Supporting Information

Binuclear Methylphosphinidine Complexes of Cyclopentadienylruthenium Carbonyls: Effects of the Higher Ligand Field Strength of Ruthenium Derivatives Relative to Iron Derivatives

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Complete Gaussian09 Reference (reference 20)

Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

Table S1. The initial $(Me_6C_6)_2Mn_2(CO)_n$ structures:

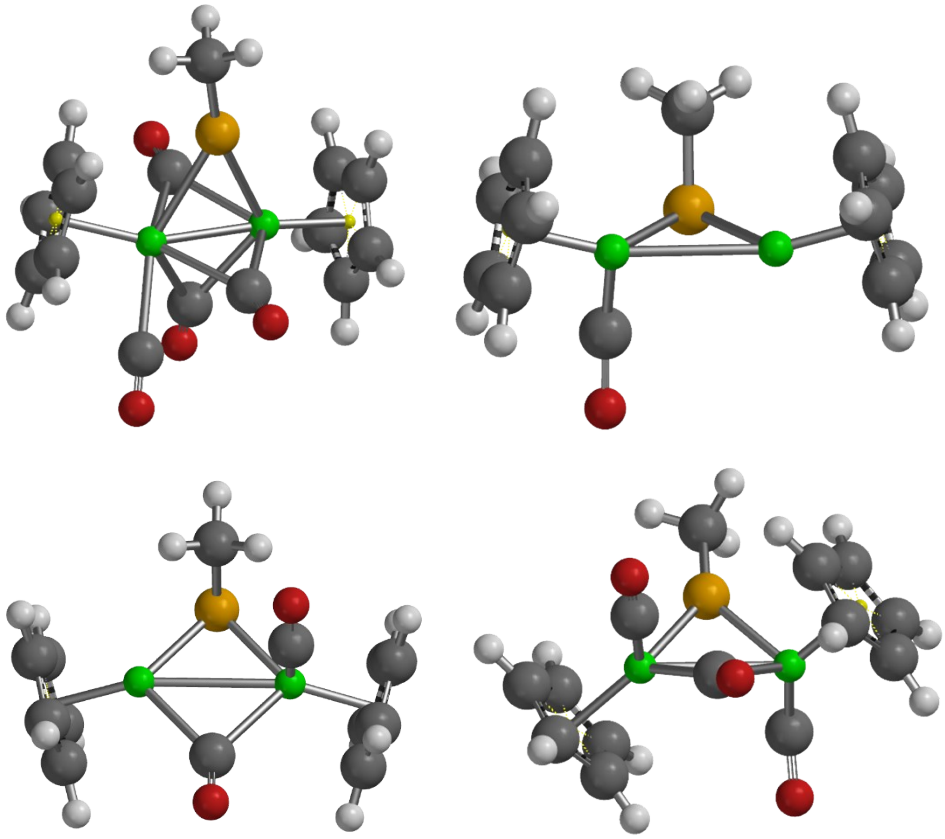
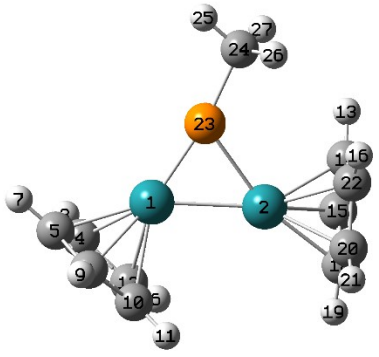


Table S2. Distance matrix for the lowest energy $MePCp_2Ru_2$ structures as optimized at the PBE0/def2TZVP level. Included are the ranking order, spin multiplicity (S, T or Q), total energy (in a.u.), relative energy (in kcal/mol), symmetry point group Wiberg bond indices for the Fe-Fe bonds, Mulliken charges and the spin density (Cp moieties are omitted for clarity).



1S -957.512043 0.00 C1
WBI 0.86

		1	2	3	4	5
1	Ru	0.000000				
2	Ru	2.463203	0.000000			
3	H	2.915267	4.722565	0.000000		
4	C	2.172637	4.164049	1.078778	0.000000	
5	C	2.173074	4.563865	2.238651	1.424658	0.000000
6	H	2.951259	3.548027	2.695578	2.238210	3.345451
7	H	2.885104	5.347308	2.694027	2.234267	1.079314
8	C	2.176872	4.204159	3.352780	2.309869	1.424126
9	H	2.918824	4.786295	4.362976	3.352943	2.238388
10	C	2.202451	3.524145	3.348165	2.305991	2.301690
11	H	2.951286	3.597963	4.357765	3.349053	3.344659
12	C	2.201075	3.495703	2.239616	1.427699	2.302336
13	H	4.800379	2.859878	6.574336	6.379488	6.909567

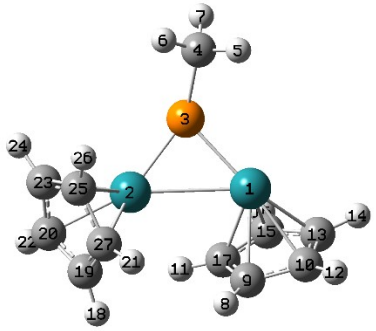
Charge densities

	1
1 Ru	0.258874
2 Ru	0.381879
4 C	-0.049401
5 C	-0.058330
8 C	-0.050110
10 C	-0.037669
12 C	-0.042786
14 C	-0.030811
15 C	-0.042423
18 C	-0.032015
20 C	-0.046521
22 C	-0.039966
23 P	-0.243618
24 C	0.032897

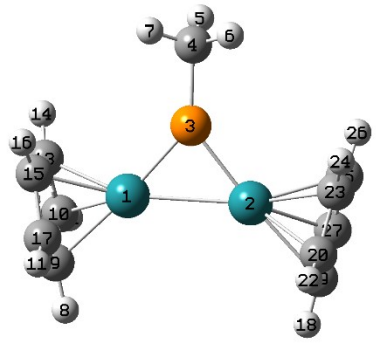
14	C	4.386583	2.112407	6.331514	6.000421	6.524620
15	C	4.397960	2.149353	5.921243	5.615916	6.369020
16	H	4.798024	2.860503	7.408621	6.834501	6.910031
17	H	4.810826	2.905078	5.799812	5.671460	6.620099
18	C	4.417687	2.178856	6.190355	5.670792	6.288935
19	H	4.792049	2.910539	6.249977	5.712797	6.414158
20	C	4.396443	2.149940	6.710203	6.056358	6.370368
21	H	4.806830	2.904977	7.240025	6.468772	6.621019
22	C	4.385800	2.113334	6.801421	6.260139	6.525504
23	P	2.101739	2.334732	4.480614	4.058253	4.008928
24	C	3.919917	3.648497	6.052210	5.776846	5.671390
25	H	4.326015	4.561474	6.243662	6.025597	5.755942
26	H	4.461873	3.832191	6.884073	6.488105	6.298249
27	H	4.447088	3.860479	6.261330	6.134144	6.253516

		6	7	8	9	10
6	H	0.000000				
7	H	4.355216	0.000000			
8	C	3.349085	2.234081	0.000000		
9	H	4.357507	2.694244	1.078796	0.000000	
10	C	2.232121	3.344727	1.427042	2.238680	0.000000
11	H	2.687916	4.354432	2.237299	2.693925	1.079228
12	C	1.079253	3.345305	2.306072	3.348082	1.420165
13	H	5.856078	7.481944	6.857444	7.424539	6.316213
14	C	5.231710	7.212511	6.293858	6.845369	5.614185
15	C	4.380361	7.194167	6.126894	6.808754	5.181634
16	H	6.376311	7.504236	6.366775	6.570931	5.950282
17	H	4.334285	7.438612	6.556040	7.350784	5.565973
18	C	4.202603	7.211586	5.748472	6.321797	4.667485
19	H	3.923856	7.412550	5.813913	6.421772	4.564977
20	C	4.962286	7.214893	5.657908	6.014593	4.798621
21	H	5.387804	7.474873	5.704162	5.899521	4.873799
22	C	5.544316	7.225337	6.015990	6.368293	5.399494
23	P	4.671790	4.351645	4.063064	4.485493	4.175818
24	C	6.416776	5.812232	5.783905	6.061372	5.987896
25	H	6.999427	5.691877	6.006233	6.204919	6.441165
26	H	6.950228	6.495545	6.185127	6.331668	6.343979
27	H	6.608899	6.433168	6.479454	6.883602	6.534943

		11	12	13	14	15
11	H	0.000000				
12	C	2.231976	0.000000			
13	H	6.449410	6.001456	0.000000		
14	C	5.613987	5.413994	1.078984	0.000000	
15	C	5.111869	4.813199	2.236757	1.428616	0.000000
16	H	5.780355	6.262147	2.711406	2.247202	3.358930
17	H	5.597914	4.933144	2.694174	2.241258	1.079030
18	C	4.320184	4.609159	3.341317	2.299368	1.421760

	19 H 4.090690 4.485955 4.350521 3.342437 2.229843 20 C 4.376655 5.089486 3.357154 2.313255 2.313781 21 H 4.261885 5.429709 4.368365 3.356837 3.356074 22 C 5.215397 5.568427 2.246513 1.432514 2.314886 23 P 4.671886 4.174236 3.468691 3.399817 4.073920 24 C 6.419134 5.985026 3.361688 3.734989 4.856951 25 H 6.975212 6.453606 4.398331 4.813175 5.888852 26 H 6.615727 6.528665 3.454006 3.725537 4.987260 27 H 6.976863 6.328049 2.802734 3.456575 4.601979 16 17 18 19 20 16 H 0.000000 17 H 4.370187 0.000000 18 C 3.342322 2.236696 0.000000 19 H 4.351285 2.688510 1.080680 0.000000 20 C 2.236652 3.356078 1.422207 2.230283 0.000000 21 H 2.693292 4.364664 2.237151 2.688988 1.079090 22 C 1.079017 3.358436 2.300316 3.343216 1.428234 23 P 3.529875 4.633819 4.469080 5.243605 4.118793 24 C 3.496398 5.425736 5.477404 6.426651 4.937407 25 H 4.498185 6.402948 6.499487 7.412700 5.952992 26 H 2.866661 5.711916 5.444830 6.440568 4.658605 27 H 3.710823 5.024122 5.471982 6.450981 5.120913 21 22 23 24 25 21 H 0.000000 22 C 2.240386 0.000000 23 P 4.707102 3.433280 0.000000 24 C 5.560492 3.799815 1.830439 0.000000 25 H 6.513230 4.861776 2.423058 1.091347 0.000000 26 H 5.161590 3.452194 2.435402 1.092101 1.777739 27 H 5.895376 3.882326 2.432674 1.092222 1.776984 26 27 26 H 0.000000 27 H 1.778321 0.000000
 2S -957.494547 10.97 WBI 0.42 Charge densities	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.840223 0.000000 3 P 2.248732 2.193507 0.000000 4 C 3.545716 3.743269 1.848210 0.000000 5 H 3.488348 4.323100 2.468565 1.092564 0.000000 6 H 4.261980 3.835818 2.444029 1.091316 1.779146 7 H 4.214418 4.470953 2.439936 1.092386 1.769069 8 H 2.923190 3.531529 4.582746 6.002841 5.966508 9 C 2.163886 3.453761 4.082425 5.559348 5.512414 10 C 2.216680 4.466288 4.457048 5.662470 5.383882 11 H 2.880189 2.697877 3.750843 5.576206 5.943695 12 H 2.970456 5.238729 5.172460 6.144553 5.697778

1 1 Ru 0.375014 2 Ru 0.420114 3 P -0.344417 4 C -0.003341 9 C -0.030133 10 C -0.013227 13 C -0.069732 15 C -0.015914 17 C -0.002525 19 C -0.045853 20 C -0.055744 23 C -0.061841 25 C -0.073805 27 C -0.078597	13 C 2.168676 4.686329 4.220212 5.435322 5.224050 14 H 2.911152 5.593843 4.791007 5.755932 5.423255 15 C 2.088034 3.894809 3.649349 5.180840 5.263008 16 H 2.829868 4.325969 3.852395 5.345583 5.542958 17 C 2.087314 2.979931 3.549878 5.265194 5.448412 18 H 4.674846 2.963384 5.059902 6.654833 7.086706 19 C 4.411487 2.197637 4.381615 5.856921 6.357882 20 C 4.868521 2.163441 4.201351 5.617571 6.331563 21 H 4.183156 2.897942 4.526958 5.563398 5.730502 22 H 5.481762 2.929182 4.779648 6.267094 7.055676 23 C 4.926335 2.117976 3.765500 4.795488 5.559780 24 H 5.574122 2.862413 4.031337 4.803186 5.692367 25 C 4.470335 2.085036 3.639406 4.480090 5.013971 26 H 4.818269 2.835009 3.834981 4.217935 4.665861 27 C 4.126361 2.138568 4.049083 5.210949 5.578615 6 7 8 9 10 6 H 0.000000 7 H 1.774920 0.000000 8 H 6.371683 6.855590 0.000000 9 C 6.092888 6.307197 1.078225 0.000000 10 C 6.352030 6.340133 2.226070 1.413112 0.000000 11 H 6.063160 6.112297 2.717013 2.257469 3.351499 12 H 6.794653 6.877306 2.678126 2.222971 1.080114 13 C 6.293746 5.892086 3.345841 2.304038 1.423144 14 H 6.702820 6.089926 4.353990 3.346173 2.237165 15 C 5.996889 5.557609 3.365547 2.322818 2.308992 16 H 6.216800 5.518222 4.378992 3.368017 3.351547 17 C 5.868763 5.837045 2.250232 1.441424 2.309032 18 H 6.692556 7.422417 3.106316 3.641193 5.051913 19 C 5.783773 6.637944 3.415961 3.871251 5.223708 20 C 5.464641 6.239769 4.596137 4.820765 6.100484 21 H 5.402901 6.565187 2.927527 3.671464 4.750441 22 H 6.175932 6.754449 5.253527 5.384018 6.668486 23 C 4.418812 5.444396 5.155157 5.355817 6.487463 24 H 4.311819 5.294252 6.152890 6.263123 7.321881 25 C 4.052817 5.346782 4.501047 4.845980 5.894052 26 H 3.595620 5.131649 5.102868 5.438420 6.322582 27 C 5.014053 6.132115 3.318657 3.871236 5.056748 11 12 13 14 15 11 H 0.000000 12 H 4.363039 0.000000 13 C 3.355179 2.232363 0.000000 14 H 4.365194 2.689748 1.079832 0.000000 15 C 2.251509 3.350520 1.425446 2.232895 0.000000 16 H 2.713448 4.358969 2.238016 2.688651 1.079297 17 C 1.081645 3.352767 2.313187 3.356205 1.440286

	18 H 2.841764 5.732307 5.690320 6.766635 4.934207 19 C 3.069873 5.903370 5.803319 6.850240 5.032463 20 C 3.500724 6.887028 6.412340 7.403482 5.431248 21 H 4.173875 5.056251 5.711576 6.678855 5.464158 22 H 3.682672 7.537424 6.832510 7.809067 5.697652 23 C 4.374716 7.187501 6.796475 7.711439 5.941390 24 H 5.150619 8.045879 7.496697 8.348427 6.585210 25 C 4.506128 6.422131 6.432183 7.337980 5.853197 26 H 5.375692 6.730765 6.885632 7.710783 6.456744 27 C 3.775450 5.553326 5.797980 6.788183 5.297488 16 17 18 19 20 16 H 0.000000 17 C 2.253472 0.000000 18 H 5.533265 3.514800 0.000000 19 C 5.591499 3.689275 1.080655 0.000000 20 C 5.750202 4.274717 2.238127 1.427516 0.000000 21 H 6.289463 4.232442 2.689695 2.233010 3.351048 22 H 5.855410 4.618048 2.693798 2.239390 1.079675 23 C 6.263941 4.932345 3.353934 2.310771 1.426324 24 H 6.773870 5.720088 4.362776 3.353526 2.238071 25 C 6.384192 4.804279 3.354570 2.309317 2.309068 26 H 7.006236 5.528658 4.362862 3.350883 3.352860 27 C 5.982958 4.052153 2.230424 1.418135 2.306953 21 22 23 24 25 21 H 0.000000 22 H 4.359805 0.000000 23 C 3.360313 2.237026 0.000000 24 H 4.371941 2.693257 1.079189 0.000000 25 C 2.247703 3.352559 1.430816 2.243586 0.000000 26 H 2.704305 4.363530 2.244131 2.705112 1.079170 27 C 1.079409 3.349172 2.317808 3.362230 1.438252 26 27 26 H 0.000000 27 C 2.248625 0.000000
 3T -957.490781 13.34 C2	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.727153 0.000000 3 P 2.157054 2.157057 0.000000 4 C 3.751766 3.751740 1.823939 0.000000 5 H 4.212730 4.212422 2.417752 1.092386 0.000000 6 H 4.510099 3.934702 2.425198 1.091109 1.776482 7 H 3.934615 4.510219 2.425210 1.091108 1.776488 8 H 2.967861 4.839514 5.093306 6.713272 7.111952 9 C 2.237040 4.574823 4.390129 5.878558 6.270758 10 C 2.181508 4.612012 4.074830 5.370890 5.536103 11 H 2.933904 5.001943 4.628242 5.915710 6.626991

WBI 0.57

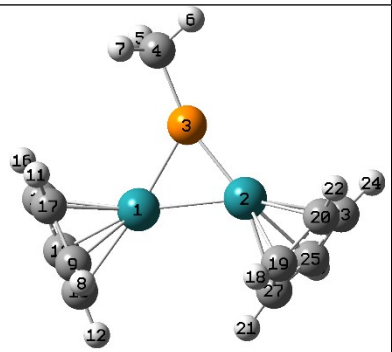
Charges and spin densities

		1	2
1	Ru	0.367336	0.920492
2	Ru	0.367345	0.920502
3	P	-0.318472	-0.041664
4	C	0.042422	-0.002391
9	C	-0.020550	0.141781
10	C	-0.056676	-0.035580
13	C	-0.047989	0.015039
15	C	-0.048844	0.015311
17	C	-0.055257	-0.035020
19	C	-0.020550	0.141782
20	C	-0.055266	-0.035021
23	C	-0.048849	0.015317
25	C	-0.047985	0.015032
27	C	-0.056666	-0.035579

		1	2	3	4	5
12	H	2.931712	4.970208	4.621287	5.894908	5.887340
13	C	2.159287	4.771419	3.583036	4.498495	4.691077
14	H	2.896508	5.240069	3.772149	4.302178	4.283888
15	C	2.160677	4.782620	3.586403	4.507792	5.003088
16	H	2.898399	5.259308	3.778106	4.320550	4.909551
17	C	2.183512	4.630668	4.079433	5.383297	5.962101
18	H	4.839545	2.967865	5.093318	6.713242	7.111504
19	C	4.574843	2.237043	4.390133	5.878514	6.270255
20	C	4.630619	2.183508	4.079518	5.383409	5.961754
21	H	4.970315	2.931714	4.621132	5.894562	5.886487
22	H	5.001860	2.933904	4.628395	5.915956	6.626814
23	C	4.782571	2.160664	3.586437	4.507823	5.002600
24	H	5.259227	2.898389	3.778185	4.320689	4.909174
25	C	4.771455	2.159295	3.582963	4.498292	4.690308
26	H	5.240126	2.896517	3.772020	4.301838	4.282924
27	C	4.612079	2.181513	4.074737	5.370663	5.535366

		6	7	8	9	10
6	H	0.000000				
7	H	1.782077	0.000000			
8	H	7.464102	6.794444	0.000000		
9	C	6.695822	5.867561	1.080383	0.000000	
10	C	6.312772	5.390731	2.229581	1.419765	0.000000
11	H	6.547343	5.669819	2.688293	2.234057	3.346600
12	H	6.848532	6.031050	2.688661	2.234359	1.079016
13	C	5.505367	4.298605	3.348420	2.304568	1.432939
14	H	5.375832	4.054274	4.354814	3.344967	2.239917
15	C	5.384837	4.135395	3.348367	2.304549	2.308498
16	H	5.138279	3.717338	4.354730	3.344957	3.353791
17	C	6.141829	5.179514	2.229445	1.419571	2.303650
18	H	6.794575	7.464289	5.358275	5.697017	6.116515
19	C	5.867703	6.696002	5.697008	5.839327	6.113072
20	C	5.179717	6.142291	6.142602	6.141530	6.505877
21	H	6.031094	6.848195	6.235560	6.283786	6.076836
22	H	5.670054	6.548032	6.282349	6.334673	6.901639
23	C	4.135599	5.385183	6.854094	6.655044	6.763552
24	H	3.717595	5.138807	7.536675	7.240478	7.348847
25	C	4.298738	5.505321	6.839855	6.638963	6.499797
26	H	4.054368	5.375574	7.512169	7.212490	6.881431
27	C	5.390824	6.312654	6.116807	6.113269	6.054657

		11	12	13	14	15
11	H	0.000000				
12	H	4.356344	0.000000			
13	C	3.350069	2.242907	0.000000		
14	H	4.362814	2.693710	1.078780	0.000000	
15	C	2.242628	3.350382	1.421836	2.237975	0.000000
16	H	2.693400	4.363222	2.238111	2.704261	1.078832

	17 C 1.079041 3.346619 2.308143 3.353354 1.432673 18 H 6.282921 6.235009 6.839702 7.511893 6.854293 19 C 6.335042 6.283424 6.638856 7.212298 6.655183 20 C 6.161167 6.878529 6.776272 7.348368 6.547486 21 H 7.384188 5.906730 6.651426 6.968143 7.117244 22 H 6.017714 7.383716 7.153381 7.817375 6.723141 23 C 6.723014 7.117164 6.807026 7.189184 6.675357 24 H 7.053313 7.794292 7.203490 7.529499 6.950184 25 C 7.153439 6.651532 6.638452 6.897897 6.807034 26 H 7.817369 6.968456 6.897935 6.992214 7.189142 27 C 6.901973 6.076764 6.499720 6.881226 6.763630 16 17 18 19 20 16 H 0.000000 17 C 2.239716 0.000000 18 H 7.537000 6.142925 0.000000 19 C 7.240706 6.141740 1.080383 0.000000 20 C 6.942517 6.114488 2.229448 1.419572 0.000000 21 H 7.794312 6.878868 2.688656 2.234359 3.346620 22 H 7.053651 6.161101 2.688299 2.234059 1.079041 23 C 6.950229 6.547390 3.348369 2.304550 1.432675 24 H 7.062018 6.942289 4.354733 3.344958 2.239718 25 C 7.203455 6.776331 3.348419 2.304568 2.308145 26 H 7.529342 7.348408 4.354814 3.344969 3.353357 27 C 7.348910 6.506107 2.229578 1.419765 2.303651 21 22 23 24 25 21 H 0.000000 22 H 4.356345 0.000000 23 C 3.350382 2.242629 0.000000 24 H 4.363223 2.693400 1.078833 0.000000 25 C 2.242907 3.350071 1.421836 2.238113 0.000000 26 H 2.693712 4.362817 2.237976 2.704263 1.078782 27 C 1.079016 3.346601 2.308497 3.353791 1.432937 26 27 26 H 0.000000 27 C 2.239918 0.000000
 4T -957.489244 14.30 C2 WBI 0.82	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.498216 0.000000 3 P 2.226778 2.144103 0.000000 4 C 3.656456 3.916080 1.829803 0.000000 5 H 3.953072 4.518055 2.424538 1.092356 0.000000 6 H 4.528969 4.244501 2.433292 1.091008 1.780944 7 H 3.825383 4.443608 2.427453 1.092164 1.773785 8 H 2.901288 4.396430 4.633771 5.790811 6.303204 9 C 2.188007 4.196060 4.139558 5.248975 5.607429 10 C 2.297771 4.379540 4.518102 5.774770 5.934893

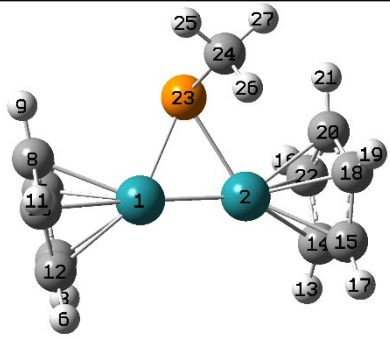
Charges and spin densities

		1	2
1	Ru	0.362602	1.604958
2	Ru	0.291252	0.417883
3	P	-0.242232	-0.117109
4	C	0.027262	-0.005531
9	C	-0.072552	-0.023691
10	C	-0.036255	0.088188
13	C	-0.005830	0.007140
15	C	-0.008821	0.021381
17	C	-0.065527	-0.015353
19	C	-0.050564	-0.006321
20	C	-0.057015	0.016260
23	C	-0.049558	0.033532
25	C	-0.040030	-0.013947
27	C	-0.052732	-0.007390

11	H	2.912201	4.863593	3.823164	4.120124	4.489674
12	H	3.028275	4.681535	5.230225	6.648827	6.825217
13	C	2.323713	4.689608	4.293904	5.272934	5.185513
14	H	3.050063	5.197463	4.843358	5.795778	5.540665
15	C	2.315815	4.787747	3.819864	4.385121	4.304287
16	H	3.052883	5.381067	4.045647	4.192556	3.885970
17	C	2.198394	4.465340	3.675279	4.330721	4.586566
18	H	4.198084	2.900352	4.581932	6.147169	6.968224
19	C	3.937689	2.164042	4.132871	5.804128	6.550260
20	C	4.544000	2.189101	4.013510	5.514823	6.289072
21	H	3.665750	2.945182	4.802878	6.623456	7.096690
22	H	5.210308	2.922818	4.359869	5.604713	6.480919
23	C	4.621638	2.204481	4.041868	5.589397	6.167831
24	H	5.327426	2.934105	4.393983	5.726760	6.238224
25	C	4.071157	2.177019	4.163219	5.903944	6.345587
26	H	4.426714	2.915173	4.629268	6.320684	6.594807
27	C	3.643500	2.194143	4.261172	6.072370	6.620744

		6	7	8	9	10
6	H	0.000000				
7	H	1.781361	0.000000			
8	H	6.615416	5.473781	0.000000		
9	C	6.170703	4.997203	1.079318	0.000000	
10	C	6.731179	5.732091	2.232947	1.417889	0.000000
11	H	5.061231	3.478442	2.703489	2.248212	3.348954
12	H	7.554716	6.684810	2.697370	2.234165	1.079220
13	C	6.302011	5.288004	3.331080	2.285859	1.417302
14	H	6.806058	5.946048	4.340727	3.328464	2.224728
15	C	5.462294	4.197126	3.353774	2.313118	2.311562
16	H	5.281012	3.992460	4.366618	3.358574	3.352033
17	C	5.333028	3.934142	2.250229	1.440356	2.308188
18	H	6.416816	6.285313	4.037368	4.542931	5.064105
19	C	6.033528	6.125322	4.483286	4.760435	5.062358
20	C	5.496920	5.989834	5.621438	5.782539	6.100687
21	H	7.121634	6.984191	4.172235	4.244499	3.936966
22	H	5.416024	6.015420	6.148858	6.383914	6.877274
23	C	5.575600	6.273610	6.247720	6.198807	6.226036
24	H	5.550014	6.526546	7.200597	7.079582	7.079977
25	C	6.134815	6.555694	5.665666	5.538725	5.298734
26	H	6.593212	7.056249	6.243942	5.980380	5.497022
27	C	6.435714	6.510214	4.544635	4.609457	4.499638

		11	12	13	14	15
11	H	0.000000				
12	H	4.362869	0.000000			
13	C	3.327105	2.230747	0.000000		
14	H	4.336968	2.678666	1.080927	0.000000	
15	C	2.231298	3.352081	1.415952	2.223236	0.000000

	16 H 2.695598 4.357324 2.229854 2.677926 1.078617 17 C 1.079402 3.354656 2.281964 3.324882 1.417357 18 H 5.640854 5.047779 6.038617 6.763576 6.240975 19 C 5.870706 5.033138 5.877746 6.477996 6.160505 20 C 6.529920 6.185308 6.691313 7.228350 6.834287 21 H 6.013372 3.510069 4.847797 5.219382 5.618851 22 H 6.854019 7.048011 7.449980 8.055144 7.428889 23 C 7.041625 6.252261 6.628008 6.965777 6.916707 24 H 7.746084 7.154042 7.331465 7.592533 7.560466 25 C 6.752012 5.163160 5.752405 5.986005 6.297809 26 H 7.268270 5.284719 5.798310 5.834117 6.488918 27 C 6.059413 4.285481 5.260957 5.672110 5.832959 16 17 18 19 20 16 H 0.000000 17 C 2.233847 0.000000 18 H 7.108864 5.379199 0.000000 19 C 6.967313 5.508752 1.079318 0.000000 20 C 7.491430 6.273635 2.238050 1.430463 0.000000 21 H 6.527367 5.293973 2.698222 2.237702 3.355820 22 H 8.032495 6.759008 2.689552 2.239323 1.078941 23 C 7.495570 6.639656 3.342396 2.301458 1.416345 24 H 8.026336 7.382962 4.353803 3.346222 2.231022 25 C 6.963190 6.155882 3.341122 2.296296 2.299369 26 H 7.094529 6.570160 4.352816 3.340286 3.340680 27 C 6.657424 5.461741 2.236065 1.423091 2.312605 21 22 23 24 25 21 H 0.000000 22 H 4.363132 0.000000 23 C 3.353920 2.231870 0.000000 24 H 4.361150 2.693599 1.079175 0.000000 25 C 2.238778 3.343952 1.425846 2.234742 0.000000 26 H 2.696762 4.351914 2.234521 2.685446 1.079351 27 C 1.078314 3.353402 2.311881 3.352989 1.425718 26 27 26 H 0.000000 27 C 2.237232 0.000000
	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.314101 0.000000 3 H 2.921529 4.140885 0.000000 4 C 2.206252 3.948569 1.078847 0.000000 5 C 2.209434 4.002371 2.233456 1.421185 0.000000 6 H 2.970037 4.783844 2.699919 2.239414 3.343969 7 H 2.922075 4.232916 2.695827 2.236482 1.078777 8 C 2.275076 4.426217 3.345755 2.302137 1.428285 9 H 3.003639 4.949220 4.353459 3.343331 2.235842

5T. -957.469678 26.58 C1
WBI 1.14

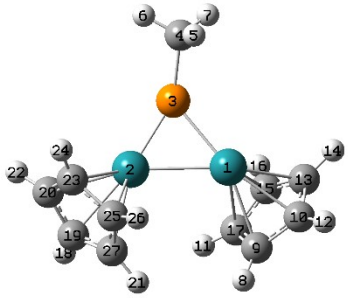
Charge and spin density

		1	2
1	Ru	0.192685	1.214154
2	Ru	0.348337	0.529530
4	C	-0.065214	0.005078
5	C	-0.001032	0.003663
8	C	-0.015895	0.021384
10	C	0.011026	0.110714
12	C	-0.068956	0.000232
14	C	-0.060697	-0.007917
15	C	-0.039321	0.011140
18	C	-0.028805	-0.020178
20	C	-0.007878	0.034607
22	C	-0.002824	0.039869
23	P	-0.266767	0.044273
24	C	0.005340	0.013451

10	C	2.305457	4.613492	3.346590	2.304007	2.301734
11	H	3.033826	5.248131	4.356353	3.347052	3.345329
12	C	2.250642	4.326955	2.239697	1.426328	2.299873
13	H	4.740401	2.910094	4.969130	5.401666	5.864128
14	C	4.328253	2.186364	5.186121	5.409892	5.691979
15	C	4.291038	2.188690	5.708952	5.753395	6.083404
16	H	4.794957	2.938891	5.582273	5.740854	5.531355
17	H	4.671869	2.910495	5.952750	6.032519	6.562419
18	C	4.270132	2.183935	6.265857	6.096100	6.127234
19	H	4.668091	2.926315	6.956557	6.667349	6.667922
20	C	4.321403	2.198644	6.156590	6.008453	5.791492
21	H	4.742759	2.937418	6.760238	6.503674	6.061021
22	C	4.350401	2.198553	5.495512	5.580804	5.501646
23	P	2.283231	2.339301	4.715930	4.089497	3.364849
24	C	3.444904	3.398020	6.266212	5.526263	4.881825
25	H	3.860135	4.319306	6.631804	5.773523	4.977098
26	H	3.450116	3.359915	6.356076	5.632115	5.237649
27	H	4.354308	3.820950	7.076326	6.414410	5.723465

		6	7	8	9	10
6	H	0.000000				
7	H	4.356867	0.000000			
8	C	3.334068	2.237816	0.000000		
9	H	4.343764	2.688304	1.078846	0.000000	
10	C	2.228687	3.342334	1.413018	2.227018	0.000000
11	H	2.682235	4.351947	2.225821	2.683855	1.079620
12	C	1.079667	3.344785	2.292149	3.335660	1.418617
13	H	6.258767	5.877122	6.750748	7.444606	6.867073
14	C	6.251962	5.726410	6.412967	7.002163	6.577478
15	C	6.150613	6.319869	6.524929	7.085933	6.480889
16	H	7.216247	5.162357	6.367097	6.721709	6.991087
17	H	6.061378	6.930323	6.946854	7.589263	6.686586
18	C	6.595549	6.317658	6.359614	6.719126	6.460196
19	H	6.922112	6.951637	6.683710	6.962511	6.684220
20	C	6.970911	5.743539	6.166498	6.419342	6.573050
21	H	7.574058	5.923556	6.317080	6.389249	6.874299
22	C	6.766959	5.337913	6.191514	6.593973	6.636593
23	P	5.230449	3.457919	3.306442	3.331414	4.000381
24	C	6.115868	5.146132	4.361203	4.154679	4.760844
25	H	6.322186	5.261475	4.200223	3.757690	4.660808
26	H	5.838545	5.674347	4.666479	4.623708	4.743338
27	H	7.127548	5.839330	5.323990	5.058835	5.820945

		11	12	13	14	15
11	H	0.000000				
12	C	2.230260	0.000000			
13	H	7.631759	6.078783	0.000000		
14	C	7.271748	5.986698	1.079670	0.000000	

	15 C 6.991427 6.001418 2.234547 1.421903 0.000000 16 H 7.798523 6.642777 2.693923 2.239764 3.350815 17 H 7.114122 6.101919 2.692346 2.234841 1.079599 18 C 6.879679 6.289530 3.347699 2.304463 1.424059 19 H 6.942447 6.660953 4.357785 3.347637 2.237760 20 C 7.127109 6.472594 3.339517 2.296510 2.299231 21 H 7.383960 6.971978 4.348466 3.339130 3.341981 22 C 7.355920 6.285966 2.234995 1.425993 2.308160 23 P 4.537417 4.416185 5.060682 4.305114 4.318754 24 C 4.898119 5.445701 6.196261 5.270639 4.812997 25 H 4.658406 5.594369 7.175019 6.290271 5.869291 26 H 4.747971 5.338166 6.115261 5.191015 4.469285 27 H 5.989846 6.453686 6.376412 5.375290 4.936891 16 17 18 19 20 16 H 0.000000 17 H 4.360862 0.000000 18 C 3.355222 2.233929 0.000000 19 H 4.364120 2.692754 1.078854 0.000000 20 C 2.235979 3.342779 1.426566 2.240197 0.000000 21 H 2.688562 4.352256 2.235990 2.695396 1.078903 22 C 1.078548 3.351367 2.312740 3.354957 1.422113 23 P 3.945846 5.079669 3.637103 3.970238 3.152412 24 C 5.194045 5.443029 3.751966 3.557408 3.644782 25 H 6.096100 6.461462 4.843547 4.609614 4.696708 26 H 5.562866 4.916029 3.470985 3.064929 3.786169 27 H 5.073455 5.663594 3.680205 3.427165 3.396077 21 22 23 24 25 21 H 0.000000 22 C 2.230368 0.000000 23 P 3.071481 3.627957 0.000000 24 C 3.322194 4.658154 1.862826 0.000000 25 H 4.295108 5.651028 2.434300 1.094914 0.000000 26 H 3.687806 4.847689 2.515265 1.089824 1.779624 27 H 2.801498 4.580134 2.449168 1.095432 1.758058 26 27 26 H 0.000000 27 H 1.784634 0.000000
	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.571540 0.000000 3 P 2.277816 2.149217 0.000000 4 C 3.715756 3.771834 1.834564 0.000000 5 H 3.859553 4.106582 2.430874 1.092273 0.000000 6 H 4.579454 4.066037 2.434253 1.091374 1.780361 7 H 4.048555 4.556042 2.435974 1.091763 1.774679 8 H 3.000840 4.159979 5.074722 6.665752 6.717570

6Q -957.46389 30.21 C1
WBI 0.69

Charges and spin densities

		1	2
1	Ru	0.321215	2.668203
2	Ru	0.344053	0.990427
3	P	-0.240653	0.036427
4	C	0.018188	0.014382
9	C	-0.092940	0.053729
10	C	-0.078294	0.040478
13	C	-0.062925	0.029342
15	C	0.002237	0.123638
17	C	-0.009326	0.032390
19	C	-0.011952	0.022488
20	C	-0.019784	0.023439
23	C	-0.096234	-0.035470
25	C	-0.045809	-0.007675
27	C	-0.027776	0.008202

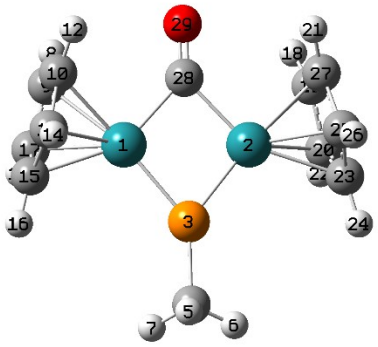
9	C	2.306608	3.960011	4.459097	6.012472	6.144197
10	C	2.283150	4.615579	4.504168	5.738346	5.749366
11	H	3.120820	3.665025	4.399607	6.164409	6.647897
12	H	2.975447	5.297938	5.158861	6.200290	6.029149
13	C	2.354286	4.764699	4.142724	5.251904	5.452748
14	H	3.061376	5.526225	4.528159	5.297173	5.456388
15	C	2.457752	4.278044	3.899745	5.289443	5.731118
16	H	3.163910	4.653447	4.027127	5.295443	5.904287
17	C	2.407723	3.713361	4.082557	5.741780	6.123125
18	H	4.975972	3.053740	4.991523	6.648034	7.112775
19	C	4.451668	2.312936	4.405395	5.990557	6.337138
20	C	4.794181	2.262182	4.114662	5.394187	5.719905
21	H	3.901078	3.013161	4.931655	6.599488	6.713554
22	H	5.557065	2.994717	4.518141	5.621879	6.062728
23	C	4.431292	2.166272	3.841750	4.909995	4.973738
24	H	4.993052	2.895556	4.093245	4.765188	4.704739
25	C	3.779556	2.152038	3.984312	5.277909	5.225311
26	H	3.857999	2.877124	4.343899	5.456568	5.193805
27	C	3.838354	2.278888	4.363492	5.957083	6.098974

		6	7	8	9	10
6	H	0.000000				
7	H	1.778489	0.000000			
8	H	7.445543	7.048030	0.000000		
9	C	6.848059	6.267218	1.079822	0.000000	
10	C	6.708598	5.829272	2.235110	1.421207	0.000000
11	H	6.770641	6.396981	2.687347	2.232288	3.341279
12	H	7.210642	6.303231	2.697416	2.236851	1.079873
13	C	6.229090	5.111690	3.339851	2.294711	1.423737
14	H	6.320275	4.962701	4.351199	3.338713	2.234926
15	C	6.118010	5.198679	3.334529	2.292800	2.298422
16	H	6.037120	5.061888	4.343505	3.335560	3.341124
17	C	6.486816	5.903408	2.233142	1.421603	2.298791
18	H	6.731997	7.352745	4.888633	5.086472	6.305294
19	C	6.088079	6.790205	4.628269	4.848744	5.958561
20	C	5.281440	6.303721	5.638680	5.746786	6.654146
21	H	7.023117	7.319371	2.837670	3.449384	4.652756
22	H	5.313247	6.504636	6.597749	6.628035	7.514034
23	C	4.887921	5.917545	5.455545	5.601346	6.315158
24	H	4.603030	5.835781	6.313736	6.412282	6.967811
25	C	5.538744	6.204129	4.232518	4.541181	5.307599
26	H	5.828019	6.372790	4.194489	4.573106	5.152527
27	C	6.254616	6.765314	3.609732	4.011299	5.088440

		11	12	13	14	15
11	H	0.000000				
12	H	4.352993	0.000000			
13	C	3.330166	2.237225	0.000000		

	14 H 4.338987 2.692949 1.079915 0.000000 15 C 2.222009 3.340721 1.414602 2.227126 0.000000 16 H 2.675426 4.350209 2.225813 2.681147 1.079601 17 C 1.078984 3.343332 2.287612 3.330444 1.409577 18 H 3.845025 7.093574 6.588604 7.557909 5.666452 19 C 4.039276 6.653744 6.335460 7.272642 5.599990 20 C 5.075652 7.298792 6.926718 7.749542 6.283766 21 H 3.488195 5.159006 5.458273 6.476109 5.025516 22 H 5.720007 8.212466 7.642713 8.419546 6.901865 23 C 5.487833 6.785666 6.730607 7.486360 6.372715 24 H 6.429340 7.357689 7.342990 7.999010 7.095587 25 C 4.811302 5.688007 5.965396 6.795797 5.741492 26 H 5.315285 5.329800 5.972918 6.742883 5.999431 27 C 3.856885 5.631626 5.733518 6.692382 5.259352 16 17 18 19 20 16 H 0.000000 17 C 2.221188 0.000000 18 H 5.940836 4.600790 0.000000 19 C 5.979350 4.577472 1.080140 0.000000 20 C 6.576589 5.480575 2.226809 1.418995 0.000000 21 H 5.749062 3.762794 2.676508 2.223071 3.341271 22 H 7.047748 6.199925 2.673969 2.227534 1.079555 23 C 6.810853 5.637681 3.340338 2.299041 1.420362 24 H 7.503006 6.493164 4.351430 3.343171 2.237982 25 C 6.372890 4.854352 3.335384 2.291585 2.303084 26 H 6.742864 5.169707 4.344786 3.333944 3.345238 27 C 5.871231 4.146397 2.221330 1.409739 2.299407 21 22 23 24 25 21 H 0.000000 22 H 4.345541 0.000000 23 C 3.358114 2.235440 0.000000 24 H 4.366040 2.703076 1.078718 0.000000 25 C 2.237569 3.349668 1.437653 2.247443 0.000000 26 H 2.696986 4.360122 2.247191 2.703355 1.079012 27 C 1.078623 3.339011 2.314550 3.355370 1.425943 26 27 26 H 0.000000 27 C 2.238274 0.000000

Table S3. Distance matrix for the lowest energy $MePCp_2Ru_2(CO)$ structures as optimized at the PBE0/def2TZVP level. Included are the ranking order, spin multiplicity (S, T or Q), total energy (in a.u.), relative energy (in kcal/mol), symmetry point group Wiberg bond indices for the Fe-Fe bonds, Mulliken charges and the spin density (Cp moieties are omitted for clarity).



1S -1070.854173 0.00 C2v
WBI 0.49

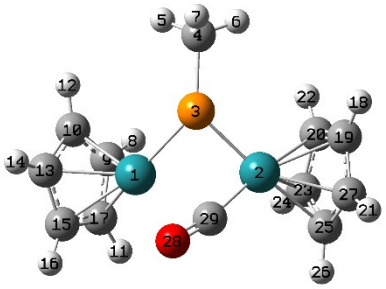
Charge and spin densities

		1
1	Ru	0.408759
2	Ru	0.408834
3	P	-0.334380
4	C	0.045373
9	C	0.004487
10	C	0.004920
13	C	-0.018783
15	C	-0.063912
17	C	-0.016459
19	C	0.004122
20	C	-0.015121
23	C	-0.066355
25	C	-0.017154
27	C	0.004547
28	C	-0.105497
29	O	-0.243379

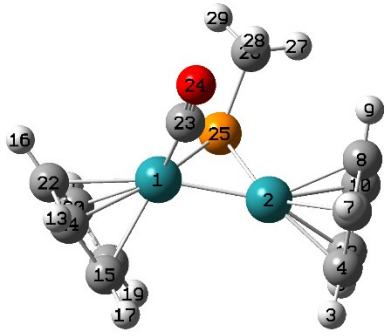
		1	2	3	4	5
1	Ru	0.000000				
2	Ru	2.731067	0.000000			
3	P	2.167998	2.166816	0.000000		
4	C	3.762059	3.766351	1.824690	0.000000	
5	H	4.141862	4.297780	2.411691	1.092645	0.000000
6	H	4.552864	3.928389	2.433599	1.090554	1.777813
7	H	3.985416	4.482501	2.425271	1.091373	1.772968
8	H	2.922526	4.786964	4.931943	6.486104	6.982277
9	C	2.199103	4.534658	4.299014	5.757653	6.152896
10	C	2.198802	4.532157	4.299545	5.755349	5.913729
11	H	2.908878	5.139699	4.207142	5.140860	5.724739
12	H	2.921540	4.781636	4.932213	6.481752	6.579432
13	C	2.170680	4.710135	3.850211	4.964551	4.953158
14	H	2.908421	5.133036	4.209056	5.133204	4.889258
15	C	2.182993	4.851504	3.578293	4.439757	4.609777
16	H	2.916567	5.364475	3.712524	4.108335	4.190610
17	C	2.171357	4.714388	3.849495	4.969065	5.405784
18	H	4.786108	2.922759	4.931147	6.491509	7.162059
19	C	4.534166	2.199354	4.298176	5.764373	6.375124
20	C	4.714574	2.171659	3.849043	4.978318	5.685940
21	H	4.780767	2.921631	4.931045	6.486592	6.768751
22	H	5.139918	2.909063	4.206794	5.150150	5.996695
23	C	4.851782	2.182926	3.577530	4.450504	4.957671
24	H	5.365068	2.916415	3.711946	4.121091	4.599851
25	C	4.710524	2.171015	3.849574	4.973378	5.256420
26	H	5.133263	2.908414	4.208081	5.141456	5.202845
27	C	4.531796	2.199072	4.298606	5.761844	6.144065
28	C	2.004138	2.004211	3.150124	4.974755	5.422359
29	O	2.976942	2.977047	4.328482	6.153107	6.582216

		6	7	8	9	10
6	H	0.000000				
7	H	1.783614	0.000000			
8	H	7.218253	6.460297	0.000000		
9	C	6.586609	5.716099	1.078958	0.000000	
10	C	6.646671	5.881288	2.228528	1.417916	0.000000
11	H	5.943289	4.700830	2.692139	2.235627	3.343256
12	H	7.321073	6.734478	2.681302	2.228382	1.078960
13	C	5.963677	5.023763	3.343856	2.301799	1.425625
14	H	6.145632	5.290517	4.351473	3.343465	2.235706
15	C	5.458300	4.214876	3.347672	2.304866	2.304807

16	H	5.165485	3.705733	4.357825	3.348054	3.347930	
17	C	5.854670	4.704014	2.237374	1.425645	2.301580	
18	H	6.473747	7.060767	5.261347	5.608459	5.934159	
19	C	5.677014	6.446584	5.608792	5.757563	5.925740	
20	C	4.675534	5.659269	6.224378	6.241010	6.493500	
21	H	6.590013	7.310198	5.898190	5.929929	5.596411	
22	H	4.753125	5.678912	6.468429	6.546203	6.998677	
23	C	4.059298	5.326783	6.883060	6.700123	6.696192	
24	H	3.507642	5.019145	7.619294	7.345439	7.341614	
25	C	4.813519	5.925598	6.697249	6.491751	6.231160	
26	H	5.007287	6.171982	7.308114	6.992823	6.532140	
27	C	5.747630	6.592401	5.934950	5.926065	5.749947	
28	C	5.459526	5.447130	3.060985	2.965632	2.961485	
29	O	6.621213	6.608388	2.979495	3.205250	3.199776	
		11	12	13	14	15	
11	H	0.000000					
12	H	4.351199	0.000000				
13	C	3.346889	2.237317	0.000000			
14	H	4.358406	2.692255	1.079105	0.000000		
15	C	2.237924	3.347640	1.424412	2.238146	0.000000	
16	H	2.696601	4.357715	2.236350	2.696556	1.078976	
17	C	1.079133	3.343602	2.302915	3.346849	1.424171	
18	H	6.468167	5.897538	6.696167	7.307062	6.882507	
19	C	6.545993	5.929891	6.490990	6.992154	6.699757	
20	C	6.581701	6.694160	6.806443	7.294054	6.789913	
21	H	7.308472	5.244920	6.209464	6.449610	6.874153	
22	H	6.574545	7.308796	7.298475	7.878094	7.085367	
23	C	7.085167	6.874958	6.783107	7.073837	6.873918	
24	H	7.488494	7.611494	7.245932	7.477080	7.224694	
25	C	7.298612	6.210652	6.398462	6.563513	6.783242	
26	H	7.877955	6.450939	6.563362	6.550676	7.073675	
27	C	6.998588	5.596830	6.230477	6.531456	6.695830	
28	C	4.283107	3.052494	3.658886	4.274359	4.057328	
29	O	4.867047	2.967469	4.237082	4.855982	4.788817	
		16	17	18	19	20	
16	H	0.000000					
17	C	2.236326	0.000000				
18	H	7.618723	6.223932	0.000000			
19	C	7.344962	6.240708	1.078951	0.000000		
20	C	7.252639	6.411739	2.237320	1.425552	0.000000	
21	H	7.610404	6.693702	2.681330	2.228468	3.343597	
22	H	7.488697	6.581700	2.692250	2.235634	1.079120	
23	C	7.224485	6.789783	3.347591	2.304768	1.424179	
24	H	7.423786	7.252587	4.357719	3.347933	2.236270	
25	C	7.245744	6.806620	3.343854	2.301829	2.302995	
26	H	7.476477	7.293993	4.351504	3.343527	3.346897	

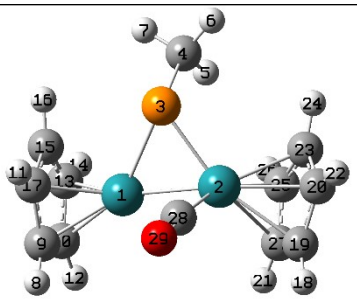
	27 C 7.340994 6.493335 2.228588 1.418027 2.301601 28 C 4.900412 3.664629 3.059743 2.964678 3.664095 29 O 5.739686 4.244057 2.977689 3.203901 4.243109 21 22 23 24 25 21 H 0.000000 22 H 4.351252 0.000000 23 C 3.347541 2.237843 0.000000 24 H 4.357648 2.696373 1.078984 0.000000 25 C 2.237235 3.346917 1.424417 2.236392 0.000000 26 H 2.692269 4.358372 2.238108 2.696551 1.079098 27 C 1.078955 3.343318 2.304706 3.347850 1.425540 28 C 3.051631 4.282595 4.056897 4.900160 3.658789 29 O 2.966429 4.866123 4.788085 5.739130 4.236716 26 27 28 29 26 H 0.000000 27 C 2.235691 0.000000 28 C 4.274275 2.960860 0.000000 29 O 4.855779 3.198897 1.178358 0.000000
 2S -1070.815996 23.96 C1 WBI 0.35 Charges and spin densities 1 1 Ru 0.481279 2 Ru 0.521327 3 P -0.270334 4 C 0.007079 9 C -0.040288 10 C -0.065049 13 C -0.054437 15 C 0.010334 17 C -0.049292 19 C -0.027170 20 C -0.035053 23 C -0.058204 25 C -0.026045 27 C -0.049314 28 O -0.168144	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.974834 0.000000 3 P 2.209511 2.200629 0.000000 4 C 3.706434 3.630982 1.832406 0.000000 5 H 3.756723 4.326647 2.434802 1.091792 0.000000 6 H 4.400916 3.653753 2.445825 1.090882 1.787625 7 H 4.336198 4.282340 2.418416 1.093116 1.769078 8 H 2.837655 4.182606 3.778545 4.389866 3.984796 9 C 2.099352 4.180566 3.571701 4.438423 4.052986 10 C 2.105843 4.711672 3.429377 4.065260 3.521584 11 H 2.952060 4.505424 4.832749 6.180355 6.051416 12 H 2.855511 5.150949 3.535671 3.659886 2.892538 13 C 2.164158 5.133136 3.969508 4.939966 4.557352 14 H 2.927888 5.852391 4.468762 5.311900 4.914261 15 C 2.216870 4.941673 4.402841 5.704359 5.475016 16 H 2.951231 5.473791 5.123968 6.558412 6.413687 17 C 2.192671 4.366545 4.202727 5.461546 5.243240 18 H 5.646276 2.938138 3.920779 4.170882 5.120645 19 C 5.086562 2.213246 3.705434 4.320172 5.177890 20 C 4.668639 2.222892 3.614716 4.173437 4.790146 21 H 5.746424 2.939094 4.775879 5.871058 6.803904 22 H 4.926065 2.961482 3.771632 3.892076 4.360228 23 C 4.438469 2.213280 4.060732 5.061418 5.576040 24 H 4.513727 2.951724 4.551987 5.535870 5.866561 25 C 4.777838 2.229582 4.416266 5.667450 6.341574 26 H 5.099205 2.954317 5.118948 6.538361 7.173090 27 C 5.131756 2.199828 4.189821 5.253698 6.109517

29 C -0.176689	28 O 2.352768 3.010048 3.262415 5.066867 5.514154 29 C 2.267673 1.843377 2.606476 4.425540 4.983374 6 7 8 9 10 6 H 0.000000 7 H 1.773759 0.000000 8 H 4.674391 5.387011 0.000000 9 C 4.944341 5.316857 1.079288 0.000000 10 C 4.821292 4.746212 2.243078 1.432058 0.000000 11 H 6.594774 7.029596 2.704762 2.247946 3.364730 12 H 4.439834 4.279135 2.703702 2.245376 1.079189 13 C 5.809567 5.437921 3.355117 2.311733 1.430238 14 H 6.284283 5.616690 4.368028 3.356672 2.245466 15 C 6.444828 6.309828 3.336027 2.293612 2.302157 16 H 7.319802 7.084694 4.346413 3.337323 3.343775 17 C 6.001782 6.260887 2.243967 1.434577 2.321559 18 H 3.520790 4.539142 6.310379 6.614809 7.028646 19 C 3.780895 4.872779 5.656223 5.968761 6.554280 20 C 3.609587 4.986425 4.577171 5.072011 5.847928 21 H 5.602214 6.215247 6.997017 7.057362 7.627724 22 H 3.174875 4.782654 4.350906 5.006106 5.737224 23 C 4.719366 5.919002 4.336472 4.755848 5.763723 24 H 5.246929 6.487518 3.864756 4.389146 5.580850 25 C 5.417958 6.356885 5.364313 5.561219 6.463319 26 H 6.387732 7.212971 5.797200 5.892967 6.855483 27 C 4.927891 5.758770 6.062226 6.222063 6.888426 28 O 5.667265 5.409237 4.937722 4.259750 4.369253 29 C 4.848162 4.887550 4.491637 4.045953 4.366399 11 12 13 14 15 11 H 0.000000 12 H 4.375250 0.000000 13 C 3.357453 2.241893 0.000000 14 H 4.362291 2.705795 1.078801 0.000000 15 C 2.228423 3.345728 1.425936 2.238371 0.000000 16 H 2.679206 4.354089 2.230147 2.684587 1.080680 17 C 1.078782 3.364665 2.315244 3.354731 1.412372 18 H 7.267231 7.118602 7.707658 8.331579 7.761588 19 C 6.388732 6.782861 7.199094 7.912535 7.088322 20 C 5.549026 6.089552 6.661461 7.496308 6.507387 21 H 6.912676 8.060126 7.895095 8.520426 7.546937 22 H 5.818779 5.821199 6.740477 7.579391 6.737571 23 C 4.660037 6.239811 6.407954 7.323613 5.955011 24 H 4.099723 6.119864 6.266836 7.260741 5.700676 25 C 5.145403 7.027863 6.852246 7.682534 6.291180 26 H 5.056352 7.543260 7.072125 7.901785 6.317540 27 C 6.168228 7.308585 7.292387 8.003771 6.951638 28 O 3.989112 5.123512 3.870742 4.286371 3.433932

	29 C 3.949986 5.036352 4.252098 4.835550 3.879460 16 17 18 19 20 16 H 0.000000 17 C 2.220786 0.000000 18 H 8.367547 7.127337 0.000000 19 C 7.666051 6.359126 1.079334 0.000000 20 C 7.193687 5.571281 2.230594 1.416310 0.000000 21 H 7.834531 7.025102 2.686036 2.236045 3.344073 22 H 7.539822 5.749612 2.692557 2.231682 1.078950 23 C 6.522840 4.923444 3.345653 2.300734 1.430172 24 H 6.291929 4.506283 4.354763 3.342709 2.240589 25 C 6.663715 5.460232 3.343227 2.301249 2.302283 26 H 6.533697 5.528686 4.352930 3.344659 3.345554 27 C 7.348178 6.288288 2.232892 1.425510 2.303063 28 O 3.430543 3.707961 5.675524 5.089727 5.191921 29 C 4.128946 3.747450 4.568972 3.930529 4.027012 21 22 23 24 25 21 H 0.000000 22 H 4.354815 0.000000 23 C 3.344730 2.239597 0.000000 24 H 4.355154 2.694699 1.078961 0.000000 25 C 2.239781 3.343519 1.416480 2.229626 0.000000 26 H 2.697827 4.352949 2.227292 2.684047 1.079208 27 C 1.078600 3.347131 2.301771 3.345055 1.425154 28 O 4.763649 5.859552 4.731181 5.076421 4.343781 29 C 3.808093 4.736114 3.630267 4.092065 3.287179 26 27 28 29 26 H 0.000000 27 C 2.236081 0.000000 28 O 4.337918 4.550703 0.000000 29 C 3.468055 3.457817 1.178307 0.000000
 3S -1070.807612 29.22 C1 WBI 1.04 Charges and spin densities 1	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.350069 0.000000 3 H 4.694375 2.875325 0.000000 4 C 4.308927 2.153336 1.079666 0.000000 5 C 4.319444 2.155721 2.234516 1.419964 0.000000 6 H 4.678952 2.882918 2.691003 2.239446 3.347874 7 H 4.717370 2.881961 2.697346 2.235632 1.079435 8 C 4.302545 2.148776 3.346765 2.302396 1.427117 9 H 4.703625 2.883083 4.355840 3.344707 2.237846 10 C 4.313294 2.169448 3.342661 2.300909 2.303364 11 H 4.706363 2.900812 4.350339 3.342954 3.346295 12 C 4.286999 2.147681 2.235133 1.427312 2.305687 13 H 2.969166 4.793983 6.140799 6.188923 6.180020 14 C 2.264026 4.278851 5.804376 5.795500 5.937716

1 Ru 0.156445 2 Ru 0.362208 4 C -0.040674 5 C 0.005397 8 C 0.002939 10 C 0.015165 12 C 0.002846 14 C -0.076724 15 C -0.010137 18 C -0.016125 20 C -0.008428 22 C -0.014061 23 C -0.029550 24 O -0.181007 25 P -0.167847 26 C -0.000449	15 C 2.297050 3.766665 4.847183 4.967518 5.423786 16 H 2.996751 5.339592 7.526648 7.268782 7.223662 17 H 3.025100 3.909465 4.303729 4.643284 5.224269 18 C 2.309188 3.792789 5.201962 5.164251 5.742245 19 H 3.027465 3.933715 5.009568 5.012004 5.812100 20 C 2.301472 4.328538 6.286843 6.075235 6.413944 21 H 3.009719 4.858873 6.967130 6.659803 7.005918 22 C 2.287400 4.612565 6.615244 6.428904 6.535643 23 C 1.840515 2.648311 5.047753 4.519400 3.940011 24 O 2.991606 3.465849 5.673460 5.112783 4.248726 25 P 2.280170 2.437103 5.156010 4.401096 4.375641 26 C 3.510448 3.381733 6.154886 5.229096 4.718107 27 H 4.375649 3.738187 6.272498 5.265742 4.764651 28 H 3.543005 3.352839 6.063962 5.151281 4.384596 29 H 3.985391 4.340150 7.165289 6.272310 5.792364 6 7 8 9 10 6 H 0.000000 7 H 4.359297 0.000000 8 C 3.346645 2.235675 0.000000 9 H 4.356537 2.689468 1.079265 0.000000 10 C 2.234276 3.345211 1.422518 2.236826 0.000000 11 H 2.686695 4.354366 2.233849 2.694242 1.078707 12 C 1.078807 3.350050 2.304049 3.347230 1.421089 13 H 7.035033 6.129551 6.648175 7.007402 6.955982 14 C 6.331113 6.076733 6.285913 6.719404 6.389882 15 C 5.291648 5.705931 5.882709 6.519359 5.775486 16 H 7.501294 7.448774 7.166889 7.361735 7.210287 17 H 5.169375 5.428121 5.922316 6.653799 5.863473 18 C 4.895301 6.251998 5.924359 6.576725 5.514033 19 H 4.342299 6.449153 5.976340 6.736265 5.339199 20 C 5.800042 6.900729 6.361671 6.823333 6.017070 21 H 6.085637 7.588485 6.762843 7.174931 6.272331 22 C 6.612559 6.816076 6.585352 6.921701 6.542193 23 C 5.502542 4.026231 3.861637 3.898444 4.438072 24 O 6.337871 4.106510 4.141602 3.912872 4.994810 25 P 4.031785 5.117301 3.664804 3.939750 3.218013 26 C 5.207602 5.314923 3.647919 3.387601 3.618673 27 H 5.050184 5.459498 3.489609 3.168453 3.299125 28 H 5.582465 4.786065 3.409687 2.947596 3.804144 29 H 6.120385 6.353736 4.741469 4.431336 4.661975 11 12 13 14 15 11 H 0.000000 12 C 2.229637 0.000000 13 H 7.538354 6.662220 0.000000 14 C 6.888021 6.067596 1.079396 0.000000 15 C 6.321982 5.188748 2.233280 1.421681 0.000000

	16 H 7.424345 7.241652 2.688751 2.235418 3.348311 17 H 6.543444 5.077272 2.691282 2.234444 1.078428 18 C 5.847490 4.988296 3.334695 2.291073 1.417640 19 H 5.618992 4.656042 4.346529 3.335538 2.230907 20 C 6.186342 5.798594 3.332836 2.290319 2.298176 21 H 6.257055 6.171000 4.344042 3.334668 3.339294 22 C 6.827126 6.413754 2.232283 1.422852 2.306039 23 C 4.911313 4.783034 3.398430 3.249355 3.718678 24 O 5.471653 5.503584 4.019390 4.118153 4.740868 25 P 3.094717 3.716480 5.218634 4.446249 4.263199 26 C 3.310553 4.644940 6.190557 5.635595 5.764795 27 H 2.739856 4.511597 7.164157 6.581039 6.559374 28 H 3.737357 4.848424 5.936314 5.559168 5.828093 29 H 4.251570 5.648030 6.480871 5.911529 6.199480 16 17 18 19 20 16 H 0.000000 17 H 4.356871 0.000000 18 C 3.341137 2.231835 0.000000 19 H 4.348324 2.691372 1.079146 0.000000 20 C 2.230133 3.341147 1.419824 2.229258 0.000000 21 H 2.688700 4.348525 2.228705 2.679103 1.079121 22 C 1.078771 3.348061 2.297642 3.338682 1.415182 23 C 3.715269 4.222654 4.105296 4.839709 3.946094 24 O 4.411466 5.168400 5.235230 5.991032 5.008080 25 P 4.448878 4.928915 3.615992 3.801778 3.413029 26 C 5.276150 6.421030 5.323963 5.632223 4.902682 27 H 6.324294 7.136195 6.047842 6.197747 5.751682 28 H 5.318198 6.416415 5.648717 6.084316 5.269256 29 H 5.122617 6.979216 5.657022 6.024012 4.973301 21 22 23 24 25 21 H 0.000000 22 C 2.228156 0.000000 23 C 4.575945 3.431602 0.000000 24 O 5.605658 4.328453 1.155971 0.000000 25 P 3.419318 3.983572 3.001110 3.891598 0.000000 26 C 4.846909 5.124289 3.220029 3.595213 1.857710 27 H 5.630348 6.113374 4.127412 4.444351 2.440735 28 H 5.394025 5.221997 2.682101 2.754787 2.530771 29 H 4.741199 5.162242 3.769624 4.090217 2.418147 26 27 28 29 26 C 0.000000 27 H 1.094820 0.000000 28 H 1.089165 1.782782 0.000000 29 H 1.094749 1.754624 1.774646 0.000000



4S -1070.806729 29.77 C1
WBI 1.03

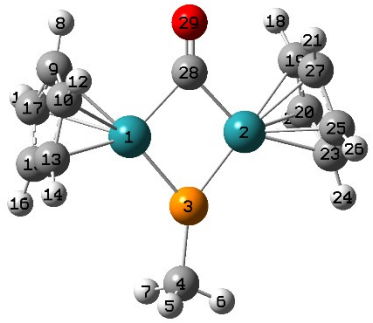
Charges and spin densities

		1
1	Ru	0.312491
2	Ru	0.173673
3	P	-0.166967
4	C	-0.019714
9	C	-0.000459
10	C	-0.026777
13	C	-0.001601
15	C	-0.001751
17	C	0.029750
19	C	-0.066560
20	C	-0.012438
23	C	-0.040922
25	C	-0.036953
27	C	0.000218
28	C	0.031045
29	O	-0.173036

		1	2	3	4	5
1	Ru	0.000000				
2	Ru	2.370834	0.000000			
3	P	2.446979	2.280952	0.000000		
4	C	3.532881	3.349534	1.863130	0.000000	
5	H	3.566900	3.286107	2.527045	1.089793	0.000000
6	H	4.482555	3.861703	2.433621	1.094989	1.781902
7	H	3.851183	4.230836	2.444817	1.094959	1.778135
8	H	2.881036	4.713355	4.950535	6.291990	6.418468
9	C	2.151803	4.322729	4.272134	5.429545	5.543708
10	C	2.162932	4.356032	4.480138	5.209066	5.067455
11	H	2.855858	4.642543	3.618012	4.973488	5.516465
12	H	2.889016	4.759962	5.281966	5.922625	5.615714
13	C	2.150261	4.330707	3.891646	4.218688	4.100194
14	H	2.893317	4.747843	4.338088	4.207113	3.881670
15	C	2.150526	4.307630	3.229679	3.814263	4.072427
16	H	2.882987	4.692960	3.126976	3.380648	3.810129
17	C	2.128702	4.275683	3.487363	4.644893	4.999470
18	H	4.817872	2.978589	5.197005	6.160553	5.888224
19	C	4.291170	2.270067	4.486686	5.232147	4.884765
20	C	4.607806	2.267542	4.019653	4.556221	4.313901
21	H	3.920073	3.051196	5.088677	5.565132	4.933791
22	H	5.338331	2.972384	4.411708	5.039513	4.969508
23	C	4.295843	2.270482	3.573456	3.563555	3.113091
24	H	4.826353	2.981428	3.616377	3.183650	2.792990
25	C	3.767649	2.307164	3.859574	3.814026	3.098369
26	H	3.900894	3.032220	4.132313	3.689169	2.759294
27	C	3.772861	2.316910	4.417595	4.865401	4.289112
28	C	2.654176	1.848382	2.858660	4.543250	4.795092
29	O	3.471676	2.995885	3.726939	5.520853	5.874023

		6	7	8	9	10
6	H	0.000000				
7	H	1.754982	0.000000			
8	H	7.221577	6.406723	0.000000		
9	C	6.410489	5.457331	1.079372	0.000000	
10	C	6.270148	5.218054	2.234375	1.418735	0.000000
11	H	5.767183	4.834167	2.693315	2.239366	3.343160
12	H	6.978391	6.013880	2.693074	2.231671	1.079966
13	C	5.308864	4.035651	3.350904	2.306954	1.426770
14	H	5.290804	3.961683	4.359547	3.348927	2.238827
15	C	4.827673	3.492722	3.349136	2.306817	2.300272
16	H	4.313581	2.804322	4.357000	3.348646	3.343722
17	C	5.571331	4.516017	2.236595	1.427284	2.300508
18	H	6.471537	7.128485	6.145265	6.197194	6.233150
19	C	5.538549	6.223276	6.082450	5.945359	5.836293
20	C	4.608246	5.627296	6.796023	6.520077	6.454983

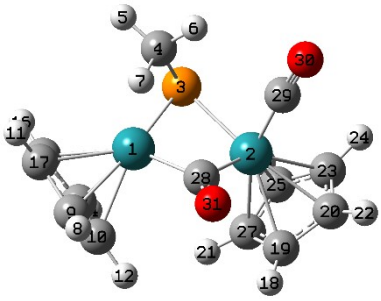
	21 H 6.193356 6.353713 5.461764 5.253984 4.698941 22 H 4.898276 6.115703 7.422581 7.204008 7.291779 23 C 3.646149 4.629136 6.865863 6.380739 6.087246 24 H 2.990576 4.245293 7.550460 6.970435 6.671782 25 C 4.243781 4.736421 6.239120 5.728826 5.190321 26 H 4.223916 4.460625 6.437837 5.798883 5.035769 27 C 5.367076 5.761036 5.722311 5.439297 5.015526 28 C 5.029542 5.236530 3.904337 3.860890 4.467732 29 O 5.961938 6.134913 3.917746 4.134637 5.017026 11 12 13 14 15 11 H 0.000000 12 H 4.353892 0.000000 13 C 3.347386 2.234823 0.000000 14 H 4.357752 2.690184 1.079177 0.000000 15 C 2.238437 3.342176 1.420729 2.234632 0.000000 16 H 2.691975 4.351890 2.232737 2.692528 1.078663 17 C 1.078848 3.344472 2.305424 3.349089 1.426577 18 H 6.980656 6.199906 6.696060 7.082969 6.959246 19 C 6.675164 5.864766 6.097192 6.379385 6.381217 20 C 6.842333 6.664524 6.433122 6.659615 6.513181 21 H 6.638804 4.383521 5.109572 5.210607 5.864102 22 H 7.276580 7.571404 7.261321 7.549913 7.181970 23 C 6.718801 6.328386 5.800180 5.834730 5.961136 24 H 7.061963 7.009430 6.174433 6.126066 6.213371 25 C 6.502992 5.257109 4.999040 4.933249 5.474050 26 H 6.665913 5.063708 4.662196 4.375927 5.295229 27 C 6.483499 4.919044 5.219139 5.338702 5.766511 28 C 3.872040 4.973761 4.788824 5.531317 4.460106 29 O 3.937631 5.529799 5.499217 6.354089 5.045321 16 17 18 19 20 16 H 0.000000 17 C 2.235492 0.000000 18 H 7.535257 6.643402 0.000000 19 C 6.871658 6.267334 1.079487 0.000000 20 C 6.789735 6.539491 2.231015 1.421754 0.000000 21 H 6.534281 5.924563 2.689532 2.233513 3.347525 22 H 7.388581 7.118114 2.688007 2.234912 1.078713 23 C 6.118369 6.291755 3.333474 2.290682 1.417829 24 H 6.183582 6.688377 4.343888 3.334458 2.229229 25 C 5.796367 5.877559 3.332860 2.289527 2.299235 26 H 5.562870 5.930126 4.343217 3.333152 3.341431 27 C 6.303390 5.869432 2.232222 1.420889 2.305645 28 C 4.971007 3.836539 3.322160 3.196419 3.435740 29 O 5.584577 4.137763 3.885008 4.028804 4.328926 21 22 23 24 25 21 H 0.000000

	22 H 4.356253 0.000000 23 C 3.341351 2.232528 0.000000 24 H 4.349756 2.689180 1.079102 0.000000 25 C 2.229465 3.342858 1.421483 2.232780 0.000000 26 H 2.685074 4.351784 2.232732 2.687759 1.079231 27 C 1.078473 3.347934 2.298209 3.340087 1.415356 28 C 4.128117 3.745538 3.955097 4.621345 4.079493 29 O 5.013595 4.453447 5.022566 5.673913 5.193687 26 27 28 29 26 H 0.000000 27 C 2.226645 0.000000 28 C 4.819468 3.654806 0.000000 29 O 5.956144 4.636450 1.153651 0.000000
 5T. -1070.806524 29.90 C2v WBI 1.00 Charge and spin density 1 1 Ru 0.312491 2 Ru 0.173673 3 P -0.166967 4 C -0.019714 9 C -0.000459 10 C -0.026777 13 C -0.001601 15 C -0.001751 17 C 0.029750 19 C -0.066560 20 C -0.012438 23 C -0.040922 25 C -0.036953 27 C 0.000218 28 C 0.031045 29 O -0.173036	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.769997 0.000000 3 P 2.205566 2.143262 0.000000 4 C 3.723059 3.795525 1.824365 0.000000 5 H 4.006648 4.426809 2.422574 1.092157 0.000000 6 H 4.559304 3.980299 2.426037 1.090862 1.780593 7 H 3.974117 4.405522 2.422423 1.092149 1.773611 8 H 3.069191 5.015440 5.216730 6.722023 6.992231 9 C 2.363541 4.757699 4.541250 5.901517 6.092660 10 C 2.312349 4.831385 4.373519 5.618194 5.567343 11 H 3.122983 5.248073 4.686045 5.689749 6.111425 12 H 3.010114 5.167757 4.955777 6.260725 6.123229 13 C 2.261150 4.947630 3.865203 4.714982 4.538736 14 H 2.960344 5.406462 4.105173 4.657308 4.234675 15 C 2.295602 4.959231 3.739234 4.461457 4.526905 16 H 3.009672 5.426393 3.879058 4.160279 4.209561 17 C 2.412293 4.901867 4.238310 5.309933 5.580662 18 H 4.768875 2.937977 4.919172 6.535075 7.292371 19 C 4.538305 2.211336 4.290471 5.833314 6.567583 20 C 4.749793 2.187607 3.871033 5.096174 5.948091 21 H 4.801466 2.938135 4.920616 6.553392 6.981322 22 H 5.169123 2.922440 4.233738 5.262973 6.227744 23 C 4.905221 2.182384 3.600378 4.606112 5.323691 24 H 5.430236 2.909875 3.746354 4.315400 5.037962 25 C 4.779954 2.189819 3.874883 5.118529 5.620235 26 H 5.219037 2.923812 4.237915 5.301388 5.620224 27 C 4.558504 2.213089 4.292910 5.845480 6.387055 28 C 2.027076 1.994525 3.132822 4.952493 5.401382 29 O 2.976473 2.974608 4.308723 6.127629 6.552455 6 7 8 9 10 6 H 0.000000

	7 H 1.780688 0.000000 8 H 7.572512 6.767642 0.000000 9 C 6.821454 5.916620 1.079669 0.000000 10 C 6.572329 5.795994 2.227390 1.421163 0.000000 11 H 6.585725 5.315964 2.681066 2.224531 3.343092 12 H 7.159851 6.577826 2.676447 2.230880 1.079519 13 C 5.751460 4.791873 3.334023 2.293009 1.418013 14 H 5.687159 4.821004 4.347520 3.339269 2.236398 15 C 5.511201 4.238173 3.328083 2.284278 2.299023 16 H 5.219851 3.719299 4.339637 3.328482 3.340507 17 C 6.270570 5.086246 2.225319 1.411576 2.300218 18 H 6.626924 6.927686 5.431622 5.743421 6.326558 19 C 5.824858 6.342991 5.782090 5.919166 6.300315 20 C 4.892454 5.567479 6.524208 6.475203 6.826593 21 H 6.643567 7.284894 5.821982 6.003443 6.001734 22 H 5.019440 5.548019 6.861865 6.808664 7.311157 23 C 4.236493 5.301056 7.120234 6.926386 6.993821 24 H 3.714287 5.020701 7.899127 7.596825 7.598562 25 C 4.913811 5.948721 6.808934 6.676581 6.571355 26 H 5.056581 6.248951 7.364364 7.164750 6.852560 27 C 5.835866 6.553216 5.982165 6.056522 6.131409 28 C 5.476491 5.384366 3.179669 3.146673 3.389408 29 O 6.642924 6.539076 2.953352 3.300270 3.684173 11 12 13 14 15 11 H 0.000000 12 H 4.348412 0.000000 13 C 3.348477 2.235782 0.000000 14 H 4.354966 2.704625 1.079449 0.000000 15 C 2.229548 3.345888 1.430237 2.239008 0.000000 16 H 2.689637 4.354959 2.237978 2.688776 1.079501 17 C 1.079924 3.340444 2.304045 3.344105 1.416074 18 H 6.113481 6.558997 6.925209 7.651918 6.773531 19 C 6.351243 6.518033 6.750767 7.357681 6.681710 20 C 6.555926 7.187914 6.998036 7.527796 6.774372 21 H 7.149305 5.842679 6.670465 7.121985 7.061287 22 H 6.535418 7.793824 7.401280 7.984775 6.972997 23 C 7.217135 7.265285 7.029593 7.366257 6.997345 24 H 7.735493 7.923446 7.450750 7.687432 7.370314 25 C 7.403911 6.636981 6.783963 7.068632 7.024522 26 H 8.065529 6.805690 7.011858 7.144940 7.423583 27 C 6.903123 6.147805 6.615275 7.071706 6.839926 28 C 4.183250 3.640451 4.002321 4.704046 4.157723 29 O 4.574174 3.731452 4.623137 5.386769 4.851543 16 17 18 19 20 16 H 0.000000 17 C 2.230253 0.000000

	18 H 7.392717 6.106276 0.000000 19 C 7.238497 6.232198 1.078808 0.000000 20 C 7.132890 6.506323 2.233652 1.420707 0.000000 21 H 7.798507 6.727798 2.683755 2.232578 3.343780 22 H 7.223877 6.651649 2.690624 2.232380 1.078961 23 C 7.308225 6.993158 3.343834 2.300152 1.425489 24 H 7.540009 7.521785 4.353763 3.342952 2.236707 25 C 7.497352 7.015440 3.343939 2.303001 2.307761 26 H 7.888101 7.564549 4.352590 3.345705 3.351096 27 C 7.462907 6.564938 2.233197 1.424102 2.302995 28 C 4.951275 3.725728 3.018538 2.919364 3.639709 29 O 5.752532 4.171017 2.939238 3.159398 4.218157 21 22 23 24 25 21 H 0.000000 22 H 4.352397 0.000000 23 C 3.343505 2.238862 0.000000 24 H 4.353370 2.696235 1.079044 0.000000 25 C 2.233085 3.351156 1.425665 2.236838 0.000000 26 H 2.690204 4.361751 2.238927 2.696195 1.078972 27 C 1.078829 3.345696 2.299734 3.342460 1.419936 28 C 3.005381 4.267867 4.024953 4.874692 3.631810 29 O 2.899857 4.854640 4.750694 5.707422 4.195628 26 27 28 29 26 H 0.000000 27 C 2.231760 0.000000 28 C 4.253466 2.914202 0.000000 29 O 4.816390 3.141851 1.176094 0.000000

Table S4. Distance matrix for the lowest energy $MePCp_2Ru_2(CO)_2$ structures as optimized at the PBE0/def2TZVP level. Included are the ranking order, spin multiplicity (S, T or Q), total energy (in a.u.), relative energy (in kcal/mol), symmetry point group Wiberg bond indices for the Fe-Fe bonds, Mulliken charges and the spin density (Cp moieties are omitted for clarity).

 1S -1184.12183 0.00 C1 WBI 0.37	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.752127 0.000000 3 P 2.294285 2.339567 0.000000 4 C 2.350371 3.258717 1.843662 0.000000 5 H 2.995565 4.282599 2.476385 1.088979 0.000000 6 H 3.139723 3.378567 2.507522 1.089851 1.794772 7 H 1.825726 3.389591 2.567433 1.189212 1.808049 8 H 2.969370 5.020744 5.260394 4.858732 5.316741 9 C 2.243150 4.585644 4.504717 4.308062 4.704599 10 C 2.163149 3.993800 4.098036 4.501424 5.016038

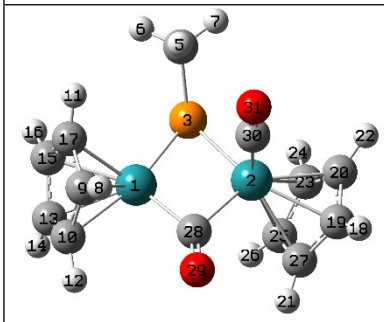
Charge and spin densities

	1
1 Ru	0.244728
2 Ru	0.306428
3 P	-0.200694
4 C	0.137361
9 C	0.034990
10 C	-0.065086
13 C	-0.014545
15 C	-0.027759
17 C	0.002684
19 C	0.005632
20 C	0.003243
23 C	-0.036288
25 C	0.027926
27 C	0.001861
28 C	0.007168
29 C	-0.055160
30 O	-0.148637
31 O	-0.223851

11 H	2.971071	5.684111	4.752757	3.940336	3.821071
12 H	2.896637	4.014589	4.639252	5.225220	5.868437
13 C	2.179558	4.135714	3.520277	4.185010	4.498008
14 H	2.913413	4.270301	3.625215	4.693317	5.004189
15 C	2.218502	4.740675	3.579707	3.705213	3.715779
16 H	2.961333	5.322644	3.723027	3.841538	3.573604
17 C	2.233565	4.965464	4.185480	3.770834	3.855001
18 H	4.349672	2.991726	5.035529	5.892955	6.887891
19 C	4.146375	2.272610	4.342179	5.412689	6.409066
20 C	4.777009	2.241610	4.455958	5.457098	6.497192
21 H	3.735034	3.010927	3.907553	5.353988	6.111009
22 H	5.458268	2.962910	5.234868	5.990034	7.062115
23 C	4.847245	2.210149	3.862463	5.154463	6.100645
24 H	5.592718	2.936020	4.275681	5.486700	6.385827
25 C	4.312952	2.266091	3.350438	4.959270	5.793995
26 H	4.650979	2.983642	3.309719	5.085338	5.769329
27 C	3.805297	2.276625	3.665844	5.096484	5.966343
28 C	1.975535	2.083774	3.258987	3.228680	4.202273
29 C	3.627738	1.838339	2.966496	3.021190	4.058215
30 O	4.528427	2.985881	3.819598	3.477458	4.398814
31 O	2.982693	3.007052	4.419783	4.195009	5.140026

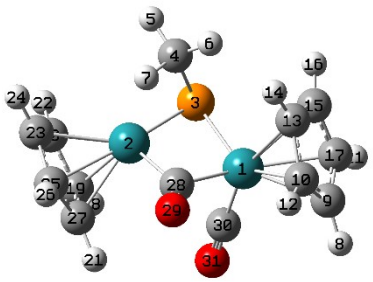
	6	7	8	9	10
6 H	0.000000				
7 H	1.721660	0.000000			
8 H	5.420393	3.792759	0.000000		
9 C	5.037534	3.384340	1.078932	0.000000	
10 C	5.288810	3.852437	2.240279	1.428018	0.000000
11 H	4.731937	3.089223	2.678459	2.219940	3.332000
12 H	5.905857	4.600511	2.693270	2.236208	1.079574
13 C	5.144751	3.844436	3.359343	2.316965	1.429173
14 H	5.651226	4.580084	4.369005	3.359658	2.243083
15 C	4.739757	3.320170	3.351351	2.307765	2.298633
16 H	4.922432	3.712116	4.357625	3.347980	3.343962
17 C	4.646709	2.973520	2.225870	1.409778	2.287533
18 H	6.086977	5.564191	5.035557	4.925079	4.057688
19 C	5.593452	5.297378	5.466429	5.184775	4.241638
20 C	5.392933	5.527215	6.409102	6.160550	5.370206
21 H	5.926281	5.335572	5.293934	4.649730	3.334162
22 H	5.754693	5.995171	6.845099	6.745148	6.100097
23 C	5.135620	5.521883	7.020903	6.578495	5.714127
24 H	5.319264	6.010024	7.911419	7.467745	6.675173
25 C	5.236754	5.332445	6.590503	5.980239	4.932229
26 H	5.455090	5.630389	7.145611	6.412989	5.339945
27 C	5.490485	5.160099	5.586221	5.039996	3.886515
28 C	3.418152	2.599630	3.175027	3.051242	2.979949
29 C	2.521455	3.272499	5.758704	5.510013	5.328960

30	O	2.649836	3.764798	6.492918	6.341703	6.327454	
31	O	4.227150	3.408105	3.111340	3.374283	3.511246	
		11	12	13	14	15	
11	H	0.000000					
12	H	4.340226	0.000000				
13	C	3.344074	2.240111	0.000000			
14	H	4.355250	2.700798	1.079020	0.000000		
15	C	2.236943	3.342047	1.420484	2.234300	0.000000	
16	H	2.691813	4.355070	2.234640	2.695118	1.079240	
17	C	1.080179	3.329551	2.301866	3.346338	1.428630	
18	H	6.852509	3.309264	4.847003	4.920568	5.942250	
19	C	6.914031	3.672457	4.738489	4.678281	5.808303	
20	C	7.657015	4.943819	5.755905	5.700128	6.663320	
21	H	6.282203	2.899264	3.309785	2.845735	4.599385	
22	H	8.235529	5.644410	6.626364	6.666568	7.467664	
23	C	7.816738	5.464993	5.744232	5.518335	6.581602	
24	H	8.533963	6.495705	6.619959	6.381369	7.346529	
25	C	7.230172	4.725824	4.738595	4.330393	5.686398	
26	H	7.449669	5.267362	4.854736	4.284462	5.721912	
27	C	6.611078	3.479396	3.969332	3.648822	5.113731	
28	C	4.332563	3.100566	3.691924	4.305678	4.082093	
29	C	6.166070	5.489511	5.518617	5.824408	5.755839	
30	O	6.775902	6.527849	6.536098	6.896550	6.626439	
31	O	4.801726	3.433333	4.518352	5.197883	4.912175	
		16	17	18	19	20	
16	H	0.000000					
17	C	2.240228	0.000000				
18	H	6.824307	5.961824	0.000000			
19	C	6.574056	6.017752	1.079351	0.000000		
20	C	7.332338	6.859720	2.219431	1.408503	0.000000	
21	H	5.235627	5.250457	2.696391	2.238089	3.337459	
22	H	8.173984	7.509111	2.676017	2.222967	1.079092	
23	C	7.065091	7.024183	3.340579	2.296520	1.434256	
24	H	7.735072	7.808757	4.348873	3.338161	2.244679	
25	C	6.116276	6.347232	3.345721	2.303311	2.308535	
26	H	5.972355	6.582402	4.356665	3.347498	3.352497	
27	C	5.742140	5.646562	2.240441	1.427836	2.296574	
28	C	4.922093	3.717125	3.103838	3.099804	3.563559	
29	C	6.234579	5.725676	4.314616	3.725395	3.121992	
30	O	7.047516	6.484099	5.279503	4.745290	3.971392	
31	O	5.830857	4.285691	3.136062	3.460516	3.914455	
		21	22	23	24	25	
21	H	0.000000					
22	H	4.348362	0.000000				
23	C	3.333387	2.245974	0.000000			
24	H	4.343055	2.703203	1.079252	0.000000		

	25 C 2.226489 3.350691 1.419022 2.230876 0.000000 26 H 2.684733 4.361447 2.231166 2.687195 1.079409 27 C 1.078825 3.340992 2.290610 3.333639 1.415419 28 C 3.810798 3.958317 4.131640 4.907120 4.112932 29 C 4.847321 3.304352 3.094498 3.279986 3.730579 30 O 5.991289 3.904196 3.949390 3.886812 4.755985 31 O 4.534852 4.046062 4.792589 5.563737 4.954620 26 27 28 29 30 26 H 0.000000 27 C 2.229702 0.000000 28 C 4.845495 3.482959 0.000000 29 C 4.321862 4.048834 2.699684 0.000000 30 O 5.295514 5.165313 3.572023 1.149345 0.000000 31 O 5.799638 4.194164 1.173885 3.333341 4.000314 31 31 O 0.000000
 2S -1184.115889 3.72 C1 WBI 0.36 Charges and spin densities 1 1 Ru 0.444270 2 Ru 0.261536 3 P -0.224793 4 C -0.012177 9 C -0.019293 10 C 0.026017 13 C -0.003941 15 C -0.026614 17 C -0.018848 19 C -0.014979 20 C -0.032544 23 C 0.027586 25 C 0.000346 27 C 0.023948 28 C -0.056663 29 O -0.225802 30 C 0.001945	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.730863 0.000000 3 P 2.259243 2.336627 0.000000 4 C 3.465275 3.597498 1.852252 0.000000 5 H 3.534628 3.682198 2.491565 1.090272 0.000000 6 H 3.793320 4.501570 2.429828 1.093253 1.780309 7 H 4.389441 3.940420 2.441560 1.092444 1.776554 8 H 2.869775 4.529640 4.659463 5.002049 4.418331 9 C 2.138835 4.354327 4.099840 4.614736 4.239432 10 C 2.244884 4.645566 4.475530 5.418418 5.271299 11 H 2.870606 4.822772 3.638205 3.268193 2.850333 12 H 2.970133 4.978305 5.221582 6.308395 6.138048 13 C 2.207853 4.862752 4.096516 5.105617 5.214495 14 H 2.940624 5.388369 4.621853 5.815300 6.066352 15 C 2.194792 4.842173 3.518361 4.088424 4.207897 16 H 2.930781 5.364423 3.633451 4.043576 4.365928 17 C 2.139883 4.519541 3.506438 3.695301 3.449666 18 H 5.452604 2.955844 5.218453 6.185030 6.074795 19 C 4.822868 2.244369 4.416166 5.568291 5.625719 20 C 4.879614 2.219609 3.803247 4.794648 5.029425 21 H 4.503119 2.980702 4.965433 6.519648 6.618303 22 H 5.576367 2.946791 4.239964 4.844523 5.030342 23 C 4.436248 2.283932 3.236038 4.578151 5.075146 24 H 4.771934 2.997645 3.165475 4.367726 5.054972 25 C 4.012933 2.293219 3.547764 5.203659 5.630470 26 H 4.030500 3.031452 3.773611 5.564843 6.094835 27 C 4.285193 2.270036 4.265944 5.771976 5.947107 28 C 1.980621 2.048128 3.327343 4.589088 4.439491 29 O 2.976460 2.996177 4.502546 5.700238 5.443759

31 O -0.149994	30 C 3.340401 1.838709 3.025585 3.323747 2.878020 31 O 4.115529 2.986552 3.862487 3.651060 2.907475 6 7 8 9 10 6 H 0.000000 7 H 1.764323 0.000000 8 H 5.294613 5.984618 0.000000 9 C 4.773697 5.657100 1.079396 0.000000 10 C 5.530060 6.441727 2.235890 1.424027 0.000000 11 H 3.091972 4.328463 2.697231 2.245677 3.359065 12 H 6.512163 7.290529 2.692297 2.234718 1.078677 13 C 5.010284 6.119836 3.327587 2.284051 1.410105 14 H 5.676869 6.769021 4.338003 3.327790 2.220752 15 C 3.803408 5.138971 3.345358 2.303895 2.313272 16 H 3.511935 5.020581 4.360270 3.350798 3.351651 17 C 3.597721 4.785633 2.245717 1.437796 2.318969 18 H 7.213699 6.226528 6.444374 6.630515 6.873275 19 C 6.553784 5.612859 6.267604 6.279735 6.426481 20 C 5.780234 4.619837 6.677195 6.569247 6.822213 21 H 7.326624 6.859515 5.940529 5.834035 5.514309 22 H 5.867976 4.459816 7.212850 7.173378 7.587136 23 C 5.400209 4.480436 6.731160 6.398019 6.442710 24 H 5.074611 4.124155 7.254812 6.820468 6.883101 25 C 5.944097 5.370391 6.308913 5.932786 5.710408 26 H 6.147132 5.821289 6.524127 6.000399 5.552217 27 C 6.625612 5.993479 6.010652 5.859237 5.705157 28 C 5.257137 5.297650 3.056936 2.931605 2.979104 29 O 6.368938 6.405923 3.201522 3.320832 3.219001 30 C 4.325234 3.662604 4.022444 4.204131 5.002927 31 O 4.606322 3.943631 4.116808 4.511796 5.537933 11 12 13 14 15 11 H 0.000000 12 H 4.367317 0.000000 13 C 3.345980 2.225657 0.000000 14 H 4.354321 2.679209 1.080051 0.000000 15 C 2.235993 3.356229 1.432182 2.237859 0.000000 16 H 2.705247 4.360064 2.241108 2.688338 1.078809 17 C 1.079389 3.361157 2.298323 3.339126 1.416799 18 H 7.433224 6.835936 7.420345 7.877155 7.636872 19 C 6.997537 6.467539 6.794609 7.177928 6.995035 20 C 6.842770 7.067705 6.954055 7.340941 6.910319 21 H 7.143919 5.254019 5.942390 6.104130 6.583556 22 H 7.193660 7.903070 7.721242 8.179168 7.520999 23 C 6.646695 6.738186 6.317393 6.543118 6.313907 24 H 6.774722 7.296532 6.555942 6.734163 6.396263 25 C 6.622215 5.831933 5.650198 5.752659 5.955914 26 H 6.760772 5.651055 5.307074 5.216894 5.740447

	27 C 6.846474 5.645297 5.989334 6.210044 6.415179 28 C 4.299295 3.072281 3.632966 4.224912 4.048535 29 O 5.061742 2.930420 4.173661 4.708373 4.821103 30 C 4.327598 5.430002 5.476095 6.263109 5.174838 31 O 4.404045 5.991677 6.119169 7.006485 5.688834 16 17 18 19 20 16 H 0.000000 17 C 2.234817 0.000000 18 H 8.266019 7.161405 0.000000 19 C 7.541569 6.678563 1.079052 0.000000 20 C 7.275679 6.659982 2.245056 1.432771 0.000000 21 H 7.243998 6.514209 2.676187 2.219356 3.338143 22 H 7.833609 7.163631 2.704115 2.244227 1.079173 23 C 6.551215 6.351296 3.349826 2.306978 1.421002 24 H 6.455154 6.552494 4.360070 3.350200 2.231838 25 C 6.318516 6.112571 3.345941 2.301858 2.294851 26 H 6.030857 6.138904 4.353395 3.342871 3.338113 27 C 6.973940 6.329697 2.223351 1.408614 2.294074 28 C 4.889328 3.670009 3.895805 3.491062 4.078890 29 O 5.757554 4.384589 4.004176 3.844054 4.750555 30 C 5.769782 4.363164 3.377142 3.193969 3.171676 31 O 6.294475 4.654556 4.056344 4.101110 4.081987 21 22 23 24 25 21 H 0.000000 22 H 4.347366 0.000000 23 C 3.339566 2.232617 0.000000 24 H 4.349542 2.687999 1.078864 0.000000 25 C 2.240061 3.336822 1.412904 2.224274 0.000000 26 H 2.697628 4.346521 2.226111 2.680813 1.078933 27 C 1.079472 3.336328 2.297458 3.340992 1.429673 28 C 2.957451 4.880135 4.042582 4.783805 3.378263 29 O 2.903784 5.565365 4.865623 5.718751 4.040366 30 C 4.331467 3.374241 3.782402 4.361973 4.083802 31 O 5.322877 4.057638 4.836751 5.358602 5.217567 26 27 28 29 30 26 H 0.000000 27 C 2.241542 0.000000 28 C 3.703696 2.977975 0.000000 29 O 4.351742 3.293369 1.175622 0.000000 30 C 4.870120 3.760038 2.718952 3.448524 0.000000 31 O 6.017912 4.811676 3.582088 4.141080 1.147860 31 31 O 0.000000



3S -1184.115276 4.11 C1
WBI 0.33

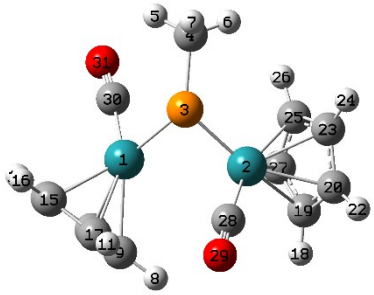
Charges and spin densities

		1
1	Ru	0.335759
2	Ru	0.206895
3	P	-0.212968
4	C	0.150783
9	C	-0.042057
10	C	0.045573
13	C	-0.052904
15	C	-0.002162
17	C	-0.024252
19	C	0.006554
20	C	-0.023467
23	C	0.006847
25	C	0.030416
27	C	-0.038347
28	C	0.003302
29	O	-0.229667
30	C	0.002665
31	O	-0.162967

		1	2	3	4	5
1	Ru	0.000000				
2	Ru	2.772454	0.000000			
3	P	2.355187	2.287730	0.000000		
4	C	3.133396	2.352609	1.853888	0.000000	
5	H	4.180690	3.011868	2.489359	1.090132	0.000000
6	H	3.159823	3.133440	2.507482	1.089553	1.797133
7	H	3.274079	1.835837	2.574663	1.184660	1.805409
8	H	2.947887	5.568351	5.123568	5.953991	7.008907
9	C	2.240432	4.952364	4.376433	5.031207	6.081289
10	C	2.272616	4.547273	4.405181	4.537665	5.606030
11	H	2.955766	5.519927	4.001884	5.081662	5.932691
12	H	2.979497	4.846617	5.155751	5.131260	6.196660
13	C	2.294322	4.236531	3.758015	3.536633	4.532475
14	H	3.043640	4.334473	4.119608	3.377720	4.272509
15	C	2.282461	4.496157	3.270018	3.515691	4.418988
16	H	3.010362	4.783224	3.204065	3.311318	4.015766
17	C	2.232048	4.910476	3.691672	4.487171	5.432511
18	H	4.385536	2.907027	3.603038	4.715917	5.072917
19	C	4.233511	2.174826	3.496748	4.202005	4.551246
20	C	4.785925	2.212058	3.536425	3.723594	3.766681
21	H	4.140893	2.888054	4.636245	5.216057	5.883736
22	H	5.346997	2.951467	3.660924	3.863407	3.636646
23	C	4.988060	2.227942	4.150922	3.771911	3.867552
24	H	5.675977	2.965717	4.711844	3.935851	3.814925
25	C	4.641653	2.241747	4.492366	4.302919	4.709160
26	H	5.067001	2.971094	5.256936	4.846735	5.304641
27	C	4.101285	2.160939	4.092428	4.504018	5.041732
28	C	2.072019	1.980955	3.310914	3.305789	4.279325
29	O	3.006550	2.976242	4.479603	4.295326	5.236703
30	C	1.834068	3.183448	2.994946	4.361117	5.265708
31	O	2.984106	3.906876	3.827604	5.326291	6.147126

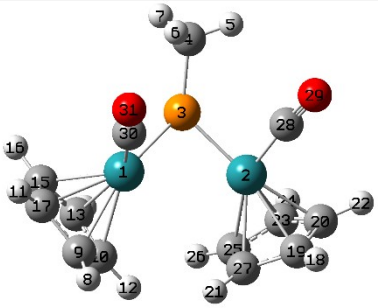
		6	7	8	9	10
6	H	0.000000				
7	H	1.721884	0.000000			
8	H	5.679484	6.075093	0.000000		
9	C	4.667079	5.212121	1.079372	0.000000	
10	C	4.036884	4.497610	2.223291	1.409231	0.000000
11	H	4.805459	5.718680	2.699196	2.244042	3.341911
12	H	4.661931	4.853470	2.681291	2.223367	1.079118
13	C	2.825858	3.691025	3.341436	2.296786	1.428885
14	H	2.504494	3.384154	4.347835	3.337122	2.237024
15	C	2.906381	4.075580	3.342310	2.299887	2.298670
16	H	2.653935	4.118160	4.350835	3.342536	3.344240
17	C	4.109167	4.985261	2.239557	1.430605	2.299911
18	H	5.648081	4.603696	6.608617	6.359073	6.510864

	19	C	5.145317	3.867618	6.670669	6.322200	6.237413
	20	C	4.758364	3.355853	7.520918	7.000856	6.734700
	21	H	5.872863	4.589276	5.868429	5.758736	5.578973
	22	H	4.948393	3.753498	8.152384	7.580940	7.383331
	23	C	4.660957	2.995488	7.686228	7.121929	6.585428
	24	H	4.755462	3.111818	8.431321	7.782409	7.116277
	25	C	5.033782	3.387228	7.014736	6.584033	6.020829
	26	H	5.413038	3.785207	7.213659	6.802380	6.071796
	27	C	5.276349	3.857283	6.293623	6.009833	5.738264
	28	C	3.498351	2.678457	4.208887	3.670503	3.006840
	29	O	4.355244	3.506657	4.458319	4.057486	3.191358
	30	C	4.716373	4.446366	3.238680	3.113334	3.645568
	31	O	5.785359	5.389657	3.857487	3.990559	4.661276
			11	12	13	14	15
	11	H	0.000000				
	12	H	4.353252	0.000000			
	13	C	3.340074	2.238462	0.000000		
	14	H	4.351654	2.689811	1.079381	0.000000	
	15	C	2.233244	3.340197	1.414458	2.231371	0.000000
	16	H	2.682162	4.352765	2.229929	2.694042	1.079669
	17	C	1.078828	3.344038	2.297917	3.342496	1.420170
	18	H	6.446428	6.863232	6.515947	6.919580	6.374753
	19	C	6.661519	6.495447	6.175199	6.432147	6.231456
	20	C	7.247011	7.022558	6.393701	6.445586	6.474592
	21	H	6.763962	5.505648	5.983116	6.298622	6.386676
	22	H	7.539469	7.779929	6.893774	6.932611	6.806832
	23	C	7.730963	6.693808	6.251127	6.111647	6.628852
	24	H	8.387068	7.205697	6.631498	6.324821	7.069304
	25	C	7.533827	5.952993	5.979411	5.923532	6.532610
	26	H	8.018051	5.821797	6.116433	5.955775	6.876135
	27	C	6.827562	5.768788	5.881831	6.083428	6.238081
	28	C	4.987544	3.025240	3.166568	3.361625	3.889510
	29	O	5.746456	2.794797	3.630406	3.703494	4.621743
	30	C	3.517364	4.146537	4.064831	4.857929	3.864417
	31	O	4.236514	5.074516	5.193141	6.000883	4.939864
			16	17	18	19	20
	16	H	0.000000				
	17	C	2.227097	0.000000			
	18	H	6.639980	6.253472	0.000000		
	19	C	6.510033	6.301335	1.078972	0.000000	
	20	C	6.571752	6.831584	2.239679	1.421942	0.000000
	21	H	6.992907	6.243284	2.688371	2.235021	3.339617
	22	H	6.740354	7.222615	2.702884	2.235938	1.079271
	23	C	6.803701	7.134851	3.349127	2.303250	1.428039
	24	H	7.147824	7.745671	4.358409	3.345252	2.235824
	25	C	6.925857	6.868652	3.359818	2.318600	2.308243

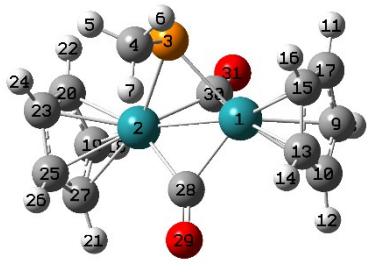
	26 H 7.347202 7.252940 4.367730 3.360404 3.352030 27 C 6.703305 6.296679 2.238281 1.427556 2.297263 28 C 4.567979 4.145158 4.201933 3.610948 4.055608 29 O 5.400005 4.832547 5.042586 4.390790 4.857688 30 C 4.519095 3.252888 3.390882 3.610346 4.624984 31 O 5.562404 4.172777 3.204538 3.689861 4.913961 21 22 23 24 25 21 H 0.000000 22 H 4.352093 0.000000 23 C 3.330733 2.239317 0.000000 24 H 4.342555 2.689659 1.080222 0.000000 25 C 2.239822 3.348433 1.410722 2.221316 0.000000 26 H 2.698159 4.358373 2.227722 2.681838 1.078765 27 C 1.079560 3.342577 2.287428 3.332365 1.429121 28 C 2.955068 4.906571 3.718763 4.368577 3.015981 29 O 3.198480 5.795551 4.266713 4.835836 3.293662 30 C 3.368445 5.224330 5.142213 6.062810 4.646486 31 O 3.359655 5.496960 5.580522 6.585428 5.028844 26 27 28 29 30 26 H 0.000000 27 C 2.241226 0.000000 28 C 3.157740 2.881233 0.000000 29 O 3.050163 3.348155 1.174217 0.000000 30 C 5.230080 3.600964 2.855908 3.678759 0.000000 31 O 5.663438 3.764744 3.752756 4.454642 1.150275 31 31 O 0.000000
 4S -1184.111335 6.58 C1 WBI 0.38 Charges and spin densities 1 1 Ru 0.510098 2 Ru 0.475170 3 P -0.244217 4 C 0.028561 9 C -0.004869 10 C -0.009096	1 2 3 4 5 1 Ru 0.000000 2 Ru 3.021677 0.000000 3 P 2.187098 2.179435 0.000000 4 C 3.611967 3.575996 1.828367 0.000000 5 H 3.643575 4.319023 2.445231 1.090798 0.000000 6 H 4.263883 3.575858 2.437192 1.091497 1.793622 7 H 4.302820 4.182755 2.399935 1.093899 1.772736 8 H 3.010257 3.560698 4.354020 6.132996 6.462256 9 C 2.276268 3.767610 3.998774 5.707070 5.888854 10 C 2.239225 4.372071 4.342024 5.802261 5.744118 11 H 2.985791 4.293291 3.948216 5.605001 5.907346 12 H 2.983312 4.722313 4.967600 6.333056 6.243447 13 C 2.203731 5.034280 4.349076 5.583129 5.330444 14 H 2.915247 5.822367 4.959501 5.924195 5.478960 15 C 2.200952 4.906245 3.986476 5.312548 5.191901 16 H 2.931240 5.628626 4.371718 5.464972 5.254723 17 C 2.259321 4.151736 3.770060 5.413108 5.572938 18 H 5.054642 2.971733 5.079367 6.427565 7.064959

13 C -0.040437 15 C -0.010274 17 C -0.034356 19 C -0.029149 20 C -0.031735 23 C -0.011438 25 C -0.046671 27 C -0.000713 28 C -0.107699 29 O -0.162574 30 C -0.112749 31 O -0.167850	19 C 4.687924 2.234334 4.352334 5.530914 6.209848 20 C 5.168436 2.201967 4.224406 5.209959 6.072121 21 H 4.104004 2.952871 4.299721 5.205559 5.524084 22 H 5.886482 2.936924 4.883877 5.909577 6.845400 23 C 5.039018 2.212154 3.692301 4.221710 5.090896 24 H 5.664824 2.946284 3.980376 4.155991 5.110729 25 C 4.434665 2.228536 3.458004 3.916016 4.544581 26 H 4.610653 2.972893 3.563529 3.547459 4.020307 27 C 4.180183 2.230006 3.893190 4.812111 5.329441 28 C 3.322249 1.851880 2.955176 4.654167 5.397455 29 O 4.019822 3.000540 3.873415 5.573826 6.300621 30 C 1.832377 3.910034 2.732237 3.229887 2.795049 31 O 2.982523 4.806421 3.601045 3.572200 2.865971 6 7 8 9 10 6 H 0.000000 7 H 1.768642 0.000000 8 H 6.562205 6.720851 0.000000 9 C 6.267071 6.297658 1.078035 0.000000 10 C 6.343595 6.540058 2.230326 1.422736 0.000000 11 H 6.377136 5.814938 2.671805 2.221959 3.343005 12 H 6.737007 7.175536 2.690108 2.236970 1.078209 13 C 6.303893 6.226309 3.335525 2.293434 1.424836 14 H 6.640310 6.604315 4.346290 3.337359 2.234826 15 C 6.170887 5.733582 3.341550 2.300016 2.310058 16 H 6.430079 5.730433 4.350651 3.342391 3.352283 17 C 6.165817 5.802299 2.220613 1.411449 2.301826 18 H 6.221440 7.116380 3.775527 4.576443 5.147307 19 C 5.232712 6.226192 4.090792 4.711867 5.216503 20 C 4.822652 5.712354 4.897960 5.465580 6.138262 21 H 4.907859 6.167905 4.314670 4.569063 4.426359 22 H 5.567975 6.260348 5.299780 5.965742 6.813681 23 C 3.635802 4.750668 5.574787 5.910391 6.389399 24 H 3.465905 4.486933 6.435359 6.713835 7.231827 25 C 3.316986 4.719930 5.298089 5.497865 5.670245 26 H 2.797983 4.429831 5.977750 6.014871 5.988949 27 C 4.439684 5.673936 4.372388 4.718385 4.864858 28 C 4.952339 4.970372 2.816787 3.192658 4.315770 29 O 5.964301 5.754390 2.933379 3.392541 4.717273 30 C 3.757240 4.139879 4.603994 3.882726 3.253755 31 O 3.961418 4.508040 5.671808 4.953681 4.147606 11 12 13 14 15 11 H 0.000000 12 H 4.350240 0.000000 13 C 3.340810 2.238947 0.000000 14 H 4.352020 2.694884 1.079699 0.000000 15 C 2.241294 3.352047 1.420802 2.230202 0.000000

16	H	2.704256	4.360974	2.234201	2.687566	1.078558
17	C	1.078811	3.343158	2.297133	3.341078	1.429454
18	H	5.819598	5.003343	6.365873	7.171685	6.593028
19	C	5.809117	5.153270	6.288291	7.049111	6.474330
20	C	6.072200	6.258227	7.039745	7.836436	6.986916
21	H	6.177930	4.066090	5.420860	5.902185	6.037325
22	H	6.322390	6.999242	7.723097	8.590004	7.531643
23	C	6.449061	6.535356	7.091176	7.766006	7.062856
24	H	6.984958	7.458463	7.805958	8.463105	7.657831
25	C	6.414210	5.672801	6.365408	6.907023	6.587996
26	H	6.927972	5.971621	6.514350	6.909490	6.811205
27	C	6.011677	4.706685	5.812575	6.407737	6.192627
28	C	3.060398	4.907352	4.965891	5.950725	4.459008
29	O	2.764469	5.390024	5.329401	6.376507	4.632913
30	C	4.752429	3.597961	2.934997	3.004932	3.420722
31	O	5.872513	4.310160	3.739611	3.501362	4.369480
		16	17	18	19	20
16	H	0.000000				
17	C	2.243620	0.000000			
18	H	7.556169	5.595174	0.000000		
19	C	7.371680	5.584852	1.078853	0.000000	
20	C	7.760443	6.056478	2.242954	1.429527	0.000000
21	H	6.955475	5.586318	2.681417	2.225421	3.340068
22	H	8.274315	6.470831	2.702382	2.241408	1.079227
23	C	7.736310	6.363244	3.351303	2.308472	1.421358
24	H	8.224691	6.998425	4.360075	3.350738	2.231478
25	C	7.311151	6.094016	3.345587	2.302812	2.298648
26	H	7.454320	6.531671	4.351383	3.343076	3.343275
27	C	7.063732	5.590958	2.227153	1.414329	2.296482
28	C	5.145124	3.309072	3.423610	3.190393	3.096759
29	O	5.251320	3.316668	4.071092	4.064317	3.948883
30	C	3.881629	3.976363	5.952547	5.408617	5.909940
31	O	4.708024	5.076032	6.751764	6.153638	6.659383
		21	22	23	24	25
21	H	0.000000				
22	H	4.350067	0.000000			
23	C	3.344304	2.231322	0.000000		
24	H	4.356073	2.683703	1.079162	0.000000	
25	C	2.234704	3.341131	1.422426	2.237586	0.000000
26	H	2.686375	4.352870	2.237927	2.701721	1.079137
27	C	1.078978	3.339433	2.302494	3.347169	1.425431
28	C	4.368360	3.272274	3.662756	4.228877	4.028257
29	O	5.373520	3.865626	4.677900	5.172942	5.150549
30	C	4.165836	6.804328	5.402046	5.949122	4.449859
31	O	4.636395	7.613957	5.991220	6.477440	4.903468
		26	27	28	29	30

	26 H 0.000000 27 C 2.234427 0.000000 28 C 4.822138 3.758576 0.000000 29 O 5.968174 4.804877 1.150757 0.000000 30 C 4.196824 4.449266 4.836428 5.699435 0.000000 31 O 4.414246 5.023313 5.914600 6.819809 1.152575 31 31 O 0.000000
 5S. -1184.103865 11.27 Cs WBI 0.38 Charge and spin density 1 1 Ru 0.480085 2 Ru 0.523127 3 P -0.243540 4 C 0.053910 9 C -0.029350 10 C -0.000524 13 C -0.060087 15 C -0.031236 17 C -0.046421 19 C -0.011739 20 C -0.036770 23 C -0.013166 25 C -0.056051 27 C -0.010387 28 C -0.106155 29 O -0.152627 30 C -0.095543 31 O -0.163526	1 2 3 4 5 1 Ru 0.000000 2 Ru 3.087916 0.000000 3 P 2.182074 2.166979 0.000000 4 C 3.587529 3.586252 1.823184 0.000000 5 H 4.435586 3.664065 2.444700 1.089939 0.000000 6 H 3.639578 4.110371 2.423458 1.092612 1.791533 7 H 4.012079 4.367840 2.396794 1.093391 1.779415 8 H 3.018605 5.059568 5.091650 6.510586 7.294045 9 C 2.267153 4.646545 4.390823 5.848251 6.689039 10 C 2.298519 4.050382 4.005706 5.684285 6.441475 11 H 2.900131 5.933117 4.892889 5.782507 6.793652 12 H 3.049871 3.947972 4.434746 6.216274 6.843785 13 C 2.267127 4.286869 3.634663 5.170830 6.007954 14 H 2.999587 4.391625 3.773120 5.289767 6.041610 15 C 2.185887 4.969543 3.803524 4.981171 5.968416 16 H 2.913342 5.621134 4.119154 4.982989 6.015550 17 C 2.192989 5.170738 4.277747 5.438049 6.413749 18 H 5.126882 2.978195 4.991743 6.213069 6.134414 19 C 4.618932 2.246956 4.367486 5.745618 5.705673 20 C 5.140140 2.218912 4.312752 5.542446 5.313391 21 H 3.640584 2.987354 4.440856 6.127584 6.471823 22 H 5.993667 2.939677 4.903230 5.855839 5.429457 23 C 4.764001 2.217783 3.951091 5.368450 5.281949 24 H 5.374591 2.939758 4.290157 5.543455 5.374224 25 C 3.913117 2.246558 3.775514 5.475862 5.662840 26 H 3.869825 2.983170 3.983151 5.741459 6.065248 27 C 3.805752 2.259081 4.045388 5.702105 5.904607 28 C 4.083543 1.838649 2.712751 3.175194 2.850796 29 O 5.012767 2.986015 3.588517 3.518512 2.950285 30 C 1.831391 3.881831 2.795374 3.356993 4.200685 31 O 2.981141 4.737293 3.665201 3.745619 4.506277 6 7 8 9 10 6 H 0.000000 7 H 1.766357 0.000000 8 H 6.358315 7.000842 0.000000 9 C 5.797123 6.222607 1.078373 0.000000 10 C 5.899124 5.995143 2.235281 1.419250 0.000000

	11 H 5.446951 5.954429 2.696886 2.235210 3.331795 12 H 6.519946 6.605104 2.684036 2.224364 1.078478 13 C 5.494936 5.236838 3.346246 2.304970 1.411104 14 H 5.802693 5.233362 4.354698 3.347328 2.226287 15 C 5.075338 4.951635 3.355599 2.313213 2.296513 16 H 5.076951 4.729317 4.363346 3.354474 3.339480 17 C 5.294587 5.625446 2.239598 1.424565 2.287421 18 H 6.442833 7.153343 5.581256 5.729173 5.394019 19 C 6.126888 6.595033 5.372767 5.338203 4.771845 20 C 6.133417 6.306354 6.441224 6.214947 5.440274 21 H 6.381161 6.834761 3.429285 3.485853 2.966240 22 H 6.456267 6.645475 7.418161 7.210746 6.482671 23 C 6.109411 5.932332 6.246233 5.825931 4.803565 24 H 6.415747 5.961035 7.095432 6.567428 5.447886 25 C 6.093152 6.010308 4.985640 4.571871 3.489963 26 H 6.390570 6.108995 4.863261 4.305865 3.019543 27 C 6.099080 6.418052 4.318869 4.194777 3.470734 28 C 3.500753 4.184665 6.177459 5.884390 5.599554 29 O 3.676200 4.551092 7.066985 6.838785 6.672823 30 C 2.856048 3.954702 3.669270 3.306534 3.913491 31 O 2.942497 4.364178 4.403134 4.215157 4.991900 11 12 13 14 15 11 H 0.000000 12 H 4.340326 0.000000 13 C 3.341988 2.219611 0.000000 14 H 4.352290 2.677076 1.079217 0.000000 15 C 2.231050 3.338704 1.429942 2.240290 0.000000 16 H 2.686772 4.348690 2.244874 2.703526 1.078471 17 C 1.079616 3.329281 2.298776 3.342338 1.423401 18 H 7.409979 4.878526 6.269588 6.567556 7.031341 19 C 7.092230 4.216205 5.525630 5.698663 6.413539 20 C 7.866881 4.913223 5.899659 5.830569 6.862015 21 H 5.537711 2.292581 4.080483 4.488967 4.998939 22 H 8.766201 5.987496 6.886311 6.785762 7.793183 23 C 7.498376 4.272451 5.046674 4.774024 6.151698 24 H 8.132804 4.970263 5.454745 4.984506 6.576435 25 C 6.414596 2.864369 3.922012 3.779907 5.113989 26 H 6.141809 2.393500 3.272490 2.962020 4.603571 27 C 6.126838 2.822602 4.307530 4.506593 5.312969 28 C 6.763686 5.629847 5.789338 5.976229 6.159788 29 O 7.535641 6.735965 6.853623 7.064565 7.105712 30 C 3.017092 4.650746 3.990372 4.765758 3.420556 31 O 3.539933 5.724395 5.095100 5.886496 4.379701 16 17 18 19 20 16 H 0.000000 17 C 2.235848 0.000000

	18 H 7.915052 6.742851 0.000000 19 C 7.269604 6.316142 1.078561 0.000000 20 C 7.590832 7.034187 2.241889 1.428761 0.000000 21 H 6.004029 4.708849 2.668113 2.216673 3.335603 22 H 8.468664 7.976172 2.699885 2.239860 1.079247 23 C 6.820438 6.563759 3.347114 2.304930 1.416535 24 H 7.121927 7.177847 4.356409 3.347622 2.227910 25 C 5.904254 5.434718 3.342803 2.300460 2.297719 26 H 5.359567 5.096866 4.353270 3.343785 3.337977 27 C 6.229466 5.255172 2.227068 1.414547 2.296283 28 C 6.678719 6.225002 3.359388 3.124457 2.988230 29 O 7.561924 7.108357 3.972308 3.968041 3.793560 30 C 3.871619 2.950220 5.559859 5.357134 5.977281 31 O 4.705846 3.773629 6.154842 6.111128 6.762402 21 22 23 24 25 21 H 0.000000 22 H 4.343571 0.000000 23 C 3.346699 2.227425 0.000000 24 H 4.358901 2.681261 1.078905 0.000000 25 C 2.239103 3.340983 1.426016 2.239538 0.000000 26 H 2.707774 4.347054 2.232992 2.691008 1.078398 27 C 1.077949 3.338937 2.302033 3.345756 1.422425 28 C 4.400631 3.116584 3.571047 4.119100 3.998949 29 O 5.401883 3.635376 4.551772 5.021483 5.103943 30 C 4.713109 6.649673 5.958559 6.619370 5.327537 31 O 5.614940 7.331249 6.898512 7.569160 6.358013 26 27 28 29 30 26 H 0.000000 27 C 2.239265 0.000000 28 C 4.808082 3.753342 0.000000 29 O 5.943782 4.785436 1.150316 0.000000 30 C 5.516103 4.916606 4.074072 4.658580 0.000000 31 O 6.621148 5.837890 4.539101 4.869774 1.151397 31 31 O 0.000000
 6S. -1184.100111 13.68 Cs WBI 0.57	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.505866 0.000000 3 P 2.378727 2.378682 0.000000 4 C 3.433722 3.433564 1.863940 0.000000 5 H 4.368850 3.831364 2.445821 1.095313 0.000000 6 H 3.831118 4.368567 2.445831 1.095314 1.758757 7 H 3.395525 3.395082 2.516705 1.090134 1.779888 8 H 2.926153 4.814194 4.829811 6.188950 7.116291 9 C 2.213687 4.473468 4.247414 5.387286 6.378361 10 C 2.268237 4.495286 4.581406 5.339054 6.377876

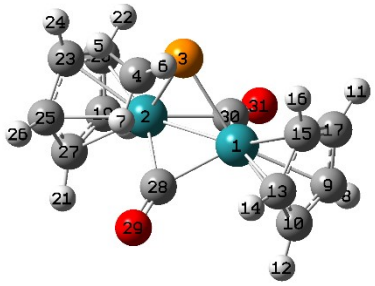
Charges and spin densities

		1
1	Ru	0.199127
2	Ru	0.198979
3	P	-0.077287
4	C	-0.014687
9	C	0.015363
10	C	0.027871
13	C	0.002726
15	C	-0.012983
17	C	0.000956
19	C	0.015443
20	C	0.001027
23	C	-0.013119
25	C	0.002818
27	C	0.027767
28	C	-0.118810
29	O	-0.235758
30	C	0.144621
31	O	-0.164055

11	H	2.932049	4.987937	3.683403	4.848964	5.740617
12	H	2.994377	4.839067	5.366271	6.097457	7.102989
13	C	2.232353	4.534151	4.136370	4.449105	5.533311
14	H	2.949080	4.915470	4.638320	4.553080	5.609416
15	C	2.201947	4.581540	3.476110	3.905737	4.980669
16	H	2.926679	5.026529	3.501985	3.523006	4.562495
17	C	2.219948	4.575315	3.587991	4.604686	5.597381
18	H	4.813955	2.926014	4.827489	6.187284	6.353009
19	C	4.473354	2.213602	4.245946	5.386223	5.483158
20	C	4.575269	2.219981	3.586677	4.602638	4.480791
21	H	4.839240	2.994423	5.366534	6.099310	6.351120
22	H	4.987837	2.932086	3.681126	4.845378	4.635573
23	C	4.581297	2.201733	3.476436	3.905145	3.671040
24	H	5.026271	2.926498	3.502960	3.522116	3.015496
25	C	4.534101	2.232243	4.137518	4.450797	4.439222
26	H	4.915397	2.948936	4.640391	4.556325	4.544217
27	C	4.495327	2.268217	4.581454	5.340067	5.488098
28	C	1.996718	1.996565	3.362757	3.937206	4.673793
29	O	3.004743	3.004714	4.478384	4.783229	5.495100
30	C	2.037732	2.038481	2.567370	4.278326	4.878889
31	O	3.038426	3.038701	3.416369	5.237753	5.765810

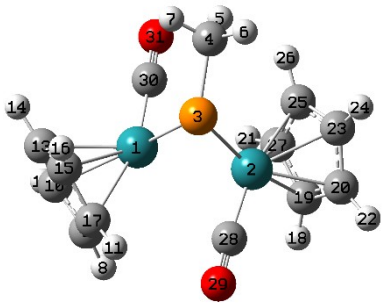
		6	7	8	9	10
6	H	0.000000				
7	H	1.779880	0.000000			
8	H	6.354744	6.273180	0.000000		
9	C	5.484093	5.412373	1.079780	0.000000	
10	C	5.486502	5.080713	2.229940	1.418567	0.000000
11	H	4.639736	5.284281	2.687522	2.238391	3.352952
12	H	6.348659	5.710953	2.690195	2.233873	1.079160
13	C	4.436498	4.130102	3.328990	2.285172	1.416289
14	H	4.539492	4.008890	4.339672	3.329199	2.227882
15	C	3.670969	3.930700	3.334311	2.292511	2.306425
16	H	3.015598	3.643704	4.346299	3.337624	3.347116
17	C	4.482897	4.823493	2.232224	1.425892	2.312009
18	H	7.114410	6.272167	5.831660	6.027679	6.327741
19	C	6.377191	5.411559	6.027649	6.030326	6.186137
20	C	5.595504	4.821177	6.499388	6.368342	6.613878
21	H	7.104559	5.713279	6.390911	6.305057	5.985823
22	H	5.737267	5.280647	6.718480	6.648748	7.092875
23	C	4.980282	3.928929	6.977578	6.640844	6.635776
24	H	4.562056	3.640824	7.600331	7.164619	7.159083
25	C	5.534861	4.131093	6.878850	6.534293	6.273704
26	H	5.612442	4.011328	7.402991	6.948961	6.484216
27	C	6.378686	5.081824	6.325663	6.184972	6.011067
28	C	4.673393	3.444120	4.240090	3.703913	3.135776
29	O	5.494596	4.085181	4.883003	4.359036	3.469423

30	C	4.878574	4.532988	3.202942	3.153754	3.768897	
31	O	5.765705	5.609340	3.243728	3.530161	4.429090	
		11	12	13	14	15	
11	H	0.000000					
12	H	4.362392	0.000000				
13	C	3.346687	2.230264	0.000000			
14	H	4.355853	2.685524	1.079835	0.000000		
15	C	2.235174	3.349699	1.427082	2.236505	0.000000	
16	H	2.696760	4.356517	2.237208	2.689921	1.078952	
17	C	1.078481	3.355162	2.302120	3.344261	1.419391	
18	H	6.714925	6.394623	6.880301	7.405440	6.976854	
19	C	6.646758	6.307049	6.535257	6.950592	6.640608	
20	C	6.531661	6.935298	6.707984	7.113244	6.569073	
21	H	7.515675	5.766862	6.390008	6.544373	6.955360	
22	H	6.497556	7.517744	7.182042	7.685292	6.844042	
23	C	6.845295	6.953943	6.485854	6.689089	6.441406	
24	H	7.112876	7.575868	6.812755	6.952805	6.640094	
25	C	7.182618	6.387753	6.215473	6.286979	6.486886	
26	H	7.686506	6.540268	6.286733	6.171455	6.690724	
27	C	7.091566	5.985739	6.274990	6.486582	6.636646	
28	C	4.917671	3.243865	3.197956	3.363523	3.829102	
29	O	5.847966	3.249183	3.568535	3.451472	4.520207	
30	C	3.532011	4.272002	4.185881	4.960559	3.952305	
31	O	3.713386	4.900371	5.028921	5.902964	4.684771	
		16	17	18	19	20	
16	H	0.000000					
17	C	2.232989	0.000000				
18	H	7.598862	6.497483	0.000000			
19	C	7.163993	6.367270	1.079783	0.000000		
20	C	6.895122	6.387035	2.232154	1.425816	0.000000	
21	H	7.578165	6.934127	2.690183	2.233905	3.355166	
22	H	7.110228	6.531758	2.687451	2.238326	1.078479	
23	C	6.640182	6.569605	3.334267	2.292459	1.419436	
24	H	6.664275	6.896367	4.346259	3.337573	2.233039	
25	C	6.814685	6.708172	3.328959	2.285155	2.302179	
26	H	6.956042	7.113708	4.339646	3.329191	3.344319	
27	C	7.160488	6.613112	2.229959	1.418617	2.312034	
28	C	4.458000	4.127501	4.241858	3.705038	4.127614	
29	O	5.159326	4.952641	4.886041	4.361025	4.953062	
30	C	4.606810	3.334646	3.202271	3.153801	3.336381	
31	O	5.360667	3.765902	3.241497	3.529096	3.767356	
		21	22	23	24	25	
21	H	0.000000					
22	H	4.362392	0.000000				
23	C	3.349709	2.235220	0.000000			
24	H	4.356525	2.696827	1.078953	0.000000		

	25 C 2.230247 3.346747 1.427122 2.237242 0.000000 26 H 2.685527 4.355914 2.236535 2.689949 1.079835 27 C 1.079157 3.352979 2.306423 3.347108 1.416247 28 C 3.245450 4.917795 3.827896 4.456116 3.197068 29 O 3.252126 5.848398 4.518805 5.156841 3.567480 30 C 4.270672 3.534435 3.953810 4.608880 4.186266 31 O 4.897459 3.716159 4.686094 5.362957 5.028616 26 27 28 29 30 26 H 0.000000 27 C 2.227848 0.000000 28 C 3.361888 3.136607 0.000000 29 O 3.449044 3.471016 1.176633 0.000000 30 C 4.960717 3.768394 2.876267 3.965339 0.000000 31 O 5.902482 4.427371 3.959776 4.984333 1.160778 31 31 O 0.000000
 7T. -1184.097507 15.26 Cs WBI 0.44 Charges and spin densities 1 2 1 Ru 0.226688 0.662103 2 Ru 0.226687 0.662170 3 P -0.069020 0.184265 4 C 0.008646 0.000678 9 C 0.008140 0.012302 10 C 0.002818 0.032070 13 C -0.009516 0.069929 15 C 0.010549 -0.021078 17 C -0.008545 0.076435 19 C 0.008119 0.012293 20 C -0.008550 0.076424 23 C 0.010550 -0.021078 25 C -0.009512 0.069954 27 C 0.002833 0.032080 28 C -0.033232 0.011244 29 O -0.196069 0.065452 30 C 0.022640 0.010831	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.496012 0.000000 3 P 2.372241 2.372228 0.000000 4 C 3.413241 3.413179 1.857828 0.000000 5 H 4.348449 3.810945 2.436457 1.095048 0.000000 6 H 3.810878 4.348347 2.436454 1.095049 1.757009 7 H 3.384603 3.384450 2.521583 1.090204 1.778432 8 H 2.966129 4.874464 5.115279 6.318430 7.280827 9 C 2.254944 4.521043 4.410479 5.445636 6.455292 10 C 2.259143 4.522038 4.483597 5.058850 6.117737 11 H 2.968820 4.976893 4.009965 5.328113 6.213839 12 H 2.973895 4.878674 5.236041 5.676612 6.706142 13 C 2.256138 4.573389 3.887802 4.111350 5.205279 14 H 2.972044 4.971829 4.244399 3.979621 5.048623 15 C 2.247172 4.601649 3.374042 3.953282 4.999106 16 H 2.966481 5.031179 3.318367 3.671997 4.645653 17 C 2.254771 4.577142 3.755352 4.852861 5.834989 18 H 4.874568 2.966129 5.115313 6.318327 6.517424 19 C 4.521100 2.254942 4.410482 5.445484 5.555234 20 C 4.577193 2.254761 3.755350 4.852689 4.783003 21 H 4.878646 2.973903 5.235994 5.676415 5.868709 22 H 4.976983 2.968810 4.009998 5.327986 5.232506 23 C 4.601631 2.247172 3.373984 3.953020 3.693031 24 H 5.031153 2.966486 3.318298 3.671709 3.155448 25 C 4.573336 2.256153 3.887725 4.111069 3.994139 26 H 4.971723 2.972057 4.244287 3.979283 3.782084 27 C 4.522026 2.259151 4.483555 5.058642 5.159778 28 C 2.009392 2.009504 3.016539 3.300295 4.046965 29 O 3.014788 3.014811 3.998122 3.820464 4.513664

31 O -0.193226 0.063925	30 C 2.014536 2.014461 2.962090 4.546673 5.180433 31 O 3.019423 3.019412 3.933591 5.631297 6.220251 6 7 8 9 10 6 H 0.000000 7 H 1.778430 0.000000 8 H 6.517444 6.269934 0.000000 9 C 5.555281 5.397756 1.079486 0.000000 10 C 5.159812 4.759570 2.230476 1.416800 0.000000 11 H 5.232623 5.714786 2.689998 2.236324 3.342634 12 H 5.868711 5.198181 2.689737 2.230926 1.079412 13 C 3.994223 3.878386 3.342336 2.298358 1.423307 14 H 3.782172 3.560099 4.351646 3.340957 2.235297 15 C 3.693179 4.105571 3.338342 2.295776 2.296648 16 H 3.155668 4.021764 4.347028 3.338328 3.340099 17 C 4.783108 5.061265 2.232253 1.422831 2.299848 18 H 7.280736 6.269685 5.994755 6.168056 6.467621 19 C 6.455154 5.397434 6.168016 6.151941 6.310987 20 C 5.834881 5.060918 6.564270 6.413316 6.661048 21 H 6.705876 5.197799 6.569445 6.468542 6.164868 22 H 6.213810 5.714504 6.749667 6.657944 7.104522 23 C 4.998905 4.105097 7.062052 6.709278 6.707616 24 H 4.645463 4.021273 7.652110 7.200192 7.199146 25 C 5.204992 3.877857 7.012779 6.654859 6.403487 26 H 5.048247 3.559474 7.555701 7.093262 6.642514 27 C 6.117500 4.759163 6.467554 6.310951 6.147817 28 C 4.046769 2.737740 4.399958 3.839372 3.239293 29 O 4.513467 2.972263 5.107466 4.540586 3.632007 30 C 5.180406 4.683169 3.260472 3.184765 3.763456 31 O 6.220227 5.834308 3.288126 3.544642 4.420489 11 12 13 14 15 11 H 0.000000 12 H 4.353434 0.000000 13 C 3.344006 2.233361 0.000000 14 H 4.354008 2.689041 1.079200 0.000000 15 C 2.233152 3.339226 1.419345 2.233506 0.000000 16 H 2.686148 4.349265 2.231195 2.690656 1.079001 17 C 1.078894 3.343712 2.301494 3.344809 1.420269 18 H 6.749707 6.569507 7.012872 7.555816 7.062143 19 C 6.657934 6.468581 6.654922 7.093357 6.709332 20 C 6.465292 7.019483 6.752843 7.186440 6.563897 21 H 7.567000 5.992459 6.556055 6.735664 7.061459 22 H 6.392618 7.567054 7.191253 7.722899 6.803426 23 C 6.803341 7.061471 6.555588 6.790097 6.460430 24 H 7.036026 7.652443 6.850053 7.024534 6.625994 25 C 7.191160 6.556054 6.340294 6.443348 6.555562 26 H 7.722770 6.735636 6.443305 6.364340 6.790024

27	C	7.104468	6.164880	6.403506	6.642567	6.707618	
28	C	4.976142	3.363462	3.264138	3.413314	3.872948	
29	O	5.920320	3.465114	3.641399	3.489171	4.553651	
30	C	3.520835	4.275722	4.189115	4.969511	3.946832	
31	O	3.677110	4.906520	5.026493	5.907987	4.665420	
		16	17	18	19	20	
16	H	0.000000					
17	C	2.229640	0.000000				
18	H	7.652207	6.564330	0.000000			
19	C	7.200251	6.413331	1.079487	0.000000		
20	C	6.857500	6.356737	2.232254	1.422831	0.000000	
21	H	7.652430	7.019448	2.689739	2.230927	3.343712	
22	H	7.036126	6.465324	2.690001	2.236325	1.078894	
23	C	6.626000	6.563847	3.338342	2.295776	1.420269	
24	H	6.615596	6.857440	4.347029	3.338328	2.229639	
25	C	6.850028	6.752779	3.342337	2.298358	2.301494	
26	H	7.024457	7.186338	4.351646	3.340957	3.344810	
27	C	7.199150	6.661017	2.230478	1.416800	2.299847	
28	C	4.467367	4.194025	4.400066	3.839471	4.194120	
29	O	5.139418	5.035448	5.107440	4.540536	5.035406	
30	C	4.586671	3.324351	3.260541	3.184792	3.324360	
31	O	5.324728	3.737058	3.288354	3.544817	3.737206	
		21	22	23	24	25	
21	H	0.000000					
22	H	4.353435	0.000000				
23	C	3.339224	2.233152	0.000000			
24	H	4.349264	2.686146	1.079002	0.000000		
25	C	2.233359	3.344006	1.419344	2.231195	0.000000	
26	H	2.689038	4.354008	2.233506	2.690658	1.079201	
27	C	1.079412	3.342634	2.296646	3.340097	1.423306	
28	C	3.363518	4.976244	3.873023	4.467434	3.264202	
29	O	3.464996	5.920303	4.553583	5.139362	3.641294	
30	C	4.275711	3.520868	3.946801	4.586634	4.189079	
31	O	4.906624	3.677281	4.665508	5.324795	5.026571	
		26	27	28	29	30	
26	H	0.000000					
27	C	2.235296	0.000000				
28	C	3.413339	3.239370	0.000000			
29	O	3.489029	3.631911	1.169502	0.000000		
30	C	4.969453	3.763446	2.927972	4.040531	0.000000	
31	O	5.908031	4.420603	4.034529	5.101026	1.168077	
		31					
31	O	0.000000					



8T. -1184.093642 17.69 Cs
WBI 0.46

Charges and spin densities

		1	2
1	Ru	0.379243	0.929524
2	Ru	0.368773	0.381673
3	P	-0.124242	0.507859
4	C	0.011777	0.029432
9	C	-0.018481	0.083769
10	C	-0.025753	-0.007944
13	C	-0.030575	0.002106
15	C	0.041521	0.025202
17	C	-0.007333	0.001035
19	C	-0.024990	0.029493
20	C	-0.036497	-0.016867
23	C	0.001592	0.041050
25	C	-0.054092	-0.003477
27	C	0.003904	-0.012194
28	C	-0.065450	0.005129
29	O	-0.173918	0.015775
30	C	-0.079257	-0.024952
31	O	-0.166222	0.013388

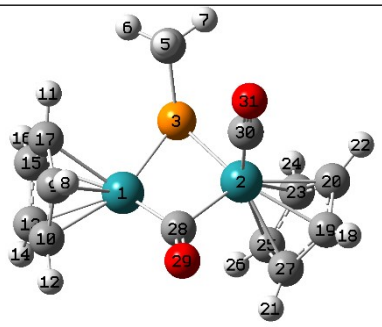
		1	2	3	4	5
1	Ru	0.000000				
2	Ru	2.750712	0.000000			
3	P	2.304445	2.229678	0.000000		
4	C	3.565337	3.556719	1.839236	0.000000	
5	H	3.697033	3.651675	2.467657	1.091636	0.000000
6	H	4.484157	3.925237	2.422610	1.092219	1.780644
7	H	3.832261	4.439957	2.433849	1.092477	1.773442
8	H	3.009555	4.290008	4.812627	6.436442	6.636006
9	C	2.299098	4.166463	4.189982	5.724190	5.980110
10	C	2.252815	4.742794	4.446417	5.630259	5.738312
11	H	3.044157	4.028093	3.646258	5.362450	5.981222
12	H	2.971267	5.339249	5.257595	6.306203	6.251463
13	C	2.247661	4.950813	3.982968	4.925398	5.172235
14	H	2.960832	5.680992	4.498617	5.068087	5.232496
15	C	2.290804	4.540821	3.360008	4.561494	5.081697
16	H	3.010378	4.973627	3.380532	4.354417	5.042002
17	C	2.312590	4.011789	3.500792	5.095220	5.592279
18	H	4.746605	2.971060	5.161125	6.353149	6.145511
19	C	4.341735	2.242928	4.417307	5.435981	5.188773
20	C	4.877570	2.223535	4.236905	5.124236	5.011331
21	H	3.695854	2.998291	4.459809	5.106410	4.536902
22	H	5.653403	2.953109	4.877694	5.850786	5.865592
23	C	4.711927	2.240538	3.675933	4.094206	3.868863
24	H	5.368327	2.964804	3.904252	4.014955	3.885998
25	C	4.022668	2.254600	3.492085	3.749384	3.228414
26	H	4.187512	2.996030	3.588233	3.334028	2.564344
27	C	3.763279	2.260997	3.993333	4.691580	4.226035
28	C	3.188470	1.843292	3.033324	4.775968	5.158311
29	O	3.955906	2.993363	3.956785	5.750810	6.224671
30	C	1.826072	3.383728	2.896779	3.199781	2.808719
31	O	2.978026	4.183670	3.714061	3.479193	2.774342

		6	7	8	9	10
6	H	0.000000				
7	H	1.772077	0.000000			
8	H	7.216090	6.724009	0.000000		
9	C	6.561001	5.882478	1.079843	0.000000	
10	C	6.605612	5.628910	2.233914	1.420086	0.000000
11	H	5.927689	5.517056	2.675603	2.225710	3.339098
12	H	7.321731	6.322586	2.697225	2.236061	1.079245
13	C	5.911040	4.687273	3.344149	2.299074	1.427127
14	H	6.095268	4.648394	4.354463	3.342004	2.238260
15	C	5.392680	4.357134	3.336802	2.294240	2.298233
16	H	5.082653	3.973687	4.344053	3.335888	3.341974
17	C	5.828263	5.168023	2.223224	1.414313	2.297416
18	H	6.712384	7.258853	4.763405	5.256439	5.932069

19	C	5.743850	6.392157	5.029787	5.312336	5.876640
20	C	5.161330	6.163978	5.880172	6.050409	6.704875
21	H	5.731142	5.886634	4.906376	4.980289	4.991017
22	H	5.757032	6.884052	6.351026	6.603455	7.416122
23	C	4.045860	5.176635	6.409147	6.352143	6.782094
24	H	3.683035	5.101172	7.245526	7.107883	7.536937
25	C	4.028943	4.752577	5.976544	5.844318	6.009716
26	H	3.663911	4.265657	6.517602	6.240281	6.183721
27	C	5.152630	5.598229	5.100241	5.168583	5.394312
28	C	5.099303	5.466677	3.470675	3.552903	4.611748
29	O	6.039521	6.352221	3.434396	3.680311	4.952648
30	C	4.227393	3.459212	4.518962	3.887840	3.306754
31	O	4.462626	3.687566	5.573215	4.972644	4.240791

		11	12	13	14	15
11	H	0.000000				
12	H	4.349510	0.000000			
13	C	3.339942	2.237620	0.000000		
14	H	4.350365	2.693287	1.079198	0.000000	
15	C	2.234980	3.340160	1.415152	2.228825	0.000000
16	H	2.689572	4.350532	2.227755	2.685971	1.078871
17	C	1.078210	3.341076	2.298168	3.341797	1.422848
18	H	5.771233	6.120965	6.749343	7.548597	6.656438
19	C	5.686849	6.144021	6.497324	7.224578	6.370363
20	C	5.924394	7.137278	7.100052	7.821750	6.738163
21	H	6.042483	4.971389	5.623925	6.111470	5.965745
22	H	6.220152	7.905134	7.821985	8.608369	7.320266
23	C	6.214352	7.235652	6.941463	7.511424	6.624363
24	H	6.718311	8.063987	7.534290	8.055176	7.104895
25	C	6.151658	6.322124	6.202317	6.659758	6.159282
26	H	6.622851	6.457034	6.208321	6.497021	6.278593
27	C	5.832037	5.568632	5.903842	6.467260	5.997223
28	C	2.844152	5.356582	4.950622	5.897483	4.226979
29	O	2.628391	5.728248	5.359178	6.379862	4.508843
30	C	4.853502	3.571945	3.164862	3.316401	3.690409
31	O	5.998239	4.312476	4.053613	3.954063	4.711594

		16	17	18	19	20
16	H	0.000000				
17	C	2.232723	0.000000			
18	H	7.379134	5.753676	0.000000		
19	C	6.993336	5.638773	1.079277	0.000000	
20	C	7.173672	6.059398	2.241230	1.430156	0.000000
21	H	6.685052	5.590111	2.683268	2.227134	3.345797
22	H	7.711609	6.523853	2.698969	2.241801	1.078974
23	C	6.929656	6.234968	3.343671	2.301105	1.417524
24	H	7.259163	6.814727	4.354130	3.344888	2.228805
25	C	6.566433	5.926111	3.339408	2.295910	2.298132

	26 H 6.606020 6.285740 4.346271 3.336859 3.341612 27 C 6.613676 5.549801 2.227316 1.414824 2.302424 28 C 4.698809 3.232471 3.350941 3.160779 3.171127 29 O 4.971119 3.300895 3.966557 4.021727 4.037529 30 C 4.208815 4.086524 5.189009 4.586688 5.165207 31 O 5.141009 5.219117 5.785146 5.114621 5.680034 21 22 23 24 25 21 H 0.000000 22 H 4.354412 0.000000 23 C 3.344460 2.230742 0.000000 24 H 4.354447 2.685967 1.079340 0.000000 25 C 2.233820 3.341493 1.422111 2.234895 0.000000 26 H 2.685306 4.352119 2.236444 2.695767 1.079019 27 C 1.078666 3.344344 2.302294 3.345667 1.422727 28 C 4.314192 3.383753 3.751548 4.351954 4.046951 29 O 5.284350 4.011769 4.787176 5.336432 5.170992 30 C 3.202578 6.135361 4.622380 5.243221 3.519860 31 O 3.429928 6.710672 4.955002 5.510691 3.695952 26 27 28 29 30 26 H 0.000000 27 C 2.231301 0.000000 28 C 4.838208 3.724951 0.000000 29 O 5.986987 4.753050 1.152244 0.000000 30 C 3.251062 3.498711 4.548289 5.506823 0.000000 31 O 3.129770 3.835409 5.560377 6.570972 1.152299 31 31 O 0.000000
 9T. -1184.093046 18.06 Cs WBI 0.33 Charges and spin densities 1 2 1 Ru 0.403466 1.295694 2 Ru 0.293425 0.034664 3 P -0.172825 0.415380 4 C 0.007896 0.039328 9 C 0.006821 0.063360 10 C -0.026016 0.009230	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.747754 0.000000 3 P 2.243201 2.280590 0.000000 4 C 3.545142 3.573704 1.841906 0.000000 5 H 3.662769 3.679197 2.469236 1.091320 0.000000 6 H 3.865505 4.476969 2.428883 1.092347 1.782850 7 H 4.446065 3.891835 2.430213 1.092663 1.776429 8 H 3.019008 4.786447 4.615678 4.915012 4.353955 9 C 2.306158 4.577235 4.077701 4.572252 4.237291 10 C 2.252097 4.743233 4.423432 5.371973 5.252784 11 H 3.032635 4.960160 3.560147 3.221023 2.936516 12 H 2.964173 5.111992 5.202879 6.271165 6.104813 13 C 2.268844 4.973812 4.136967 5.173486 5.324229 14 H 2.987263 5.510943 4.732294 5.943358 6.218729 15 C 2.263703 4.890055 3.491417 4.136889 4.336066 16 H 2.980220 5.367753 3.612439 4.125123 4.535925 17 C 2.301748 4.657126 3.463588 3.686027 3.528923 18 H 5.428363 2.965832 5.198313 6.204989 6.100073

13	C	-0.052424	0.096906
15	C	-0.045576	0.048669
17	C	0.002074	0.018329
19	C	-0.009585	-0.000580
20	C	-0.032627	-0.003047
23	C	0.010245	0.011933
25	C	0.004758	-0.007132
27	C	0.033800	0.005485
28	C	-0.054054	-0.042662
29	O	-0.212504	0.010710
30	C	-0.008692	0.000203
31	O	-0.148182	0.003532

19	C	4.769186	2.250152	4.416453	5.612213	5.674576
20	C	4.863845	2.213389	3.851261	4.910969	5.164237
21	H	4.326002	2.996558	4.941271	6.502979	6.581019
22	H	5.613668	2.941569	4.300933	4.998861	5.218170
23	C	4.361307	2.274064	3.325268	4.718016	5.218827
24	H	4.719283	2.988549	3.307828	4.571476	5.259606
25	C	3.843163	2.287731	3.591801	5.270562	5.687876
26	H	3.791578	3.022382	3.819487	5.619233	6.131740
27	C	4.145072	2.281774	4.266711	5.795457	5.960305
28	C	1.947925	2.106496	3.240307	4.461118	4.276932
29	O	2.972257	3.015232	4.395926	5.493556	5.163470
30	C	3.530833	1.837617	2.928873	3.237225	2.832668
31	O	4.372199	2.985279	3.766758	3.544108	2.846470

		6	7	8	9	10
6	H	0.000000				
7	H	1.769229	0.000000			
8	H	5.120460	5.927483	0.000000		
9	C	4.653108	5.632249	1.079226	0.000000	
10	C	5.449586	6.398000	2.235798	1.427298	0.000000
11	H	2.924112	4.289717	2.681427	2.220668	3.336914
12	H	6.443244	7.262085	2.683655	2.234170	1.079567
13	C	5.054293	6.174883	3.350577	2.309764	1.422242
14	H	5.796768	6.883022	4.361166	3.353927	2.238402
15	C	3.826828	5.164414	3.339660	2.293752	2.285755
16	H	3.594197	5.063612	4.347877	3.334985	3.330341
17	C	3.510315	4.777847	2.220945	1.405099	2.291748
18	H	7.228388	6.242670	6.774574	6.884257	6.957307
19	C	6.588665	5.659125	6.548890	6.493279	6.475238
20	C	5.881118	4.738747	6.960125	6.790400	6.880315
21	H	7.300457	6.860829	6.087575	5.924825	5.463224
22	H	6.006365	4.613652	7.543080	7.438902	7.683476
23	C	5.521683	4.635799	6.925116	6.539957	6.438702
24	H	5.258832	4.352424	7.431692	6.950171	6.876761
25	C	5.996937	5.457025	6.432505	6.005318	5.643712
26	H	6.187129	5.903695	6.558643	5.986486	5.411971
27	C	6.638800	6.030697	6.196769	5.987216	5.683094
28	C	5.132008	5.174266	3.170731	3.060990	3.056948
29	O	6.178472	6.197250	3.278979	3.450316	3.384943
30	C	4.262619	3.506086	4.445054	4.583793	5.240697
31	O	4.534338	3.737953	4.632207	4.972453	5.852469

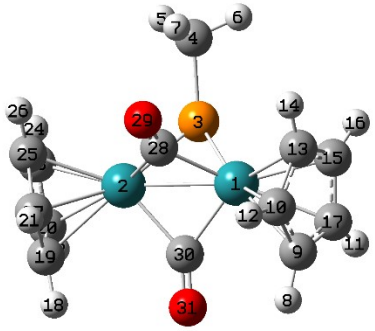
		11	12	13	14	15
11	H	0.000000				
12	H	4.342933	0.000000			
13	C	3.349803	2.236214	0.000000		
14	H	4.359870	2.700304	1.079198	0.000000	
15	C	2.243088	3.330687	1.414435	2.228915	0.000000

16	H	2.696875	4.342869	2.225758	2.683646	1.079686
17	C	1.079079	3.331719	2.309252	3.353186	1.432880
18	H	7.637347	6.945927	7.493995	7.934425	7.678755
19	C	7.156511	6.548606	6.834961	7.208326	6.998538
20	C	7.022228	7.156888	7.007994	7.386903	6.930323
21	H	7.166225	5.246395	5.880849	6.043146	6.478755
22	H	7.437708	8.022582	7.816216	8.260719	7.592520
23	C	6.734049	6.776581	6.306333	6.534697	6.258645
24	H	6.854861	7.332758	6.543267	6.726982	6.340300
25	C	6.626326	5.817225	5.570695	5.681375	5.826035
26	H	6.675126	5.572462	5.143551	5.066644	5.525249
27	C	6.906958	5.666657	5.957083	6.177378	6.338163
28	C	4.316851	3.193647	3.759041	4.390821	4.079567
29	O	5.048092	3.176355	4.384939	4.983870	4.899209
30	C	4.656403	5.673256	5.731972	6.511241	5.394783
31	O	4.851126	6.296864	6.451431	7.322083	6.003119

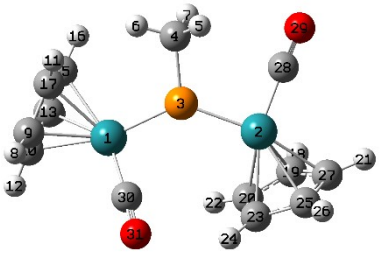
		16	17	18	19	20
16	H	0.000000				
17	C	2.242159	0.000000			
18	H	8.264262	7.327256	0.000000		
19	C	7.501213	6.805532	1.079111	0.000000	
20	C	7.247100	6.807533	2.245366	1.434311	0.000000
21	H	7.109880	6.513243	2.675817	2.218328	3.339618
22	H	7.855636	7.366711	2.702562	2.244756	1.079128
23	C	6.446839	6.418577	3.349648	2.307223	1.420873
24	H	6.346650	6.616516	4.360211	3.350884	2.232000
25	C	6.147775	6.099802	3.343899	2.299437	2.294352
26	H	5.778004	6.039875	4.351072	3.340160	3.337543
27	C	6.859819	6.366838	2.222355	1.407172	2.295536
28	C	4.905243	3.710991	3.917349	3.525688	4.122517
29	O	5.824139	4.419614	3.965480	3.848063	4.754656
30	C	5.941461	4.677479	3.371019	3.184957	3.153875
31	O	6.561300	5.067312	4.032927	4.078857	4.050235

		21	22	23	24	25
21	H	0.000000				
22	H	4.347810	0.000000			
23	C	3.341163	2.233653	0.000000		
24	H	4.351388	2.689983	1.079039	0.000000	
25	C	2.239765	3.336958	1.413730	2.225872	0.000000
26	H	2.696136	4.346948	2.226652	2.682432	1.078867
27	C	1.079349	3.336929	2.299234	3.342994	1.429295
28	C	2.996981	4.920011	4.099438	4.846420	3.433858
29	O	3.026911	5.539064	4.927159	5.787072	4.149849
30	C	4.336933	3.355458	3.769071	4.352363	4.074202
31	O	5.323753	4.019158	4.815889	5.342297	5.204202

		26	27	28	29	30

	26 H 0.000000 27 C 2.240344 0.000000 28 C 3.755653 3.027179 0.000000 29 O 4.497875 3.382625 1.173488 0.000000 30 C 4.859802 3.759920 2.738359 3.347122 0.000000 31 O 6.007152 4.804688 3.595319 4.004920 1.147875 31 31 O 0.000000
 10T. -1184.09086 19.43 C2V WBI 0.34 Charges and spin densities 1 2 1 Ru 0.272348 0.508359 2 Ru 0.272454 0.508162 3 P -0.119179 0.559733 4 C 0.030961 0.046269 9 C 0.030877 -0.011991 10 C 0.008443 0.023175 13 C -0.017142 0.034281 15 C -0.028821 -0.006563 17 C -0.032810 0.121161 19 C 0.030992 -0.012013 20 C -0.032835 0.121463 23 C -0.028924 -0.006777 25 C -0.016841 0.034286 27 C 0.008158 0.023150 28 C 0.028962 0.022160 29 O -0.207825 0.044842 30 C 0.010819 -0.027764 31 O -0.209638 0.018067	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.624446 0.000000 3 P 2.281041 2.281065 0.000000 4 C 3.603954 3.603958 1.838832 0.000000 5 H 4.500360 3.949013 2.439024 1.091915 0.000000 6 H 3.949284 4.500441 2.439023 1.091913 1.774785 7 H 3.674548 3.674742 2.438125 1.092782 1.779270 8 H 3.011680 4.830990 5.176320 6.603889 7.501278 9 C 2.296124 4.545094 4.515374 5.780825 6.740311 10 C 2.275447 4.473363 4.461754 5.375402 6.388018 11 H 2.994046 5.217073 4.428422 5.750969 6.627293 12 H 2.999604 4.729279 5.106515 5.934599 6.909363 13 C 2.224340 4.630110 3.946458 4.496275 5.572195 14 H 2.931646 5.012992 4.237963 4.348078 5.422756 15 C 2.215727 4.791880 3.662208 4.411802 5.453154 16 H 2.930843 5.308495 3.739699 4.195646 5.203622 17 C 2.271495 4.751676 4.059685 5.266840 6.226181 18 H 4.831693 3.011478 5.174975 6.603401 6.826658 19 C 4.545564 2.296023 4.514587 5.780543 5.917536 20 C 4.752393 2.271653 4.058366 5.264640 5.191712 21 H 4.728944 2.999653 5.108008 5.938263 6.224721 22 H 5.218278 2.994282 4.426155 5.747177 5.614143 23 C 4.791845 2.215843 3.662100 4.410358 4.185009 24 H 5.308381 2.931002 3.739512 4.192797 3.715453 25 C 4.629431 2.224272 3.947704 4.497914 4.462879 26 H 5.011599 2.931436 4.240031 4.351168 4.273426 27 C 4.473021 2.275327 4.462494 5.377380 5.549662 28 C 2.012345 2.012196 2.621539 3.332272 4.065883 29 O 2.999828 2.999772 3.563370 3.774167 4.479889 30 C 2.019703 2.019789 3.069312 4.780308 5.375964 31 O 3.005934 3.005995 4.153391 5.914546 6.475514 6 7 8 9 10 6 H 0.000000 7 H 1.779269 0.000000 8 H 6.828084 6.620811 0.000000 9 C 5.918564 5.777307 1.079751 0.000000 10 C 5.547857 5.121098 2.224645 1.412493 0.000000

11	H	5.619363	6.128810	2.682912	2.232748	3.341188	
12	H	6.221160	5.517383	2.683235	2.227326	1.079121	
13	C	4.460952	4.263338	3.338942	2.295020	1.426556	
14	H	4.269276	3.912833	4.347264	3.336945	2.236936	
15	C	4.186860	4.522704	3.338263	2.296135	2.302289	
16	H	3.718873	4.443654	4.347540	3.339139	3.345963	
17	C	5.194891	5.474232	2.227996	1.419929	2.299424	
18	H	7.500671	6.621849	5.438202	5.749431	5.976002	
19	C	6.739973	5.778103	5.748747	5.863359	5.928723	
20	C	6.224022	5.472657	6.409295	6.399200	6.543744	
21	H	6.912975	5.522223	5.903529	5.898903	5.472369	
22	H	6.623468	6.125883	6.713388	6.767859	7.107146	
23	C	5.451873	4.520925	6.967871	6.752982	6.646226	
24	H	5.201094	4.439860	7.713716	7.410669	7.305571	
25	C	5.573784	4.264776	6.729464	6.487189	6.125887	
26	H	5.425713	3.915231	7.287383	6.930558	6.369454	
27	C	6.389922	5.123868	5.971083	5.925734	5.651503	
28	C	4.066242	2.910912	4.373028	3.804072	3.145807	
29	O	4.480288	3.030841	5.076264	4.478911	3.502194	
30	C	5.376078	4.957469	3.060709	3.045396	3.512241	
31	O	6.475612	6.125785	2.920333	3.294849	4.054965	
		11	12	13	14	15	
11	H	0.000000					
12	H	4.350558	0.000000				
13	C	3.345854	2.237194	0.000000			
14	H	4.357488	2.691781	1.079120	0.000000		
15	C	2.237595	3.344846	1.421771	2.236293	0.000000	
16	H	2.694443	4.355411	2.234249	2.695247	1.079120	
17	C	1.079176	3.342621	2.302076	3.346175	1.423587	
18	H	6.707984	5.911319	6.733432	7.293377	6.967788	
19	C	6.764102	5.903511	6.489991	6.935038	6.753063	
20	C	6.880599	6.708676	6.856561	7.281451	6.905630	
21	H	7.370484	5.093166	6.084413	6.274133	6.799072	
22	H	6.957327	7.375732	7.410393	7.925755	7.270590	
23	C	7.270784	6.798237	6.725449	6.951388	6.878499	
24	H	7.694511	7.547876	7.202256	7.366011	7.246069	
25	C	7.408788	6.081358	6.282180	6.382704	6.725705	
26	H	7.924327	6.267579	6.381421	6.298163	6.951547	
27	C	7.103177	5.472686	6.127915	6.373873	6.646568	
28	C	4.992846	3.256698	3.153491	3.277886	3.818861	
29	O	5.886806	3.335701	3.454699	3.247673	4.425462	
30	C	3.727726	3.919507	4.063693	4.826473	3.998881	
31	O	3.913063	4.395182	4.839576	5.703811	4.697893	
		16	17	18	19	20	
16	H	0.000000					
17	C	2.234607	0.000000				

	18 H 7.712574 6.406964 0.000000 19 C 7.410230 6.397476 1.079779 0.000000 20 C 7.384823 6.638272 2.227964 1.419905 0.000000 21 H 7.549971 6.705240 2.683345 2.227432 3.342746 22 H 7.692569 6.881562 2.682907 2.232771 1.079199 23 C 7.246214 6.905670 3.338277 2.296132 1.423631 24 H 7.464135 7.385761 4.347571 3.339158 2.234668 25 C 7.203702 6.855103 3.338989 2.295035 2.302113 26 H 7.368255 7.279586 4.347347 3.336992 3.346235 27 C 7.306669 6.541180 2.224727 1.412574 2.299541 28 C 4.432101 4.178857 4.375731 3.805710 4.179024 29 O 5.014574 4.969301 5.080327 4.481396 4.969457 30 C 4.734910 3.401802 3.060158 3.045240 3.403965 31 O 5.485184 3.787489 2.918997 3.294356 3.790483 21 22 23 24 25 21 H 0.000000 22 H 4.350711 0.000000 23 C 3.344978 2.237643 0.000000 24 H 4.355565 2.694495 1.079144 0.000000 25 C 2.237334 3.345903 1.421764 2.234259 0.000000 26 H 2.691936 4.357555 2.236298 2.695246 1.079147 27 C 1.079140 3.341334 2.302389 3.346082 1.426627 28 C 3.258846 4.993166 3.817160 4.429370 3.151915 29 O 3.339760 5.887013 4.423077 5.010527 3.452758 30 C 3.916376 3.731358 4.000248 4.736993 4.062893 31 O 4.390343 3.918450 4.699845 5.488257 4.838558 26 27 28 29 30 26 H 0.000000 27 C 2.237003 0.000000 28 C 3.274924 3.146751 0.000000 29 O 3.243522 3.504102 1.172078 0.000000 30 C 4.824992 3.510320 2.780162 3.870488 0.000000 31 O 5.702001 4.052145 3.858177 4.878275 1.169646 31 31 O 0.000000
 11T. -1184.084612 23.35 Cs WBI 0.09	1 2 3 4 5 1 Ru 0.000000 2 Ru 4.053345 0.000000 3 P 2.219217 2.208415 0.000000 4 C 3.378831 3.416954 1.842135 0.000000 5 H 4.238164 3.466418 2.444175 1.091401 0.000000 6 H 3.296409 4.362880 2.462366 1.088193 1.781944 7 H 3.902246 3.687290 2.423470 1.094222 1.763340 8 H 2.955859 6.612677 4.731256 5.330079 5.990766 9 C 2.234987 6.144513 4.144656 4.691550 5.489997 10 C 2.264031 6.286702 4.438922 5.215797 6.151639

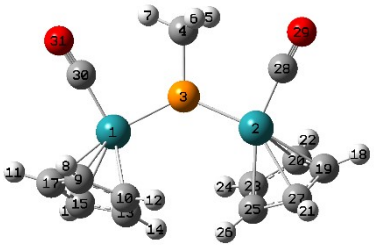
Charges and spin densities

		1	2
1	Ru	0.391311	0.825304
2	Ru	0.407504	0.866538
3	P	-0.051183	0.067508
4	C	0.004530	-0.000359
9	C	-0.023472	0.017227
10	C	-0.044955	-0.034416
13	C	0.000445	0.114029
15	C	-0.046521	-0.030370
17	C	-0.050608	0.021290
19	C	-0.004617	-0.000594
20	C	-0.038067	0.047336
23	C	-0.027227	-0.042410
25	C	0.009793	0.113434
27	C	-0.052802	-0.022458
28	C	-0.084784	0.001599
29	O	-0.150328	0.022802
30	C	-0.067210	0.009076
31	O	-0.171808	0.024465

11	H	2.985974	5.908745	3.745969	3.383224	4.024771
12	H	2.993484	6.855194	5.206630	6.178658	7.098308
13	C	2.283033	5.978100	4.085613	4.613782	5.656635
14	H	3.004892	6.286981	4.607133	5.179457	6.256974
15	C	2.267532	5.622691	3.509541	3.532194	4.554319
16	H	3.006936	5.672642	3.637336	3.224665	4.260442
17	C	2.254108	5.750319	3.569908	3.609163	4.439619
18	H	5.510661	2.955401	4.353002	5.496984	5.834464
19	C	5.118432	2.231731	3.899184	5.237986	5.490189
20	C	4.136411	2.250646	3.388948	5.057091	5.432895
21	H	6.857308	2.992542	5.165509	6.129037	5.982274
22	H	3.597097	2.962205	3.418204	5.133944	5.701825
23	C	4.490402	2.275593	3.626683	5.303396	5.466065
24	H	4.343550	3.011804	3.872159	5.604974	5.782525
25	C	5.600199	2.295829	4.256636	5.646809	5.573230
26	H	6.310672	3.018110	4.913628	6.177438	5.939417
27	C	5.924748	2.269641	4.403754	5.610073	5.587506
28	C	5.045108	1.842088	2.893487	3.049303	2.841706
29	O	5.894132	2.991040	3.764489	3.399632	3.069033
30	C	1.842075	3.949766	2.907714	4.495582	5.065372
31	O	2.991827	4.358097	3.781110	5.411087	5.835856

		6	7	8	9	10
6	H	0.000000				
7	H	1.776427	0.000000			
8	H	4.715867	6.082940	0.000000		
9	C	4.086979	5.314462	1.079305	0.000000	
10	C	4.771759	5.621433	2.238949	1.428065	0.000000
11	H	2.447588	4.075918	2.679810	2.227574	3.347589
12	H	5.802244	6.579860	2.697453	2.240621	1.078942
13	C	4.218350	4.769244	3.337612	2.294905	1.414749
14	H	4.915394	5.134965	4.349661	3.339922	2.227489
15	C	2.951744	3.732980	3.338658	2.295326	2.298637
16	H	2.672168	3.152873	4.349746	3.339326	3.339566
17	C	2.846380	4.176991	2.227988	1.417382	2.305596
18	H	6.425064	5.233608	8.402096	7.737216	7.333887
19	C	6.163765	5.189324	7.894902	7.339624	7.065414
20	C	5.824927	5.228230	6.753662	6.282097	5.994304
21	H	7.171914	6.105052	9.480571	9.025145	8.983684
22	H	5.762527	5.274560	6.216098	5.682036	5.200775
23	C	6.047877	5.710769	6.731115	6.464903	6.430345
24	H	6.203302	6.167283	6.187092	6.074997	6.121006
25	C	6.530747	5.982079	7.884446	7.613125	7.677734
26	H	7.038894	6.609121	8.356339	8.195092	8.397276
27	C	6.598028	5.684216	8.523768	8.088097	8.016669
28	C	4.136662	2.934527	7.602620	7.018475	7.229967
29	O	4.445964	3.023367	8.401119	7.767277	7.996716

30	C	4.598676	5.187122	3.287085	3.130133	3.259687	
31	O	5.567279	6.155258	3.885085	3.988496	4.157110	
		11	12	13	14	15	
11	H	0.000000					
12	H	4.355652	0.000000				
13	C	3.345388	2.229134	0.000000			
14	H	4.355159	2.686240	1.079947	0.000000		
15	C	2.240809	3.341845	1.420017	2.229692	0.000000	
16	H	2.703651	4.348655	2.229828	2.680772	1.079213	
17	C	1.079120	3.347679	2.301005	3.343780	1.424500	
18	H	7.924342	7.682969	6.761223	6.584873	6.833669	
19	C	7.561119	7.401681	6.674174	6.650684	6.714914	
20	C	6.803423	6.234520	5.824379	5.894613	6.012357	
21	H	8.892475	9.400181	8.616663	8.698686	8.422115	
22	H	6.463742	5.356194	5.032724	5.015351	5.424741	
23	C	6.923941	6.662906	6.500048	6.765533	6.573830	
24	H	6.722808	6.267113	6.423601	6.794766	6.559446	
25	C	7.762973	7.996406	7.634876	7.893678	7.540643	
26	H	8.249417	8.721888	8.447100	8.789224	8.276481	
27	C	8.121481	8.389667	7.730393	7.837875	7.619687	
28	C	6.257050	7.963133	6.636454	6.893201	5.994411	
29	O	6.769029	8.793463	7.269860	7.482784	6.509077	
30	C	4.221499	3.512752	3.837425	4.468375	4.054723	
31	O	5.147310	4.201901	4.900864	5.500275	5.178826	
		16	17	18	19	20	
16	H	0.000000					
17	C	2.238452	0.000000				
18	H	6.762173	7.463782	0.000000			
19	C	6.765941	7.149106	1.078867	0.000000		
20	C	6.277099	6.308209	2.234093	1.420430	0.000000	
21	H	8.370529	8.700444	2.698200	2.240484	3.344274	
22	H	5.769023	5.824303	2.691177	2.232177	1.079411	
23	C	6.934562	6.569389	3.343867	2.300823	1.420420	
24	H	7.068478	6.366672	4.352255	3.342571	2.231612	
25	C	7.758425	7.544410	3.339646	2.297887	2.297102	
26	H	8.514311	8.135178	4.350541	3.342156	3.340312	
27	C	7.669460	7.863764	2.241296	1.429580	2.301294	
28	C	5.713167	6.274445	3.480422	3.235033	3.819554	
29	O	6.052837	6.870860	4.152938	4.125062	4.874729	
30	C	4.841049	3.673446	5.567179	4.891781	3.618855	
31	O	5.985289	4.681932	5.970547	5.165368	3.818317	
		21	22	23	24	25	
21	H	0.000000					
22	H	4.355377	0.000000				
23	C	3.341847	2.231564	0.000000			
24	H	4.350009	2.686647	1.078328	0.000000		

	25 C 2.224923 3.340520 1.423229 2.236567 0.000000 26 H 2.679399 4.350128 2.233573 2.692010 1.079991 27 C 1.079367 3.345441 2.298298 3.339901 1.411067 28 C 3.326578 4.441744 4.060258 4.842258 3.701590 29 O 3.937938 5.457860 5.185558 5.988424 4.719838 30 C 6.497114 3.216532 3.501443 2.976741 4.767052 31 O 6.598406 3.556569 3.352391 2.528592 4.623824 26 27 28 29 30 26 H 0.000000 27 C 2.223182 0.000000 28 C 4.238988 3.162477 0.000000 29 O 5.184607 4.025776 1.150299 0.000000 30 C 5.339014 5.469594 5.446310 6.487658 0.000000 31 O 5.046639 5.557234 6.023783 7.122960 1.151287 31 31 O 0.000000
 12T. -1184.081055 25.59 C2 WBI 0.10 Charges and spin densities 1 2 1 Ru 0.379316 0.857109 2 Ru 0.392377 0.837976 3 P -0.041978 0.092047 4 C 0.020398 -0.001720 9 C -0.001662 0.000908 10 C -0.036688 0.038612 13 C -0.048594 -0.041088 15 C 0.007205 0.115416 17 C -0.054573 -0.028453 19 C -0.058604 -0.021272 20 C -0.004651 -0.001749 23 C -0.041253 0.037135 25 C -0.049758 -0.028068 27 C 0.001439 0.103712 28 C -0.084645 -0.002786 29 O -0.151499 0.021574 30 C -0.078605 -0.001367 31 O -0.148223 0.022016	1 2 3 4 5 1 Ru 0.000000 2 Ru 4.030697 0.000000 3 P 2.220760 2.223301 0.000000 4 C 3.451177 3.406090 1.838243 0.000000 5 H 4.195454 3.494264 2.424017 1.092106 0.000000 6 H 4.114282 3.586259 2.426450 1.093592 1.758061 7 H 3.395395 4.378717 2.476024 1.087546 1.778242 8 H 2.952797 5.717563 4.378279 5.420154 6.422047 9 C 2.230904 5.233462 3.921635 5.200656 6.109178 10 C 2.247100 4.196356 3.402999 5.023257 5.797960 11 H 2.992659 6.874719 5.181848 6.151149 6.980774 12 H 2.951325 3.732272 3.422500 5.054314 5.811698 13 C 2.276688 4.380161 3.635257 5.335402 5.929333 14 H 3.022650 4.152185 3.890828 5.670774 6.103175 15 C 2.298924 5.488801 4.266530 5.704057 6.333999 16 H 3.024225 6.130278 4.921600 6.272246 6.785274 17 C 2.270185 5.931753 4.420137 5.627118 6.437765 18 H 6.898988 2.985587 5.157708 6.004228 5.705037 19 C 5.971863 2.266374 4.409011 5.507850 5.316985 20 C 5.301704 2.233881 3.889552 5.024133 4.734517 21 H 6.158296 3.021374 4.972460 6.309257 6.474274 22 H 5.787331 2.957459 4.318329 5.168615 4.665490 23 C 4.294629 2.252290 3.406159 4.928307 4.896049 24 H 3.867711 2.960202 3.422929 4.952326 4.933029 25 C 4.458312 2.281927 3.685929 5.344828 5.527868 26 H 4.244526 3.031239 3.975925 5.754311 6.105127 27 C 5.530745 2.294953 4.298551 5.688328 5.765927 28 C 5.117027 1.838294 2.919698 3.011274 2.769894 29 O 6.025038 2.986609 3.805544 3.361877 2.915036

30	C	1.839551	5.119899	2.928188	3.107212	3.968520
31	O	2.987470	6.024653	3.816847	3.480919	4.319182
		6	7	8	9	10
6	H	0.000000				
7	H	1.777038	0.000000			
8	H	5.564038	5.325756	0.000000		
9	C	5.526849	5.156810	1.078805	0.000000	
10	C	5.368015	5.255090	2.232789	1.419453	0.000000
11	H	6.703666	5.752931	2.697437	2.239979	3.343768
12	H	5.221258	5.467465	2.686162	2.228948	1.079251
13	C	5.916332	5.534926	3.342805	2.299664	1.421558
14	H	6.284828	6.008500	4.353612	3.342926	2.237098
15	C	6.389137	5.633243	3.339696	2.298085	2.298609
16	H	7.068668	6.137156	4.350349	3.342242	3.342102
17	C	6.172054	5.407621	2.240894	1.429258	2.301018
18	H	6.049047	7.051165	8.468421	7.955744	6.719543
19	C	5.672901	6.506264	7.583003	7.004589	5.737919
20	C	5.455397	5.917585	7.366387	6.653521	5.448242
21	H	6.254432	7.262522	6.877823	6.463359	5.155142
22	H	5.686615	6.018931	8.111123	7.374560	6.254679
23	C	5.460037	5.686909	6.279519	5.476432	4.228744
24	H	5.658599	5.542775	6.120664	5.211030	4.081528
25	C	5.659999	6.142725	5.777567	5.084901	3.711191
26	H	6.061647	6.441574	5.135772	4.431155	3.013126
27	C	5.793283	6.631094	6.683631	6.143916	4.811333
28	C	2.874658	4.097017	6.822302	6.513157	5.709370
29	O	3.047379	4.386592	7.713666	7.479861	6.772315
30	C	3.710313	2.502204	3.431078	3.196944	3.793163
31	O	3.953623	2.604511	4.076847	4.067138	4.837867
		11	12	13	14	15
11	H	0.000000				
12	H	4.353242	0.000000			
13	C	3.340208	2.235451	0.000000		
14	H	4.344591	2.699919	1.077980	0.000000	
15	C	2.224519	3.342848	1.422645	2.229915	0.000000
16	H	2.678680	4.353324	2.233857	2.683588	1.079977
17	C	1.079345	3.344051	2.296642	3.335457	1.410882
18	H	9.646309	6.091197	6.717571	6.117609	7.967719
19	C	8.653665	5.170106	5.662480	5.040301	6.918651
20	C	8.008882	5.140459	5.082007	4.407654	6.183466
21	H	8.438867	4.293097	5.455685	4.963462	6.858305
22	H	8.539536	6.050631	5.777976	5.111185	6.734723
23	C	6.787192	4.045502	3.723917	2.993444	4.861824
24	H	6.201521	4.178978	3.267134	2.510601	4.195795
25	C	6.743629	3.228566	3.559139	2.908387	4.915261
26	H	6.142736	2.526057	2.923233	2.325966	4.337034

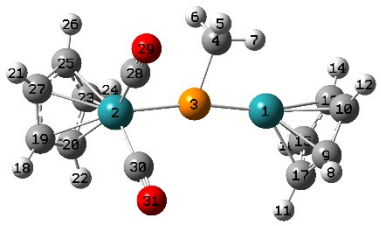
27	C	7.962436	4.111752	4.896185	4.319795	6.261454
28	C	8.058091	5.249807	6.010006	5.893093	6.956730
29	O	8.957011	6.319712	7.101826	7.014246	7.979690
30	C	3.293042	4.407194	4.051087	4.850834	3.691694
31	O	3.873026	5.415004	5.168510	5.993457	4.695962

		16	17	18	19	20
16	H	0.000000				
17	C	2.222906	0.000000			
18	H	8.469208	8.641564	0.000000		
19	C	7.412764	7.637869	1.079415	0.000000	
20	C	6.522025	7.040882	2.238535	1.428277	0.000000
21	H	7.557831	7.379713	2.678240	2.223240	3.343121
22	H	6.951517	7.632619	2.696980	2.240803	1.078657
23	C	5.215287	5.792175	3.341906	2.298929	1.420364
24	H	4.380952	5.265434	4.350714	3.341503	2.228149
25	C	5.480917	5.681857	3.340380	2.296787	2.301171
26	H	4.976894	5.064226	4.344893	3.335737	3.344631
27	C	6.873945	6.906607	2.224404	1.411297	2.299355
28	C	7.577351	7.231020	3.253689	3.112924	3.234204
29	O	8.578912	8.190436	3.820674	3.948931	4.114239
30	C	4.240905	3.132843	8.073275	7.268616	6.606293
31	O	5.173814	3.973539	8.962801	8.221805	7.578560

		21	22	23	24	25
21	H	0.000000				
22	H	4.351263	0.000000			
23	C	3.341198	2.233862	0.000000		
24	H	4.353145	2.684930	1.079306	0.000000	
25	C	2.235508	3.343846	1.419967	2.234392	0.000000
26	H	2.685581	4.354741	2.236344	2.699908	1.078156
27	C	1.079859	3.341039	2.297570	3.342256	1.423739
28	C	4.174903	3.496867	3.830444	4.468162	4.048343
29	O	5.086355	4.165116	4.885154	5.494346	5.164447
30	C	7.570628	6.934896	5.831382	5.428504	6.082868
31	O	8.551447	7.840476	6.898679	6.509580	7.168103

		26	27	28	29	30
26	H	0.000000				
27	C	2.230910	0.000000			
28	C	4.846557	3.650459	0.000000		
29	O	5.986182	4.644478	1.150482	0.000000	
30	C	5.971704	6.980472	5.664519	6.315699	0.000000
31	O	7.083765	7.990570	6.311921	6.807132	1.150055

		31
31	O	0.000000



13S. -1184.07395 30.04 C1
WBI 0.07

Charges and spin densities

		1
1	Ru	0.365383
2	Ru	0.325134
3	P	-0.170619
4	C	0.022329
9	C	-0.066723
10	C	-0.055294
13	C	-0.053279
15	C	-0.069982
17	C	-0.084241
19	C	-0.005378
20	C	0.001777
23	C	0.053426
25	C	-0.015998
27	C	-0.003916
28	C	-0.033987
29	O	-0.109720
30	C	0.004009
31	O	-0.102919

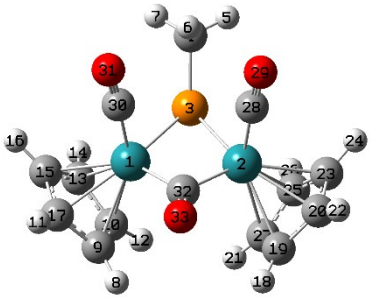
		1	2	3	4	5
1	Ru	0.000000				
2	Ru	4.482039	0.000000			
3	P	2.138701	2.362728	0.000000		
4	C	2.494333	3.550277	1.862833	0.000000	
5	H	3.218679	3.793458	2.511265	1.090134	0.000000
6	H	3.242908	3.793088	2.509120	1.090873	1.794007
7	H	2.007915	4.540949	2.475188	1.138666	1.765682
8	H	2.873370	6.185891	4.273530	4.877158	5.116695
9	C	2.127010	6.056868	3.918112	4.392413	4.814560
10	C	2.163909	6.503989	4.191548	4.045809	4.441528
11	H	2.853361	5.850133	4.086825	5.227067	5.926810
12	H	2.923336	6.989250	4.736420	4.269997	4.429888
13	C	2.179505	6.612921	4.263234	4.059949	4.730876
14	H	2.937880	7.169852	4.846276	4.283498	4.951279
15	C	2.148062	6.240513	4.036441	4.406042	5.234545
16	H	2.901828	6.519404	4.474943	4.899287	5.842237
17	C	2.103233	5.866261	3.799880	4.590827	5.274480
18	H	7.095974	2.985360	5.131074	6.469581	6.756538
19	C	6.372381	2.264258	4.368093	5.580613	5.928447
20	C	5.448810	2.262646	3.661524	4.985265	5.571569
21	H	7.311544	2.987951	5.184524	5.785439	5.812717
22	H	5.461728	2.991344	3.960413	5.480691	6.162584
23	C	4.983232	2.277739	3.217293	4.086836	4.733736
24	H	4.493307	2.980634	3.094859	3.777756	4.608701
25	C	5.685818	2.262880	3.723086	4.200734	4.566417
26	H	5.907546	2.995894	4.073827	4.056754	4.330787
27	C	6.499985	2.266525	4.401745	5.170521	5.376416
28	C	4.867146	1.857230	2.944621	3.370659	3.044154
29	O	5.434258	2.999334	3.754458	3.755704	3.101575
30	C	4.628633	1.862119	2.926376	4.491120	4.626959
31	O	5.090249	3.002421	3.734709	5.334500	5.421475

		6	7	8	9	10
6	H	0.000000				
7	H	1.758700	0.000000			
8	H	5.855778	4.376558	0.000000		
9	C	5.268606	3.752139	1.079194	0.000000	
10	C	4.820376	3.124094	2.235532	1.423590	0.000000
11	H	5.904084	4.857632	2.704232	2.244547	3.351973
12	H	5.070898	3.312301	2.691604	2.235109	1.079437
13	C	4.560435	3.078355	3.354044	2.310687	1.431535
14	H	4.582776	3.218665	4.362858	3.353057	2.242000
15	C	4.871549	3.682739	3.362033	2.318279	2.310539
16	H	5.165695	4.263268	4.373050	3.361861	3.353764
17	C	5.287276	4.045322	2.245228	1.432942	2.309163
18	H	6.528894	7.433679	8.526100	8.474367	9.156519

19	C	5.544901	6.559055	8.088425	7.931057	8.484815	
20	C	4.912387	5.825135	7.365093	7.064701	7.595082	
21	H	5.606513	6.904753	9.139345	9.013957	9.337305	
22	H	5.492395	6.178038	7.194521	6.886990	7.547277	
23	C	3.776216	4.951892	7.308746	6.870886	7.138524	
24	H	3.352492	4.466897	7.034552	6.456050	6.602641	
25	C	3.810409	5.235327	7.968711	7.613799	7.779533	
26	H	3.467301	5.088476	8.329659	7.923611	7.901402	
27	C	4.985690	6.247789	8.434221	8.238906	8.588505	
28	C	3.773307	4.412576	6.278869	6.299638	6.563188	
29	O	4.196012	4.724770	6.625989	6.728706	6.876425	
30	C	5.081639	5.261731	5.440129	5.597646	6.391834	
31	O	6.037993	5.977282	5.294161	5.638749	6.616454	
		11	12	13	14	15	
11	H	0.000000					
12	H	4.362739	0.000000				
13	C	3.349572	2.243002	0.000000			
14	H	4.360172	2.698791	1.079672	0.000000		
15	C	2.246125	3.352452	1.419126	2.230056	0.000000	
16	H	2.705791	4.361900	2.231479	2.685540	1.079269	
17	C	1.079171	3.352953	2.307229	3.351084	1.434804	
18	H	7.654146	9.766908	9.162021	9.768108	8.481221	
19	C	7.213958	9.086833	8.405516	8.937692	7.789612	
20	C	6.163465	8.301465	7.348118	7.862668	6.625181	
21	H	8.768727	9.731150	9.352888	9.748632	9.034813	
22	H	5.671939	8.351975	7.251670	7.835418	6.350233	
23	C	6.267041	7.776601	6.774217	7.125954	6.240460	
24	H	5.840006	7.285484	6.060046	6.324648	5.522793	
25	C	7.324942	8.263423	7.549607	7.840165	7.223591	
26	H	7.867613	8.287140	7.639403	7.798595	7.489384	
27	C	7.854108	9.067194	8.516036	8.927035	8.111243	
28	C	6.711351	6.767101	6.945327	7.441387	6.925894	
29	O	7.444471	6.903611	7.396926	7.842504	7.564119	
30	C	5.282787	6.896929	6.777934	7.552624	6.287918	
31	O	5.257708	7.117184	7.146347	8.019116	6.602345	
		16	17	18	19	20	
16	H	0.000000					
17	C	2.246917	0.000000				
18	H	8.536995	8.010869	0.000000			
19	C	7.822900	7.459976	1.079465	0.000000		
20	C	6.547393	6.415782	2.241010	1.430202	0.000000	
21	H	9.176332	8.805453	2.679692	2.224207	3.344440	
22	H	6.191362	6.077334	2.702213	2.244231	1.078955	
23	C	6.148372	6.291229	3.341276	2.298625	1.415958	
24	H	5.327013	5.780308	4.349949	3.341135	2.223806	
25	C	7.249380	7.251925	3.342628	2.298269	2.297030	

	26 H 7.532208 7.658164 4.351338 3.340236 3.339455 27 C 8.195652 7.918030 2.223760 1.410981 2.300273 28 C 7.417999 6.520785 4.302543 3.736762 4.069820 29 O 8.149049 7.157451 5.268246 4.768492 5.194833 30 C 6.711843 5.507204 3.332397 3.169476 3.247617 31 O 7.089169 5.611929 3.957288 4.040013 4.143860 21 22 23 24 25 21 H 0.000000 22 H 4.354046 0.000000 23 C 3.342941 2.227723 0.000000 24 H 4.354650 2.676739 1.079348 0.000000 25 C 2.241798 3.338927 1.416666 2.229718 0.000000 26 H 2.700140 4.347359 2.229839 2.688115 1.079005 27 C 1.079341 3.342859 2.300163 3.344666 1.430277 28 C 3.382069 4.847264 3.809929 4.395685 3.238013 29 O 4.030314 5.988705 4.860220 5.397860 4.135449 30 C 4.257520 3.485312 3.831680 4.432717 4.068263 31 O 5.201197 4.169934 4.884706 5.444867 5.188466 26 27 28 29 30 26 H 0.000000 27 C 2.242149 0.000000 28 C 3.468400 3.200269 0.000000 29 O 4.147721 4.084204 1.142323 0.000000 30 C 4.852608 3.707497 2.631505 3.542719 0.000000 31 O 5.990282 4.724764 3.544099 4.276178 1.140649 31 31 O 0.000000

Table S5. Distance matrix for the lowest energy $MePCp_2Ru_2(CO)_3$ structures as optimized at the PBE0/def2TZVP level. Included are the ranking order, spin multiplicity (S, T or Q), total energy (in a.u.), relative energy (in kcal/mol), symmetry point group Wiberg bond indices for the Fe-Fe bonds, Mulliken charges and the spin density (Cp moieties are omitted for clarity).

 1S -1297.415564 0.00 Cs WBI 0.33	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.761340 0.000000 3 P 2.346915 2.348805 0.000000 4 C 3.522091 3.521487 1.853592 0.000000 5 H 4.441047 3.854754 2.420200 1.094116 0.000000 6 H 3.623915 3.623841 2.540749 1.089249 1.774185 7 H 3.856013 4.440651 2.418758 1.094121 1.758986 8 H 3.002026 4.262170 4.861655 6.408976 7.196276 9 C 2.283073 4.135310 4.212836 5.704900 6.552796 10 C 2.294835 3.970920 3.487154 5.123903 5.875661 11 H 2.966741 5.335229 5.286246 6.243526 7.262826

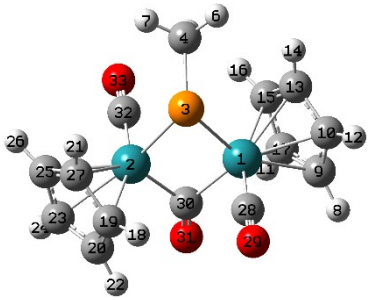
Charge densities

		1
1	Ru	0.300802
2	Ru	0.315585
3	P	-0.087519
4	C	-0.023375
9	C	0.014061
10	C	0.006208
13	C	0.030560
15	C	-0.031213
17	C	0.016254
19	C	0.016911
20	C	0.004611
23	C	-0.031865
25	C	0.052711
27	C	-0.007776
28	C	-0.042015
29	O	-0.129050
30	C	-0.041499
31	O	-0.129387
32	C	-0.023989
33	O	-0.210017

12	H	3.033379	3.981160	3.633672	5.418048	6.006936
13	C	2.273968	4.513116	3.309778	4.606861	5.458004
14	H	2.988037	4.936427	3.284269	4.431728	5.186757
15	C	2.212920	4.922580	3.941451	4.904206	5.904964
16	H	2.929918	5.661191	4.443051	5.037453	6.079901
17	C	2.252744	4.740172	4.471084	5.603857	6.587970
18	H	4.460088	3.001125	5.039468	6.484538	6.831581
19	C	4.247780	2.284618	4.328418	5.754444	5.983139
20	C	4.819663	2.242270	4.433441	5.501884	5.538873
21	H	3.944979	3.049147	3.893963	5.684972	5.969342
22	H	5.470687	2.955321	5.222143	6.068728	6.090452
23	C	4.884599	2.213053	3.808434	4.787990	4.609168
24	H	5.599518	2.933000	4.213494	4.821365	4.420272
25	C	4.404098	2.282060	3.281120	4.663223	4.587196
26	H	4.737443	2.994395	3.209410	4.527586	4.325026
27	C	3.947215	2.300088	3.630118	5.269378	5.457289
28	C	3.536871	1.836386	2.987627	3.103269	3.364248
29	O	4.393952	2.981580	3.833177	3.405648	3.566332
30	C	1.837062	3.533490	2.993460	3.114233	4.149738
31	O	2.982414	4.388243	3.839681	3.419293	4.411579
32	C	2.023672	2.023183	3.342280	4.387648	5.096043
33	O	2.985877	2.990010	4.510917	5.447792	6.155193

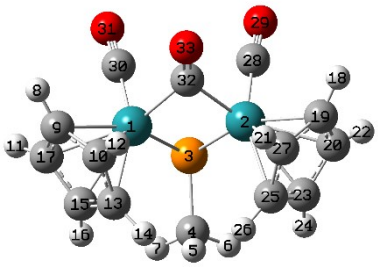
		6	7	8	9	10
6	H	0.000000				
7	H	1.774033	0.000000			
8	H	6.543986	6.779570	0.000000		
9	C	5.902107	5.947395	1.079744	0.000000	
10	C	5.572442	5.275951	2.235741	1.424007	0.000000
11	H	6.128182	6.342779	2.679520	2.227649	3.344922
12	H	5.989889	5.643527	2.697316	2.238611	1.078157
13	C	5.088758	4.484339	3.340639	2.297884	1.415523
14	H	5.088364	4.130957	4.350046	3.340851	2.227651
15	C	5.108908	4.749172	3.334407	2.290297	2.290559
16	H	5.168202	4.692530	4.343826	3.333052	3.333471
17	C	5.657171	5.685648	2.220892	1.411687	2.301077
18	H	6.545979	7.322069	3.654888	4.279735	4.617206
19	C	5.907024	6.631192	4.086118	4.480992	4.517258
20	C	5.555807	6.502202	5.292796	5.570904	5.545104
21	H	6.181830	6.294964	3.537992	3.681808	3.150629
22	H	5.951490	7.113476	5.915276	6.267692	6.409818
23	C	5.045536	5.772774	5.872135	5.926859	5.562310
24	H	5.051347	5.833748	6.880156	6.869797	6.451479
25	C	5.165791	5.484584	5.221278	5.185790	4.574754
26	H	5.221908	5.223842	5.777036	5.588226	4.725697
27	C	5.676196	6.028229	4.018574	4.174368	3.775714
28	C	2.704492	4.140296	5.599056	5.394811	5.385625

29	O	2.716382	4.399790	6.576824	6.353475	6.406065	
30	C	2.711990	3.379387	4.509089	3.852223	4.054767	
31	O	2.726062	3.586819	5.538991	4.909610	5.169842	
32	C	4.182777	5.096813	3.063128	3.043418	3.571455	
33	O	5.106498	6.154676	3.195657	3.465470	4.330302	
		11	12	13	14	15	
11	H	0.000000					
12	H	4.353895	0.000000				
13	C	3.352308	2.222944	0.000000			
14	H	4.362675	2.676854	1.078668	0.000000		
15	C	2.243849	3.331608	1.419881	2.233445	0.000000	
16	H	2.700192	4.340425	2.230697	2.689098	1.079556	
17	C	1.078796	3.342895	2.309932	3.353237	1.430412	
18	H	5.748875	4.385054	5.794619	6.502145	6.158056	
19	C	6.069061	4.185590	5.589275	6.152845	6.110665	
20	C	6.943250	5.267203	6.421063	6.880982	6.900805	
21	H	5.774503	2.399676	4.321672	4.717166	5.250509	
22	H	7.411153	6.222278	7.261088	7.775816	7.595106	
23	C	7.423747	5.179544	6.263506	6.503164	6.939022	
24	H	8.261425	6.091530	7.014556	7.154312	7.680805	
25	C	6.951765	4.022398	5.324699	5.483522	6.213071	
26	H	7.402883	4.089790	5.303836	5.249589	6.349593	
27	C	6.063611	3.211564	4.814431	5.203767	5.624728	
28	C	5.986567	5.606260	5.594095	5.958129	5.691172	
29	O	6.662646	6.695832	6.482920	6.811539	6.440682	
30	C	3.498733	4.846613	3.624187	4.133067	3.041732	
31	O	4.181900	5.982748	4.621081	5.043960	3.889640	
32	C	3.655394	4.019252	4.123896	4.903176	3.987806	
33	O	3.694068	4.810628	4.972831	5.855259	4.630988	
		16	17	18	19	20	
16	H	0.000000					
17	C	2.240235	0.000000				
18	H	7.127289	5.350489	0.000000			
19	C	7.052751	5.534257	1.079588	0.000000		
20	C	7.739897	6.449451	2.219016	1.408773	0.000000	
21	H	6.265571	4.950569	2.693821	2.235988	3.337496	
22	H	8.389824	7.048985	2.676727	2.224247	1.079046	
23	C	7.723082	6.777027	3.338962	2.294804	1.434071	
24	H	8.382963	7.624626	4.347461	3.336644	2.244316	
25	C	7.058861	6.160156	3.342532	2.299905	2.308075	
26	H	7.138775	6.518276	4.352166	3.343024	3.351603	
27	C	6.585058	5.315074	2.238510	1.426087	2.297436	
28	C	6.169580	5.602570	4.353844	3.756332	3.141795	
29	O	6.777538	6.392934	5.329224	4.783827	4.003905	
30	C	3.161148	3.245478	5.648750	5.423214	5.622572	
31	O	3.737197	4.135216	6.566388	6.347202	6.385121	

	32 C 4.715625 3.361676 3.043198 3.032143 3.474290 33 O 5.325566 3.707954 3.065958 3.403362 3.865519 21 22 23 24 25 21 H 0.000000 22 H 4.348327 0.000000 23 C 3.333161 2.245862 0.000000 24 H 4.342711 2.702853 1.079270 0.000000 25 C 2.225486 3.350290 1.418951 2.231185 0.000000 26 H 2.681910 4.360795 2.230979 2.688150 1.078753 27 C 1.078319 3.341848 2.290757 3.333729 1.414321 28 C 4.882685 3.324306 3.092865 3.263282 3.732212 29 O 6.024602 3.944860 3.954994 3.877476 4.757617 30 C 5.597918 6.029280 5.679865 6.155869 5.561618 31 O 6.695278 6.659129 6.440571 6.786809 6.480668 32 C 3.813176 3.858645 4.056088 4.829899 4.062310 33 O 4.508117 3.995223 4.758238 5.536616 4.920988 26 27 28 29 30 26 H 0.000000 27 C 2.226823 0.000000 28 C 4.309273 4.069966 0.000000 29 O 5.278894 5.187047 1.146276 0.000000 30 C 5.895163 5.373242 3.304209 3.709415 0.000000 31 O 6.805156 6.396286 3.705760 3.762532 1.146348 32 C 4.803464 3.443559 2.685012 3.563569 2.675173 33 O 5.769413 4.151450 3.400441 4.088391 3.382749 31 32 33 31 O 0.000000 32 C 3.551346 0.000000 33 O 4.066727 1.172372 0.000000
 2S -1297.412194 2.11 C1 WBI 0.33 Charge densities 1 1 Ru 0.330540 2 Ru 0.309839 3 P -0.075682 4 C -0.044751	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.774020 0.000000 3 P 2.365269 2.349653 0.000000 4 C 3.435731 3.488334 1.859090 0.000000 5 H 3.443682 3.606393 2.543646 1.090099 0.000000 6 H 3.864732 4.439293 2.438161 1.094022 1.782354 7 H 4.343948 3.742726 2.414599 1.094563 1.770213 8 H 2.966477 5.447715 5.267336 6.099947 5.888750 9 C 2.250696 4.856640 4.481903 5.117629 4.856209 10 C 2.214014 4.950384 3.881065 4.362882 4.282199 11 H 3.004258 4.561100 5.046857 5.400104 4.784808 12 H 2.931383 5.624721 4.294115 4.882246 4.987309 13 C 2.262694 4.556716 3.334938 3.265015 3.014564 14 H 2.987130 4.937881 3.292605 2.808377 2.701398 15 C 2.290800 4.146164 3.658946 3.517258 2.901436 16 H 3.033232 4.204016 3.899484 3.344604 2.463123

9 C -0.003551 10 C -0.021328 13 C 0.026736 15 C -0.041210 17 C 0.040033 19 C 0.012446 20 C 0.022795 23 C 0.007496 25 C -0.031776 27 C 0.039413 28 C 0.016397 29 O -0.149910 30 C -0.044721 31 O -0.215288 32 C -0.025260 33 O -0.152217	17 C 2.290880 4.364679 4.356842 4.690466 4.172107 18 H 4.133426 3.026903 3.537516 5.313755 5.908594 19 C 4.100341 2.294850 3.410229 5.026394 5.508671 20 C 4.272985 2.291217 4.178424 5.652353 5.886678 21 H 4.978115 2.983406 3.172790 4.254664 4.962918 22 H 4.427299 3.005959 4.836226 6.378236 6.544550 23 C 4.809161 2.256363 4.445832 5.544078 5.645564 24 H 5.391306 2.972930 5.281659 6.209882 6.146869 25 C 4.958012 2.216808 3.896788 4.800683 5.058650 26 H 5.659227 2.932771 4.405937 4.925323 5.115010 27 C 4.575009 2.269863 3.221226 4.468025 4.997277 28 C 1.838897 3.337510 2.937057 4.568181 4.915471 29 O 2.985761 4.120431 3.754985 5.486798 5.949452 30 C 2.025462 2.014665 3.374495 4.500253 4.335735 31 O 2.985441 2.981337 4.547035 5.613308 5.343085 32 C 3.361838 1.833709 3.039385 3.132321 2.734636 33 O 4.140160 2.982474 3.885026 3.446708 2.749712 6 7 8 9 10 6 H 0.000000 7 H 1.755469 0.000000 8 H 6.261622 7.121739 0.000000 9 C 5.271408 6.158780 1.078898 0.000000 10 C 4.264728 5.442851 2.244402 1.432212 0.000000 11 H 5.882254 6.291703 2.677434 2.219494 3.336994 12 H 4.603465 5.934317 2.702225 2.243078 1.079249 13 C 3.178100 4.356955 3.348200 2.305832 1.417973 14 H 2.409553 3.865988 4.357021 3.348027 2.227946 15 C 3.801978 4.513660 3.343208 2.299707 2.295648 16 H 3.757206 4.201311 4.349193 3.339862 3.339750 17 C 5.038469 5.668798 2.225761 1.410192 2.293359 18 H 5.909819 5.495963 6.308749 6.073087 5.993319 19 C 5.785854 5.110645 6.475391 6.150041 6.170484 20 C 6.527054 5.800396 6.333257 6.097835 6.432374 21 H 4.965908 3.895864 7.797679 7.222581 6.878388 22 H 7.208126 6.654518 6.002911 5.945897 6.468322 23 C 6.544074 5.514222 7.062660 6.685134 7.020747 24 H 7.251354 6.186612 7.411182 7.067013 7.562103 25 C 5.791932 4.539050 7.595616 7.062397 7.122843 26 H 5.942824 4.466091 8.365285 7.748583 7.760888 27 C 5.302236 4.268934 7.286919 6.780153 6.646038 28 C 4.880934 5.326799 3.392770 3.187322 3.095722 29 O 5.734366 6.163090 4.046667 4.069258 3.965533 30 C 5.273390 5.126769 3.788379 3.405364 4.017336 31 O 6.389312 6.230710 3.873866 3.740617 4.674981 32 C 4.185786 3.332824 5.851910 5.068902 5.189179 33 O 4.444065 3.576455 6.386965 5.539689 5.669940

		11	12	13	14	15	
11	H	0.000000					
12	H	4.346148	0.000000				
13	C	3.338942	2.230165	0.000000			
14	H	4.349049	2.683486	1.078242	0.000000		
15	C	2.232402	3.338714	1.419457	2.232299	0.000000	
16	H	2.685259	4.349987	2.234770	2.694905	1.078972	
17	C	1.079507	3.335760	2.296282	3.339445	1.422146	
18	H	6.601224	6.188735	6.155214	6.463103	6.290126	
19	C	6.320926	6.536533	6.143153	6.468333	6.065216	
20	C	5.851285	6.952159	6.430990	6.932432	6.058996	
21	H	7.421995	7.210364	6.475103	6.444374	6.548419	
22	H	5.697308	6.969442	6.664337	7.294757	6.254044	
23	C	6.051111	7.673489	6.754143	7.189564	6.188621	
24	H	6.110064	8.301277	7.267918	7.772888	6.516364	
25	C	6.612453	7.723065	6.665943	6.889803	6.259529	
26	H	7.144064	8.407295	7.134985	7.264962	6.665899	
27	C	6.789973	7.073651	6.320582	6.464588	6.213900	
28	C	4.403227	3.252705	3.700487	4.269662	4.068473	
29	O	5.401376	3.871572	4.726308	5.229510	5.191401	
30	C	2.926540	4.804086	4.015167	4.788257	3.370728	
31	O	2.848479	5.476682	4.822982	5.704581	4.012429	
32	C	4.203586	6.061910	4.383001	4.692042	3.598593	
33	O	4.393253	6.609933	4.681001	4.921227	3.730668	
		16	17	18	19	20	
16	H	0.000000					
17	C	2.232133	0.000000				
18	H	6.712679	6.250825	0.000000			
19	C	6.335256	6.081505	1.079035	0.000000		
20	C	6.271805	5.856434	2.234458	1.421047	0.000000	
21	H	6.592277	7.025036	2.685262	2.229454	3.337743	
22	H	6.575871	5.803434	2.688568	2.231163	1.079706	
23	C	6.155988	6.157235	3.343412	2.301771	1.412232	
24	H	6.391430	6.394291	4.353259	3.345165	2.228409	
25	C	6.132388	6.536233	3.337990	2.294912	2.291216	
26	H	6.372135	7.089879	4.347695	3.337974	3.334055	
27	C	6.273961	6.518164	2.231183	1.419056	2.295385	
28	C	4.868964	3.796292	3.084656	3.499931	3.920134	
29	O	6.013531	4.840218	2.915224	3.628569	4.163627	
30	C	3.733609	2.942219	3.851925	3.445867	2.944896	
31	O	4.357780	3.236666	4.563233	4.145159	3.296211	
32	C	3.192095	4.130619	4.844154	4.068344	3.866808	
33	O	3.015640	4.409345	5.987682	5.196944	4.938242	
		21	22	23	24	25	
21	H	0.000000					
22	H	4.346677	0.000000				

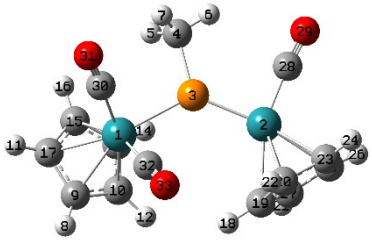
	23 C 3.351413 2.221216 0.000000 24 H 4.361081 2.680316 1.078816 0.000000 25 C 2.232921 3.335104 1.430684 2.243755 0.000000 26 H 2.689653 4.344722 2.240994 2.700739 1.079434 27 C 1.078573 3.338118 2.307840 3.350289 1.419257 28 C 4.776003 3.904145 4.922739 5.676594 5.151227 29 O 5.044036 4.030174 5.364754 6.170713 5.626394 30 C 4.836108 2.936459 3.335570 3.669612 3.974791 31 O 5.769237 2.951822 3.664777 3.713191 4.618963 32 C 4.171320 4.505495 3.278121 3.533575 3.098142 33 O 5.108337 5.542876 4.194831 4.248202 3.980348 26 27 28 29 30 26 H 0.000000 27 C 2.230779 0.000000 28 C 6.061193 4.394680 0.000000 29 O 6.606682 4.706464 1.147496 0.000000 30 C 4.736759 4.053090 2.766139 3.661306 0.000000 31 O 5.371511 4.878566 3.541654 4.281684 1.172767 32 C 3.234543 3.658214 4.635427 5.615406 2.742256 33 O 3.860961 4.679341 5.616730 6.650566 3.629232 31 32 33 31 O 0.000000 32 C 3.515494 0.000000 33 O 4.242714 1.148980 0.000000
 3S -1297.408871 4.20 Cs WBI 0.33 Charges and spin densities 1 1 Ru 0.317868 2 Ru 0.317874 3 P -0.069765 4 C -0.068050 9 C 0.006357 10 C 0.028403 13 C -0.043810 15 C 0.014522 17 C -0.013592	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.766536 0.000000 3 P 2.368010 2.368042 0.000000 4 C 3.411703 3.411968 1.865030 0.000000 5 H 3.440386 3.440463 2.549648 1.091055 0.000000 6 H 4.357856 3.761529 2.432894 1.094339 1.778352 7 H 3.760713 4.357905 2.432843 1.094339 1.778336 8 H 2.961708 5.386996 5.282173 6.104831 5.923705 9 C 2.246673 4.776876 4.514319 5.133076 4.897568 10 C 2.280604 4.189641 4.374047 4.714062 4.221054 11 H 2.931521 5.650673 4.378938 4.898388 5.018688 12 H 2.997619 4.342992 5.042502 5.421349 4.832869 13 C 2.288086 3.978807 3.716065 3.566714 2.968776 14 H 3.034559 3.992258 3.955746 3.410731 2.545592 15 C 2.269608 4.491421 3.440918 3.319104 3.074849 16 H 2.995934 4.902477 3.434241 2.885525 2.766060 17 C 2.211756 4.922298 3.955097 4.384931 4.321155 18 H 5.388678 2.961631 5.281435 6.104591 5.923970 19 C 4.777847 2.246571 4.513803 5.133016 4.897733 20 C 4.921938 2.211782 3.953611 4.383059 4.319062 21 H 4.345242 2.997611 5.044195 5.424618 4.836742

19 C 0.006197 20 C -0.013627 23 C 0.014908 25 C -0.043916 27 C 0.028451 28 C 0.008136 29 O -0.123592 30 C 0.008194 31 O -0.123606 32 C -0.038741 33 O -0.212213	22 H 5.650079 2.931592 4.376478 4.895010 5.015257 23 C 4.490178 2.269680 3.440451 3.318208 3.072854 24 H 4.900206 2.995985 3.433307 2.883066 2.761697 25 C 3.978424 2.288088 3.717257 3.568935 2.970582 26 H 3.991616 3.034647 3.958036 3.414915 2.549631 27 C 4.190898 2.280603 4.375062 4.716180 4.223419 28 C 3.533064 1.844604 2.873674 4.473356 4.862754 29 O 4.386804 2.987701 3.680010 5.369508 5.879476 30 C 1.844601 3.532991 2.873585 4.473079 4.862659 31 O 2.987704 4.386665 3.679861 5.369196 5.879351 32 C 2.018920 2.018891 3.326162 4.570836 4.474339 33 O 2.982015 2.982095 4.488636 5.724617 5.556578 6 7 8 9 10 6 H 0.000000 7 H 1.751320 0.000000 8 H 7.147867 6.186171 0.000000 9 C 6.194109 5.206997 1.078832 0.000000 10 C 5.723373 4.993298 2.226190 1.410500 0.000000 11 H 5.943732 4.533589 2.701296 2.241902 3.334510 12 H 6.354376 5.841252 2.677820 2.219775 1.079627 13 C 4.585376 3.783562 3.343413 2.299550 1.423941 14 H 4.297200 3.768708 4.350164 3.339960 2.234701 15 C 4.409853 3.152132 3.350817 2.308670 2.299020 16 H 3.921267 2.417353 4.359417 3.350727 3.342441 17 C 5.468227 4.202131 2.244561 1.431839 2.292118 18 H 6.185790 7.147584 7.322263 6.944077 6.138075 19 C 5.207115 6.193986 6.942861 6.425319 5.540030 20 C 4.200593 5.466383 7.496605 6.851850 6.038249 21 H 5.844718 6.357581 5.772714 5.281074 4.139429 22 H 4.530110 5.940399 8.309072 7.694663 6.984138 23 C 3.152504 4.408944 7.137689 6.339307 5.431995 24 H 2.416638 3.918992 7.668057 6.793263 5.952423 25 C 3.786903 4.587280 6.260466 5.466112 4.372184 26 H 3.774183 4.300958 6.057821 5.172954 3.979038 27 C 4.995835 5.725342 6.135800 5.539547 4.466673 28 C 4.686808 5.264166 5.966204 5.588594 5.397938 29 O 5.508888 6.072621 6.609507 6.356963 6.335091 30 C 5.264003 4.686086 3.402186 3.185931 3.805818 31 O 6.072357 5.508195 4.048617 4.056549 4.845915 32 C 5.263236 5.262780 3.711837 3.383016 3.010214 33 O 6.411033 6.410501 3.773327 3.732206 3.393145 11 12 13 14 15 11 H 0.000000 12 H 4.345062 0.000000 13 C 3.334516 2.235753 0.000000 14 H 4.344106 2.691294 1.078592 0.000000

15	C	2.229490	3.341892	1.417500	2.229387	0.000000
16	H	2.683467	4.352365	2.231528	2.689296	1.078219
17	C	1.079420	3.336039	2.291473	3.334407	1.418317
18	H	8.310488	5.774628	6.264363	6.062842	7.141111
19	C	7.695834	5.280541	5.468724	5.176570	6.342132
20	C	7.753246	6.007120	5.657902	5.301885	6.320600
21	H	7.002433	3.573301	4.325459	3.995919	5.531393
22	H	8.433915	6.999943	6.588479	6.274503	7.123582
23	C	7.123879	5.525397	4.773133	4.260963	5.427725
24	H	7.284974	6.191240	5.077721	4.519895	5.538400
25	C	6.589599	4.319095	3.829353	3.236811	4.775473
26	H	6.275892	3.986926	3.236003	2.431474	4.263722
27	C	6.985919	4.137370	4.375869	3.984497	5.436193
28	C	6.154423	5.602820	5.390602	5.629848	5.592518
29	O	6.761082	6.548955	6.407120	6.719778	6.487633
30	C	3.192562	4.435714	4.060627	4.869455	3.668171
31	O	3.775532	5.438399	5.173792	6.006969	4.673299
32	C	4.754389	3.017501	3.498274	3.919082	4.086833
33	O	5.396670	3.079620	4.224712	4.659015	4.930969

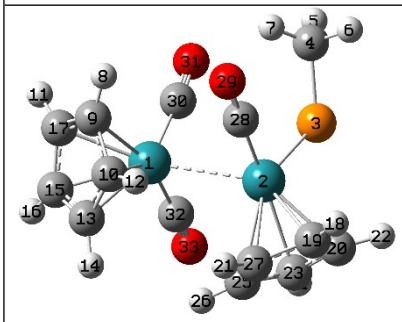
		16	17	18	19	20
16	H	0.000000				
17	C	2.229056	0.000000			
18	H	7.672165	7.498514	0.000000		
19	C	6.797174	6.853155	1.078835	0.000000	
20	C	6.556959	6.989002	2.244580	1.431884	0.000000
21	H	6.198833	6.010052	2.677796	2.219751	3.336093
22	H	7.285346	7.752854	2.701334	2.241962	1.079416
23	C	5.540286	6.319962	3.350770	2.308630	1.418284
24	H	5.439068	6.555213	4.359379	3.350694	2.229020
25	C	5.082544	5.658320	3.343390	2.299519	2.291487
26	H	4.526038	5.302239	4.350136	3.339925	3.334429
27	C	5.958317	6.040078	2.226161	1.410468	2.292172
28	C	5.975114	5.680490	3.400340	3.184809	3.054692
29	O	6.847375	6.425299	4.046039	4.055088	3.901662
30	C	4.223433	3.054139	5.966965	5.588949	5.680361
31	O	5.156257	3.900995	6.609772	6.357000	6.425229
32	C	4.869578	4.003273	3.714320	3.384442	4.004155
33	O	5.818383	4.660904	3.777098	3.734311	4.662591

		21	22	23	24	25
21	H	0.000000				
22	H	4.345110	0.000000			
23	C	3.341906	2.229468	0.000000		
24	H	4.352368	2.683442	1.078217	0.000000	
25	C	2.235787	3.334527	1.417496	2.231498	0.000000
26	H	2.691308	4.344126	2.229413	2.689296	1.078599
27	C	1.079625	3.334558	2.299031	3.342442	1.423968

	28 C 4.434052 3.193687 3.669310 4.225311 4.060747 29 O 5.436132 3.777023 4.674728 5.158763 5.173926 30 C 5.603552 6.154274 5.591999 5.974153 5.390315 31 O 6.549067 6.761100 6.487372 6.846930 6.406838 32 C 3.017510 4.755765 4.086244 4.868541 3.496953 33 O 3.078600 5.399261 4.930634 5.817637 4.222990 26 27 28 29 30 26 H 0.000000 27 C 2.234708 0.000000 28 C 4.869768 3.804772 0.000000 29 O 6.007344 4.844526 1.144261 0.000000 30 C 5.629486 5.398323 3.281983 3.680901 0.000000 31 O 6.719486 6.335102 3.680792 3.729239 1.144263 32 C 3.916869 3.010268 2.679273 3.558994 2.679257 33 O 4.655906 3.392815 3.389761 4.079477 3.389649 31 32 33 31 O 0.000000 32 C 3.558957 0.000000 33 O 4.079364 1.172932 0.000000
 4S -1297.391410 15.16 C1 WBI 0.06 Charges and spin densities 1 1 Ru 0.373288 2 Ru 0.471448 3 P -0.154001 4 C 0.029371 9 C 0.005076 10 C -0.018000 13 C 0.077322 15 C -0.026616 17 C 0.000176 19 C -0.075912 20 C -0.021106 23 C -0.025801 25 C -0.033513 27 C -0.040688 28 C -0.115291 29 O -0.168046	1 2 3 4 5 1 Ru 0.000000 2 Ru 4.098189 0.000000 3 P 2.378045 2.154779 0.000000 4 C 3.364257 3.548585 1.838112 0.000000 5 H 3.385464 4.258319 2.446777 1.093091 0.000000 6 H 4.357233 3.529166 2.434529 1.090194 1.779116 7 H 3.556644 4.219052 2.445575 1.092789 1.767056 8 H 2.988178 6.269641 5.131155 6.266499 6.067177 9 C 2.266938 5.681266 4.364153 5.361206 5.073032 10 C 2.261911 4.675782 3.635522 4.778506 4.510403 11 H 2.991255 7.025165 5.201053 5.539898 5.065487 12 H 2.989773 4.442310 3.922852 5.306563 5.161737 13 C 2.276453 4.578746 3.186943 3.847582 3.350527 14 H 2.984799 4.207924 3.057215 3.567855 3.040371 15 C 2.264761 5.519604 3.719125 3.934210 3.283473 16 H 2.998673 6.008920 4.076909 3.783355 2.933816 17 C 2.269682 6.129623 4.408203 4.922791 4.457725 18 H 3.947832 2.973344 3.740518 5.565974 5.979444 19 C 4.418536 2.231309 3.584233 5.351904 5.890579 20 C 4.927715 2.238145 3.793675 5.443743 6.197486 21 H 5.439831 2.948734 4.372796 5.813821 6.101854 22 H 4.936761 2.964203 4.086591 5.703837 6.513006 23 C 5.884950 2.232952 4.254446 5.641074 6.449232 24 H 6.639583 2.968749 4.883755 6.072711 6.975861 25 C 6.024192 2.223104 4.343784 5.676494 6.314968 26 H 6.864717 2.943407 5.018638 6.119467 6.724447

30 C -0.037541 31 O -0.110245 32 C -0.016553 33 O -0.113370	27 C 5.184294 2.210453 3.939703 5.484919 5.951762 28 C 5.187950 1.842960 2.834522 3.232321 4.003823 29 O 6.105824 2.993355 3.735567 3.618350 4.337173 30 C 1.855404 4.947758 2.998133 3.228147 3.403803 31 O 2.998034 5.736576 3.823030 3.664637 3.893986 32 C 1.857294 3.903886 2.942163 4.388688 4.789195 33 O 2.998783 4.225325 3.747876 5.268619 5.794039 6 7 8 9 10 6 H 0.000000 7 H 1.775223 0.000000 8 H 7.226553 6.511638 0.000000 9 C 6.315451 5.677910 1.079431 0.000000 10 C 5.586216 5.344052 2.240440 1.429713 0.000000 11 H 6.599763 5.542102 2.679887 2.224166 3.343888 12 H 5.990217 5.959926 2.702833 2.244476 1.078730 13 C 4.631701 4.502354 3.341879 2.299285 1.416719 14 H 4.142583 4.422319 4.350321 3.341754 2.224251 15 C 4.875831 4.305966 3.342265 2.297895 2.296542 16 H 4.680815 4.079224 4.350627 3.339647 3.339424 17 C 5.944038 5.108253 2.223520 1.410664 2.299637 18 H 5.989559 6.123570 4.591017 4.455578 3.630611 19 C 5.591965 5.951485 5.540155 5.284593 4.343578 20 C 5.583824 5.867574 6.411565 6.183108 5.403122 21 H 5.837407 6.700372 6.399273 5.954326 4.654759 22 H 5.947818 5.938732 6.375584 6.258679 5.706642 23 C 5.502531 6.147123 7.616947 7.269730 6.332181 24 H 5.820796 6.469449 8.526680 8.180391 7.298583 25 C 5.463568 6.396926 7.618230 7.180789 6.039408 26 H 5.733455 6.897551 8.527595 8.027045 6.809224 27 C 5.502234 6.267031 6.414479 6.009922 4.827661 28 C 2.649570 3.936220 7.712358 6.972866 5.945197 29 O 2.740215 4.259360 8.728215 7.933689 6.906772 30 C 4.270965 2.817971 4.301368 3.734390 4.065790 31 O 4.626654 2.931369 5.261485 4.762092 5.190249 32 C 5.228517 4.438521 3.349523 3.182389 3.259029 33 O 6.011718 5.260651 3.982547 4.058900 4.162009 11 12 13 14 15 11 H 0.000000 12 H 4.353868 0.000000 13 C 3.343135 2.227032 0.000000 14 H 4.355685 2.674768 1.079548 0.000000 15 C 2.241384 3.337807 1.416553 2.231172 0.000000 16 H 2.698478 4.346654 2.230198 2.690752 1.079139 17 C 1.079325 3.342380 2.300553 3.345800 1.430130 18 H 6.404799 2.927755 4.445358 4.557408 5.501695 19 C 7.115192 3.699399 4.899712 4.807052 5.995331

	20	C	7.790076	4.917808	5.849625	5.768145	6.780019
	21	H	7.859240	3.867731	4.932453	4.450781	6.284678
	22	H	7.730256	5.323796	6.233220	6.306250	6.995827
	23	C	8.824881	5.837736	6.558993	6.257234	7.557327
	24	H	9.615409	6.862819	7.458540	7.142937	8.378181
	25	C	8.857929	5.444755	6.182498	5.708642	7.346573
	26	H	9.666490	6.220395	6.815575	6.203993	8.007189
	27	C	7.843242	4.126303	5.135096	4.748868	6.384087
	28	C	7.983344	5.873115	5.445514	4.834079	6.243753
	29	O	8.785514	6.890611	6.253394	5.552966	6.968278
	30	C	3.378607	4.843820	3.804544	4.397715	3.233787
	31	O	4.019125	5.985421	4.856123	5.403320	4.130318
	32	C	4.259406	3.501000	3.835118	4.440614	4.068671
	33	O	5.205430	4.195110	4.892672	5.456799	5.191580
			16	17	18	19	20
	16	H	0.000000				
	17	C	2.241372	0.000000			
	18	H	6.400215	5.509547	0.000000		
	19	C	6.787971	6.198833	1.078975	0.000000	
	20	C	7.484904	6.967363	2.229275	1.418484	0.000000
	21	H	6.983831	6.813063	2.707024	2.245195	3.347905
	22	H	7.708800	7.016969	2.684108	2.230162	1.079288
	23	C	8.148452	7.956974	3.341879	2.300238	1.419377
	24	H	8.902837	8.793613	4.349597	3.342095	2.231218
	25	C	7.928859	7.894607	3.341447	2.298115	2.296717
	26	H	8.509034	8.680509	4.351996	3.341575	3.339702
	27	C	7.080412	6.844648	2.241898	1.429399	2.303990
	28	C	6.441608	7.132316	4.799077	4.007879	3.806557
	29	O	7.015993	7.967632	5.941727	5.127865	4.865047
	30	C	3.465190	3.196725	5.384761	5.689610	5.797048
	31	O	4.144027	4.075868	6.391468	6.629396	6.563475
	32	C	4.850239	3.711554	3.126136	3.647547	3.857169
	33	O	5.989187	4.732160	3.097494	3.596781	3.552471
			21	22	23	24	25
	21	H	0.000000				
	22	H	4.358823	0.000000			
	23	C	3.347687	2.229417	0.000000		
	24	H	4.356434	2.684476	1.078618	0.000000	
	25	C	2.229352	3.339849	1.424855	2.238821	0.000000
	26	H	2.681068	4.349352	2.235648	2.695833	1.079296
	27	C	1.078901	3.347386	2.305929	3.348358	1.418526
	28	C	4.108336	4.457896	3.216778	3.486435	3.061508
	29	O	5.019312	5.487613	4.100350	4.158119	3.901286
	30	C	6.939040	5.571137	6.669458	7.197360	7.073419
	31	O	7.953034	6.234199	7.372907	7.773735	7.892528
	32	C	5.340100	3.551768	5.069798	5.760139	5.554415

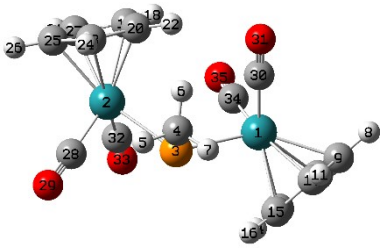
	33 O 5.594372 2.985494 4.878889 5.488719 5.574056 26 27 28 29 30 26 H 0.000000 27 C 2.228113 0.000000 28 C 3.191854 3.576739 0.000000 29 O 3.757706 4.575185 1.152257 0.000000 30 C 7.884157 6.514381 5.658868 6.399714 0.000000 31 O 8.675429 7.464840 6.238724 6.856658 1.142957 32 C 6.547713 4.814072 5.354091 6.397140 2.615296 33 O 6.622492 4.937547 5.780323 6.847994 3.524407 31 32 33 31 O 0.000000 32 C 3.523670 0.000000 33 O 4.249563 1.141765 0.000000
 5S. -1297.366150 31.01 C1 WBI 0.45 Charge and spin density 1 1 Ru 0.509474 2 Ru 0.326225 3 P -0.107981 4 C 0.020109 9 C -0.023723 10 C 0.033626 13 C -0.059105 15 C -0.009156 17 C -0.002594 19 C -0.025831 20 C 0.016363 23 C -0.010887 25 C 0.026156 27 C -0.059291 28 C -0.040815 29 O -0.173202 30 C -0.100102 31 O -0.132275 32 C -0.044555	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.813798 0.000000 3 P 3.895212 2.162955 0.000000 4 C 4.551952 3.437215 1.841426 0.000000 5 H 5.008542 4.261527 2.415602 1.093476 0.000000 6 H 5.482792 3.953656 2.398577 1.096745 1.755686 7 H 4.167129 3.506204 2.524142 1.089043 1.783847 8 H 2.996067 4.447293 5.415833 5.131658 5.725872 9 C 2.264216 4.159195 5.371208 5.431766 6.008415 10 C 2.287474 3.659976 5.352933 5.806261 6.520307 11 H 2.948408 5.592610 6.311565 6.262347 6.478412 12 H 3.016954 3.501142 5.361287 5.836391 6.682679 13 C 2.264480 4.111126 5.822801 6.553526 7.153876 14 H 3.007168 4.378781 6.252138 7.207590 7.842074 15 C 2.230596 4.808538 6.124197 6.677934 7.088158 16 H 2.952684 5.554769 6.766571 7.413257 7.721087 17 C 2.230189 4.833372 5.864622 6.026215 6.400157 18 H 5.497448 2.921793 4.170196 5.218328 6.213081 19 C 4.733980 2.209228 3.715315 5.035853 5.958610 20 C 4.799268 2.260399 3.149463 4.794500 5.540267 21 H 4.300610 3.032887 5.140489 6.251467 7.189971 22 H 5.571130 2.959310 3.119130 4.715650 5.379583 23 C 4.115131 2.321357 3.456723 5.219595 5.834891 24 H 4.409690 3.051618 3.694387 5.515357 5.950664 25 C 3.572790 2.338169 4.163280 5.712783 6.432122 26 H 3.404378 3.076172 4.875873 6.369866 7.014003 27 C 4.049838 2.311740 4.331074 5.648383 6.537785 28 C 3.085005 1.816471 2.859525 3.088939 4.075472 29 O 3.770007 2.968672 3.727886 3.414469 4.390805 30 C 1.846799 3.350728 3.280840 3.454216 3.582302 31 O 2.990682 4.157855 3.485618 3.243525 3.035202

33 O -0.142437	32 C 1.845055 3.159106 3.951098 5.123938 5.398886 33 O 2.991303 3.878767 4.450962 5.801621 5.968899 6 7 8 9 10 6 H 0.000000 7 H 1.777764 0.000000 8 H 5.834563 4.203117 0.000000 9 C 6.221633 4.639736 1.078716 0.000000 10 C 6.512400 5.171643 2.226884 1.416283 0.000000 11 H 7.233930 5.529513 2.703346 2.239286 3.338995 12 H 6.386862 5.228911 2.674173 2.223118 1.078456 13 C 7.357997 6.053846 3.339853 2.299014 1.415746 14 H 7.964986 6.813071 4.347950 3.341444 2.229793 15 C 7.607884 6.137645 3.346070 2.302551 2.298089 16 H 8.390093 6.947323 4.356803 3.345977 3.341092 17 C 6.955168 5.324995 2.243400 1.427606 2.295825 18 H 5.116034 5.382666 6.353272 6.226002 5.376064 19 C 5.142348 5.229163 6.036450 5.753953 4.855374 20 C 4.967779 5.239208 6.643558 6.293406 5.527624 21 H 6.565646 6.087068 5.230304 4.761284 3.511494 22 H 4.726263 5.347943 7.371321 7.110122 6.461667 23 C 5.654882 5.585670 6.443474 5.891984 5.084211 24 H 6.026342 5.984510 7.027018 6.423170 5.726504 25 C 6.216329 5.816547 5.706304 5.048518 4.017321 26 H 6.991375 6.386520 5.705836 4.889915 3.812928 27 C 5.972596 5.650209 5.464492 4.985338 3.871102 28 C 3.501189 2.651560 3.259497 3.385863 3.223503 29 O 3.686081 2.697706 2.911483 3.381512 3.470004 30 C 4.524742 3.127417 3.495038 3.238304 3.837073 31 O 4.331800 2.992835 4.180638 4.126502 4.896906 32 C 6.061013 5.111337 4.839386 4.061874 3.818110 33 O 6.707327 5.953708 5.983759 5.187188 4.874399 11 12 13 14 15 11 H 0.000000 12 H 4.346941 0.000000 13 C 3.343364 2.227293 0.000000 14 H 4.352263 2.686227 1.079077 0.000000 15 C 2.227355 3.341483 1.428785 2.240298 0.000000 16 H 2.682969 4.351676 2.241182 2.699093 1.079180 17 C 1.079356 3.337454 2.299741 3.342058 1.416059 18 H 8.109214 4.644849 5.995481 5.934897 7.101852 19 C 7.491469 4.274948 5.276656 5.163150 6.344460 20 C 7.712545 5.180938 5.729901 5.615192 6.597178 21 H 6.662181 2.785296 3.842679 3.536790 5.175992 22 H 8.455573 6.121683 6.716230 6.654374 7.499633 23 C 7.055831 4.959867 4.955787 4.742513 5.727578 24 H 7.284104 5.762056 5.417146 5.200337 5.986362

	25 C 6.388764 3.845527 3.818136 3.473101 4.807411 26 H 6.014828 3.842771 3.249864 2.722668 4.193218 27 C 6.718899 3.333848 4.096150 3.836619 5.286055 28 C 5.142051 2.911472 4.234678 4.793369 4.879495 29 O 5.223916 3.085089 4.712154 5.380185 5.293398 30 C 3.231760 4.482795 4.047718 4.843760 3.630904 31 O 3.792061 5.519042 5.159629 5.977442 4.615426 32 C 4.247831 4.436480 3.244749 3.496474 3.157070 33 O 5.195648 5.452732 4.139976 4.177095 4.026677 16 17 18 19 20 16 H 0.000000 17 C 2.228675 0.000000 18 H 7.907228 7.221877 0.000000 19 C 7.073024 6.594134 1.079109 0.000000 20 C 7.185504 6.905769 2.238962 1.428410 0.000000 21 H 5.932602 5.625108 2.694110 2.236214 3.348563 22 H 8.074858 7.719754 2.692564 2.237454 1.078933 23 C 6.162907 6.249597 3.338293 2.297329 1.408882 24 H 6.261566 6.570786 4.350872 3.342690 2.226083 25 C 5.303242 5.461092 3.328487 2.285687 2.288942 26 H 4.542254 5.079329 4.340037 3.329723 3.327710 27 C 5.979975 5.736126 2.238828 1.426444 2.306039 28 C 5.833219 4.451488 3.403297 3.201041 3.777630 29 O 6.315990 4.623218 4.075841 4.103291 4.830464 30 C 4.165970 3.091253 6.218649 5.552608 5.348015 31 O 5.060311 3.924487 6.957803 6.357182 6.037879 32 C 3.332577 3.694453 5.824307 4.856299 4.441939 33 O 3.953304 4.715751 6.345315 5.314986 4.651868 21 22 23 24 25 21 H 0.000000 22 H 4.356845 0.000000 23 C 3.347936 2.222497 0.000000 24 H 4.353570 2.685422 1.078882 0.000000 25 C 2.224356 3.333934 1.427288 2.237849 0.000000 26 H 2.682005 4.338754 2.230695 2.682464 1.078291 27 C 1.078972 3.348060 2.303289 3.342793 1.406017 28 C 3.516425 4.338894 4.099762 4.867237 3.819410 29 O 4.194569 5.332715 5.235541 6.019929 4.871465 30 C 5.721669 5.827522 4.863439 4.958506 4.813469 31 O 6.753065 6.351704 5.656650 5.649888 5.798608 32 C 4.779456 5.138578 3.366717 3.230218 3.184656 33 O 5.407231 5.254747 3.412948 2.932658 3.489560 26 27 28 29 30 26 H 0.000000 27 C 2.218325 0.000000 28 C 4.420300 3.294077 0.000000

	29	O	5.418267	4.194421	1.153010	0.000000
	30	C	4.864387	5.287913	3.418775	3.969999	0.000000
	31	O	5.912977	6.264873	4.116525	4.536599	1.146864
	32	C	2.855559	4.225404	4.261026	5.200786	2.585122
	33	O	3.089250	4.744471	5.225923	6.230241	3.496840
			31	32	33		
	31	O	0.000000				
	32	C	3.495733	0.000000			
	33	O	4.219728	1.147463	0.000000		

Table S6. Distance matrix for the lowest energy $MePCp_2Ru_2(CO)_4$ structures as optimized at the PBE0/def2TZVP level. Included are the ranking order, spin multiplicity (S, T or Q), total energy (in a.u.), relative energy (in kcal/mol), symmetry point group Wiberg bond indices for the Fe-Fe bonds, Mulliken charges and the spin density (Cp moieties are omitted for clarity).



1S -1410.661647 0.00 C1
WBI 0.02

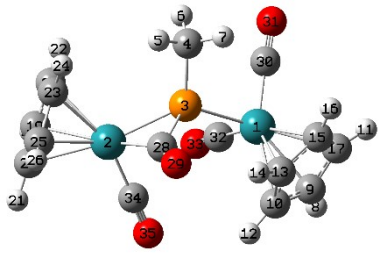
Charge densities

		1
1	Ru	0.418165
2	Ru	0.347581
3	P	-0.047391
4	C	-0.013154
9	C	-0.009422
10	C	-0.017304
13	C	-0.001942
15	C	0.076708
17	C	-0.037147
19	C	-0.018732
20	C	0.016195
23	C	-0.026712
25	C	-0.000036
27	C	-0.006075
28	C	-0.014735
29	O	-0.123181

		1	2	3	4	5
1	Ru	0.000000				
2	Ru	4.202078	0.000000			
3	P	2.451225	2.454570	0.000000		
4	C	3.431563	3.356901	1.862661	0.000000	
5	H	4.420649	3.449647	2.434245	1.093947	0.000000
6	H	3.667106	3.484658	2.540037	1.091865	1.770982
7	H	3.453488	4.368403	2.440159	1.094445	1.767822
8	H	2.991684	7.157030	5.299664	5.746560	6.797240
9	C	2.273703	6.465812	4.478596	5.109699	6.114377
10	C	2.266503	6.148566	4.360766	5.468245	6.398470
11	H	3.001274	6.505281	4.190098	4.066660	4.956009
12	H	2.980282	6.604696	5.110405	6.343142	7.278076
13	C	2.276109	5.535591	3.584405	4.860159	5.638568
14	H	3.000226	5.495567	3.809602	5.329465	5.977035
15	C	2.291300	5.511408	3.186988	3.999965	4.760869
16	H	2.984954	5.390726	3.008809	3.685505	4.243111
17	C	2.273007	6.082633	3.798593	4.162194	5.085689
18	H	4.514806	3.001933	4.362097	5.149183	5.682037
19	C	4.697584	2.272917	3.992494	4.582825	4.955122
20	C	4.432126	2.279237	3.497595	3.534249	3.891685
21	H	6.436451	2.987088	5.334930	6.157276	6.233968
22	H	3.967156	3.008114	3.458390	3.215399	3.796557
23	C	5.390446	2.259036	3.841799	3.617650	3.557031
24	H	5.804163	2.990609	4.107586	3.403286	3.132561
25	C	6.129307	2.260619	4.502195	4.713837	4.557378
26	H	7.043340	2.976564	5.206439	5.356349	4.998979
27	C	5.767880	2.268334	4.581219	5.203830	5.298776
28	C	5.169710	1.850264	2.852098	3.535833	3.122811

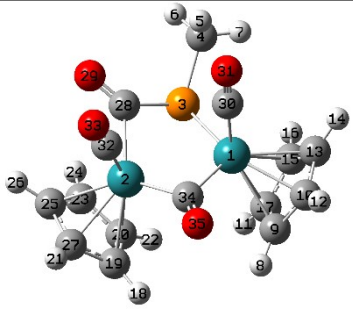
30 C -0.068962 31 O -0.150146 32 C -0.024772 33 O -0.123665 34 C -0.036297 35 O -0.138977	29 O 6.004147 2.993553 3.609762 4.098599 3.451021 30 C 1.839202 4.306574 3.049586 3.140750 4.208311 31 O 2.986973 4.775668 3.864000 3.499067 4.494386 32 C 4.163776 1.853819 2.928376 4.516857 4.730769 33 O 4.556994 2.997399 3.702160 5.442459 5.692587 34 C 1.846823 3.705867 3.104847 4.425936 5.291924 35 O 2.991299 3.907728 3.958273 5.319978 6.105308 6 7 8 9 10 6 H 0.000000 7 H 1.769353 0.000000 8 H 5.825130 5.299258 0.000000 9 C 5.359681 4.678880 1.079063 0.000000 10 C 5.837924 5.228965 2.225414 1.411158 0.000000 11 H 4.417776 3.246150 2.701139 2.241475 3.336643 12 H 6.641037 6.200498 2.679547 2.222619 1.079633 13 C 5.465488 4.641074 3.346991 2.303136 1.429238 14 H 6.016277 5.243096 4.356398 3.345520 2.244089 15 C 4.686084 3.538380 3.343143 2.300454 2.294741 16 H 4.555334 3.183941 4.354253 3.344288 3.336620 17 C 4.585372 3.544418 2.242862 1.429997 2.293898 18 H 4.744723 6.008401 6.854684 6.531219 6.245100 19 C 4.172068 5.546774 7.260877 6.856232 6.644483 20 C 2.939054 4.504866 6.945894 6.558768 6.607456 21 H 5.957530 7.199250 9.161669 8.640605 8.167927 22 H 2.419979 4.024584 6.199375 5.917930 6.164727 23 C 3.153077 4.682005 8.044082 7.560876 7.597074 24 H 2.899083 4.406481 8.351696 7.872671 8.049548 25 C 4.440662 5.806677 8.928986 8.383378 8.200829 26 H 5.175613 6.444091 9.897111 9.303141 9.087658 27 C 4.930199 6.256804 8.506339 8.001993 7.675118 28 C 4.048353 4.445056 8.115533 7.280579 6.945164 29 O 4.742939 4.876400 8.877472 7.988521 7.653775 30 C 2.804870 3.259199 3.459432 3.242220 3.784312 31 O 2.819644 3.650145 4.132664 4.138607 4.834663 32 C 4.881188 5.323182 7.058927 6.265068 5.558736 33 O 5.882389 6.138952 7.261496 6.435311 5.508060 34 C 4.466471 4.825820 4.125846 3.623122 3.115758 35 O 5.275979 5.841522 5.005781 4.604523 3.961649 11 12 13 14 15 11 H 0.000000 12 H 4.347969 0.000000 13 C 3.338107 2.239373 0.000000 14 H 4.345940 2.701241 1.078782 0.000000 15 C 2.227258 3.337618 1.415364 2.228009 0.000000 16 H 2.684894 4.345590 2.221868 2.675794 1.079017 17 C 1.079426 3.338409 2.295585 3.337497 1.414271

	18	H	7.243215	6.325730	6.296024	6.431859	6.619574
	19	C	7.252333	6.875217	6.506453	6.631961	6.649443
	20	C	6.545500	7.031764	6.422757	6.709503	6.264112
	21	H	9.113481	8.296243	7.830546	7.669142	8.133641
	22	H	5.822563	6.638994	6.125520	6.577642	5.858034
	23	C	7.257216	8.108061	7.193888	7.388952	6.904240
	24	H	7.258405	8.665802	7.589574	7.849402	7.104961
	25	C	8.302040	8.600481	7.726828	7.736664	7.633292
	26	H	9.119769	9.509106	8.506032	8.441049	8.380237
	27	C	8.298982	7.912536	7.341842	7.301844	7.492113
	28	C	6.947351	7.537660	6.000672	5.814565	5.779911
	29	O	7.468846	8.300124	6.572601	6.317946	6.255523
	30	C	3.400406	4.380196	4.065494	4.837657	3.751960
	31	O	4.058207	5.377670	5.196163	5.985196	4.793541
	32	C	6.767735	5.828243	4.856366	4.501249	5.252173
	33	O	7.191843	5.630179	4.786388	4.216503	5.438028
	34	C	4.822122	3.242278	3.299563	3.580697	3.884407
	35	O	5.951387	3.817758	4.212512	4.307862	4.959682
			16	17	18	19	20
	16	H	0.000000				
	17	C	2.227294	0.000000			
	18	H	6.967859	6.741483	0.000000		
	19	C	6.839518	6.843110	1.078698	0.000000	
	20	C	6.362813	6.328526	2.228895	1.414893	0.000000
	21	H	8.188561	8.605602	2.695749	2.240015	3.340983
	22	H	6.045754	5.703281	2.684041	2.225471	1.077894
	23	C	6.787554	7.118627	3.339109	2.296280	1.417488
	24	H	6.880786	7.268254	4.347987	3.338621	2.230622
	25	C	7.499903	8.026848	3.338284	2.297042	2.298286
	26	H	8.140706	8.864563	4.349184	3.341440	3.341206
	27	C	7.527814	7.877678	2.239136	1.428759	2.298541
	28	C	5.318432	6.603249	4.841002	4.056795	3.833667
	29	O	5.624365	7.179204	5.979018	5.175834	4.890957
	30	C	4.292410	3.201068	4.080311	4.189476	3.578675
	31	O	5.272685	4.091956	4.236384	4.290564	3.492184
	32	C	5.223757	6.085895	3.472807	3.246601	3.805532
	33	O	5.467652	6.387980	4.164422	4.152905	4.862673
	34	C	4.517699	4.046012	3.143923	3.633185	3.921213
	35	O	5.575155	5.159374	2.661234	3.398857	4.077254
			21	22	23	24	25
	21	H	0.000000				
	22	H	4.350102	0.000000			
	23	C	3.343229	2.226388	0.000000		
	24	H	4.352094	2.683134	1.078959	0.000000	
	25	C	2.224222	3.340301	1.428880	2.241695	0.000000
	26	H	2.680114	4.349778	2.239682	2.698683	1.079536

	27 C 1.079237 3.340979 2.299145 3.341183 1.410853 28 C 4.200770 4.480679 3.234747 3.488644 3.123867 29 O 5.128484 5.503531 4.130065 4.174512 3.983412 30 C 6.298012 2.758945 4.676494 4.984809 5.694285 31 O 6.509232 2.475956 4.595564 4.803461 5.746362 32 C 3.385957 4.416997 4.063824 4.843368 3.734741 33 O 4.039687 5.426522 5.191896 5.986090 4.768285 34 C 5.183099 3.737863 5.054378 5.772125 5.461206 35 O 4.677510 4.082549 5.241004 6.104437 5.404104 26 27 28 29 30 26 H 0.000000 27 C 2.223844 0.000000 28 C 3.266748 3.664983 0.000000 29 O 3.869117 4.672727 1.143755 0.000000 30 C 6.686729 5.456549 5.534449 6.458987 0.000000 31 O 6.747726 5.600191 6.069077 7.004523 1.148072 32 C 4.296415 3.204433 2.612129 3.526119 4.929769 33 O 5.261124 4.093711 3.514457 4.243420 5.609536 34 C 6.425788 4.715440 5.104221 6.109042 2.604376 35 O 6.361357 4.407182 5.457666 6.509558 3.515402 31 32 33 34 35 31 O 0.000000 32 C 5.686657 0.000000 33 O 6.467167 1.143773 0.000000 34 C 3.516554 3.329094 3.604650 0.000000 35 O 4.241724 3.325179 3.457642 1.145918 0.000000
 2S -1410.643481 11.4 C1 WBI 0.04 Charge densities 1 1 Ru 0.303141 2 Ru 0.494750 3 P 0.056128 4 C -0.003370 9 C 0.009567 10 C -0.000651 13 C 0.116850	1 2 3 4 5 1 Ru 0.000000 2 Ru 4.276910 0.000000 3 P 2.374708 2.328655 0.000000 4 C 3.526801 3.517893 1.835987 0.000000 5 H 4.460518 3.407814 2.414794 1.091493 0.000000 6 H 3.841638 3.986117 2.447016 1.091891 1.771729 7 H 3.551804 4.402496 2.449214 1.091841 1.779046 8 H 2.966388 6.427618 5.117580 6.472945 7.354796 9 C 2.247635 5.859841 4.358916 5.633896 6.494520 10 C 2.259309 4.877151 3.655919 5.110355 5.798950 11 H 2.972922 7.200757 5.184223 5.824950 6.818510 12 H 2.985317 4.627790 3.945028 5.592989 6.160198 13 C 2.287380 4.804903 3.227427 4.314803 4.954795 14 H 2.999075 4.439429 3.114357 4.094447 4.517495 15 C 2.265478 5.726493 3.733623 4.390247 5.205475 16 H 3.002759 6.211544 4.092000 4.295334 5.071181 17 C 2.249743 6.313992 4.398257 5.246171 6.176808 18 H 6.277537 3.050997 4.784852 5.674945 5.588341 19 C 6.066074 2.314634 4.263422 5.049570 4.810800

15 C -0.016963 17 C -0.003203 19 C -0.025201 20 C 0.016949 23 C -0.100917 25 C -0.000307 27 C -0.050529 28 C 0.014348 29 O -0.292411 30 C -0.034749 31 O -0.108790 32 C 0.021809 33 O -0.092793 34 C -0.130451 35 O -0.173206	20 C 5.823775 2.297772 3.747118 4.050320 3.680492 21 H 6.920379 2.953249 5.264325 6.380025 6.056508 22 H 5.818349 3.024285 3.871392 3.856399 3.599197 23 C 6.071011 2.247610 3.765374 3.917267 3.245378 24 H 6.322087 2.982881 3.950660 3.633407 2.741672 25 C 6.444410 2.225491 4.289905 4.885185 4.284090 26 H 6.976297 2.942870 4.850188 5.410934 4.722035 27 C 6.414235 2.235445 4.541863 5.468117 5.094096 28 C 3.673531 1.963142 1.867680 2.971328 2.912098 29 O 4.319157 3.033625 2.866944 3.678070 3.509821 30 C 1.857252 5.118100 3.005998 3.243861 4.329810 31 O 2.999538 5.898115 3.835296 3.597725 4.658599 32 C 1.863441 4.074475 2.973289 4.348663 5.194739 33 O 3.002400 4.376960 3.785965 5.144257 5.912972 34 C 3.926665 1.842204 2.982457 4.692029 4.876177 35 O 4.161458 2.994065 3.828578 5.628454 5.913503 6 7 8 9 10 6 H 0.000000 7 H 1.776841 0.000000 8 H 6.794567 6.400273 0.000000 9 C 6.058392 5.478685 1.079470 0.000000 10 C 5.732265 5.045116 2.240433 1.429798 0.000000 11 H 6.075804 5.355874 2.682039 2.225861 3.345241 12 H 6.238345 5.686961 2.701035 2.243777 1.079337 13 C 5.080180 4.035895 3.342804 2.300116 1.418189 14 H 5.017589 3.840093 4.353129 3.344401 2.227358 15 C 4.992265 3.862761 3.344042 2.299498 2.297257 16 H 4.902663 3.536027 4.353077 3.341623 3.339568 17 C 5.639594 4.850981 2.225689 1.412698 2.301126 18 H 5.588740 6.728923 8.081814 7.842717 7.163711 19 C 5.099976 6.101805 8.087427 7.713041 6.898794 20 C 4.032663 5.126524 8.239804 7.730020 6.950183 21 H 6.738130 7.302358 8.444146 8.097168 7.037129 22 H 3.555993 4.940382 8.363500 7.868916 7.253259 23 C 4.213880 4.883809 8.543280 7.900591 6.938343 24 H 3.971116 4.498620 8.962499 8.227287 7.276481 25 C 5.343321 5.778031 8.574214 7.980804 6.869914 26 H 6.012855 6.182400 9.005797 8.360470 7.140352 27 C 5.781225 6.431832 8.269632 7.839038 6.817135 28 C 3.875504 3.437053 5.866113 5.053763 3.894952 29 O 4.702848 3.866426 6.238945 5.349843 4.075275 30 C 3.075816 3.178481 4.254746 3.697302 4.059552 31 O 3.133623 3.476701 5.206197 4.719087 5.181412 32 C 4.358775 4.762077 3.277486 3.132684 3.249496 33 O 5.019790 5.692309 3.898837 4.004448 4.153507 34 C 5.181477 5.385725 5.263763 4.888090 3.877740

35	O	6.112560	6.221753	4.788473	4.591902	3.634663	
		11	12	13	14	15	
11	H	0.000000					
12	H	4.355197	0.000000				
13	C	3.343370	2.230612	0.000000			
14	H	4.357290	2.680627	1.081462	0.000000		
15	C	2.243002	3.339560	1.415049	2.230503	0.000000	
16	H	2.701724	4.347859	2.227468	2.687102	1.078988	
17	C	1.079391	3.344116	2.300734	3.347431	1.431052	
18	H	9.191127	6.792158	7.451210	7.311970	8.229012	
19	C	9.033836	6.556494	7.011779	6.736632	7.839272	
20	C	8.761942	6.805483	6.802780	6.472877	7.475920	
21	H	9.785390	6.407343	7.271457	6.848504	8.392853	
22	H	8.669760	7.239340	7.069390	6.841322	7.553910	
23	C	8.948262	6.785982	6.587888	6.046608	7.360911	
24	H	9.068667	7.246099	6.721933	6.108152	7.386446	
25	C	9.322581	6.510815	6.664318	6.053754	7.657685	
26	H	9.745454	6.738621	6.852055	6.111169	7.926698	
27	C	9.346653	6.336032	6.898601	6.461129	7.918413	
28	C	6.248660	3.851630	3.374020	2.727171	4.372531	
29	O	6.514231	4.029143	3.343631	2.410762	4.426069	
30	C	3.317795	4.839822	3.816203	4.422471	3.225031	
31	O	3.942613	5.980267	4.865649	5.429103	4.116487	
32	C	4.210893	3.490508	3.852755	4.474347	4.067510	
33	O	5.144530	4.188527	4.911124	5.495519	5.186675	
34	C	6.653106	3.318746	4.302777	4.159069	5.403991	
35	O	6.585865	2.844876	4.395148	4.405379	5.541579	
		16	17	18	19	20	
16	H	0.000000					
17	C	2.242940	0.000000				
18	H	8.795325	8.459593	0.000000			
19	C	8.330737	8.245772	1.078828	0.000000		
20	C	7.800995	8.024650	2.221843	1.406208	0.000000	
21	H	8.988581	8.855359	2.700183	2.239887	3.328708	
22	H	7.812499	8.039255	2.674724	2.217060	1.079663	
23	C	7.593131	8.131509	3.344012	2.300193	1.426570	
24	H	7.465189	8.286608	4.350499	3.340551	2.238344	
25	C	8.012716	8.409692	3.356800	2.315143	2.306694	
26	H	8.244472	8.785332	4.365711	3.357531	3.350830	
27	C	8.427177	8.450845	2.244381	1.430464	2.286325	
28	C	4.731357	5.288664	5.010783	4.244756	3.918056	
29	O	4.683172	5.519446	6.069342	5.249298	4.928212	
30	C	3.464105	3.148792	6.708771	6.551449	6.025947	
31	O	4.137988	4.019768	7.234732	7.111351	6.453787	
32	C	4.857245	3.671153	5.183164	5.275333	5.333804	
33	O	5.992162	4.684771	4.778379	5.099238	5.365923	

	34 C 6.157292 5.709551 3.630141 3.330173 3.876153 35 O 6.424666 5.642911 4.356068 4.248307 4.953846 21 22 23 24 25 21 H 0.000000 22 H 4.340195 0.000000 23 C 3.332408 2.235805 0.000000 24 H 4.343166 2.691639 1.079329 0.000000 25 C 2.226129 3.348839 1.424503 2.235814 0.000000 26 H 2.683474 4.360058 2.240174 2.698880 1.078550 27 C 1.079702 3.331189 2.288999 3.332950 1.418360 28 C 4.484524 4.474766 3.352189 3.546198 3.362567 29 O 5.145762 5.533589 4.122693 4.149312 3.959246 30 C 7.888692 5.687373 6.441532 6.532876 7.167104 31 O 8.657504 5.939320 6.943173 6.942566 7.829140 32 C 6.265352 5.287963 5.967044 6.476640 6.275419 33 O 6.132721 5.296579 6.208577 6.847530 6.461759 34 C 3.210094 4.542592 4.020201 4.802318 3.580875 35 O 3.816633 5.593820 5.148417 5.944784 4.590750 26 27 28 29 30 26 H 0.000000 27 C 2.232838 0.000000 28 C 3.555596 3.909026 0.000000 29 O 3.827656 4.686616 1.191726 0.000000 30 C 7.825297 7.203889 4.745442 5.489190 0.000000 31 O 8.534985 7.899269 5.629725 6.386183 1.142678 32 C 6.996113 5.854336 4.329674 5.251794 2.627614 33 O 7.267176 5.807690 5.051078 6.048952 3.530794 34 C 4.080037 3.082163 2.619426 3.456655 5.258288 35 O 4.993768 3.953891 3.499214 4.142275 5.685866 31 32 33 34 35 31 O 0.000000 32 C 3.537479 0.000000 33 O 4.258036 1.139141 0.000000 34 C 6.231721 3.457891 3.653171 0.000000 35 O 6.721761 3.564601 3.652360 1.152128 0.000000
 3S -1410.629176 20.4 C1 WBI 0.32	1 2 3 4 5 1 Ru 0.000000 2 Ru 2.866983 0.000000 3 P 2.394413 3.015917 0.000000 4 C 3.516070 4.544319 1.851914 0.000000 5 H 3.641185 4.631560 2.496533 1.090294 0.000000 6 H 4.471719 5.043442 2.421737 1.092549 1.774560 7 H 3.713975 5.294384 2.437382 1.092368 1.777915 8 H 2.987787 4.218278 4.940091 6.370083 6.619367 9 C 2.271144 4.176948 4.242293 5.521186 5.803648 10 C 2.244380 4.752995 4.454353 5.311418 5.404602

Charges and spin densities

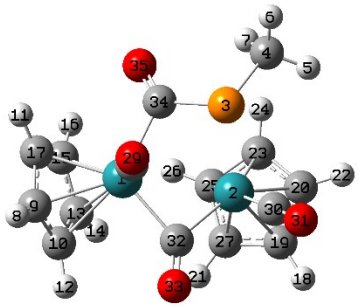
	1
1 Ru	0.231741
2 Ru	0.287587
3 P	0.000378
4 C	0.005154
9 C	0.013966
10 C	0.035419
13 C	-0.005399
15 C	0.025591
17 C	-0.007771
19 C	-0.002894
20 C	0.029911
23 C	0.017205
25 C	0.019550
27 C	0.027262
28 C	0.118660
29 O	-0.269763
30 C	-0.033938
31 O	-0.127427
32 C	-0.019769
33 O	-0.110484
34 C	-0.032170
35 O	-0.202812

11 H	3.028538	4.243466	3.643626	5.147445	5.809375
12 H	2.962560	5.262490	5.288997	6.030269	5.956448
13 C	2.226326	5.067788	3.856512	4.368145	4.562997
14 H	2.944622	5.801810	4.319233	4.377775	4.436947
15 C	2.264322	4.753415	3.188872	3.997018	4.513849
16 H	2.984816	5.256415	3.100308	3.624361	4.320818
17 C	2.286504	4.173066	3.470354	4.793277	5.317281
18 H	4.370591	3.030944	5.306554	7.079541	7.339052
19 C	4.208397	2.309214	4.682629	6.463390	6.749434
20 C	3.907500	2.310630	3.780464	5.612575	6.090853
21 H	5.496413	2.950682	5.911514	7.451655	7.475225
22 H	3.838038	3.052686	3.732376	5.567647	6.182681
23 C	4.459184	2.290462	3.659995	5.324705	5.773889
24 H	4.824361	3.006629	3.476694	4.981632	5.552971
25 C	4.961410	2.204669	4.465497	5.991540	6.210977
26 H	5.710992	2.914962	4.980154	6.290729	6.425964
27 C	4.841253	2.241670	5.040791	6.670394	6.816817
28 C	3.171312	2.098327	1.795221	2.840232	2.988270
29 O	4.304040	2.958065	2.752619	3.244200	3.242528
30 C	1.838842	3.487467	2.982490	3.243588	2.796845
31 O	2.984076	4.275689	3.792107	3.582353	2.810266
32 C	3.735180	1.848389	3.974587	4.932650	4.611394
33 O	4.602250	2.989443	4.857107	5.513787	4.996557
34 C	2.040640	2.002189	3.701637	5.010435	4.922101
35 O	2.965653	2.964887	4.857869	6.087749	5.909795

	6	7	8	9	10
6 H	0.000000				
7 H	1.772305	0.000000			
8 H	7.252101	6.413881	0.000000		
9 C	6.440829	5.458266	1.079549	0.000000	
10 C	6.343507	5.128561	2.222369	1.416643	0.000000
11 H	5.798476	5.073675	2.695459	2.235426	3.346868
12 H	7.094358	5.880031	2.676945	2.230385	1.078822
13 C	5.396083	3.969037	3.334226	2.291891	1.427384
14 H	5.420429	3.829542	4.344296	3.335633	2.238730
15 C	4.879038	3.602019	3.335885	2.291550	2.302975
16 H	4.375264	3.048931	4.346089	3.334793	3.346545
17 C	5.602016	4.650600	2.231171	1.418734	2.304383
18 H	7.649540	7.568465	3.288904	3.967906	5.103505
19 C	6.923616	7.055351	3.871485	4.318472	5.395422
20 C	5.961177	6.165641	4.086790	4.237066	5.346278
21 H	7.837377	8.239736	5.525918	6.018020	6.819907
22 H	5.945816	5.947852	3.769409	3.824033	5.033429
23 C	5.453614	6.059309	5.320591	5.339901	6.272036
24 H	4.917983	5.716383	6.004887	5.870819	6.742921
25 C	6.148076	6.843895	5.787081	5.945401	6.776229

26	H	6.314849	7.236224	6.790824	6.907740	7.640307	
27	C	7.025369	7.430940	5.027241	5.414234	6.303209	
28	C	3.094057	3.799047	5.559435	5.132336	5.413416	
29	O	3.165273	4.314843	6.725761	6.319552	6.544144	
30	C	4.240144	3.584362	4.507494	3.859137	3.265693	
31	O	4.498404	3.953388	5.548464	4.928434	4.174735	
32	C	5.415905	5.808892	5.424000	5.367497	5.552704	
33	O	5.958988	6.415972	6.339839	6.285557	6.302471	
34	C	5.830904	5.490632	2.917485	2.928365	3.213968	
35	O	6.945668	6.517520	2.947586	3.244143	3.427489	
		11	12	13	14	15	
11	H	0.000000					
12	H	4.355585	0.000000				
13	C	3.339331	2.242953	0.000000			
14	H	4.348059	2.702009	1.079524	0.000000		
15	C	2.230717	3.346528	1.417012	2.228800	0.000000	
16	H	2.684216	4.357356	2.229578	2.684665	1.079374	
17	C	1.078007	3.346375	2.298725	3.341604	1.421275	
18	H	4.081097	5.515934	5.952435	6.948570	5.563648	
19	C	4.103261	5.908926	6.036102	6.992180	5.529644	
20	C	3.354122	6.075228	5.668416	6.613343	4.880166	
21	H	6.205948	7.088873	7.544027	8.372097	7.289925	
22	H	2.489737	5.875319	5.255025	6.239053	4.291876	
23	C	4.408454	6.994366	6.412978	7.242160	5.620993	
24	H	4.651371	7.549121	6.663319	7.424315	5.742210	
25	C	5.464588	7.327051	7.092000	7.882767	6.528295	
26	H	6.446385	8.155873	7.890732	8.606348	7.364599	
27	C	5.317630	6.721523	6.897758	7.757502	6.490697	
28	C	4.793186	6.056019	5.163980	5.639826	4.723107	
29	O	5.940992	7.134508	6.246528	6.621870	5.836605	
30	C	4.844204	3.529274	3.085083	3.215726	3.629402	
31	O	5.980602	4.240054	3.947848	3.814539	4.632974	
32	C	5.892010	5.787179	5.884248	6.387582	5.925712	
33	O	6.975458	6.394578	6.635760	7.014038	6.831418	
34	C	4.039848	3.461086	3.925386	4.654442	4.106103	
35	O	4.758202	3.341777	4.447402	5.141091	4.851559	
		16	17	18	19	20	
16	H	0.000000					
17	C	2.231780	0.000000				
18	H	6.299905	4.325569	0.000000			
19	C	6.135904	4.414947	1.079437	0.000000		
20	C	5.277493	3.868309	2.239604	1.427091	0.000000	
21	H	7.919676	6.341936	2.678744	2.223031	3.338363	
22	H	4.627889	3.212621	2.697750	2.238632	1.078332	
23	C	5.848641	4.866618	3.345328	2.303416	1.412861	
24	H	5.768934	5.168396	4.354475	3.346427	2.225755	

25	C	6.881834	5.765650	3.343358	2.298647	2.288834	
26	H	7.653993	6.714673	4.352361	3.340544	3.331617	
27	C	7.046120	5.542403	2.219757	1.407311	2.293061	
28	C	4.831667	4.691669	4.984750	4.161467	3.531571	
29	O	5.849072	5.874936	5.876182	4.967208	4.381625	
30	C	4.139085	4.057697	5.649322	5.393512	5.248884	
31	O	5.052435	5.177966	6.599300	6.315231	6.235545	
32	C	6.441111	5.604920	4.369689	3.776587	4.093610	
33	O	7.342340	6.614830	5.337217	4.799945	5.208844	
34	C	4.927892	3.547702	3.126799	3.084748	3.491995	
35	O	5.781754	4.215923	3.261093	3.527636	4.273475	
		21	22	23	24	25	
21	H	0.000000					
22	H	4.346930	0.000000				
23	C	3.350109	2.219864	0.000000			
24	H	4.361638	2.673683	1.079034	0.000000		
25	C	2.246104	3.329797	1.419819	2.232910	0.000000	
26	H	2.705163	4.338466	2.231338	2.689464	1.079173	
27	C	1.079240	3.334417	2.308386	3.352935	1.436378	
28	C	4.759094	3.982699	2.922679	2.878578	3.235201	
29	O	5.168021	4.935257	3.453743	3.233304	3.518496	
30	C	6.080882	5.416884	5.444240	5.746069	5.628024	
31	O	6.710539	6.485137	6.283424	6.546529	6.317357	
32	C	3.310927	4.898853	3.774430	4.366940	3.115306	
33	O	3.935252	6.037362	4.804893	5.345636	3.987476	
34	C	3.827354	3.877602	4.078871	4.824354	4.032498	
35	O	3.955035	4.673171	4.972020	5.820198	4.738756	
		26	27	28	29	30	
26	H	0.000000					
27	C	2.248397	0.000000				
28	C	3.493042	4.011275	0.000000			
29	O	3.402980	4.526904	1.195695	0.000000		
30	C	6.114665	5.621292	3.267961	4.073691	0.000000	
31	O	6.653807	6.362597	3.836325	4.372136	1.145739	
32	C	3.279780	3.146799	2.603478	2.921870	3.400028	
33	O	3.912674	4.012823	3.429650	3.447869	3.865427	
34	C	4.781780	3.461445	3.471029	4.457422	2.670742	
35	O	5.468205	3.869489	4.584249	5.495874	3.391033	
		31	32	33	34	35	
31	O	0.000000					
32	C	3.711207	0.000000				
33	O	3.845242	1.141783	0.000000			
34	C	3.536929	2.573188	3.429104	0.000000		
35	O	4.086125	3.181325	3.800952	1.172710	0.000000	



4S -1410.621176 25.40 C1
WBI 0.32

Charges and spin densities

		1
1	Ru	0.284005
2	Ru	0.127838
3	P	0.030399
4	C	-0.027386
9	C	0.008262
10	C	0.037465
13	C	-0.027731
15	C	0.041564
17	C	-0.000452
19	C	0.030472
20	C	-0.041876
23	C	0.058662
25	C	0.025493
27	C	0.002969
28	C	-0.020575
29	O	-0.114566
30	C	0.028796
31	O	-0.121138
32	C	0.004105
33	O	-0.199136
34	C	0.193387
35	O	-0.320556

		1	2	3	4	5
1	Ru	0.000000				
2	Ru	2.827048	0.000000			
3	P	3.121165	2.439586	0.000000		
4	C	4.678444	3.512384	1.853588	0.000000	
5	H	5.303629	3.542932	2.466565	1.091485	0.000000
6	H	5.337224	4.471289	2.423677	1.092659	1.766551
7	H	4.722009	3.785888	2.470520	1.091506	1.789783
8	H	2.962298	5.629754	5.798748	7.436931	8.157758
9	C	2.254841	4.950351	5.277461	6.807659	7.516073
10	C	2.320778	4.435520	5.405161	6.874212	7.427026
11	H	2.921695	5.580520	5.032795	6.206976	7.134306
12	H	3.030452	4.707463	5.985367	7.522093	7.968419
13	C	2.307935	4.017540	5.042831	6.218314	6.762690
14	H	3.051415	3.995292	5.410961	6.409158	6.818074
15	C	2.277801	4.379070	4.707835	5.741396	6.466772
16	H	2.960409	4.605448	4.731210	5.427468	6.179334
17	C	2.216589	4.912511	4.831380	6.109171	6.932257
18	H	5.376849	2.932863	5.181338	5.755876	5.283754
19	C	4.694306	2.217071	4.462030	4.949715	4.572353
20	C	4.877566	2.212208	3.794744	3.812105	3.302250
21	H	4.059145	2.973448	5.275569	6.126369	6.093180
22	H	5.694406	2.944462	4.079366	3.801700	3.023520
23	C	4.312012	2.280462	3.450983	3.325091	3.147538
24	H	4.715379	3.009504	3.402519	2.759668	2.656067
25	C	3.662294	2.294348	3.940475	4.303003	4.355067
26	H	3.540585	3.037762	4.300247	4.664150	4.919711
27	C	3.940415	2.251818	4.524148	5.180349	5.076660
28	C	1.851821	3.614000	3.031979	4.827577	5.489781
29	O	2.990330	4.496566	3.610848	5.364437	6.015114
30	C	3.851439	1.841976	2.802837	4.005001	3.827093
31	O	4.768910	2.984434	3.553020	4.674743	4.399965
32	C	2.024002	2.032185	3.519587	5.115166	5.359908
33	O	2.973344	2.986423	4.585740	6.198575	6.360205
34	C	2.094822	2.883726	1.810360	2.874993	3.727359
35	O	2.947222	3.864870	2.739339	3.163480	4.119469

		6	7	8	9	10
6	H	0.000000				
7	H	1.769376	0.000000			
8	H	7.902512	7.476934	0.000000		
9	C	7.365101	6.740247	1.079706	0.000000	
10	C	7.602458	6.771151	2.219162	1.405183	0.000000
11	H	6.544744	5.966020	2.703995	2.247621	3.341608
12	H	8.289109	7.503634	2.674361	2.218234	1.079103
13	C	7.024206	5.926670	3.333155	2.287770	1.426764
14	H	7.316298	6.056296	4.338883	3.327548	2.232618

15	C	6.411797	5.342207	3.344872	2.302510	2.303257
16	H	6.083596	4.847766	4.350429	3.342664	3.348686
17	C	6.610728	5.878575	2.243694	1.434244	2.299953
18	H	6.757101	5.994925	7.757290	7.092783	6.130062
19	C	5.997842	5.066813	7.265023	6.510417	5.602004
20	C	4.857121	3.915754	7.719312	6.935132	6.238300
21	H	7.175469	6.022502	6.059774	5.233277	4.039083
22	H	4.739597	4.064793	8.563637	7.831938	7.209938
23	C	4.412925	3.066889	7.195410	6.309088	5.701132
24	H	3.786507	2.260351	7.616913	6.724250	6.287577
25	C	5.371724	3.971521	6.316082	5.364820	4.575123
26	H	5.667638	4.142716	5.975987	4.949909	4.214048
27	C	6.250514	5.084026	6.363209	5.509906	4.496412
28	C	5.189061	5.201510	3.116305	3.027026	3.611530
29	O	5.536970	5.876894	3.595673	3.805417	4.543149
30	C	4.717994	4.694063	6.269399	5.864218	5.509429
31	O	5.220394	5.506484	6.921624	6.657580	6.375413
32	C	5.910341	5.402215	4.049154	3.563081	3.001528
33	O	6.976507	6.537807	4.237863	3.942144	3.247460
34	C	3.447325	2.792821	4.688813	3.999490	4.244445
35	O	3.608460	2.702301	5.190949	4.435924	4.765717

		11	12	13	14	15
11	H	0.000000				
12	H	4.352370	0.000000			
13	C	3.331176	2.239918	0.000000		
14	H	4.342066	2.689632	1.079103	0.000000	
15	C	2.230242	3.345039	1.412483	2.226152	0.000000
16	H	2.673749	4.358040	2.232733	2.695868	1.078620
17	C	1.078938	3.343722	2.288337	3.332273	1.417873
18	H	8.184162	5.963016	5.741367	5.229751	6.579937
19	C	7.394995	5.611327	5.028033	4.520361	5.738694
20	C	7.401396	6.458138	5.511432	5.114112	5.895543
21	H	6.464573	3.933658	3.456087	2.723778	4.533752
22	H	8.211510	7.418338	6.534557	6.181285	6.847533
23	C	6.472907	6.127745	4.744040	4.375425	4.902186
24	H	6.525189	6.845388	5.253625	4.984065	5.131215
25	C	5.791603	4.973034	3.537729	3.024219	3.931694
26	H	5.186244	4.767989	2.962469	2.444458	3.191697
27	C	6.438219	4.577299	3.771215	3.151902	4.578545
28	C	3.445833	4.104389	4.054684	4.861361	3.863495
29	O	4.111990	4.935322	5.137813	5.972215	4.908572
30	C	6.631013	5.582880	5.477744	5.581387	5.858215
31	O	7.472809	6.354326	6.496517	6.638267	6.885196
32	C	4.884480	3.021937	3.236961	3.497629	3.918356
33	O	5.631184	2.866164	3.811028	4.002814	4.716345
34	C	3.422596	5.057519	3.698841	4.217499	3.045860

35	O	3.305656	5.702393	4.000340	4.493364	3.012743	
		16	17	18	19	20	
16	H	0.000000					
17	C	2.220960	0.000000				
18	H	6.815864	7.337381	0.000000			
19	C	5.873220	6.582193	1.079166	0.000000		
20	C	5.821383	6.742255	2.245345	1.432598	0.000000	
21	H	4.858834	5.482250	2.675347	2.220602	3.340727	
22	H	6.739946	7.621921	2.704031	2.243844	1.079205	
23	C	4.644790	5.873609	3.347729	2.304500	1.420147	
24	H	4.681314	6.078918	4.358039	3.347454	2.231000	
25	C	3.801715	5.037402	3.345576	2.301607	2.294807	
26	H	2.914539	4.450716	4.356215	3.344535	3.333906	
27	C	4.738493	5.552340	2.225652	1.411909	2.297432	
28	C	4.503787	3.198690	6.235604	5.720586	5.780948	
29	O	5.542375	4.061421	7.019673	6.598335	6.621874	
30	C	6.213583	6.061724	3.245536	3.085823	3.106529	
31	O	7.285249	6.956208	3.854415	3.945282	3.975883	
32	C	4.594796	4.073345	3.830611	3.470788	4.071984	
33	O	5.507336	4.772322	3.981601	3.915728	4.787919	
34	C	2.996379	3.237377	5.760466	4.882078	4.436277	
35	O	2.580778	3.335670	6.603886	5.637751	5.071115	
		21	22	23	24	25	
21	H	0.000000					
22	H	4.349301	0.000000				
23	C	3.339874	2.233417	0.000000			
24	H	4.348427	2.689856	1.078041	0.000000		
25	C	2.243823	3.336837	1.410170	2.218969	0.000000	
26	H	2.711902	4.341069	2.215981	2.663047	1.077792	
27	C	1.079558	3.339625	2.296394	3.338300	1.429543	
28	C	5.521888	6.363514	5.466701	5.769094	5.161421	
29	O	6.542605	7.087076	6.419131	6.677771	6.229209	
30	C	4.276474	3.308006	3.760252	4.375576	4.068041	
31	O	5.235545	3.938933	4.793030	5.359659	5.183693	
32	C	3.074733	4.838269	4.106313	4.862073	3.514899	
33	O	3.326265	5.510812	5.030796	5.879454	4.368207	
34	C	4.958558	5.052364	3.591966	3.516678	3.545572	
35	O	5.600189	5.685414	3.975284	3.641306	3.930305	
		26	27	28	29	30	
26	H	0.000000					
27	C	2.246297	0.000000				
28	C	5.223807	5.326745	0.000000			
29	O	6.341904	6.341765	1.143319	0.000000		
30	C	4.876749	3.696464	3.780917	4.257916	0.000000	
31	O	6.016180	4.717183	4.339822	4.547613	1.143190	
32	C	3.900284	3.057337	2.696761	3.572986	2.564853	

	33	O	4.785670	3.587783	3.388107	4.060731	3.081814
	34	C	3.436752	4.396827	2.716322	3.613535	3.984955
	35	O	3.555462	5.034053	3.696570	4.536230	5.112648
			31	32	33	34	35
	31	O	0.000000				
	32	C	3.407634	0.000000			
	33	O	3.653604	1.170912	0.000000		
	34	C	4.922620	3.448273	4.595370	0.000000	
	35	O	6.064853	4.518612	5.659578	1.203491	0.000000

Table S7. Orbital energies and the HOMO-LUMO gaps.

Structure	HOMO energy (Hartree)	LUMO energy (Hartree)	HOMO/LUMO Gap (Hartree)	HOMO/LUMO Gap (eV)
Ru2PCO0-1S	-0.19330	-0.07037	0.12293	3.35
Ru2PCO0-2S	-0.18523	-0.07996	0.10527	2.86
Ru2PCO0-3T	-0.18603	-0.04538	0.14065	3.83
Ru2PCO0-4T	-0.18149	-0.06896	0.11253	3.06
Ru2PCO0-5T	-0.17812	-0.07340	0.10472	2.85
Ru2PCO0-6Q	-0.17544	-0.05980	0.11564	3.15
Ru2PCO1-1S	-0.20566	-0.05170	0.15396	4.19
Ru2PCO1-2S	-0.19437	-0.06949	0.12488	3.40
Ru2PCO1-3S	-0.19874	-0.08089	0.11785	3.21
Ru2PCO1-4S	-0.19590	-0.08067	0.11523	3.14
Ru2PCO1-5T	-0.15883	-0.05167	0.10716	2.92
Ru2PCO2-1S	-0.20228	-0.04698	0.15530	4.23
Ru2PCO2-2S	-0.19069	-0.08247	0.10822	2.94
Ru2PCO2-3S	-0.19954	-0.04549	0.15405	4.19
Ru2PCO2-4S	-0.20892	-0.08343	0.12549	3.41
Ru2PCO2-5S	-0.20889	-0.08403	0.12486	3.40
Ru2PCO2-6S	-0.18655	-0.09698	0.08957	2.44
Ru2PCO2-7T	-0.18264	-0.05060	0.13204	3.59
Ru2PCO2-8T	-0.19153	-0.04471	0.14682	4.00
Ru2PCO2-9T	-0.17416	-0.04639	0.12777	3.48
Ru2PCO2-10T	-0.17722	-0.03822	0.13900	3.78
Ru2PCO2-11T	-0.18564	-0.06731	0.11833	3.22
Ru2PCO2-12S	-0.18725	-0.06735	0.11990	3.26
Ru2PCO2-13S	-0.18104	-0.04120	0.13984	3.81
Ru2PCO3-1S	-0.20516	-0.05109	0.15407	4.19
Ru2PCO3-2S	-0.20376	-0.05273	0.15103	4.11

Ru2PCO3-3S	-0.20123	-0.05411	0.14712	4.00
Ru2PCO3-4S	-0.19927	-0.05067	0.14860	4.04
Ru2PCO3-5S	-0.21178	-0.08005	0.13173	3.58
Ru2PCO4-1S	-0.18309	-0.03332	0.14977	4.08
Ru2PCO4-2S	-0.18506	-0.05059	0.13447	3.66
Ru2PCO4-3S	-0.20037	-0.05844	0.14193	3.86
Ru2PCO4-4S	-0.20139	-0.06424	0.13715	3.73