26231474134448
H	3.13816948028469	4.08790228533981	0.40805125770850
H	2.12342561710645	-0.32512173549344	2.21917747590586
H	4.00839142746697	0.94449338293331	3.20256516431665
H	1.13897199266568	4.99345474975514	-0.10550506386422
H	-0.21411118063205	5.83407413586691	-2.01150610044157
H	-1.14053030203038	4.18240177533049	-3.65594324523255
H	-0.671111407729659	1.75884538327314	-3.29400948083424
H	1.16048759707589	-5.73085362719187	3.13585646432598
H	2.43611817775065	-4.93518643097350	1.18238799850820
H	-1.36889247589914	-2.28055367573385	2.73276811273485
H	-0.81322625384998	-4.39793149180672	3.93290040694111
H	3.06009438059911	-4.39855362130654	-0.71052817360253
H	4.21284754804800	-3.41213550411647	-2.65604740732923

H	3.65250523095872	-1.05251043003696	-3.32574543140712
H	1.93591779882027	0.17403229797342	-2.00160637961500
H	-4.75615894816556	1.77725625766118	0.81543074426408
H	-4.84020924959888	-0.87949532162900	-1.53786636244719
H	-4.03909833337836	3.12421003683113	3.32797147544455
H	-3.81274071441006	4.27953769994032	1.98282600324507
H	-2.45446946749061	3.89464721109949	3.07180067660237
H	-4.14223416760437	-3.78390515353209	-2.37641086099715
H	-2.71498373984111	-3.48420480863599	-3.40194710597377
H	-4.20826951453714	-2.54820878435229	-3.66600194920276

## Atomic coordinates for 2<sup>3</sup>MECP(B)

61

Coordinates from ORCA-job 2MCb\_GS\_MECP\_defSD

C	1.83248514468416	-4.91617430665097	-1.48721667861218
C	1.10929326043115	-4.60869230870462	-0.33842520714507
C	0.90280607109025	-3.26665021261468	-0.00332994552711
N	1.36876611970812	-2.27104604581323	-0.77973731450321
C	2.06489904104271	-2.57217826606340	-1.88034634114702
C	2.32959735583664	-3.88070100534312	-2.27188305289795
C	-0.12760436117582	-3.72642168561959	2.25283241958632
C	-0.78047280064988	-3.27561346402271	3.39300973976989
C	-1.11309851223582	-1.92853589642123	3.48532214597038
C	-0.77643355245153	-1.08974192710448	2.43380168675633
N	-0.14488624122772	-1.52004868074143	1.32258814710940
C	0.18248667239248	-2.83614130814430	1.22109365377357
C	1.68880326611061	3.53700370168584	-3.20713493125936
C	2.45852456017386	3.14653925440451	-2.11962404334633
C	2.02758799838521	2.10211687824380	-1.30120324113991
N	0.84566719075653	1.46264239757853	-1.54671988459449
C	0.10509480320346	1.84947089278182	-2.60525086969226
C	0.48990250404036	2.87288433264201	-3.45650943601399
C	3.97786280292618	2.15379101448516	0.31007441543864
C	4.62569387717788	1.58778206539487	1.40127691836787
C	4.07280297516317	0.46291126902660	2.00845329979428
C	2.88799855453247	-0.05035936032744	1.50462369107674
N	2.24428401741343	0.50079598912934	0.45870808288453
C	2.78600289911067	1.59349462295564	-0.15083129609175
N	-2.16753873545394	-1.03649879886300	-1.58625478696788
N	-3.46648881668876	-0.81404706186091	-1.74440049193550
C	-3.88346121905050	0.23409079983477	-0.99707731172381
C	-2.75674348682432	0.68528496500399	-0.33791166276355
N	-1.72958791495528	-0.13178226205692	-0.73824562809852
N	-1.54137397867981	3.00754224306393	2.05957406333630
N	-2.78966157422040	3.48311954250107	1.91363941127577
C	-3.48508269491671	2.74908806144690	1.01738585524811
C	-2.59288330635031	1.77741490130292	0.60424529816495
N	-1.41753230158967	1.97921341371552	1.27157602148152
C	-4.26036474736793	-1.67688589726676	-2.62488086862232
C	-3.25037757220349	4.61625210297087	2.71739525719172
Ru	0.33697754973312	-0.06626459660578	-0.22789201203960
H	2.00606379499540	-5.95006066968732	-1.76499937886318
H	0.70783940226505	-5.40756571957606	0.27148461937364
H	2.42784609842067	-1.73220769973398	-2.46405263901457
H	2.90390955269801	-4.07939721929622	-3.16876707604987
H	0.16214251672156	-4.76598959771384	2.17812159359921
H	-1.01747914511913	-3.96389103495962	4.19655750344038
H	-1.61730564035057	-1.52392190302128	4.35468437185855
H	-1.00896241873211	-0.03228747653013	2.46282736417485
H	2.02160760168168	4.34345710279100	-3.85066715215424
H	3.39633159912793	3.64710465882481	-1.91892524968964
H	-0.81872560282308	1.30885745616769	-2.76259137531492
H	-0.14145283166246	3.14163456983445	-4.29462628173791
H	4.39893895345185	3.02679450118977	-0.17076213023682
H	5.54686725366483	2.02085703535906	1.77326139767830

H	4.55068450572528	-0.01481219287448	2.85480934161171
H	2.42381299876794	-0.92296252686728	1.94347004222400
H	-4.90941207832708	0.56446084848873	-0.98162214769935
H	-4.50545680617449	2.97416500013815	0.75197754965050
H	-4.84210088588279	-1.05990420121592	-3.30871015640830
H	-4.92484738826880	-2.30105424124606	-2.02685579321574
H	-3.56996325705848	-2.30227071640151	-3.18478484286309
H	-3.70275897836505	5.36821741857958	2.07129677532751
H	-2.38255732816525	5.03441563612611	3.22172841055120
H	-3.97532199446147	4.27590291768083	3.45757268065327

## Atomic coordinates for 2<sup>3</sup>MECP(F)

61

Coordinates from ORCA-job 2MCflat\_GS\_MECP\_defSD

C	1.17958377658535	-4.13464821968424	2.37514643052717
C	-0.12238207544827	-3.83145271049510	1.99530310326446
C	-0.42270865387525	-2.56260439184244	1.50363268583696
N	0.55002090226874	-1.61724152257581	1.37433809757453
C	1.80312516827480	-1.91189165430320	1.76394344102509
C	2.15940245722278	-3.15257468580931	2.26986744058038
C	-2.91220441286772	-2.93654743140362	1.23313083814047
C	-4.14798211309817	-2.45046943552259	0.82637256368224
C	-4.21932348460669	-1.17791788497729	0.26772300888335
C	-3.05353050085227	-0.43502223944016	0.15362049064620
N	-1.85517612976823	-0.89154730367932	0.56295741447272
C	-1.77276786979729	-2.14393247745981	1.09040860908040
C	4.05114536947845	2.79412060414804	0.66988136245660
C	2.88104298731476	3.23171306823930	1.27824356853274
C	1.71645309305973	2.46867199223442	1.18133584319739
N	1.71431401678836	1.28661277515611	0.50400662191754
C	2.84405529990995	0.88298810783435	-0.10792087023048
C	4.02875913936475	1.60339971784005	-0.04961536388571
C	0.26799261765859	4.04670977783295	2.53359451639835
C	-0.97013163483400	4.34042076696921	3.09567863359289
C	-2.02241354150224	3.44795453894975	2.92231331930264
C	-1.79507754999953	2.29927089109033	2.17757143900308
N	-0.60632461387783	2.01484347421861	1.62337472701423
C	0.43267545218107	2.87013077748385	1.80060062515722
Ru	-0.07729242675800	0.19341230013006	0.47087744363860
N	1.57721241845115	-2.62728071267573	-2.08844680836712
N	1.42801324837072	-2.80934832806825	-3.40985977522458
C	0.72379199678453	-1.79461829896919	-3.96111587512543
C	0.43858873926290	-0.95861905020983	-2.89986354117331
N	0.98213425533435	-1.51105050110897	-1.77790452716217
N	-1.24353994213862	1.99200187164345	-1.80058943929909
N	-1.42292756948087	2.11655853219877	-3.11361782924815
C	-0.85476683845090	1.08954326673983	-3.78699421092006
C	-0.29585351858500	0.28718523441343	-2.81339676084973
N	-0.56298176386564	0.88579685016005	-1.61132180347934
C	2.02337492280177	-3.97114949717777	-4.07139916854396
C	-2.12616299223130	3.27804088586025	-3.66222322397644
H	1.42349909370448	-5.11970734158041	2.75625443086845
H	-0.89475648117771	-4.58470543542455	2.07975518063956
H	2.53454490121119	-1.12200983212130	1.65780531417824
H	3.18313629158281	-3.34211085737172	2.56880324459557
H	-2.84097154213905	-3.92464254251623	1.66817346073443
H	-5.03895870371570	-3.05635814402725	0.94479497503426
H	-5.15867191641940	-0.76017005155086	-0.07412315517559
H	-3.05719683313052	0.55800405510882	-0.27908892294086
H	4.96034030154503	3.37851001723243	0.75413411492835
H	2.88256280053722	4.16379868012039	1.82684563680648
H	2.76871006505549	-0.04816730528158	-0.65520241827431
H	4.91020105599176	1.22914192655106	-0.55623698706203
H	1.09246160633465	4.73272662677903	2.67457521328854
H	-1.10804985598347	5.25134686418631	3.66713755079559

H	-2.99868707425696	3.63599650431327	3.35247787343200
H	-2.58368618760912	1.57463564854003	2.01557742722850
H	0.48633989377694	-1.75726539964261	-5.01238413789610
H	-0.88768205452923	1.01158380588738	-4.86213433814427
H	2.78165839807233	-3.64494578444581	-4.78357733300861
H	1.25241502403665	-4.54345743734412	-4.58786123373798
H	2.48479499539419	-4.58378170757600	-3.30079561125222
H	-1.41518907156114	3.94978316910450	-4.14441513311196
H	-2.61835894652805	3.79016511288923	-2.83943181245620
H	-2.86906154926733	2.94249679042976	-4.38515787590954

### Atomic coordinates for 3<sup>3</sup>MLCT

61

geometry

C	-0.81883153	3.89615068	2.79337521
C	-0.49150337	4.02130222	1.47415949
C	-0.25511958	2.86742305	0.67193128
N	-0.36065679	1.59660649	1.26974013
C	-0.69328942	1.50217904	2.57921831
C	-0.92520490	2.59737567	3.37168535
C	0.22747662	4.03556887	-1.50459487
C	0.56293654	3.92394119	-2.82300045
C	0.75233792	2.63139969	-3.39365561
C	0.59002251	1.52813231	-2.59492176
N	0.25120272	1.60875888	-1.28623083
C	0.06471502	2.87359173	-0.69586472
N	0.12118841	-2.33487891	-2.13221547
N	1.08287084	-3.10957880	-2.63660110
C	2.30196541	-2.78580767	-2.13733182
C	2.05792608	-1.74385203	-1.27146179
N	0.70681030	-1.50813965	-1.31101400
N	2.82679589	0.74526352	1.09646031
N	4.06932328	0.31489936	0.89985223
C	4.11825409	-0.69746624	-0.00404060
C	2.80852881	-0.89511031	-0.37526133
N	2.06411231	0.01596084	0.33135458
C	0.75584782	-4.13317053	-3.63460981
C	5.18135147	0.93182296	1.63167099
N	0.02869611	-2.32058899	2.14448293
N	-0.88020880	-3.15076070	2.65849816
C	-2.11781724	-2.91353006	2.15600879
C	-1.94269938	-1.86693879	1.27914818
N	-0.60998714	-1.54255418	1.31539922
N	-2.87625825	0.55368034	-1.10073257
N	-4.08823020	0.04671398	-0.89642462
C	-4.06933072	-0.96228044	0.01229921
C	-2.74832472	-1.07463301	0.37900813
N	-2.06587975	-0.12179987	-0.33517882
C	-0.48272943	-4.15443709	3.65121037
C	-5.23901775	0.58277988	-1.63182863
Ru	-0.00425337	0.05282146	-0.00321117
H	-0.99521194	4.77685338	3.39960529
H	-0.40676158	5.00330874	1.02695360
H	-0.74514993	0.49859862	2.98220724
H	-1.17152062	2.46562834	4.41723299
H	0.08036687	5.01269020	-1.06292353
H	0.68317712	4.81061184	-3.43423983
H	1.00798345	2.50976982	-4.43818095
H	0.70612500	0.52757918	-2.99206881
H	3.20284482	-3.30120919	-2.42761808
H	5.04196677	-1.16968457	-0.29557239
H	1.19553797	-5.08417189	-3.33751677
H	1.13688265	-3.83343643	-4.61053723
H	-0.32651000	-4.22156054	-3.67238660
H	5.90358706	1.33689543	0.92400677

H	5.65654838	0.18913760	2.27167053
H	4.76723766	1.73303814	2.23747542
H	-2.98286267	-3.48398989	2.45233249
H	-4.96021722	-1.49025705	0.31022118
H	-1.01179067	-3.97569717	4.58663943
H	0.58759681	-4.05251590	3.80841587
H	-0.70995739	-5.15208952	3.27692796
H	-5.62485459	-0.17422572	-2.31390824
H	-4.89359666	1.44659097	-2.19315111
H	-6.01242896	0.88380310	-0.92651658

### Atomic coordinates for 3<sup>3</sup>MC(A)

61

geometry

C	-4.26351706	-0.12823735	2.71272847
C	-4.28563852	0.20578278	1.36494172
C	-3.09926557	0.20547529	0.63112306
N	-1.91548743	-0.12347977	1.22001102
C	-1.90240181	-0.44402240	2.52626512
C	-3.04844144	-0.45764257	3.30596423
C	-4.12275745	0.84266401	-1.59206397
C	-3.94451262	1.15124293	-2.93430008
C	-2.65497680	1.16537427	-3.45749432
C	-1.59267940	0.87392603	-2.61599838
N	-1.75656499	0.57574802	-1.31467597
C	-3.01548237	0.55434703	-0.79408212
N	2.10939865	-0.35482221	-2.06910618
N	3.10314835	0.34156524	-2.61839780
C	3.11536996	1.62345275	-2.17797797
C	2.05475864	1.70824054	-1.30173773
N	1.47148154	0.46686163	-1.27460776
N	0.03451251	3.52086825	0.95153103
N	0.87394086	4.51190118	0.62253964
C	1.80223588	4.09163901	-0.26983090
C	1.49555146	2.76382434	-0.48278103
N	0.40793771	2.46723373	0.28788820
C	4.01026466	-0.29936737	-3.57328702
C	0.71039062	5.84237972	1.21073013
N	2.01274974	-0.17930111	2.19200460
N	2.76982205	-1.09770467	2.79000135
C	2.48645383	-2.34509638	2.34158445
C	1.48810634	-2.16872200	1.40773461
N	1.23498418	-0.82134538	1.35763244
N	-0.79275675	-3.43538728	-0.96659696
N	-0.24620282	-4.60217914	-0.59935283
C	0.70687645	-4.42073834	0.34585090
C	0.72949900	-3.05703108	0.55151078
N	-0.20571509	-2.50378692	-0.27558604
C	3.75349430	-0.69680590	3.79853751
C	-0.70381374	-5.85369853	-1.20530022
Ru	-0.21622122	0.02160723	-0.00217301
H	-5.18046296	-0.12695932	3.29052318
H	-5.22225413	0.47258268	0.89393992
H	-0.93524551	-0.68790534	2.94512634
H	-2.98329220	-0.71944688	4.35478474
H	-5.12071363	0.81941450	-1.17515098
H	-4.80000838	1.37290410	-3.56169892
H	-2.46943852	1.39547593	-4.49933801
H	-0.57371602	0.86780223	-2.97930725
H	3.84672605	2.34256556	-2.50875357
H	2.56679401	4.74393107	-0.65937226
H	3.96546042	0.21954040	-4.53028650
H	3.68151309	-1.32770619	-3.69679942
H	5.02866094	-0.27944094	-3.18624156
H	0.50448539	6.57231506	0.42821883

H	1.61276118	6.12170561	1.75385554
H	-0.13086943	5.79187401	1.89686899
H	2.99617279	-3.22156356	2.70683938
H	1.26210258	-5.24044712	0.77196781
H	3.52507803	-1.17830194	4.74886577
H	3.68822384	0.38234415	3.90798907
H	4.75419555	-0.97653294	3.47044013
H	0.12958447	-6.35450986	-1.69713297
H	-1.46435874	-5.59919454	-1.93869571
H	-1.13110921	-6.50263354	-0.44119993

### Atomic coordinates for 3<sup>3</sup>MC(B)

61

geometry

C	1.44953572	3.97761806	-2.56773609
C	0.81350756	4.17518287	-1.34939452
C	0.37508399	3.08016396	-0.60109256
N	0.56390492	1.81714647	-1.06050908
C	1.18076483	1.62933046	-2.24058234
C	1.63866667	2.67769483	-3.02408481
C	-0.45941702	4.45142515	1.36033878
C	-1.12481260	4.49747400	2.58016705
C	-1.63223324	3.32058787	3.12113227
C	-1.44692744	2.13952324	2.41211667
N	-0.80663668	2.09161744	1.24052787
C	-0.31536786	3.22559890	0.70405825
N	-0.78257567	-2.38494739	1.82886359
N	-1.80659982	-3.22093586	1.99983113
C	-2.85675329	-2.90327157	1.20123005
C	-2.43822340	-1.79676723	0.49903359
N	-1.15874317	-1.52114420	0.92276276
N	-2.66691950	0.86258513	-1.78813117
N	-3.87971143	0.35374396	-2.00435224
C	-4.11265339	-0.73988735	-1.23605676
C	-2.95839048	-0.90312967	-0.50497940
N	-2.10626360	0.10663770	-0.88325191
C	-1.71024828	-4.31153110	2.97369489
C	-4.76588129	0.96699982	-2.99764748
N	1.11425980	-2.60224991	-2.32705799
N	2.21727877	-3.36217195	-2.27287426
C	3.02202300	-2.98097219	-1.25325620
C	2.35447012	-1.92596177	-0.66489409
N	1.19434638	-1.73352093	-1.36025738
N	2.19049950	0.53398618	1.90333377
N	3.40429001	0.05354309	2.16017148
C	3.73793967	-0.93850346	1.30038839
C	2.64759943	-1.07006606	0.46709732
N	1.72854566	-0.14277600	0.88291028
C	2.42490551	-4.43253761	-3.24910824
C	4.19548357	0.60468484	3.26244551
Ru	-0.20166097	0.13456184	0.02192967
H	1.78707923	4.82644550	-3.15126862
H	0.65049451	5.18245805	-0.99120557
H	1.29751598	0.59912054	-2.55335101
H	2.12627079	2.47179411	-3.96891447
H	-0.05462658	5.36259070	0.94051930
H	-1.24250411	5.44145438	3.10005105
H	-2.15771310	3.31318024	4.06840698
H	-1.82014021	1.19460472	2.79343807
H	-3.77485390	-3.46752968	1.20006365
H	-5.04013910	-1.28721589	-1.27414048
H	-1.88610152	-5.26449292	2.47598461
H	-2.44176225	-4.16377138	3.76769380
H	-0.70649416	-4.29099727	3.38917642
H	-5.73198237	1.18087544	-2.54248302

H	-4.89125638	0.29475558	-3.84615107
H	-4.29930403	1.89193493	-3.32535632
H	3.95820339	-3.47123685	-1.04091271
H	4.68680473	-1.44752276	1.34395529
H	3.32433798	-4.23564327	-3.83205701
H	1.55833658	-4.44533551	-3.90491814
H	2.51525305	-5.39061287	-2.73781371
H	4.39929942	-0.17471262	3.99606185
H	3.61057212	1.39766577	3.72041812
H	5.13096352	1.00988002	2.87799886

Atomic coordinates for 3<sup>3</sup>MC(F)

61

geometry

C	4.61368941	1.70205163	0.87664471
C	3.78204427	2.39796842	0.00810372
C	2.53373477	1.87309139	-0.32538460
N	2.11475309	0.68587220	0.19433863
C	2.92709155	0.01294880	1.02741798
C	4.17890457	0.48592880	1.39330243
C	1.84241424	3.73317783	-1.90105356
C	0.88428473	4.26758448	-2.75515828
C	-0.31799438	3.59103487	-2.93529787
C	-0.51599790	2.39728872	-2.25688139
N	0.41319506	1.87065756	-1.44359726
C	1.58800526	2.52765304	-1.24844748
N	-2.69506134	-0.25990356	-1.54054505
N	-3.43537020	-1.22132344	-2.09814920
C	-2.74502265	-2.38264682	-2.20798597
C	-1.50489927	-2.10325500	-1.68098288
N	-1.52859848	-0.78803707	-1.28366024
N	1.82139392	-2.81046887	-0.76885074
N	1.53788584	-3.99670779	-1.30270660
C	0.25949126	-4.04892338	-1.75885840
C	-0.25866336	-2.80599384	-1.47736878
N	0.73974494	-2.08850527	-0.87084036
C	-4.80594673	-0.93767641	-2.52990300
C	2.56551442	-5.03898790	-1.37083349
N	0.08728724	-2.16474516	2.24323818
N	-0.41529644	-2.23193663	3.48009095
C	-1.07157263	-1.09218092	3.80524701
C	-0.95095889	-0.29233207	2.68862823
N	-0.23400349	-0.99428562	1.76342480
N	-1.53668064	2.71611827	0.94910801
N	-2.16217872	3.04287178	2.08642649
C	-2.10106334	2.03162946	2.98585693
C	-1.39365382	1.04008793	2.33948781
N	-1.07398762	1.50907364	1.10033425
C	-0.22782573	-3.43432215	4.29260864
C	-2.79034031	4.35585504	2.23494662
Ru	0.24451769	0.00477580	-0.42759802
H	5.58574920	2.10228813	1.14025783
H	4.10890685	3.34233947	-0.40629836
H	2.54815486	-0.93124369	1.39475737
H	4.79610075	-0.09506166	2.06742977
H	2.77860492	4.25448259	-1.75217640
H	1.07619508	5.20180930	-3.27040169
H	-1.09267394	3.97746488	-3.58596415
H	-1.43894580	1.83871429	-2.34583588
H	-3.17474448	-3.27372374	-2.63551751
H	-0.15035932	-4.92678948	-2.23073873
H	-4.86029833	-0.93559343	-3.61852456
H	-5.07549729	0.04212770	-2.14495309
H	-5.48013583	-1.69083637	-2.12435276
H	2.83045538	-5.22945868	-2.41059902

H	2.19354566	-5.95127515	-0.90622760
H	3.43528543	-4.67632220	-0.82990642
H	-1.54780977	-0.95091225	4.76176126
H	-2.54379696	2.10132932	3.96608807
H	0.26803721	-3.17572140	5.22773679
H	0.39574292	-4.11927931	3.72430203
H	-1.19197385	-3.89842853	4.49963973
H	-3.85384475	4.23792819	2.44101902
H	-2.65496303	4.88959384	1.29803113
H	-2.31336449	4.90741343	3.04486546

### Atomic coordinates for 3<sup>3</sup>MC(P)

61

geometry

C	-3.56684946	-3.74088010	-0.30705221
C	-3.81309836	-2.53184546	0.33175351
C	-2.76737630	-1.63187500	0.53248350
N	-1.50686953	-1.92143002	0.10446646
C	-1.27457017	-3.09080940	-0.51889343
C	-2.27555852	-4.02567689	-0.73898087
C	-4.12250766	0.14403522	1.71502317
C	-4.15987296	1.38067223	2.34729452
C	-2.98502832	2.11679099	2.45527110
C	-1.81287045	1.59423773	1.92808167
N	-1.77054382	0.39542761	1.31884401
C	-2.91597902	-0.33490669	1.20728150
N	1.46230090	1.74286441	2.22752703
N	2.70677009	1.97864883	2.63222632
C	3.56591058	1.02084682	2.20158967
C	2.77879062	0.14912248	1.48519059
N	1.49843172	0.64197404	1.52769801
N	2.02777784	-2.73727151	-0.36781802
N	3.33012747	-2.97043956	-0.22074234
C	3.94247517	-1.97789376	0.47213381
C	2.93479673	-1.08835774	0.76544438
N	1.78096901	-1.60090784	0.22712497
C	2.99158163	3.13495796	3.48638952
C	3.93567154	-4.16887764	-0.80773908
N	0.05747274	-1.09060691	-2.64369822
N	0.02242976	-0.61108843	-3.88707068
C	-0.04543391	0.74000536	-3.88556106
C	-0.05238453	1.09387698	-2.55117756
N	0.01162541	-0.06746530	-1.83051736
N	-0.15135007	3.75896562	-0.22245692
N	-0.22349992	4.47789287	-1.35557263
C	-0.20095246	3.66993548	-2.43897780
C	-0.11158146	2.39452997	-1.91390146
N	-0.08444301	2.50285648	-0.55701456
C	0.05462602	-1.51749451	-5.03420979
C	-0.30888440	5.93581956	-1.30412895
Ru	-0.02801046	-0.49517273	0.56914243
H	-4.37263627	-4.44921328	-0.46172173
H	-4.81223328	-2.29890930	0.67464493
H	-0.25717723	-3.26238560	-0.84077404
H	-2.03952096	-4.95740494	-1.23799857
H	-5.02794058	-0.44080044	1.62374648
H	-5.09243740	1.75971253	2.74916617
H	-2.96685420	3.08567018	2.93857373
H	-0.87904389	2.13420547	1.97991530
H	4.61788346	1.03800209	2.43402560
H	4.99692106	-1.99083112	0.69377741
H	2.94543289	2.84195851	4.53532356
H	2.24425989	3.89645969	3.27925535
H	3.98282532	3.51629686	3.24898600
H	4.65108638	-4.59097650	-0.10413341

H	4.43631156	-3.91321874	-1.74164723
H	3.14111756	-4.88564549	-0.99692158
H	-0.08188290	1.31862596	-4.79411081
H	-0.25058685	4.05228906	-3.44562798
H	-0.85050835	-1.39610413	-5.62884712
H	0.10697888	-2.53239675	-4.64927724
H	0.93129261	-1.31028752	-5.64758594
H	0.56553851	6.38075171	-1.77914454
H	-0.34182012	6.22185779	-0.25602722
H	-1.21529139	6.27527043	-1.80507190

### Atomic coordinates for 3<sup>3</sup>MECP(A)

61

Coordinates from ORCA-job 3MCA\_GS\_MECP\_defSD

C	-4.15927031488840	0.42645281120880	2.17838598997374
C	-4.06803997164616	0.40545956407915	0.79215373054986
C	-2.82304580840621	0.20244967062894	0.19028589761122
N	-1.71247097445824	0.02037449044813	0.93962805681050
C	-1.80222003103769	0.05335881879881	2.27416322769023
C	-3.00649594250871	0.25205182838210	2.93821840221637
C	-3.65664215887759	0.26003784094733	-2.19632760154812
C	-3.38372291039997	0.21488130197564	-3.55657273937898
C	-2.06191131296431	0.08864336963608	-3.97215748059303
C	-1.06764002486710	0.01091896308190	-3.01066109540085
N	-1.32444363827768	0.04808890192763	-1.68845483616358
C	-2.61496889120823	0.17680760794224	-1.27091848703676
N	2.30414424614075	0.33236137509189	-2.46320232879021
N	3.14501546315581	1.29718721656289	-2.83513400298297
C	3.01958672402586	2.39490354446842	-2.05072852548853
C	2.03965580080450	2.06863370360482	-1.13848628630902
N	1.63783077246085	0.79447223753130	-1.43332601997805
N	0.00815834098343	2.80104057793343	1.63801923637788
N	0.54242260919228	4.02179186601214	1.48177385577269
C	1.41480406811248	4.04294556529053	0.44563025263887
C	1.39804527077313	2.75360268945410	-0.03996054659362
N	0.52309107123964	2.03665958349911	0.72208593990157
C	4.04788223989220	1.10506924422323	-3.97181768913368
C	0.12646371643111	5.12526815540110	2.34750640850445
N	2.75382915610441	-0.48369038913387	1.47911843922367
N	3.39688632186241	-1.42465681036191	2.17490483934922
C	2.70581435626610	-2.59131393475394	2.19720680218339
C	1.57371654821355	-2.34066339767328	1.45774696540579
N	1.64810555244699	-1.02811243832189	1.04794182620741
N	-1.36307782603097	-3.20479794619912	-0.27307425146912
N	-1.16526315757953	-4.38539547448525	0.31392791456193
C	-0.05763738077147	-4.37305131896019	1.10096368780109
C	0.44103207205173	-3.09569111316263	0.97425647892491
N	-0.39493248438491	-2.42612639702543	0.12042385799399
C	4.73177268633586	-1.15745993666845	2.71607738496730
C	-2.08797244155253	-5.49295140419075	0.05324098228850
Ru	0.16660140364570	-0.31126838902650	-0.28233826291634
H	-5.11849401627713	0.58652988151615	2.65828759679853
H	-4.95733738656008	0.55731802188391	0.19469554666017
H	-0.87437455129261	-0.07805092178099	2.81817676206817
H	-3.03498663258114	0.27441774885673	4.02135898880159
H	-4.68071624245328	0.35155881377426	-1.85967525525790
H	-4.19039947922228	0.27384518824981	-4.27801041371415
H	-1.79639622454942	0.04520240278511	-5.02174393472382
H	-0.02763702337492	-0.09841558422529	-3.28992439025812
H	3.61714252516395	3.28002606752703	-2.19641289632375
H	1.94319907731518	4.93422103889262	0.14831686239531
H	3.75097419601569	1.75332833268284	-4.79595973724789
H	3.97892990551788	0.06417852987231	-4.27825070549594
H	5.06828515878163	1.33466052710458	-3.66507186448290
H	-0.36016245869782	5.89871233084997	1.75244925154694

H	0.99010023300835	5.54170194733220	2.86584766882674
H	-0.57664002299652	4.72069151294802	3.07111390563118
H	3.06802975473434	-3.47141972072735	2.70292799338268
H	0.26571737453210	-5.23564404888022	1.66037826844609
H	4.75719181320190	-1.40237137516411	3.77787906040985
H	4.93630581436030	-0.09972276786050	2.57133209129578
H	5.47025546640432	-1.75297777845857	2.18016385847597
H	-1.54620362518788	-6.32451311799929	-0.39681656268241
H	-2.84437050644301	-5.12756566354736	-0.63632427755305
H	-2.55868503967863	-5.81141463379837	0.98343374982917

### Atomic coordinates for 3<sup>3</sup>MECP(B)

61

Coordinates from ORCA-job 3MCb\_GS\_MECP\_defSD

C	1.79323328532316	4.02897832463647	-2.20585859376982
C	0.91204918533988	4.25323457700213	-1.15631897080991
C	0.33745149086598	3.17715168438171	-0.47485189542049
N	0.64873931175081	1.90128131320395	-0.82645736589888
C	1.49663871792038	1.68847561343536	-1.85259933929264
C	2.08721382529544	2.71881580573767	-2.56763620939699
C	-1.09148184927907	4.62465176841890	1.04128761819339
C	-1.94096168626262	4.71759790317232	2.13855095772894
C	-2.29116034491830	3.56019112466098	2.82768521492827
C	-1.78744126599651	2.34996644720047	2.36660407976932
N	-0.97018598544873	2.25576806924289	1.31420780421951
C	-0.60318175824856	3.37041779199693	0.65900215666957
N	-0.64083855873462	-2.48023467095025	1.75535532441011
N	-1.65771635455304	-3.32537943136710	1.91190771278286
C	-2.74683817462620	-2.94938474801934	1.19510488176851
C	-2.36085187654024	-1.79421198399514	0.55816661760286
N	-1.05925353682940	-1.54867191577671	0.93577710618324
N	-2.69112620654819	1.01904619447721	-1.51630031753882
N	-3.90242125324981	0.50900005678600	-1.73403119641800
C	-4.10441750779410	-0.63429356557092	-1.03055268463453
C	-2.92703135361811	-0.83069398910661	-0.34701050802824
N	-2.09631637867164	0.21194075684725	-0.67838228234640
C	-1.54251394918152	-4.46655816326704	2.82339367456995
C	-4.84288668499054	1.18770107694206	-2.63117074170758
N	1.32444497760844	-2.63339491803933	-2.63735257321435
N	2.24795892855666	-3.56818667557881	-2.35577731956039
C	2.94821538740691	-3.23770260157033	-1.24655073316658
C	2.40473905115030	-2.03234137539185	-0.84763756476760
N	1.41732876364879	-1.70299966440456	-1.73343416616973
N	2.37061740476141	0.41598495909517	1.76961203004145
N	3.60081419244460	-0.05820587021191	1.92297067337303
C	3.87288459264686	-1.02755453499350	1.01689526535384
C	2.72091772943073	-1.16298113891985	0.27095933534277
N	1.83120626338278	-0.24728634349404	0.77368309920980
C	2.34891614551302	-4.76796004590751	-3.18600974745174
C	4.49207659153236	0.51402085545471	2.93475017995860
Ru	-0.15565294733901	0.18021782127939	0.18234527797266
H	2.24004508682001	4.86490306417898	-2.73166326777037
H	0.68274592038566	5.26789116168137	-0.86063098765581
H	1.68348168936987	0.65078840929097	-2.10128895961359
H	2.75905739367117	2.48849521187029	-3.38564199344726
H	-0.82442287077598	5.52164434571579	0.49834354805997
H	-2.32536307756615	5.68214451189783	2.45116515083689
H	-2.94269902434836	3.59178319902870	3.69279144647860
H	-2.04734682347979	1.41702810504574	2.85793494384721
H	-3.66608732771644	-3.51191666481316	1.19870078991301
H	-5.02487080837662	-1.19240499018136	-1.08093111793090
H	-1.85876114562066	-5.37333769225012	2.30904495865207
H	-2.16450814080032	-4.29768339523092	3.70234555733593
H	-0.50115484668414	-4.54974543349060	3.12251219507707
H	-5.59374628260223	1.71868462570299	-2.04563279921323

H	-5.32124662630426	0.45019629289857	-3.27462860071469
H	-4.27552890638343	1.89130297889978	-3.23499017411041
H	3.72783133237152	-3.86376010920575	-0.84282926609915
H	4.83080428942086	-1.51763101825913	0.95852606408701
H	3.37455279695515	-4.90257451998546	-3.52819635549269
H	1.69531375080188	-4.62083348623260	-4.04184318795687
H	2.02534768583307	-5.64210487487813	-2.61987128551568
H	4.97809471448903	-0.28812257900007	3.48850283097607
H	3.88545818732934	1.11394804570427	3.60864703170388
H	5.24117443146252	1.14232482420522	2.45126934806696

### Atomic coordinates for 3<sup>3</sup>MECP(F)

61

Coordinates from ORCA-job 3MCc\_GS\_MECP\_defSD

C	4.17166378681737	2.30705422869348	1.12664227940576
C	3.39604296279189	2.84697603858684	0.10756561797672
C	2.30191251943664	2.13373765682185	-0.38181405062716
N	1.98315943386516	0.91039023867214	0.12533323943994
C	2.75181398444343	0.38329362549505	1.09369000250151
C	3.84790329822699	1.04888607454542	1.62454226497096
C	1.62572884869538	3.78602826248175	-2.18062786658867
C	0.70590685191357	4.17342006429508	-3.14960035181582
C	-0.42700803350977	3.39254229514223	-3.36017124882600
C	-0.59117974844719	2.24017799294535	-2.60517577190445
N	0.30646876000240	1.85055566767697	-1.68035978260298
C	1.40331783154056	2.62450923132114	-1.44260713582174
N	-2.69697764628733	-0.41777916598101	-1.58983656382528
N	-3.42965973978304	-1.46025230140120	-1.98540190218042
C	-2.68670638209466	-2.59111421286107	-2.06930357309512
C	-1.42082085985208	-2.20561889925262	-1.69492683079088
N	-1.48052781303863	-0.86240907984451	-1.41058417109444
N	1.92879738636859	-2.79149295690782	-0.78394426765426
N	1.62168671460072	-4.04211779090310	-1.12666718545287
C	0.34212625166649	-4.13886364302445	-1.57065068254937
C	-0.14907530839245	-2.85757915077631	-1.48301328012582
N	0.86273988995281	-2.07320901555892	-0.99807076742582
C	-4.86626159117004	-1.30982586881039	-2.22006905188984
C	2.61506264045523	-5.11013363087232	-0.99294741636202
N	-0.23242736614254	-2.24793039224344	1.68312231072908
N	-0.77163422095277	-2.44882839100478	2.88335192064609
C	-1.25593387542945	-1.29416259059681	3.40593098626556
C	-0.97374254100749	-0.33611244106052	2.45254649881224
N	-0.34660160673981	-0.97428282003645	1.41946237854413
N	-1.07625551644236	2.97763094898612	1.26154012796623
N	-1.44409045917952	3.23037939216575	2.52791233750270
C	-1.52482951703820	2.08554886908600	3.24762496646453
C	-1.17712489960944	1.09433921142973	2.35395810469947
N	-0.91894726914721	1.69196919721887	1.15553362294334
C	-0.82474332978387	-3.80901230631142	3.41737773035659
C	-1.66634776620978	4.60684694573102	2.97344863860975
Ru	0.24363094976126	0.05353168023989	-0.60626271920814
H	5.01546892121759	2.85993013297077	1.52284781310415
H	3.63602160583978	3.82377134621984	-0.29116368180918
H	2.46015986092740	-0.59821366728814	1.44304990304577
H	4.43066342399162	0.58396795451610	2.41043703979308
H	2.51167470865006	4.38367621800626	-2.01050337867585
H	0.87515368050833	5.07221327165559	-3.73144823699418
H	-1.17298439294701	3.66576944801916	-4.09682931455537
H	-1.45594279178039	1.60057215041450	-2.72458293689175
H	-3.10424460031215	-3.53716736120054	-2.37321482167534
H	-0.08822647145969	-5.07074193283111	-1.89875989044014
H	-5.10957091446711	-1.62130196523542	-3.23575342221493
H	-5.11493929225432	-0.26105851052865	-2.08033144002644
H	-5.42170490521878	-1.91557540315251	-1.50457439519170
H	2.87349448492329	-5.50630218509214	-1.97448627007614

H	2.21330815911050	-5.90480455737023	-0.36452631174205
H	3.49576418765609	-4.67871404161969	-0.52487836676203
H	-1.74410794182338	-1.24749770046411	4.36557295457008
H	-1.80414060724739	2.07371880870786	4.28861108871556
H	-0.59921844115090	-3.79670479163273	4.48297923540854
H	-0.07489720909198	-4.39629368916481	2.89412559150143
H	-1.81302950703945	-4.23971494966195	3.24661206133433
H	-2.69621859185465	4.73259076561080	3.30881226015862
H	-1.47084262436331	5.25679094391215	2.12402892845916
H	-0.98150062209503	4.84827976112152	3.78592169297087

### Atomic coordinates for 3<sup>3</sup>MECP(P)

61

Coordinates from ORCA-job 3MCpenta\_GS\_MECP\_defSD\_fromgeo20

C	-3.59858829924234	-3.81432609722584	-0.42014171272926
C	-3.84968368942088	-2.59802394246140	0.20281653346743
C	-2.79338047942463	-1.72988650063130	0.47332945869316
N	-1.51495376554286	-2.05605232597534	0.12933156416363
C	-1.27852023082954	-3.23437647373577	-0.47620622864676
C	-2.29002332617844	-4.13868154621449	-0.76419654354080
C	-4.16607896795510	0.07110947164425	1.59561690800831
C	-4.20124092157745	1.27914987984825	2.28272194758639
C	-3.00982169335306	1.95968386359225	2.50831545927623
C	-1.82628965766145	1.41744310623063	2.02861623357905
N	-1.78491203737826	0.24617057027821	1.36590278949617
C	-2.94636043382579	-0.43833925740288	1.15710619480792
N	1.38306815142285	1.69774601428460	2.11398953716965
N	2.62887532319868	2.04327373448203	2.41360648760839
C	3.52354324704109	1.10703067777649	2.00075241900886
C	2.75283195820347	0.13412044093495	1.40404470960380
N	1.44751820689337	0.55357063441791	1.49494055186366
N	2.02954474350828	-2.86301285843087	-0.28161584413566
N	3.34631261738847	-3.03851994244141	-0.20069712159866
C	3.95273747564139	-1.99669439164648	0.42509486103697
C	2.92835592489800	-1.13480493810080	0.74104000401697
N	1.76815005567998	-1.71502405611072	0.28421661320593
C	2.87027104670112	3.33117595230066	3.07009882759587
C	3.96700706557887	-4.24815121824159	-0.75095452649305
N	0.02560177394070	-1.02490114885771	-2.44854814110325
N	0.00042988162468	-0.51902754964113	-3.67760076003860
C	-0.06043489249055	0.83034348719368	-3.64953975522228
C	-0.06800846221605	1.16407912193600	-2.30920792704780
N	-0.01451874380155	-0.01547204842856	-1.61143842380663
N	-0.10808324921744	3.93120585416885	-0.08571814738437
N	-0.08076352569537	4.59274297335189	-1.25742256817405
C	-0.07240107346053	3.72845895042079	-2.29442523769778
C	-0.09521477523733	2.47975524852396	-1.70022537448405
N	-0.11836373275570	2.65706241367967	-0.35161631823506
C	0.00280457962959	-1.39593478701818	-4.84800583582515
C	-0.06906738128839	6.05259175425120	-1.28705343430907
Ru	-0.04751074937826	-0.66333881716380	0.65219699507736
H	-4.41381842003714	-4.49759596807662	-0.62918469526514
H	-4.86034330130846	-2.33647373684787	0.48687523913467
H	-0.24737874162373	-3.43969981158995	-0.72862805455323
H	-2.04760380040689	-5.07728948150472	-1.24706837382766
H	-5.08493242139138	-0.46946942760437	1.41115407253876
H	-5.14426462074026	1.67898251888778	2.63802014721286
H	-2.98801082585321	2.90152856897076	3.04213648002128
H	-0.88067247529271	1.92202082620681	2.15906389644525
H	4.58441160094725	1.20683378287188	2.16235696032732
H	5.01676139589975	-1.96115164087748	0.59442195838497
H	2.68944062271905	3.24449304590375	4.14201912689082
H	2.19022133341314	4.06057461230618	2.63630993347145
H	3.90004396995724	3.63053821691313	2.88439487935646
H	4.44898991431645	-4.81266352114803	0.04720711034592

H	4.70072829324516	-3.97120501415911	-1.50732289304518
H	3.17940074901212	-4.84541876398358	-1.20313685725073
H	-0.09385969580007	1.42697264060062	-4.54645565725874
H	-0.05016680287935	4.05915784752294	-3.32038556405427
H	-0.98768652194918	-1.41233736269996	-5.30411488071576
H	0.27310583595324	-2.39380981825717	-4.51206973750372
H	0.73634450544024	-1.03848596015249	-5.56980988466425
H	0.80637140961044	6.41065581206142	-1.82889265010698
H	-0.02795101804002	6.39695662243646	-0.25681530218988
H	-0.97615580861123	6.42812738263162	-1.76122099848773

### Atomic coordinates for 3 <sup>1</sup>GS(P)

61			
geometry			
C	-3.29794207	-4.21094050	0.28900819
C	-3.65859165	-2.89730761	0.56660384
C	-2.67558577	-1.91130731	0.63451041
N	-1.36483029	-2.21412129	0.42857962
C	-1.02240302	-3.48433247	0.15353816
C	-1.95614163	-4.50923626	0.08094874
C	-4.22792371	0.00592351	1.20454108
C	-4.38920072	1.34867797	1.52544701
C	-3.26486717	2.16459992	1.58615294
C	-2.02018783	1.61188852	1.31782697
N	-1.85837769	0.31284825	1.00595923
C	-2.95269130	-0.49678112	0.95078520
N	1.21367988	2.07975221	1.69591207
N	2.43278016	2.56024735	1.91236283
C	3.39067884	1.64858473	1.61550473
C	2.69459983	0.54082885	1.19194886
N	1.36393285	0.86349775	1.24897280
N	2.23652568	-2.79290975	0.17690751
N	3.56732566	-2.81972757	0.22948612
C	4.07756985	-1.61783607	0.59943704
C	2.97686956	-0.81306256	0.77892760
N	1.87257998	-1.58287910	0.50801091
C	2.60025269	3.94341131	2.36423212
C	4.29148354	-4.06590522	-0.03441728
N	-0.03710315	-1.39324019	-2.08263872
N	-0.05694779	-1.00582621	-3.35028291
C	-0.03872096	0.33913755	-3.45025954
C	-0.00438313	0.81292732	-2.15582518
N	-0.01041267	-0.30341405	-1.34539043
N	0.96436292	4.04112438	-1.00117901
N	-0.17421929	4.36384334	-1.64706496
C	-0.76276781	3.25715890	-2.14768879
C	0.07109871	2.22080906	-1.77107334
N	1.12057291	2.75411380	-1.08088466
C	-0.12599089	-2.00098388	-4.42282650
C	-0.57877808	5.76248293	-1.77835077
Ru	-0.01686462	-0.62718256	0.67609228
H	-4.05417039	-4.98588683	0.24058324
H	-4.69829118	-2.65121399	0.73596262
H	0.03142184	-3.66503291	-0.00895174
H	-1.62840821	-5.51902341	-0.13339671
H	-5.09270460	-0.64253856	1.16217331
H	-5.37658027	1.74539611	1.73162780
H	-3.34114603	3.21343751	1.84528561
H	-1.11459152	2.20211737	1.36563652
H	4.44186426	1.85444387	1.72938255
H	5.13621778	-1.44474368	0.70178318
H	2.12666202	4.06855465	3.33668705
H	2.14743334	4.60529053	1.62808456
H	3.66423587	4.15332543	2.44397661
H	4.58521471	-4.53141090	0.90647728

H	5.17349894	-3.84934719	-0.63475331
H	3.62717265	-4.72883005	-0.58230318
H	-0.02270107	0.85937443	-4.39404558
H	-1.68508995	3.28760501	-2.70525241
H	-1.14249685	-2.05762732	-4.81225175
H	0.16437172	-2.96169883	-4.00624370
H	0.56190688	-1.72018299	-5.21866324
H	-0.46567594	6.09125422	-2.81157921
H	0.07290553	6.35155666	-1.13814339
H	-1.61447939	5.88415504	-1.46267526

### Atomic coordinates for 4 <sup>3</sup>MC(A)

61			
geometry			
C	-1.45176940	1.13569085	-2.73692515
C	-1.98430109	2.04494719	-3.63906737
C	-1.99954593	3.39628010	-3.30273809
C	-1.47340611	3.79122117	-2.07913711
C	-0.94737273	2.82814466	-1.22214816
N	-0.94342775	1.50347670	-1.54781394
C	-0.34912565	3.11402810	0.06905029
C	-0.12917172	4.23515889	0.84082334
N	0.50762964	3.77499928	1.94372205
N	0.68998616	2.45301427	1.89627722
N	0.17264950	2.05686192	0.76557911
C	0.93811640	4.53064188	3.12240907
C	-3.98105385	-2.02816554	0.54794305
N	-4.34043516	-0.98523283	1.33396850
N	-3.38303422	-0.04811350	1.36341505
N	-2.41083072	-0.47091937	0.61129096
C	-2.72789296	-1.68935356	0.08222664
C	-1.75982671	-2.32229132	-0.78910530
N	-0.57145430	-1.68248517	-1.03473347
N	0.17609783	-2.39837140	-1.83574033
N	-0.51660796	-3.50007245	-2.11841716
C	-1.72117249	-3.50443501	-1.49656592
C	-5.57954323	-0.79742187	2.08973199
C	0.05105924	-4.51727879	-3.00620420
C	4.44713062	-0.37598850	-0.14521415
N	4.44768632	0.37187393	-1.27481430
N	3.20596621	0.75246919	-1.60442529
N	2.40462102	0.25960282	-0.70710213
C	3.11881640	-0.44549077	0.21890278
C	2.39169150	-1.07077899	1.30367224
N	1.02725334	-0.94936490	1.34156589
N	0.53871331	-1.57554155	2.37928499
N	1.57637751	-2.10336251	3.02581320
C	2.74683258	-1.82216501	2.40246947
C	5.58513748	0.76958343	-2.10502000
C	1.36386728	-2.86846352	4.25559608
Ru	-0.06216761	0.18935027	-0.11012258
H	-1.41867018	0.07731689	-2.95996689
H	-2.37743904	1.69531362	-4.58560970
H	-2.41085063	4.13153844	-3.98460345
H	-1.46483995	4.83624375	-1.79317177
H	-0.36485612	5.27777467	0.70413979
H	1.63760609	3.90994272	3.67581803
H	0.07666087	4.76502022	3.74781135
H	1.42988350	5.44832183	2.80385809
H	-4.61838581	-2.88386737	0.39525116
H	-2.42456233	-4.31403530	-1.60217641
H	-5.49390102	0.14582876	2.62265381
H	-6.42943831	-0.76012632	1.40859919
H	-5.70741027	-1.61234625	2.80166103
H	1.02294391	-4.15880972	-3.33443231

H	0.16543875	-5.45683939	-2.46629411
H	-0.60001603	-4.65971898	-3.86811565
H	5.35097277	-0.77766505	0.28301081
H	3.69841167	-2.16295140	2.77603326
H	5.19453303	1.36627035	-2.92509760
H	6.08543909	-0.11468870	-2.49907852
H	6.28524677	1.36329770	-1.51773994
H	1.89105681	-2.39236154	5.08177124
H	1.72184124	-3.88916077	4.12353934
H	0.29598000	-2.87398823	4.45639260

**Atomic coordinates for 4<sup>3</sup>MC(B)**

61

geometry

C	1.21638508	0.19984522	2.80052266
C	2.00795241	0.64644067	3.84783692
C	2.80775845	1.76865628	3.64936263
C	2.77937165	2.40197309	2.41458100
C	1.95700374	1.90612138	1.40207569
N	1.18502380	0.80637665	1.60016683
C	1.86321497	2.52936060	0.08547385
C	2.49211177	3.61261618	-0.49817832
N	1.96205163	3.68635670	-1.74018964
N	1.05363742	2.71969998	-1.93798081
N	0.99916195	2.02613264	-0.84040441
C	2.25996273	4.64578389	-2.80455605
C	2.49044537	-3.25930584	-0.66492668
N	3.13313799	-2.25282684	-1.30488436
N	2.47848218	-1.10042617	-1.18425473
N	1.40953716	-1.35100592	-0.47361180
C	1.36639459	-2.67492662	-0.12255890
C	0.26989718	-3.16643003	0.68664114
N	-0.65225151	-2.27357925	1.15451210
N	-1.55869753	-2.90090685	1.84762592
N	-1.23460369	-4.20131036	1.84092968
C	-0.10297442	-4.41881289	1.12983594
C	4.38574646	-2.31115082	-2.06070380
C	-2.06529579	-5.17242321	2.55417542
C	-3.84856158	1.96217299	0.14295897
N	-3.27355988	2.56414964	1.21459888
N	-2.02606693	2.13881373	1.41206147
N	-1.78423721	1.26150709	0.47592268
C	-2.87988671	1.11300080	-0.33996269
C	-2.71810975	0.16629027	-1.41434192
N	-1.50407243	-0.47766496	-1.44839165
N	-1.45546130	-1.30895624	-2.45417459
N	-2.62906893	-1.21183382	-3.07860252
C	-3.44840850	-0.31301888	-2.47678936
C	-3.86699743	3.54498256	2.12703871
C	-2.88510979	-1.99948487	-4.28680022
Ru	-0.10103488	0.07311238	0.02744208
H	0.57615455	-0.66705809	2.90741763
H	1.99206574	0.12266242	4.79554767
H	3.44053503	2.14641268	4.44427964
H	3.38710966	3.28066186	2.23479143
H	3.24114719	4.30565935	-0.15155985
H	1.65190746	4.37583124	-3.66389460
H	3.31567927	4.59114348	-3.06866895
H	2.00924825	5.65452686	-2.47724432
H	2.86990297	-4.26769074	-0.64357568
H	0.32083119	-5.40175352	1.00328557
H	4.59019744	-1.31059872	-2.43181968
H	5.19570820	-2.63726464	-1.40888102
H	4.27941160	-3.00020342	-2.89798335
H	-2.89827922	-4.62754881	2.99054946

H	-2.43914166	-5.92388400	1.85919904
H	-1.48508105	-5.65077797	3.34293222
H	-4.85637491	2.17870160	-0.17098351
H	-4.43901723	-0.09729650	-2.84185407
H	-3.07850782	3.89779583	2.78616893
H	-4.65602457	3.07459980	2.71343736
H	-4.27181886	4.37839838	1.55445475
H	-2.91385184	-1.34392874	-5.15699760
H	-3.83221098	-2.52749472	-4.18459616
H	-2.07295625	-2.71376661	-4.39088522

### Atomic coordinates for 4<sup>3</sup>MC(C)

61			
geometry			
C	0.98131276	2.58437024	2.40605613
C	0.99237608	3.86918830	2.93988362
C	0.32882992	4.87932362	2.24899940
C	-0.32182127	4.56985807	1.05985788
C	-0.28668617	3.25357948	0.59710180
N	0.36093402	2.27784305	1.26361410
C	-0.94966122	2.82035927	-0.63298859
C	-1.68083785	3.47810626	-1.60075728
N	-2.03547938	2.51816286	-2.48619154
N	-1.57244238	1.32175660	-2.12117752
N	-0.91632383	1.50542453	-1.00738957
C	-2.82366298	2.65697158	-3.71204668
C	4.19852652	-0.03221888	-0.99781791
N	3.76305980	0.92858338	-1.85124745
N	2.46249184	1.17620964	-1.69764414
N	2.04628275	0.38214173	-0.74879473
C	3.08172416	-0.38974851	-0.27848053
C	2.73075568	-1.30471647	0.77837381
N	1.40776524	-1.28543530	1.15292655
N	1.19112145	-2.14941238	2.10841721
N	2.36322797	-2.73157290	2.36185265
C	3.35022069	-2.24684497	1.56656272
C	4.53020067	1.64340553	-2.87456000
C	2.46462080	-3.75432430	3.40605926
C	-3.54085442	-1.75669029	1.27056337
N	-3.43826659	-0.73359693	2.15376596
N	-2.33141840	-0.02217498	1.95139622
N	-1.71213541	-0.57756449	0.94299691
C	-2.41694641	-1.65714174	0.47949737
C	-1.89480568	-2.40838215	-0.64293025
N	-0.69020416	-2.03303448	-1.16543573
N	-0.37871398	-2.80879521	-2.16097113
N	-1.37591168	-3.69393280	-2.29894877
C	-2.34486730	-3.48673509	-1.37547126
C	-4.35415092	-0.37405949	3.23792597
C	-1.32018565	-4.70977931	-3.35023190
Ru	0.14694911	0.04269230	0.10129735
H	1.48461296	1.76658334	2.91189533
H	1.50779087	4.06856989	3.87167114
H	0.31569727	5.89382118	2.63100416
H	-0.84902696	5.33824461	0.50622241
H	-1.96396433	4.51016920	-1.72663680
H	-2.84705762	1.68489660	-4.19711066
H	-2.35314916	3.38590802	-4.37088142
H	-3.83727381	2.97419850	-3.46794506
H	5.22236115	-0.36761966	-0.97727462
H	4.36696466	-2.59894231	1.62565601
H	3.89820646	2.43747995	-3.26264464
H	5.42696589	2.06963548	-2.42698569
H	4.80097635	0.95969439	-3.67891552
H	1.46629434	-3.91503693	3.80365479

H	2.84612841	-4.68031020	2.97727282
H	3.12693897	-3.40841510	4.19916181
H	-4.36962316	-2.44536264	1.27604067
H	-3.23320776	-4.09479659	-1.32262189
H	-3.97599422	0.53512794	3.69745941
H	-4.38614415	-1.17486878	3.97630354
H	-5.35094125	-0.19805435	2.83495490
H	-2.17199819	-4.59856293	-4.02072048
H	-1.32242690	-5.70562972	-2.90751556
H	-0.39675129	-4.55457947	-3.90190077

**Atomic coordinates for 4<sup>3</sup>MC(F)**

61

geometry

C	-1.82762423	-0.19965947	-2.55994763
C	-2.63670518	-0.77288879	-3.53161864
C	-3.22205533	-2.01004800	-3.27891059
C	-2.98356663	-2.62814581	-2.05695191
C	-2.16419516	-1.99840873	-1.12431588
N	-1.58221252	-0.79263775	-1.37978643
C	-1.86702714	-2.52966564	0.19873975
C	-2.22590799	-3.64818985	0.91833470
N	-1.60504231	-3.50053201	2.11578882
N	-0.89816292	-2.37314268	2.17150434
N	-1.05445363	-1.78909976	1.01498491
C	-1.66227410	-4.38752632	3.28025348
C	-1.50586126	3.93920158	1.45108654
N	-2.36725408	3.85090696	0.40430395
N	-2.21482901	2.70772595	-0.26192083
N	-1.26104109	2.05078041	0.33794147
C	-0.78651882	2.76714932	1.40664405
C	0.26304891	2.14079110	2.17997930
N	0.64282519	0.87999635	1.78537552
N	1.58760489	0.42580149	2.56050513
N	1.82871620	1.37918342	3.46275760
C	1.03485345	2.46234934	3.27237693
C	-3.38732657	4.81630109	-0.01197826
C	2.83966786	1.16715281	4.50023788
C	3.45915282	-1.83378403	-1.57385109
N	3.04927319	-2.91330185	-0.86534316
N	1.88846469	-2.67092409	-0.24248227
N	1.54573876	-1.45135529	-0.53713513
C	2.47837279	-0.88940621	-1.35706114
C	2.25443645	0.47217466	-1.79359671
N	1.13000755	1.11277644	-1.35676378
N	1.08288963	2.32117114	-1.84863410
N	2.17134273	2.47457408	-2.60773813
C	2.93345898	1.35411665	-2.60692802
C	3.70069017	-4.21652589	-0.73608409
C	2.41590737	3.73801057	-3.30450494
Ru	-0.36672516	0.01930227	0.15074240
H	-1.35818638	0.76382974	-2.70994038
H	-2.80316396	-0.25116343	-4.46593709
H	-3.85848322	-2.48366036	-4.01732858
H	-3.43214302	-3.58718344	-1.82653589
H	-2.84632336	-4.50000964	0.69305156
H	-0.93045623	-4.03000128	3.99946148
H	-2.65928540	-4.35849234	3.71958641
H	-1.41685848	-5.40417068	2.97630407
H	-1.48476865	4.79026882	2.11180378
H	1.08184658	3.33380102	3.90462312
H	-3.85062283	4.43160421	-0.91647324
H	-4.13783403	4.92192623	0.77103251
H	-2.92097939	5.77962547	-0.21540445
H	3.29755958	0.19920059	4.31544850

H	3.59490726	1.95061601	4.44606303
H	2.36806635	1.17005645	5.48265489
H	4.37240278	-1.82986263	-2.14626358
H	3.85456456	1.27981504	-3.16158891
H	3.11262512	-4.80650715	-0.03815288
H	4.71101962	-4.08930228	-0.34838794
H	3.73380968	-4.71574739	-1.70442812
H	2.50764029	3.55845047	-4.37528384
H	3.32679175	4.20158589	-2.92611316
H	1.56556749	4.38701442	-3.11293215

### Atomic coordinates for 4<sup>3</sup>MC(P)

61

geometry

C	-1.55747931	-2.93626318	-0.12254275
C	-2.63745680	-3.80880901	-0.09570835
C	-3.91409666	-3.31529160	-0.34710016
C	-4.06938375	-1.96238188	-0.62565414
C	-2.94519596	-1.14244415	-0.64697400
N	-1.69649296	-1.62616643	-0.39114349
C	-2.96569636	0.27459253	-0.95774243
C	-3.91996055	1.20199233	-1.31483654
N	-3.22619697	2.35153269	-1.49897290
N	-1.92131879	2.18638648	-1.28013374
N	-1.76514258	0.93470783	-0.94847830
C	-3.73241526	3.65714536	-1.92818820
C	3.66557497	-2.02319794	-1.37066817
N	3.00235680	-3.11401269	-0.91044501
N	1.76089192	-2.81341433	-0.53485166
N	1.60685299	-1.53344339	-0.74277975
C	2.75725717	-0.99563675	-1.26438846
C	2.69014356	0.40835981	-1.57836751
N	1.48101797	1.00647447	-1.31737434
N	1.50890383	2.26126405	-1.67104718
N	2.72873713	2.48938217	-2.15266907
C	3.50394657	1.37514244	-2.11958205
C	3.48245578	-4.49612562	-0.83370052
C	3.07376688	3.81755203	-2.66445237
C	0.26216999	2.58807441	3.38028189
N	0.18653434	3.60976405	2.49541695
N	0.09999021	3.15285385	1.23652316
N	0.11840600	1.85311469	1.29521898
C	0.21762560	1.45489522	2.59497479
C	0.25442493	0.03973800	2.88890048
N	0.17844401	-0.86060739	1.86590968
N	0.22970777	-2.07449302	2.34156468
N	0.33720811	-1.97526238	3.66965891
C	0.35766028	-0.67929563	4.06132230
C	0.19125770	5.04650568	2.76172890
C	0.41265988	-3.17578446	4.50048097
Ru	-0.07486201	-0.21535083	-0.54396316
H	-0.55102990	-3.27524859	0.07737493
H	-2.47224753	-4.85725215	0.11965857
H	-4.77583160	-3.97268136	-0.33060061
H	-5.04938184	-1.54801785	-0.83046380
H	-4.98704452	1.14201787	-1.45262413
H	-2.93934777	4.38279358	-1.76988993
H	-3.99860554	3.62312176	-2.98462928
H	-4.60384921	3.92312729	-1.33175598
H	4.68215024	-2.06978848	-1.72507482
H	4.52206565	1.36507690	-2.47236435
H	2.73697477	-5.07406521	-0.29446691
H	3.60820476	-4.90048689	-1.83796085
H	4.43032842	-4.52409272	-0.29799413
H	2.26607567	4.49085033	-2.39078656

H	4.00599730	4.15244961	-2.21160369
H	3.17575477	3.78211508	-3.74896085
H	0.33631684	2.74608027	4.44397791
H	0.43924462	-0.38758402	5.09561538
H	0.09813249	5.55402751	1.80511794
H	1.12588183	5.33610388	3.24225824
H	-0.65043323	5.31120786	3.40171791
H	-0.42989189	-3.20406627	5.19126740
H	1.34916077	-3.18467640	5.05794766
H	0.37193424	-4.03583874	3.83737958

## Atomic coordinates for 4<sup>3</sup>MECP(A)

61

Coordinates from ORCA-job 4M<sub>Ca</sub>\_GS\_MECP\_defSD

C	-1.91830498569222	1.26720298187226	-2.52393705680588
C	-2.53087038216265	2.21152998475442	-3.33462671355999
C	-2.34832995973429	3.56381340655494	-3.05289430628435
C	-1.56517260634654	3.92508641052639	-1.96368952351769
C	-0.98809989395354	2.92781793908485	-1.18504120086324
N	-1.15376250108413	1.60124894475769	-1.46769461879818
C	-0.17768155351757	3.17782522101146	-0.01022020353965
C	0.25817137898458	4.28168353461564	0.69010032550679
N	0.97468622732150	3.77165891782560	1.72172668620986
N	1.01146566553608	2.43898940803369	1.69133744175825
N	0.31526368249915	2.08330325138572	0.64561648648040
C	1.67181850162227	4.49836809441432	2.78468828403695
C	-4.06255071304808	-2.38522686223496	0.39417369534348
N	-4.56308860970839	-1.47543412745509	1.26041104232449
N	-3.74597317911816	-0.41392601039335	1.37175836994545
N	-2.72782796273042	-0.62376163836986	0.59145402288101
C	-2.87357088152860	-1.82979428303977	-0.03200131653075
C	-1.83882702485448	-2.30457081464184	-0.92691107768740
N	-0.68178927562897	-1.59109020102970	-1.10918228287525
N	0.11416277430974	-2.21484333717596	-1.94696187507900
N	-0.51816283032831	-3.32296027761867	-2.31675136759280
C	-1.72744097153756	-3.43123406633446	-1.71591305877032
C	-5.79136436199907	-1.56115948763478	2.05104956601099
C	0.13177399197276	-4.27801014747924	-3.21771500188203
C	4.51449567894267	-0.50172370232581	0.01684591201812
N	4.66370940682101	0.21840752621424	-1.11956390632837
N	3.48113463708574	0.67595761938853	-1.55985326695267
N	2.57161816113158	0.26323952583134	-0.72734009061833
C	3.15744758637119	-0.46769722887772	0.26607953745916
C	2.32791581580507	-0.99244418551730	1.33147049839796
N	0.96445278980039	-0.86745638181023	1.26709483703842
N	0.40515396339274	-1.34044351738781	2.35375672266429
N	1.39366398591531	-1.77253856366129	3.12933463699522
C	2.60273137964282	-1.58860844393073	2.54415067375811
C	5.88883206026356	0.51630075397914	-1.86153085706710
C	1.10131253789242	-2.30215698527334	4.46339589861399
Ru	-0.13168475108250	0.24998350735768	-0.17525149155909
H	-2.03195810564307	0.20789945211518	-2.71499898035098
H	-3.13552041249647	1.88747706904887	-4.17284961764975
H	-2.80882599972200	4.32483543742957	-3.67196337666848
H	-1.40175244216689	4.96764851014383	-1.71536764406711
H	0.11803074457152	5.34131630257043	0.55009781305172
H	2.16765507809392	3.76359125857077	3.41371626121134
H	0.95436260450824	5.06727890482144	3.37601834100892
H	2.41062412903075	5.16808334620073	2.34475674541014
H	-4.56975774069585	-3.30805978183321	0.16366736179521
H	-2.38963583346385	-4.26232491960596	-1.89485318690077
H	-5.97448114191084	-0.58045590492060	2.48322875326573
H	-6.62288494024016	-1.84557988544356	1.40678674286848
H	-5.67226902680645	-2.29539638551408	2.84845606284860
H	0.86965134126466	-3.73685237768846	-3.80494016270085

H	0.61898638468808	-5.06181370687011	-2.63703392605695
H	-0.61726463524246	-4.71459350247310	-3.87692520529120
H	5.34600725514405	-0.96064520597784	0.52670869363740
H	3.52557795600339	-1.87585495576308	3.02055873387850
H	5.62228060120143	1.20616402840781	-2.65811424488682
H	6.30174881496561	-0.39714400545444	-2.29051005128166
H	6.61972520419515	0.98134611830805	-1.19985552367728
H	1.66604326512399	-1.74199524836411	5.20692745359167
H	1.36538986247565	-3.35881633495924	4.51467796607385
H	0.03609681586649	-2.17108695816492	4.63714618975943

## Atomic coordinates for 4 <sup>3</sup>MECP(B)

61

Coordinates from ORCA-job 4MCb\_GS\_MECP\_defSD

C	1.42467562957033	0.04949599985747	2.61064197843133
C	2.13467541330089	0.47926754886051	3.72178909638686
C	2.80448614164007	1.69784248474706	3.65619332457197
C	2.71497859018421	2.44771909772820	2.49172755868385
C	1.96059114116661	1.97527993798038	1.41674041260778
N	1.32804813842247	0.77262891119067	1.47667756997752
C	1.78463284764697	2.75203593278760	0.19387034601519
C	2.12152896580533	4.04936539203146	-0.14750811030400
N	1.62062479910071	4.21378760249201	-1.39215937583852
N	1.00630097968467	3.09783782309534	-1.81767698531844
N	1.11171483454020	2.22139914170037	-0.86363741262187
C	1.66403082321989	5.40115699936595	-2.24588114552404
C	2.14521396719212	-3.63830693136157	-0.73027705517876
N	2.80231671992500	-2.73693633305508	-1.49556551535338
N	2.31637832601587	-1.51290852187697	-1.32984947369874
N	1.33706647109763	-1.61069093700960	-0.46008729891403
C	1.18605662929896	-2.91294211137833	-0.05485218433414
C	0.18556683249714	-3.33727773017716	0.90639117421580
N	-0.62762722071283	-2.43441964668732	1.52816577189068
N	-1.41289846707895	-3.06026909816421	2.35610902187203
N	-1.11901825861575	-4.36981956437111	2.28303930599230
C	-0.13137326373161	-4.59336997989217	1.38709937984516
C	3.90439446575025	-2.97780422441921	-2.42831704558179
C	-1.83604901347636	-5.33214210022813	3.11883208760951
C	-3.57237519219460	2.14943510076342	-0.20475634619723
N	-2.99114552535816	2.76899813253695	0.85497902130471
N	-1.76985908787627	2.29691653132603	1.09846429913106
N	-1.54966562174626	1.37044393249417	0.20564045644624
C	-2.63415179670124	1.23571080591968	-0.62943220460305
C	-2.48983686434188	0.22377122222054	-1.64642760151709
N	-1.32898564235404	-0.51104055856595	-1.56045406881782
N	-1.27178218855949	-1.39570729005695	-2.52122549555506
N	-2.38191468867412	-1.24106520233609	-3.23773099243708
C	-3.17100780643181	-0.25148506036984	-2.74355702534343
C	-3.56667769050109	3.79027577696742	1.73464046982636
C	-2.57150182078405	-2.04201043246836	-4.45125598045366
Ru	0.06478704114489	0.05824195340176	-0.13160368181018
H	0.88426468912546	-0.88796414554629	2.61442750951268
H	2.16165848335506	-0.13718795319402	4.61193529889967
H	3.38229741965025	2.06216010057113	4.49823638246268
H	3.22721059649474	3.39895132844345	2.41213016657223
H	2.64296923912993	4.83749412283287	0.37071034577969
H	1.03665615635017	5.19937649611448	-3.11033477164854
H	2.68533263056464	5.59560158333965	-2.57279807460862
H	1.27636289469961	6.26054407878247	-1.69920226986775
H	2.40624682501861	-4.68405152821310	-0.71618994064453
H	0.25109769838692	-5.57952040097552	1.17879410491409
H	4.19201332108509	-2.02068584875883	-2.85547237275736
H	4.74780056294327	-3.41545693697882	-1.89461596420840
H	3.57198850922143	-3.65000119711653	-3.21917902139081
H	-2.51810038647909	-4.76622581688906	3.74869573015545

H	-2.39963105245107	-6.02521197349949	2.49373543962576
H	-1.13069095593229	-5.88232331751782	3.74183158176757
H	-4.56110796060487	2.39962359418056	-0.55211770592205
H	-4.10760162159733	0.02516540886839	-3.19851018717384
H	-2.74996673465639	4.27551384040630	2.26301696371411
H	-4.24205700309908	3.32021272941854	2.45065048843434
H	-4.10648473108160	4.51967457880502	1.13255119321375
H	-2.29032548353994	-1.45335826952764	-5.32505654496835
H	-3.61211754043371	-2.35361709615825	-4.52383667249481
H	-1.93050173421554	-2.91567179243640	-4.37257814477302

## Atomic coordinates for 4<sup>3</sup>MECP(C)

61

Coordinates from ORCA-job 4MCc\_GS\_MECP\_defSD

C	0.09568526672428	1.33681656939318	2.73428064573346
C	0.08376963855364	2.30081514638520	3.73648044140744
C	-0.15280639073760	3.62704897823322	3.38686065485278
C	-0.38594574639574	3.94115711183095	2.05336294403580
C	-0.36949155449176	2.91479785529188	1.10967492238361
N	-0.11489312811620	1.63175951390099	1.44568349338408
C	-0.65051485823174	3.11058052449544	-0.30738558830489
C	-0.80976943133154	4.20655097640300	-1.12838920341058
N	-1.03291000385305	3.68597295930394	-2.36010033230778
N	-1.01819753112358	2.35147334436162	-2.33604965482782
N	-0.78724077562581	2.00852724054214	-1.09966537842523
C	-1.25407721127475	4.39111060729547	-3.62463827297703
C	3.52177774736131	-0.49845162935767	-1.90750224598972
N	2.89100573423680	0.17726125797101	-2.89980978434641
N	1.65024580246875	0.51110371676412	-2.55117478015571
N	1.46604008568029	0.05933220884374	-1.33680392467014
C	2.59778749888546	-0.57409393672965	-0.88859220674896
C	2.57645026151494	-1.16514499463116	0.43062477685402
N	1.40297944447694	-1.12404808771106	1.12713399353990
N	1.56030844573654	-1.68574605483344	2.29185931762356
N	2.83246049163233	-2.09652374963343	2.36510223540755
C	3.50782846423591	-1.79723459832585	1.22918786080930
C	3.40713095871105	0.55981359460446	-4.21811675521369
C	3.33505044486772	-2.72411806986223	3.58886260306183
C	-3.96678842936105	-1.64689343668506	1.04246774196303
N	-4.11369619547709	-0.38507474715550	1.51766699295313
N	-3.07300721956064	0.38810315244071	1.20190219754071
N	-2.24556972465764	-0.36197246250420	0.52759474967894
C	-2.75464723149234	-1.63495771341640	0.39181594395761
C	-1.92508323250346	-2.54991679804044	-0.35702989601313
N	-0.74025194323857	-2.01812702793796	-0.80164893225062
N	-0.06489332841538	-2.90235040988047	-1.48436957669828
N	-0.80131809190652	-4.01126829281327	-1.49390958934896
C	-1.96434788455100	-3.84999055331213	-0.80736287941484
C	-5.25443304869745	0.19498001651851	2.22980930438906
C	-0.29315798593805	-5.21523584666608	-2.15729730881592
Ru	-0.36827523107788	0.01552567214439	-0.31889466004971
H	0.28699849626391	0.29646006214007	2.96387062578240
H	0.25903952336155	2.01010259633431	4.76570677231341
H	-0.16516973996756	4.40474380991560	4.14214724359369
H	-0.59356510439248	4.96153153082077	1.75162809717893
H	-0.77205999569238	5.26848280129820	-0.94723541542345
H	-1.23986257125288	3.64670639366263	-4.41665439560512
H	-0.45490603067744	5.11431308038449	-3.78332803971074
H	-2.21822757658677	4.89960328762999	-3.60906849824698
H	4.53148631233518	-0.86292862301807	-2.00298579908250
H	4.54731158161523	-2.04667826673324	1.09083417469776
H	2.57005636197042	0.93785665124524	-4.79929337180676
H	4.16534956869466	1.33613824677912	-4.11257781531149
H	3.83685975337269	-0.31216854101566	-4.71021432746592
H	2.48308242979516	-3.12246885670446	4.13460814594143

H	4.01433611196348	-3.53424330153698	3.32828223073561
H	3.85605602368102	-1.98738565525121	4.20165627800207
H	-4.70568810999541	-2.41594145496627	1.19917949192398
H	-2.69021252290440	-4.64014050013933	-0.70451942148373
H	-4.88095515443346	0.97694020921815	2.88659264771945
H	-5.73816026982621	-0.58134492608410	2.82021313390191
H	-5.96299947657657	0.61730502979856	1.51629846115770
H	-1.10185582676953	-5.69845673462947	-2.70337340361091
H	0.12255880327008	-5.90084906669527	-1.41790393722775
H	0.48372561572456	-4.90519361968103	-2.85128554757942

## Atomic coordinates for 4<sup>3</sup>MECP(F)

61

Coordinates from ORCA-job 4MCflat\_GS\_MECP\_defSD

C	-2.17598417512714	-0.54845999684994	-2.37001609819775
C	-3.12278293414994	-1.12553399120084	-3.20476309236185
C	-3.74127759750129	-2.30715856139904	-2.80617182571781
C	-3.37965842408224	-2.87763666200687	-1.59175020803055
C	-2.42134911613840	-2.24833484924644	-0.80066504293831
N	-1.83485252981619	-1.07970671030707	-1.18335737024564
C	-1.95537094574252	-2.75797917520002	0.48196650042761
C	-2.14809051051235	-3.91553449613860	1.20461532202617
N	-1.37399316135719	-3.76337097338617	2.30855578381505
N	-0.73230978833212	-2.59529206174117	2.30308503959012
N	-1.08474729268210	-1.98790687424039	1.20342069206522
C	-1.13146084536138	-4.72666840604824	3.38512012095810
C	3.06048402854162	-1.64968671510955	-1.84899775359532
N	2.33968286468941	-2.74867772001437	-1.51979319583670
N	1.20838399045824	-2.42064517987413	-0.90930466078696
N	1.19031632454535	-1.11408375798900	-0.81774769566051
C	2.31645846019184	-0.58169810746909	-1.38949177021837
C	2.54634070146630	0.85020757361780	-1.43990640087308
N	1.51752564280793	1.72390850517823	-1.23956461859575
N	1.96941685670643	2.94145891757827	-1.28212310813319
N	3.29303564797593	2.87653568997888	-1.52043543154878
C	3.69829058439708	1.59037023857204	-1.62638494885294
C	2.63206580750948	-4.15562194568481	-1.78922995681942
C	4.08590848356446	4.10246198327721	-1.60752407925136
C	-1.81003398495146	3.76687958109137	0.89116449979560
N	-2.74229852695104	3.41256702037298	-0.03390247041610
N	-2.58126697805083	2.15886540950045	-0.44351778620998
N	-1.54708266235185	1.68914973496009	0.20624045842868
C	-1.03304774262049	2.64522904777935	1.04858840785936
C	0.13111133170518	2.24638103456222	1.80068809460202
N	0.58208423248986	0.96897358282616	1.56417588982747
N	1.64783066395610	0.72452703428274	2.27371817299579
N	1.89344094876589	1.83197947510303	2.97947534542090
C	0.98217795889653	2.80341007204923	2.72368020722096
C	-3.80175334236906	4.24286025865074	-0.61088250689666
C	3.08391287731302	1.91434962593821	3.82553128913162
Ru	-0.51627813197985	-0.13978575646929	0.16929844546684
H	-1.67446692167581	0.37297199098323	-2.63636543336006
H	-3.37109952800433	-0.64976348364436	-4.14544910974003
H	-4.49027248758748	-2.77947715047268	-3.43166172697671
H	-3.84157784389733	-3.79806408245218	-1.25492614801922
H	-2.73528324720587	-4.80242001957806	1.03088502792691
H	-0.65671326295293	-4.19248088691483	4.20398312689184
H	-0.47282556096044	-5.51900074941940	3.02804915894383
H	-2.07759343703238	-5.15100485888938	3.71766986209214
H	3.99943719305669	-1.70763320358137	-2.37450618572505
H	4.72569513019798	1.31867004507184	-1.80739006452359
H	1.99108768385531	-4.75271766850467	-1.14642615034016
H	2.42270138918389	-4.38696075864184	-2.83413092183370
H	3.67613831029326	-4.36076798928075	-1.55682584204602
H	3.40557835999114	4.93572148258495	-1.45008043306066

H	4.85760080606827	4.10589134193913	-0.83717016739534
H	4.54898405084249	4.18519620888655	-2.59094817728697
H	-1.77925744306538	4.74696468942471	1.33743083257976
H	1.01215768894303	3.76925381510020	3.20037427935939
H	-4.47356878473221	3.58668623606592	-1.15873010189113
H	-3.36359216798309	4.97614868792665	-1.28913845402196
H	-4.34623355068784	4.74765826042586	0.18622161076316
H	2.87728750958490	2.57738827960137	4.66375739666439
H	3.92452125447491	2.29932246049237	3.24681359220186
H	3.31183075338999	0.91800170793280	4.19603296035284

### Atomic coordinates for 4<sup>3</sup>MECP(P)

61

Coordinates from ORCA-job 4MCpenta\_GS\_MECP\_defSD

N	-1.69577337101273	2.04310651786321	-1.58231547259901
N	-2.96832716770478	2.25581650271591	-1.90985005785562
C	-3.68987334670716	1.10402842711004	-1.92066477407478
C	-2.78644723446415	0.13075749403237	-1.56928791885722
N	-1.57704823256277	0.76174834991677	-1.37000657809427
N	-1.65070101980895	-3.09197134455639	-0.77095946774849
N	-2.90675728695441	-3.43276262407853	-1.04015630882754
C	-3.65016021390483	-2.35764028436920	-1.40881166299902
C	-2.77589349377115	-1.29421095522231	-1.35175908261064
N	-1.56370339100569	-1.80289326216332	-0.95760130271003
C	-3.43514205413646	3.62046273583857	-2.17415445418035
C	-3.29733839451359	-4.84366543322424	-0.96118305745673
N	-0.43702873909670	-1.68176950066922	2.00548876531359
N	-0.55476850558604	-1.56367865813736	3.32500781433977
C	-0.45589478250494	-0.26977284535082	3.70821378215459
C	-0.26194464074745	0.44185651050886	2.54069884934086
N	-0.25817421276335	-0.47719571445150	1.52030293444280
N	0.26451595804605	3.67225334939287	1.18591778107217
N	0.23480646081872	4.00037762904415	2.49478642163927
C	0.02402050894988	2.90520286716657	3.25728988534966
C	-0.07185454850557	1.86767040892228	2.34506307717190
N	0.07833560090418	2.39021413692405	1.09784946476015
C	-0.75511261837574	-2.74921038710587	4.15802857095662
C	0.41274168400937	5.39186657803858	2.90611222730513
Ru	0.05078454652190	-0.45572668924332	-0.81495231748967
H	-4.73776249708620	1.07595030218637	-2.17074502558245
H	-4.69103312561739	-2.43478729951602	-1.67690466521117
H	-3.76715960772468	3.70755362038626	-3.20902403442420
H	-2.59736241920206	4.28814500716532	-1.99029955520656
H	-4.25545282976730	3.86163179514546	-1.49925263309962
H	-3.06201975777868	-5.34662131464721	-1.90013328732920
H	-4.36528080781840	-4.90621616828282	-0.75881203010658
H	-2.74332976763903	-5.30499956539068	-0.14768084813085
H	-0.52830793123295	0.03724906849745	4.73876214450813
H	-0.03430437125998	2.95297321237665	4.33322394324481
H	0.04969819301898	-2.82931077099096	4.88830095625651
H	-0.74199307385239	-3.61441019956901	3.50033651992672
H	-1.71510400859685	-2.68713378664138	4.67157423814840
H	-0.51482678067397	5.78898843495806	3.32062368587741
H	0.68786983567405	5.95750754931943	2.01893999503505
H	1.20760081603344	5.46514963798026	3.64821046143362
C	2.92668440317561	0.15725314873222	-0.90071186679048
C	2.92512095391443	-1.27148306187972	-0.65135860715230
N	1.67267383945201	-1.80649310705401	-0.57257260747721
C	1.55218307135701	-3.13181694674979	-0.36992264290748
C	2.65077366259073	-3.96954525748786	-0.24423633002949
C	3.92961053426650	-3.42385307911090	-0.31612227700307
C	4.06686234276883	-2.05671174137896	-0.52117875644832
C	3.87807867899939	1.14079011258766	-1.05093180136241
N	3.16475389318238	2.27043510116914	-1.28671291527617
N	1.85271790660939	2.03936937444557	-1.29415868734178

N	1.70629436264470	0.76744159982188	-1.04863010499923
C	3.66179767976482	3.63061720800465	-1.50974066663853
H	0.54156850297661	-3.51224336020385	-0.31415290938684
H	2.49639401154553	-5.03117253534908	-0.09256221903353
H	4.80669544665313	-4.05277847735316	-0.21659802086034
H	5.04895804625480	-1.60367291151149	-0.58853056185288
H	4.95531802087823	1.13188799895075	-1.00912230579097
H	2.82682145440701	4.30880363186049	-1.35444865294858
H	4.04840961456808	3.72824173408945	-2.52462028557896
H	4.45093443239055	3.84506790653765	-0.79050769480460

### Atomic coordinates for 4 <sup>1</sup>GS(P)

61			
geometry			
N	-1.98861880	1.36094950	-1.53631738
N	-3.30292008	1.27820748	-1.71792026
C	-3.78212516	0.05000715	-1.40094456
C	-2.67446702	-0.65913070	-1.00583813
N	-1.60379238	0.19342391	-1.09894096
N	-0.81745709	-3.48211827	-0.03823160
N	-2.01698713	-4.06099276	-0.01591658
C	-3.00043209	-3.18905621	-0.35498066
C	-2.34728955	-2.00288241	-0.59531921
N	-1.01068190	-2.23779255	-0.38743044
C	-4.05930321	2.46772617	-2.11103537
C	-2.14054842	-5.48924786	0.28535279
N	0.93734429	-1.20436853	2.07802105
N	0.85450072	-0.84458196	3.35142613
C	0.14404473	0.29377093	3.49176730
C	-0.23472159	0.66201387	2.21832430
N	0.28874367	-0.29886328	1.37820978
N	-2.84418025	2.89599396	1.27749093
N	-1.96472240	3.77890761	1.79077190
C	-0.83799787	3.14854898	2.18354044
C	-1.06163878	1.81944781	1.88133258
N	-2.30910343	1.71443573	1.33811636
C	1.48112920	-1.66438556	4.39084137
C	-2.30598898	5.19651665	1.87837420
Ru	0.28720646	-0.58973276	-0.64528083
H	-4.82579294	-0.20410231	-1.48205620
H	-4.03879394	-3.47389190	-0.39530309
H	-4.94266540	2.15999525	-2.66700758
H	-3.42218311	3.08155346	-2.74293515
H	-4.34485777	3.01908226	-1.21548738
H	-2.20540108	-6.06075279	-0.64070065
H	-3.03303893	-5.65239539	0.88683441
H	-1.25958499	-5.79192091	0.84524749
H	-0.06624813	0.74274862	4.44880980
H	-0.00368895	3.66662870	2.62815378
H	2.21655668	-1.07108766	4.93310570
H	1.97105899	-2.50102923	3.90035230
H	0.71971088	-2.03207319	5.07801564
H	-2.22027566	5.53874658	2.90939830
H	-3.33587006	5.30308403	1.54727651
H	-1.65043630	5.78540281	1.23648835
C	2.87133618	0.71505319	-1.12763924
C	3.26590098	-0.66242426	-0.86542934
N	2.22082958	-1.48310439	-0.56326628
C	2.47440563	-2.77950146	-0.31759997
C	3.75650411	-3.31196522	-0.36925566
C	4.82483998	-2.47551559	-0.67733370
C	4.57464211	-1.13043752	-0.92714099
C	3.51538831	1.87952848	-1.48306021
N	2.52740672	2.80177173	-1.58400748
N	1.32902525	2.27690421	-1.31756542

N	1.53643210	1.01716365	-1.04378269
C	2.63828369	4.20626686	-1.98381272
H	1.61513593	-3.39057463	-0.07480112
H	3.90621452	-4.36626484	-0.17168909
H	5.83621552	-2.86226000	-0.72605923
H	5.38469403	-0.45422379	-1.17336168
H	4.54921021	2.11848735	-1.67180026
H	1.67850388	4.67828686	-1.79236749
H	2.87473759	4.27182428	-3.04581544
H	3.41661012	4.69307161	-1.39776669

**Atomic coordinates for 5<sup>3</sup>MLCT (*D*<sub>3</sub> symmetry)**

61

geometry

N	0.08074186	2.34520111	-2.05240619
N	-2.07137467	-1.10267606	-2.05240619
N	1.99063281	-1.24252505	-2.05240619
N	2.34520111	0.08074186	2.05240619
N	-1.10267606	-2.07137467	2.05240619
N	-1.24252505	1.99063281	2.05240619
N	0.89639820	3.37910221	-2.28370139
N	-3.37458746	-0.91324750	-2.28370139
N	2.47818926	-2.46585472	-2.28370139
N	3.37910221	0.89639820	2.28370139
N	-0.91324750	-3.37458746	2.28370139
N	-2.46585472	2.47818926	2.28370139
C	1.93171347	3.42707236	-1.41064300
C	-3.93378846	-0.04062324	-1.41064300
C	2.00207499	-3.38644912	-1.41064300
C	3.42707236	1.93171347	1.41064300
C	-0.04062324	-3.93378846	1.41064300
C	-3.38644912	2.00207499	1.41064300
C	1.74800711	2.34697437	-0.57730614
C	-2.90654298	0.34033138	-0.57730614
C	1.15853587	-2.68730575	-0.57730614
C	2.34697437	1.74800711	0.57730614
C	0.34033138	-2.90654298	0.57730614
C	-2.68730575	1.15853587	0.57730614
N	0.60319460	1.71249093	-1.01866576
N	-1.78465795	-0.33386362	-1.01866576
N	1.18146335	-1.37862732	-1.01866576
N	1.71249093	0.60319460	1.01866576
N	-0.33386362	-1.78465795	1.01866576
N	-1.37862732	1.18146335	1.01866576
C	0.64490094	4.25117621	-3.43105787
C	-4.00407707	-1.56708751	-3.43105787
C	3.35917613	-2.68408870	-3.43105787
C	4.25117621	0.64490094	3.43105787
C	-1.56708751	-4.00407707	3.43105787
C	-2.68408870	3.35917613	3.43105787
Ru	-0.00000000	-0.00000000	-0.00000000
H	2.68651051	4.19483197	-1.45104465
H	-4.97608630	0.22917037	-1.45104465
H	2.28957579	-4.42400233	-1.45104465
H	4.19483197	2.68651051	1.45104465
H	0.22917037	-4.97608630	1.45104465
H	-4.42400233	2.28957579	1.45104465
H	1.12893662	5.21004578	-3.25758658
H	-5.07650031	-1.62733510	-3.25758658
H	3.94756369	-3.58271068	-3.25758658
H	5.21004578	1.12893662	3.25758658
H	-1.62733510	-5.07650031	3.25758658
H	-3.58271068	3.94756369	3.25758658
H	-0.42905636	4.39343728	-3.52722139
H	-3.59030011	-2.56829235	-3.52722139

H	4.01935648	-1.82514493	-3.52722139
H	4.39343728	-0.42905636	3.52722139
H	-2.56829235	-3.59030011	3.52722139
H	-1.82514493	4.01935648	3.52722139
H	1.03957103	3.79392847	-4.33870578
H	-3.80542395	-0.99666931	-4.33870578
H	2.76585292	-2.79725916	-4.33870578
H	3.79392847	1.03957103	4.33870578
H	-0.99666931	-3.80542395	4.33870578
H	-2.79725916	2.76585292	4.33870578

## Atomic coordinates for 5 <sup>3</sup>MC

61			
geometry			
N	-2.22136417	0.26336136	-1.97170818
N	-3.28848159	1.02573534	-2.20169567
C	-3.40321565	2.01332252	-1.28011593
C	-2.32943910	1.83616750	-0.43545510
N	-1.63891510	0.75124228	-0.90856224
N	-0.39194016	2.77013648	2.36015688
N	-1.35067034	3.69825581	2.48483970
C	-2.27620911	3.58121796	1.50253207
C	-1.83984259	2.51370736	0.74651937
N	-0.68614939	2.05503896	1.31517098
C	-4.15896514	0.74450912	-3.34439153
C	-1.30375599	4.66353145	3.58313027
N	1.34885976	2.27436601	-1.86876435
N	2.55735196	2.79102030	-2.09013619
C	3.50188902	2.22402619	-1.29764197
C	2.81498858	1.29986711	-0.54541360
N	1.49988486	1.37259133	-0.93729817
N	2.36227372	-1.24842739	1.83365498
N	3.66930551	-1.07206866	2.02585421
C	4.17281653	-0.10560580	1.21711182
C	3.09352761	0.33213332	0.48547547
N	2.01006211	-0.40176901	0.90479367
C	2.73818992	3.82166630	-3.11503954
C	4.37358899	-1.85620959	3.04293126
N	-1.73066234	-1.34901650	2.02536642
N	-2.25131588	-2.54902544	2.27383921
C	-1.86422089	-3.46133739	1.34882608
C	-1.05144947	-2.76414086	0.48213345
N	-1.00388451	-1.47592373	0.94683304
N	1.03049111	-2.59034846	-2.35985561
N	0.67985403	-3.87919424	-2.46960516
C	-0.15379290	-4.24693619	-1.46708072
C	-0.30952429	-3.10222088	-0.71414339
N	0.43408073	-2.12077119	-1.30453445
C	-3.11955994	-2.74614843	3.43568286
C	1.19050769	-4.69047444	-3.57471214
Ru	0.15839896	0.04538218	0.00207890
H	-4.20459800	2.73342150	-1.29956565
H	-3.12896527	4.23633039	1.43006036
H	-4.17731446	1.60357216	-4.01437802
H	-5.16708420	0.52146200	-2.99602357
H	-3.74802332	-0.11713043	-3.86347784
H	-2.19495330	4.56591948	4.20261319
H	-1.23467451	5.67642668	3.18692858
H	-0.41992925	4.43870847	4.17427393
H	4.53935447	2.51251883	-1.33613887
H	5.21216950	0.17823638	1.23169494
H	3.25432328	4.67885847	-2.68466562
H	1.75098693	4.11882454	-3.45813827
H	3.31271647	3.41800271	-3.94852363
H	5.26304085	-2.30713034	2.60500999

H	3.69573206	-2.63337659	3.38520272
H	4.65164102	-1.21432918	3.87870782
H	-2.18304500	-4.49014020	1.38124798
H	-0.54903114	-5.24587735	-1.38035875
H	-2.68898512	-3.50011093	4.09392254
H	-4.11102620	-3.05860141	3.10878766
H	-3.18509160	-1.79615057	3.95909607
H	1.77372234	-5.52513274	-3.18627257
H	1.82474715	-4.04919752	-4.18105059
H	0.36204386	-5.06319028	-4.17660167