

**Supplementary Material for: Structure and  
Bonding in  
hexa-tert-butyl-hexa-peri-hexabenzocoronene  
sandwich complexes of Ruthenium**

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## Supplementary Material

Table S1: Relative energies of **2a**, **2b** and **2c** at the B3LYP/def2-TZVP//B3LYP/def2-SVP and the the BP86/def2-TZVP//BP86/def2-SVP levels of theory and HBC-Ru distances. Enthalpies are given in kcal mol<sup>-1</sup> and distances in Å.

Compound	Binding site	B3LYP		BP86	
		$\Delta H$	distance	$\Delta H$	distance
<b>2a</b>	central (1)	5.8	1.81	6.3	1.78
<b>2b</b>	intermediate (2)	17.1	1.88	16.4	1.82
<b>2c</b>	peripheral (3)	0.0	1.79	0.0	1.76

Table S2: NICS values (in ppm) and electron densities ( $\rho$ ) for the peripheral (**1-p**), intermediate (**1-i**) and central (**1-c**) ring of hexa-*tert*-butyl-hexa-*peri*-hexabenzocoronene (**1**) along with comparative data for benzene (Bz), the cyclopentadienyl anion (Cp<sup>-</sup>) and the pentamethylcyclopentadienyl anion (Cp<sup>\*-</sup>). The coordinate  $r$  denotes the distance (in Å) of the point perpendicularly above the aromatic ring at which the NICS value was calculated. Of particular interest are the two points where  $r = 0.00$  Å (the center of mass of the six-carbon atoms that make up the aromatic ring) and  $r = 1.00$  Å (the reference point most commonly used to discuss aromaticity).

$r$	<b>1-p</b>	<b>1-i</b>	<b>1-c</b>	Bz	Cp <sup>-</sup>	Cp <sup>*-</sup>
0.00	-7.61	2.88	-11.15	-8.20	-13.83	-11.39
0.25	-8.29	2.33	-11.92	-8.81	-13.76	-11.44
0.50	-9.55	1.02	-13.31	-9.94	-13.29	-11.36
1.00	-9.70	-1.55	-13.13	-9.97	-10.40	-9.29
1.50	-7.24	-2.87	-9.91	-7.41	-6.95	-6.23
2.00	-4.91	-3.23	-7.07	-4.87	-4.47	-3.96
3.00	-2.44	-2.78	-4.03	-2.01	-1.77	-1.56
4.00	-1.53	-2.11	-2.68	-0.94	-0.78	-0.69
5.00	-1.10	-1.58	-1.91	-0.50	-0.40	-0.35
$\rho$	0.0226	0.0203	0.0213	0.0231	0.0481	0.0468

Cartesian coordinates of **1** at the B3LYP/def2-SVP level (including the positions of the NICS calculations)

C	0.000000	1.423224	0.017691
C	0.000000	0.711687	-1.214507
C	0.000000	-0.711687	-1.214507
C	0.000000	-1.423224	0.017691

C	0.000000	-0.711480	1.250693
C	0.000000	0.711480	1.250693
C	0.000000	2.869412	0.018459
C	0.000000	3.593370	-1.210498
C	0.000000	4.995070	-1.174883
C	0.000000	5.724773	0.019326
C	0.000000	4.999029	1.211531
C	0.000000	3.593363	1.243998
C	0.000000	1.435592	-2.467461
C	0.000000	0.734321	-3.709487
C	0.000000	1.466484	-4.904972
C	0.000000	2.866030	-4.938811
C	0.000000	3.534416	-3.713996
C	0.000000	2.858577	-2.480770
C	0.000000	-1.435592	-2.467461
C	0.000000	-2.858577	-2.480770
C	0.000000	-3.534416	-3.713996
C	0.000000	-2.866030	-4.938811
C	0.000000	-1.466484	-4.904972
C	0.000000	-0.734321	-3.709487
C	0.000000	-2.869412	0.018459
C	0.000000	-3.593363	1.243998
C	0.000000	-4.999029	1.211531
C	0.000000	-5.724773	0.019326
C	0.000000	-4.995070	-1.174883
C	0.000000	-3.593370	-1.210498
C	0.000000	-1.433827	2.502829

C	0.000000	-0.733224	3.742260
C	0.000000	-1.464620	4.943880
C	0.000000	-2.859627	4.976286
C	0.000000	-3.530091	3.747265
C	0.000000	-2.860411	2.515560
C	0.000000	1.433827	2.502829
C	0.000000	2.860411	2.515560
C	0.000000	3.530091	3.747265
C	0.000000	2.859627	4.976286
C	0.000000	1.464620	4.943880
C	0.000000	0.733224	3.742260
C	0.000000	7.266637	-0.022253
C	1.262390	7.760708	-0.766294
C	0.000000	7.889895	1.385526
C	-1.262390	7.760708	-0.766294
C	0.000000	3.603394	-6.293798
C	1.262340	3.207431	-7.094443
C	0.000000	5.133376	-6.125258
C	-1.262340	3.207431	-7.094443
C	0.000000	-3.603394	-6.293798
C	-1.262340	-3.207431	-7.094443
C	0.000000	-5.133376	-6.125258
C	1.262340	-3.207431	-7.094443
C	0.000000	-7.266637	-0.022253
C	-1.262390	-7.760708	-0.766294
C	0.000000	-7.889895	1.385526
C	1.262390	-7.760708	-0.766294

C	0.000000	-3.665645	6.291144
C	1.262263	-4.557318	6.347293
C	0.000000	-2.756472	7.533451
C	-1.262263	-4.557318	6.347293
C	0.000000	3.665645	6.291144
C	1.262263	4.557318	6.347293
C	0.000000	2.756472	7.533451
C	-1.262263	4.557318	6.347293
H	0.000000	5.545717	-2.112939
H	0.000000	5.543460	2.150573
H	0.000000	0.930524	-5.851793
H	0.000000	4.619711	-3.714380
H	0.000000	-4.619711	-3.714380
H	0.000000	-0.930524	-5.851793
H	0.000000	-5.543460	2.150573
H	0.000000	-5.545717	-2.112939
H	0.000000	-0.923461	5.884704
H	0.000000	-4.617894	3.755371
H	0.000000	4.617894	3.755371
H	0.000000	0.923461	5.884704
H	1.277954	8.862302	-0.809774
H	1.303473	7.387160	-1.800799
H	2.178788	7.426945	-0.254127
H	0.000000	8.988238	1.305287
H	0.892037	7.602068	1.963692
H	-0.892037	7.602068	1.963692
H	-1.277954	8.862302	-0.809774

H	-1.303473	7.387160	-1.800799
H	-2.178788	7.426945	-0.254127
H	1.276965	3.721784	-8.069550
H	2.178861	3.483875	-6.549386
H	1.303637	2.124988	-7.289403
H	0.000000	5.617617	-7.114384
H	0.891995	5.487658	-5.585281
H	-0.891995	5.487658	-5.585281
H	-1.276965	3.721784	-8.069550
H	-1.303637	2.124988	-7.289403
H	-2.178861	3.483875	-6.549386
H	-1.276965	-3.721784	-8.069550
H	-1.303637	-2.124988	-7.289403
H	-2.178861	-3.483875	-6.549386
H	0.000000	-5.617617	-7.114384
H	-0.891995	-5.487658	-5.585281
H	0.891995	-5.487658	-5.585281
H	1.276965	-3.721784	-8.069550
H	1.303637	-2.124988	-7.289403
H	2.178861	-3.483875	-6.549386
H	-1.277954	-8.862302	-0.809774
H	-1.303473	-7.387160	-1.800799
H	-2.178788	-7.426945	-0.254127
H	0.000000	-8.988238	1.305287
H	0.892037	-7.602068	1.963692
H	-0.892037	-7.602068	1.963692
H	1.277954	-8.862302	-0.809774

H	1.303473	-7.387160	-1.800799
H	2.178788	-7.426945	-0.254127
H	1.278655	-5.144109	7.280614
H	1.301216	-5.267931	5.507780
H	2.178914	-3.947423	6.311741
H	0.000000	-3.372666	8.446188
H	-0.891846	-2.111530	7.571224
H	0.891846	-2.111530	7.571224
H	-1.278655	-5.144109	7.280614
H	-2.178914	-3.947423	6.311741
H	-1.301216	-5.267931	5.507780
H	1.278655	5.144109	7.280614
H	1.301216	5.267931	5.507780
H	2.178914	3.947423	6.311741
H	0.000000	3.372666	8.446188
H	-0.891846	2.111530	7.571224
H	0.891846	2.111530	7.571224
H	-1.278655	5.144109	7.280614
H	-1.301216	5.267931	5.507780
H	-2.178914	3.947423	6.311741
Bq	0.000000	0.000000	0.017959
Bq	0.000000	4.295836	0.017989
Bq	0.000000	2.148647	-1.222848
Bq	0.250000	0.000000	0.017959
Bq	0.250000	4.295836	0.017989
Bq	0.250000	2.148647	-1.222848
Bq	0.500000	0.000000	0.017959

Bq	0.500000	4.295836	0.017989
Bq	0.500000	2.148647	-1.222848
Bq	1.000000	0.000000	0.017959
Bq	1.000000	4.295836	0.017989
Bq	1.000000	2.148647	-1.222848
Bq	1.500000	0.000000	0.017959
Bq	1.500000	4.295836	0.017989
Bq	1.500000	2.148647	-1.222848
Bq	2.000000	0.000000	0.017959
Bq	2.000000	4.295836	0.017989
Bq	2.000000	2.148647	-1.222848
Bq	3.000000	0.000000	0.017959
Bq	3.000000	4.295836	0.017989
Bq	3.000000	2.148647	-1.222848
Bq	4.000000	0.000000	0.017959
Bq	4.000000	4.295836	0.017989
Bq	4.000000	2.148647	-1.222848
Bq	5.000000	0.000000	0.017959
Bq	5.000000	4.295836	0.017989
Bq	5.000000	2.148647	-1.222848

Cartesian coordinates of **2a** at the B3LYP/def2-SVP level

Ru	-0.005832	0.006136	1.253961
C	-1.047284	-0.985879	-0.562130
C	0.331275	-1.393177	-0.559390
C	1.374120	-0.402831	-0.558693
C	1.038437	0.994827	-0.561813
C	-0.340767	1.402473	-0.562228



C	-1.383256	0.412418	-0.561684
C	-2.100367	-1.986333	-0.581790
C	-1.770454	-3.366755	-0.602283
C	-2.811568	-4.311368	-0.639020
C	-4.159352	-3.946465	-0.657528
C	-4.455601	-2.576625	-0.637046
C	-3.465361	-1.585670	-0.601626
C	0.670086	-2.806105	-0.570608
C	2.033073	-3.213114	-0.578805
C	2.324242	-4.583791	-0.595287
C	1.330227	-5.571862	-0.609322
C	0.000782	-5.144209	-0.608372
C	-0.358247	-3.784620	-0.591988
C	2.767896	-0.815015	-0.568918
C	3.799524	0.159972	-0.588196
C	5.138121	-0.270117	-0.601742
C	5.494878	-1.620730	-0.603485
C	4.455813	-2.560852	-0.592159
C	3.102613	-2.197718	-0.577482
C	2.091772	1.994975	-0.581198
C	1.762913	3.375631	-0.602519
C	2.804241	4.319304	-0.638083
C	4.152351	3.953423	-0.657611
C	4.447595	2.583970	-0.637332
C	3.456425	1.593325	-0.600027
C	-0.680519	2.814150	-0.574191
C	-2.041004	3.219645	-0.582292

C	-2.337280	4.594474	-0.598990
C	-1.345692	5.578121	-0.613590
C	-0.012049	5.148574	-0.611984
C	0.350088	3.794846	-0.594575
C	-2.775771	0.825312	-0.573147
C	-3.809662	-0.151663	-0.592695
C	-5.142261	0.281145	-0.608493
C	-5.501288	1.635797	-0.609571
C	-4.466476	2.573758	-0.596295
C	-3.109333	2.205391	-0.581248
C	-5.302360	-4.979184	-0.706101
C	-4.779189	-6.426900	-0.717698
C	-6.135991	-4.755002	-1.989584
C	-6.206631	-4.800746	0.535946
C	1.726238	-7.061600	-0.632199
C	2.566572	-7.387176	0.624862
C	2.562895	-7.346967	-1.901629
C	0.498957	-7.990573	-0.645396
C	6.960813	-2.096796	-0.626217
C	7.954804	-0.921746	-0.627551
C	7.203102	-2.937372	-1.901996
C	7.238055	-2.963495	0.624435
C	5.295996	4.985466	-0.707202
C	6.201164	4.806681	0.534139
C	4.773911	6.433586	-0.718863
C	6.128564	4.760264	-1.991196
C	-1.663535	7.086146	-0.637843

C	-3.177525	7.364374	-0.633438
C	-1.043857	7.758852	0.609533
C	-1.059569	7.712489	-1.916911
C	-6.989830	2.035745	-0.632663
C	-7.696130	1.451468	0.613093
C	-7.648208	1.471112	-1.913544
C	-7.183212	3.562687	-0.624236
C	1.086551	0.565802	3.069661
C	0.860268	-0.859846	3.071304
C	-0.565717	-1.084564	3.070845
C	-1.220691	0.201914	3.068909
C	-0.199378	1.222076	3.068160
C	2.419701	1.245990	3.156102
C	1.917607	-1.918681	3.158895
C	-1.246760	-2.417202	3.158652
C	-2.698600	0.435787	3.158185
C	-0.431159	2.700356	3.156858
H	-2.561192	-5.367052	-0.657406
H	-5.501447	-2.278493	-0.655320
H	3.363769	-4.903810	-0.601531
H	-0.784068	-5.893373	-0.623668
H	5.928758	0.473398	-0.614402
H	4.719676	-3.615923	-0.599285
H	2.554564	5.375260	-0.656582
H	5.493062	2.284980	-0.655776
H	-3.376303	4.908092	-0.605234
H	0.769045	5.905098	-0.627199

H	-5.938770	-0.459169	-0.622318
H	-4.723463	3.628123	-0.602367
H	-5.627409	-7.127231	-0.750985
H	-4.195478	-6.662748	0.186009
H	-4.151803	-6.631924	-1.599139
H	-6.959584	-5.484921	-2.042171
H	-5.516260	-4.876997	-2.891916
H	-6.583512	-3.749865	-2.023117
H	-7.029286	-5.533198	0.516989
H	-5.638100	-4.954136	1.467070
H	-6.659418	-3.798273	0.579135
H	2.862701	-8.448319	0.621096
H	3.488610	-6.788121	0.674375
H	1.992649	-7.199507	1.546326
H	2.854771	-8.408806	-1.934782
H	3.487016	-6.749945	-1.932610
H	1.988318	-7.124290	-2.814533
H	0.828992	-9.040257	-0.660717
H	-0.128975	-7.857902	0.249583
H	-0.128390	-7.831982	-1.536326
H	8.985159	-1.307961	-0.641865
H	7.852915	-0.293995	0.271680
H	7.833806	-0.280459	-1.514521
H	8.247138	-3.287699	-1.934878
H	7.015631	-2.343553	-2.810483
H	6.555563	-3.826567	-1.942916
H	8.281940	-3.315665	0.620261

H	7.079034	-2.388028	1.550325
H	6.591211	-3.853212	0.665715
H	7.024274	5.538602	0.514339
H	6.653186	3.803886	0.576879
H	5.633550	4.960520	1.465745
H	5.622614	7.133285	-0.753030
H	4.146120	6.638844	-1.600029
H	4.191240	6.670247	0.185375
H	6.952599	5.489624	-2.044620
H	6.575338	3.754814	-2.024340
H	5.508309	4.882254	-2.893177
H	-3.354623	8.450401	-0.650473
H	-3.678861	6.938477	-1.516621
H	-3.668601	6.967717	0.269130
H	-1.255048	8.840017	0.604165
H	0.049506	7.636913	0.646553
H	-1.461535	7.336833	1.537496
H	-1.274582	8.792383	-1.950309
H	0.033638	7.592131	-1.961217
H	-1.485047	7.253258	-2.823106
H	-8.763530	1.724108	0.609172
H	-7.250441	1.841365	1.542075
H	-7.637057	0.352767	0.646747
H	-8.714237	1.746966	-1.947531
H	-7.164596	1.872048	-2.818250
H	-7.589849	0.372897	-1.960450
H	-8.257566	3.800741	-0.639556

H	-6.758563	4.028330	0.279066
H	-6.730713	4.041581	-1.506629
H	2.694090	1.415886	4.211906
H	3.216229	0.641452	2.700343
H	2.413054	2.223285	2.653649
H	2.146731	-2.144401	4.215017
H	2.853036	-1.602257	2.676838
H	1.597162	-2.855204	2.681662
H	-1.413378	-2.692058	4.214860
H	-0.644299	-3.213934	2.700400
H	-2.225709	-2.409341	2.659554
H	-3.012850	0.487370	4.215334
H	-3.270614	-0.373044	2.682511
H	-2.993632	1.379404	2.678432
H	-0.480742	3.015157	4.213944
H	0.377776	3.271040	2.679691
H	-1.375081	2.996596	2.678390

Cartesian coordinates of **2b** at the B3LYP/def2-SVP level

Ru	-2.091178	-0.045083	1.106329
C	-0.678522	0.710395	-0.623617
C	-0.645550	-0.725277	-0.625697
C	0.611751	-1.414031	-0.522815
C	1.810058	-0.671457	-0.442021
C	1.777457	0.767440	-0.442189
C	0.546144	1.455314	-0.520929
C	-1.946684	1.403636	-0.747290
C	-3.173448	0.668550	-0.906824

C	-4.391778	1.387187	-1.072913
C	-4.435282	2.768701	-1.104218
C	-3.215993	3.470621	-0.933982
C	-1.991353	2.845101	-0.746041
C	-1.880673	-1.474925	-0.755828
C	-1.859487	-2.916703	-0.762115
C	-3.052215	-3.596785	-0.965573
C	-4.300789	-2.950625	-1.143051
C	-4.321677	-1.568962	-1.097564
C	-3.139381	-0.796327	-0.915325
C	0.633066	-2.856311	-0.500698
C	1.870291	-3.549659	-0.383041
C	1.862897	-4.955978	-0.308211
C	0.690145	-5.708829	-0.353818
C	-0.516054	-5.006958	-0.497626
C	-0.576855	-3.611655	-0.583079
C	3.077120	-1.361826	-0.363248
C	4.298278	-0.631741	-0.311108
C	5.511383	-1.334587	-0.252023
C	5.577828	-2.731565	-0.241900
C	4.367621	-3.430299	-0.285139
C	3.120760	-2.787991	-0.340970
C	3.011163	1.514570	-0.367393
C	2.991386	2.938374	-0.349755
C	4.210390	3.641391	-0.300892
C	5.446628	2.998881	-0.263789
C	5.441919	1.595862	-0.268212

C	4.266667	0.837994	-0.316016
C	0.503094	2.896158	-0.499202
C	-0.739911	3.597129	-0.575729
C	-0.739850	4.993801	-0.494728
C	0.435583	5.748834	-0.361786
C	1.640431	5.048899	-0.320309
C	1.709533	3.643558	-0.389407
C	-5.737213	3.561349	-1.325630
C	-6.957903	2.640161	-1.497010
C	-5.595907	4.421756	-2.603654
C	-5.991263	4.480678	-0.108004
C	-5.560987	-3.800426	-1.391821
C	-5.778940	-4.759682	-0.198316
C	-5.367437	-4.623114	-2.687868
C	-6.823948	-2.935823	-1.552518
C	0.676381	-7.247090	-0.259794
C	2.089818	-7.833726	-0.093243
C	0.058089	-7.831759	-1.551560
C	-0.172064	-7.677380	0.959860
C	6.911394	-3.503174	-0.191102
C	6.934718	-4.404593	1.065456
C	8.128007	-2.561774	-0.130398
C	7.040172	-4.380168	-1.458655
C	6.784758	3.762737	-0.223050
C	6.583948	5.288787	-0.218127
C	7.558987	3.371935	1.057562
C	7.622604	3.388605	-1.468196



C	0.356172	7.285596	-0.275347
C	-0.504197	7.686012	0.946094
C	-0.292576	7.836583	-1.566998
C	1.743992	7.932880	-0.119060
C	-1.264525	-0.753169	2.987302
C	-2.619716	-1.229889	2.853779
C	-3.493995	-0.082387	2.766485
C	-2.676310	1.105323	2.859563
C	-1.299552	0.693890	2.989164
C	-0.047539	-1.601742	3.198425
C	-3.051287	-2.664266	2.882974
C	-4.990330	-0.116198	2.689188
C	-3.177825	2.516587	2.901927
C	-0.124423	1.600743	3.194660
H	-5.310700	0.825657	-1.204989
H	-3.248563	4.557184	-0.968904
H	-3.033860	-4.683295	-1.009393
H	-5.263963	-1.048792	-1.234193
H	2.808658	-5.477612	-0.202531
H	-1.440041	-5.580069	-0.539735
H	6.440193	-0.774577	-0.214461
H	4.402419	-4.517265	-0.282666
H	4.189953	4.726322	-0.300480
H	6.400104	1.082504	-0.235820
H	-1.688119	5.526119	-0.533375
H	2.563200	5.611565	-0.223765
H	-7.862378	3.247895	-1.650391

H	-7.132429	2.014832	-0.607095
H	-6.856559	1.978741	-2.371455
H	-6.520818	4.993454	-2.780021
H	-5.412829	3.791179	-3.487796
H	-4.770589	5.146319	-2.530680
H	-6.914706	5.062331	-0.256911
H	-6.109826	3.892840	0.816562
H	-5.172506	5.198676	0.052118
H	-6.673250	-5.379857	-0.367797
H	-4.928565	-5.442620	-0.050620
H	-5.929926	-4.201151	0.739514
H	-6.261115	-5.236253	-2.884895
H	-4.506790	-5.306312	-2.623785
H	-5.209615	-3.964095	-3.555966
H	-7.697394	-3.583275	-1.722340
H	-7.032035	-2.336569	-0.651922
H	-6.751147	-2.253550	-2.413709
H	2.030406	-8.930682	-0.026089
H	2.579581	-7.475482	0.825839
H	2.740219	-7.594030	-0.948926
H	0.042021	-8.932287	-1.502583
H	0.641934	-7.539869	-2.438682
H	-0.978048	-7.493147	-1.705391
H	-0.193080	-8.775785	1.041687
H	0.246887	-7.276091	1.896400
H	-1.215183	-7.333667	0.882504
H	7.882029	-4.964925	1.115756

H	6.116253	-5.140471	1.062033
H	6.845278	-3.805739	1.985708
H	9.054347	-3.154957	-0.093600
H	8.191466	-1.911424	-1.016871
H	8.112108	-1.923705	0.767239
H	7.988150	-4.941368	-1.439978
H	6.223084	-5.113423	-1.538407
H	7.028297	-3.763703	-2.371362
H	7.562574	5.791494	-0.188351
H	6.063884	5.639495	-1.123307
H	6.014862	5.627786	0.661804
H	8.519645	3.909575	1.100751
H	7.782294	2.294755	1.094809
H	6.985460	3.628173	1.962477
H	8.586389	3.922386	-1.453937
H	7.842349	2.310930	-1.510794
H	7.096922	3.661308	-2.396925
H	-0.571004	8.783012	1.022240
H	-0.064561	7.307837	1.882758
H	-1.532255	7.298359	0.875292
H	-0.355330	8.935707	-1.523524
H	0.299099	7.565410	-2.455509
H	-1.314062	7.453448	-1.714050
H	1.638046	9.026627	-0.057395
H	2.253291	7.600498	0.799058
H	2.399863	7.716293	-0.976647
H	0.102084	-1.791646	4.275765

H	-0.135312	-2.576478	2.698664
H	0.861198	-1.113062	2.820492
H	-3.272536	-2.974781	3.919040
H	-2.268499	-3.330995	2.495908
H	-3.959098	-2.829481	2.286118
H	-5.433198	-0.084584	3.699923
H	-5.348507	-1.032434	2.199138
H	-5.384668	0.742282	2.127074
H	-3.406766	2.806886	3.942252
H	-4.097291	2.642039	2.313393
H	-2.432129	3.225501	2.516264
H	0.032191	1.786310	4.271714
H	0.801733	1.163818	2.796172
H	-0.270584	2.574606	2.707016

Cartesian coordinates of **2c** at the B3LYP/def2-SVP level

Ru	-3.65304	-0.05419	0.72965
C	-0.42863	-0.00965	-0.58789
C	0.29457	-1.22775	-0.49924
C	1.70892	-1.19787	-0.34173
C	2.38837	0.05209	-0.26488
C	1.65425	1.27210	-0.34324
C	0.24154	1.24025	-0.50879
C	-1.86392	-0.04144	-0.79265
C	-2.56226	-1.29815	-0.87254
C	-3.97010	-1.29574	-1.11698
C	-4.71229	-0.10726	-1.33027
C	-4.01825	1.11639	-1.15187

C	-2.61374	1.18340	-0.90411
C	-0.39926	-2.49825	-0.56962
C	0.32490	-3.72233	-0.48187
C	-0.38177	-4.93368	-0.53963
C	-1.77076	-5.00630	-0.69093
C	-2.46267	-3.79570	-0.78877
C	-1.81119	-2.55329	-0.73193
C	2.45495	-2.43423	-0.26700
C	3.87048	-2.41502	-0.12724
C	4.57045	-3.63360	-0.08028
C	3.93517	-4.87379	-0.15879
C	2.54005	-4.87082	-0.28286
C	1.78581	-3.69152	-0.33951
C	3.82431	0.08418	-0.10776
C	4.51547	1.32587	-0.02287
C	5.91235	1.32351	0.13143
C	6.66090	0.14708	0.20339
C	5.96273	-1.06313	0.11399
C	4.57114	-1.12939	-0.03876
C	2.34311	2.53915	-0.26018
C	1.62124	3.76370	-0.33932
C	2.32042	4.98093	-0.26015
C	3.70634	5.04281	-0.10458
C	4.39691	3.82710	-0.02624
C	3.75964	2.58091	-0.10020
C	-0.50323	2.47909	-0.59877
C	-1.91653	2.47211	-0.78296

C	-2.61259	3.68273	-0.86672
C	-1.97316	4.92737	-0.76976
C	-0.59008	4.91734	-0.59296
C	0.16566	3.73129	-0.51038
C	-6.16554	-0.12888	-1.83946
C	-6.86707	-1.46799	-1.54287
C	-6.08842	0.06205	-3.37577
C	-7.00474	1.01256	-1.23290
C	-2.46985	-6.37890	-0.75199
C	-2.19133	-7.15451	0.55670
C	-1.91765	-7.18045	-1.95410
C	-3.99444	-6.24904	-0.92044
C	4.70200	-6.21058	-0.11595
C	6.22339	-6.00573	-0.00207
C	4.41804	-7.00592	-1.41164
C	4.23054	-7.03064	1.10764
C	8.19287	0.13880	0.37290
C	8.55817	-0.61339	1.67401
C	8.77903	1.55984	0.45750
C	8.83679	-0.57825	-0.83686
C	4.48104	6.37300	-0.02391
C	3.55304	7.59607	-0.13554
C	5.22404	6.45135	1.33022
C	5.50619	6.43712	-1.18040
C	-2.79724	6.22601	-0.87052
C	-3.86480	6.24610	0.24843
C	-3.49383	6.28166	-2.25037

C	-1.92302	7.48400	-0.72057
C	-2.76249	-0.40998	2.71173
C	-3.92174	-1.25348	2.55752
C	-5.07193	-0.39870	2.39067
C	-4.62017	0.97238	2.43588
C	-3.19548	0.96495	2.63992
C	-1.37034	-0.87844	3.01166
C	-3.93848	-2.74767	2.68397
C	-6.50058	-0.85367	2.37659
C	-5.49467	2.19152	2.42584
C	-2.33023	2.17145	2.84226
H	-4.48879	-2.24559	-1.18064
H	-4.57550	2.04214	-1.24583
H	0.17236	-5.86644	-0.46631
H	-3.54068	-3.82522	-0.91298
H	5.65102	-3.61174	0.01684
H	2.03094	-5.83010	-0.34395
H	6.43435	2.27267	0.19736
H	6.53280	-1.98759	0.16747
H	1.76651	5.91189	-0.32637
H	5.47728	3.85977	0.09301
H	-3.69070	3.67218	-1.01213
H	-0.07256	5.86830	-0.51938
H	-7.91154	-1.42104	-1.88523
H	-6.87815	-1.69551	-0.46674
H	-6.39862	-2.31170	-2.07156
H	-7.10041	0.04550	-3.81023

H	-5.50219	-0.73981	-3.85103
H	-5.62228	1.02373	-3.64105
H	-8.04044	0.94829	-1.59866
H	-7.02755	0.95267	-0.13522
H	-6.63173	2.00870	-1.51359
H	-2.68372	-8.13971	0.52949
H	-1.11598	-7.32770	0.71451
H	-2.57526	-6.60794	1.43292
H	-2.40523	-8.16674	-2.01176
H	-0.83365	-7.35255	-1.87343
H	-2.10380	-6.65298	-2.90291
H	-4.45090	-7.24974	-0.95838
H	-4.45942	-5.71047	-0.07917
H	-4.26410	-5.73251	-1.85517
H	6.72859	-6.98332	0.02129
H	6.50079	-5.47213	0.92049
H	6.62928	-5.44766	-0.86035
H	4.96252	-7.96376	-1.39866
H	4.74157	-6.44337	-2.30163
H	3.34832	-7.23677	-1.53115
H	4.76433	-7.99359	1.15135
H	4.42720	-6.49024	2.04714
H	3.15282	-7.25171	1.06671
H	9.65123	-0.62997	1.81179
H	8.21133	-1.65799	1.65939
H	8.11177	-0.12366	2.55393
H	9.87154	1.50350	0.57902



H	8.58182	2.14368	-0.45533
H	8.38232	2.11932	1.31924
H	9.93356	-0.59377	-0.73191
H	8.49876	-1.62176	-0.92755
H	8.59274	-0.06315	-1.77941
H	4.14807	8.52007	-0.07535
H	3.01161	7.61728	-1.09440
H	2.81425	7.62944	0.68067
H	5.78847	7.39492	1.40234
H	5.94184	5.62659	1.45700
H	4.51670	6.41341	2.17388
H	6.06841	7.38395	-1.14068
H	6.23809	5.61661	-1.13099
H	5.00428	6.38047	-2.15927
H	-4.45976	7.17169	0.19335
H	-3.39576	6.20527	1.24461
H	-4.56709	5.40114	0.16914
H	-4.09104	7.20309	-2.34081
H	-2.75524	6.27451	-3.06727
H	-4.17428	5.43013	-2.40626
H	-2.55226	8.38393	-0.79472
H	-1.41355	7.51918	0.25511
H	-1.16043	7.55313	-1.51170
H	-1.22078	-0.93944	4.10376
H	-1.17548	-1.87634	2.59563
H	-0.60911	-0.19359	2.61313
H	-4.00658	-3.04161	3.74586

H	-3.02611	-3.20152	2.27237
H	-4.79834	-3.19306	2.16402
H	-6.87972	-0.92617	3.41109
H	-6.61412	-1.84602	1.91885
H	-7.15466	-0.15427	1.83933
H	-5.79482	2.45203	3.45578
H	-6.41481	2.03420	1.84661
H	-4.97518	3.06416	2.00557
H	-2.31700	2.45392	3.90937
H	-1.29175	1.98614	2.53607
H	-2.69516	3.03794	2.27337

Cartesian coordinates of **2a** at the BP86/def2-SVP level

Ru	-0.00552	0.00610	1.21829
C	-1.06063	-0.98607	-0.55988
C	0.32483	-1.40410	-0.55722
C	1.38053	-0.41339	-0.55688
C	1.05117	0.99572	-0.55983
C	-0.33475	1.41410	-0.56064
C	-1.39021	0.42355	-0.55996
C	-2.12205	-1.98220	-0.57072
C	-1.79750	-3.37314	-0.58908
C	-2.85048	-4.31628	-0.62318
C	-4.20381	-3.94089	-0.64097
C	-4.49412	-2.56176	-0.62067
C	-3.49258	-1.57031	-0.58806
C	0.65603	-2.82208	-0.56027
C	2.02480	-3.23901	-0.56785

C	2.30881	-4.61970	-0.58418
C	1.30285	-5.60689	-0.59825
C	-0.03178	-5.16906	-0.59607
C	-0.38522	-3.80005	-0.57987
C	2.77465	-0.83479	-0.55852
C	3.81832	0.14061	-0.57541
C	5.16148	-0.30071	-0.58777
C	5.51151	-1.66155	-0.59068
C	4.46120	-2.60088	-0.57977
C	3.10228	-2.22803	-0.56615
C	2.11283	1.99148	-0.57028
C	1.78925	3.38257	-0.58916
C	2.84257	4.32480	-0.62201
C	4.19616	3.94849	-0.64156
C	4.48552	2.56969	-0.62176
C	3.48310	1.57870	-0.58678
C	-0.66685	2.83081	-0.56415
C	-2.03357	3.24633	-0.57065
C	-2.32252	4.63082	-0.58614
C	-1.31891	5.61382	-0.60101
C	0.01967	5.17433	-0.59883
C	0.37637	3.81071	-0.58232
C	-2.78312	0.84550	-0.56265
C	-3.82877	-0.13151	-0.57989
C	-5.16637	0.31257	-0.59490
C	-5.51871	1.67711	-0.59676
C	-4.47235	2.61443	-0.58326

C	-3.10986	2.23651	-0.56943
C	-5.35475	-4.96956	-0.68914
C	-4.83638	-6.42333	-0.69947
C	-6.18733	-4.73729	-1.97764
C	-6.26060	-4.78126	0.55619
C	1.68884	-7.10264	-0.62265
C	2.52913	-7.43361	0.63887
C	2.52788	-7.38959	-1.89599
C	0.45059	-8.02378	-0.63850
C	6.97745	-2.14760	-0.61583
C	7.98019	-0.97482	-0.61049
C	7.21082	-2.98533	-1.90100
C	7.24716	-3.02690	0.63349
C	5.34765	4.97654	-0.69137
C	6.25523	4.78780	0.55264
C	4.83034	6.43072	-0.70130
C	6.17829	4.74339	-1.98097
C	-1.62802	7.12690	-0.62664
C	-3.14450	7.41416	-0.62065
C	-0.99802	7.79708	0.62284
C	-1.01746	7.74629	-1.91181
C	-7.00739	2.08887	-0.62261
C	-7.72281	1.49988	0.62152
C	-7.66384	1.53108	-1.91327
C	-7.18820	3.62139	-0.60761
C	1.09903	0.56323	3.02306
C	0.86499	-0.87192	3.02336

C	-0.57248	-1.09179	3.02428
C	-1.22684	0.20702	3.02455
C	-0.19356	1.23011	3.02398
C	2.43690	1.23920	3.10148
C	1.91901	-1.93747	3.10206
C	-1.26070	-2.42324	3.10465
C	-2.70564	0.44734	3.11064
C	-0.41889	2.71130	3.11022
H	-2.60455	-5.38376	-0.64015
H	-5.54799	-2.25383	-0.63719
H	3.35657	-4.94826	-0.59061
H	-0.82850	-5.92093	-0.61083
H	5.96502	0.44443	-0.59916
H	4.72006	-3.66785	-0.58671
H	2.59752	5.39258	-0.63887
H	5.53894	2.26070	-0.63888
H	-3.36946	4.95443	-0.59166
H	0.81339	5.93274	-0.61310
H	-5.97432	-0.43059	-0.60775
H	-4.72556	3.68046	-0.58884
H	-5.69326	-7.12646	-0.73328
H	-4.24996	-6.66361	0.21177
H	-4.20470	-6.63364	-1.58732
H	-7.02466	-5.46431	-2.03138
H	-5.56389	-4.86596	-2.88663
H	-6.62854	-3.72003	-2.01218
H	-7.09645	-5.51157	0.53770

H	-5.69048	-4.93928	1.49537
H	-6.70839	-3.76707	0.59824
H	2.82535	-8.50349	0.63345
H	3.45978	-6.83235	0.69099
H	1.95091	-7.24509	1.56740
H	2.81835	-8.46051	-1.93120
H	3.46159	-6.79164	-1.92529
H	1.95145	-7.16125	-2.81633
H	0.77324	-9.08458	-0.65579
H	-0.18186	-7.88724	0.26326
H	-0.17960	-7.85749	-1.53660
H	9.01685	-1.36828	-0.62634
H	7.88077	-0.34630	0.29896
H	7.86297	-0.32325	-1.50116
H	8.25875	-3.35017	-1.93668
H	7.02822	-2.38017	-2.81307
H	6.54844	-3.87398	-1.94771
H	8.29505	-3.39339	0.62624
H	7.09414	-2.45174	1.57042
H	6.58629	-3.91722	0.67074
H	7.09144	5.51767	0.53283
H	6.70237	3.77333	0.59380
H	5.68663	4.94607	1.49270
H	5.68769	7.13320	-0.73648
H	4.19772	6.64136	-1.58847
H	4.24557	6.67175	0.21088
H	7.01611	5.46975	-2.03596

H	6.61859	3.72577	-2.01557
H	5.55374	4.87228	-2.88917
H	-3.31812	8.50931	-0.63931
H	-3.65377	6.98711	-1.50945
H	-3.64095	7.01919	0.29019
H	-1.19802	8.88894	0.61518
H	0.10249	7.66217	0.65960
H	-1.42220	7.37924	1.55956
H	-1.22213	8.83671	-1.94701
H	0.08285	7.61332	-1.95779
H	-1.45153	7.28696	-2.82396
H	-8.79761	1.77761	0.61406
H	-7.27717	1.88666	1.56161
H	-7.66746	0.39226	0.65098
H	-8.73710	1.81224	-1.95094
H	-7.17154	1.93733	-2.82105
H	-7.60828	0.42437	-1.96576
H	-8.26840	3.87198	-0.62478
H	-6.75907	4.08328	0.30594
H	-6.72645	4.10473	-1.49352
H	2.71444	1.42314	4.16291
H	3.23730	0.62038	2.65080
H	2.43488	2.21782	2.58272
H	2.15343	-2.17126	4.16406
H	2.86182	-1.62141	2.61433
H	1.59010	-2.87815	2.61856
H	-1.44679	-2.69755	4.16655

H	-0.64916	-3.22980	2.65499
H	-2.23944	-2.41305	2.58637
H	-3.02360	0.50778	4.17503
H	-3.28526	-0.36891	2.63703
H	-2.99941	1.39633	2.62105
H	-0.47800	3.02908	4.17474
H	0.40437	3.28266	2.63868
H	-1.36379	3.01575	2.61908

Cartesian coordinates of **2b** at the BP86/def2-SVP level

Cartesian coordinates of **2c** at the BP86/def2-SVP level

Ru	-3.65405	-0.05682	0.73317
C	-0.44357	-0.01042	-0.57439
C	0.28486	-1.23565	-0.48854
C	1.70837	-1.20484	-0.33509
C	2.39142	0.05300	-0.25753
C	1.65198	1.27983	-0.33325
C	0.22993	1.24721	-0.49587
C	-1.88264	-0.04286	-0.77699
C	-2.58510	-1.30916	-0.85304
C	-4.00588	-1.30672	-1.07615
C	-4.75706	-0.11019	-1.27976
C	-4.05600	1.12227	-1.11003
C	-2.63829	1.19084	-0.88485
C	-0.40901	-2.50920	-0.56103
C	0.32168	-3.74041	-0.48381



C	-0.38696	-4.95926	-0.55451
C	-1.78363	-5.03314	-0.70637
C	-2.48273	-3.81603	-0.78880
C	-1.83038	-2.56591	-0.72027
C	2.45702	-2.44308	-0.26562
C	3.88203	-2.42283	-0.12806
C	4.58671	-3.64759	-0.08751
C	3.94864	-4.89525	-0.16788
C	2.54535	-4.89380	-0.28793
C	1.78505	-3.70858	-0.34141
C	3.83033	0.08578	-0.10246
C	4.52526	1.33563	-0.01563
C	5.92979	1.33326	0.13976
C	6.68314	0.15036	0.21005
C	5.98225	-1.06708	0.11700
C	4.58281	-1.13479	-0.03636
C	2.34202	2.54959	-0.25231
C	1.61549	3.78177	-0.33453
C	2.31881	5.00561	-0.25731
C	3.71285	5.06798	-0.10189
C	4.40781	3.84595	-0.02125
C	3.76744	2.59221	-0.09277
C	-0.51635	2.48841	-0.58822
C	-1.93829	2.48151	-0.77300
C	-2.63598	3.69948	-0.87362
C	-1.99071	4.95106	-0.79049
C	-0.60065	4.94120	-0.60534

C	0.15768	3.74894	-0.50808
C	-6.22230	-0.13060	-1.76274
C	-6.90817	-1.48627	-1.48551
C	-6.17039	0.09874	-3.29986
C	-7.05769	0.99360	-1.11036
C	-2.48112	-6.40878	-0.79276
C	-2.17448	-7.22223	0.49186
C	-1.94188	-7.17257	-2.03110
C	-4.01267	-6.27787	-0.93198
C	4.71973	-6.23356	-0.12955
C	6.24576	-6.02349	-0.03383
C	4.41838	-7.03511	-1.42307
C	4.25856	-7.04962	1.10661
C	8.21816	0.14311	0.38087
C	8.58071	-0.61699	1.68382
C	8.80306	1.56882	0.47040
C	8.86217	-0.57347	-0.83521
C	4.48878	6.40136	-0.02508
C	3.55730	7.62602	-0.14535
C	5.23036	6.48215	1.33513
C	5.51983	6.45663	-1.18318
C	-2.81092	6.25296	-0.92561
C	-3.91653	6.28399	0.16163
C	-3.46501	6.29163	-2.33217
C	-1.93574	7.51328	-0.75947
C	-2.71808	-0.40649	2.69101
C	-3.88328	-1.26324	2.55522

C	-5.04948	-0.40907	2.40645
C	-4.60121	0.97444	2.44191
C	-3.16344	0.97556	2.62525
C	-1.31490	-0.86605	2.96135
C	-3.88821	-2.75969	2.68022
C	-6.47699	-0.87400	2.42328
C	-5.48259	2.19098	2.44009
C	-2.29972	2.18900	2.80457
H	-4.53169	-2.26590	-1.12448
H	-4.62217	2.05698	-1.18592
H	0.17560	-5.89997	-0.49363
H	-3.57080	-3.84691	-0.91587
H	5.67802	-3.62506	0.00626
H	2.03126	-5.86218	-0.34883
H	6.45666	2.29147	0.20845
H	6.55742	-2.00067	0.16868
H	1.75985	5.94560	-0.32547
H	5.49873	3.87817	0.09687
H	-3.72304	3.68763	-1.02896
H	-0.07702	5.90138	-0.54063
H	-7.96708	-1.44261	-1.81097
H	-6.89850	-1.74087	-0.40655
H	-6.43670	-2.31916	-2.04586
H	-7.19666	0.08324	-3.72219
H	-5.58005	-0.69173	-3.80738
H	-5.71354	1.07797	-3.55167
H	-8.10717	0.93832	-1.46388

H	-7.06199	0.89984	-0.00571
H	-6.68776	2.00656	-1.36809
H	-2.66637	-8.21638	0.44488
H	-1.08747	-7.39716	0.62615
H	-2.54673	-6.69974	1.39769
H	-2.42305	-8.17013	-2.10811
H	-0.84618	-7.33504	-1.97475
H	-2.15246	-6.61705	-2.96839
H	-4.47239	-7.28561	-0.98794
H	-4.46787	-5.75774	-0.06296
H	-4.30258	-5.73531	-1.85596
H	6.75896	-7.00658	-0.01546
H	6.53564	-5.48469	0.89214
H	6.64314	-5.46093	-0.90414
H	4.96565	-8.00108	-1.41293
H	4.73375	-6.47263	-2.32622
H	3.33884	-7.26754	-1.52980
H	4.79182	-8.02266	1.14709
H	4.47065	-6.50354	2.04924
H	3.17089	-7.26700	1.07955
H	9.68191	-0.63780	1.82381
H	8.22840	-1.66876	1.66482
H	8.13135	-0.12637	2.57212
H	9.90400	1.51483	0.59395
H	8.60520	2.15988	-0.44804
H	8.40195	2.12968	1.34018
H	9.96724	-0.59307	-0.72907

H	8.51872	-1.62385	-0.93048
H	8.61841	-0.05114	-1.78357
H	4.15493	8.55870	-0.08944
H	3.01295	7.64177	-1.11254
H	2.81176	7.66458	0.67609
H	5.80417	7.43009	1.40527
H	5.94914	5.64783	1.46878
H	4.51575	6.45125	2.18381
H	6.08921	7.40914	-1.14676
H	6.25548	5.62834	-1.12740
H	5.01724	6.39544	-2.17076
H	-4.51387	7.21584	0.07685
H	-3.47767	6.25393	1.18090
H	-4.62260	5.43256	0.06773
H	-4.06589	7.21730	-2.45342
H	-2.69527	6.27648	-3.13123
H	-4.14278	5.42936	-2.50089
H	-2.56514	8.42155	-0.85439
H	-1.44707	7.55284	0.23624
H	-1.14749	7.57952	-1.53753
H	-1.13109	-0.89960	4.05790
H	-1.12833	-1.88190	2.56282
H	-0.56010	-0.18577	2.52045
H	-3.92056	-3.05865	3.75113
H	-2.98026	-3.21248	2.23540
H	-4.76916	-3.21194	2.18434
H	-6.83464	-0.95179	3.47401

H	-6.59648	-1.87420	1.96348
H	-7.15419	-0.17263	1.89975
H	-5.77471	2.45472	3.48048
H	-6.41560	2.02696	1.86708
H	-4.96749	3.07139	2.00893
H	-2.28126	2.49059	3.87508
H	-1.25387	2.00119	2.49400
H	-2.67279	3.05315	2.22041

Cartesian coordinates of **2a'** at the B3LYP/def2-SVP level

Ru	-0.92138	-0.00324	-0.00028
C	0.89158	0.03242	1.44072
C	0.88863	1.26423	0.69396
C	0.88979	1.23397	-0.74632
C	0.89292	-0.02804	-1.44026
C	0.89480	-1.25994	-0.69370
C	0.89439	-1.22985	0.74668
C	0.90801	0.06315	2.89655
C	0.92531	1.31134	3.57971
C	0.95600	1.31224	4.98454
C	0.96962	0.12233	5.70298
C	0.95635	-1.09696	5.03535
C	0.92760	-1.15519	3.63164
C	0.90107	2.54074	1.39523
C	0.91413	3.75654	0.65597
C	0.93421	4.97376	1.35769
C	0.94222	5.00107	2.74740
C	0.93548	3.81316	3.46956

C	0.91873	2.56824	2.81812
C	0.90213	2.47982	-1.50093
C	0.92130	2.44763	-2.92358
C	0.93687	3.66390	-3.62700
C	0.93807	4.88113	-2.95566
C	0.92844	4.91252	-1.56589
C	0.91315	3.72592	-0.81334
C	0.91108	-0.05850	-2.89641
C	0.93191	-1.30685	-3.57954
C	0.96226	-1.30760	-4.98437
C	0.97493	-0.11745	-5.70274
C	0.96011	1.10171	-5.03510
C	0.92889	1.15978	-3.63146
C	0.91127	-2.53621	-1.39528
C	0.92536	-3.75208	-0.65580
C	0.94448	-4.96927	-1.35768
C	0.95462	-4.99641	-2.74759
C	0.94908	-3.80857	-3.46949
C	0.92927	-2.56376	-2.81793
C	0.90995	-2.47538	1.50099
C	0.92582	-2.44311	2.92365
C	0.94515	-3.65942	3.62707
C	0.95433	-4.87666	2.95574
C	0.94674	-4.90793	1.56605
C	0.92586	-3.72136	0.81357
C	-2.74257	0.54199	-1.09575
C	-2.74546	1.20189	0.18827

C	-2.74051	0.18450	1.21226
C	-2.73423	-1.10384	0.56096
C	-2.73605	-0.88278	-0.86521
C	-2.83684	1.21524	-2.43166
C	-2.84769	2.67975	0.41652
C	-2.83460	0.42049	2.68925
C	-2.81954	-2.43490	1.24459
C	-2.82492	-1.94418	-1.91922
H	0.97391	2.24978	5.53689
H	0.94668	5.92083	0.82189
H	0.94728	3.86844	4.55633
H	0.95000	3.67294	-4.71509
H	0.93612	5.88157	-1.07072
H	0.98152	-2.24507	-5.53679
H	0.95568	-5.91644	-0.82199
H	0.96206	-3.86374	-4.55624
H	0.95644	-3.66846	4.71521
H	0.96036	-5.87691	1.07083
H	-3.89498	1.34542	-2.71807
H	-2.37252	2.21091	-2.42104
H	-2.35076	0.62576	-3.22160
H	-3.90792	2.98491	0.45548
H	-2.36940	3.25292	-0.38987
H	-2.38218	2.98114	1.36512
H	-3.89273	0.44423	3.00308
H	-2.38241	1.37877	2.97999
H	-2.33749	-0.37363	3.26374



H	-3.87595	-2.71682	1.39682
H	-2.33572	-2.42075	2.23099
H	-2.34747	-3.23053	0.65157
H	-3.88202	-2.17975	-2.13305
H	-2.36113	-1.62282	-2.86190
H	-2.33554	-2.87639	-1.60492
H	0.97117	-5.95346	-3.27346
H	1.00125	-0.14051	-6.79431
H	0.97736	2.01530	-5.62616
H	0.95118	5.81519	-3.52146
H	0.95839	5.95812	3.27328
H	0.99543	0.14542	6.79456
H	0.97452	-2.01048	5.62653
H	0.97168	-5.81063	3.52156

Cartesian coordinates of **2a''** at the B3LYP/def2-SVP level

Ru	-0.00631	0.00591	1.46565
C	-1.04738	-0.98680	-0.33483
C	0.33254	-1.39323	-0.33260
C	1.37516	-0.40124	-0.33130
C	1.03766	0.99706	-0.33412
C	-0.34282	1.40360	-0.33468
C	-1.38499	0.41209	-0.33388
C	-2.09990	-1.98806	-0.35063
C	-1.76788	-3.36802	-0.37067
C	-2.80801	-4.31327	-0.40623
C	-4.15611	-3.94913	-0.42648
C	-4.45374	-2.57964	-0.40776

C	-3.46481	-1.58796	-0.37124
C	0.67243	-2.80568	-0.33850
C	2.03600	-3.21056	-0.34321
C	2.32819	-4.58077	-0.35480
C	1.33480	-5.56953	-0.36784
C	0.00487	-5.14336	-0.37121
C	-0.35544	-3.78443	-0.35887
C	2.76922	-0.81181	-0.33652
C	3.79913	0.16463	-0.35588
C	5.13782	-0.26410	-0.36694
C	5.49570	-1.61436	-0.36486
C	4.45782	-2.55592	-0.35379
C	3.10441	-2.19437	-0.34236
C	2.09001	1.99858	-0.35017
C	1.75908	3.37851	-0.37226
C	2.79924	4.32288	-0.40795
C	4.14763	3.95822	-0.42538
C	4.44471	2.58904	-0.40443
C	3.45483	1.59747	-0.36873
C	-0.68403	2.81548	-0.34337
C	-2.04494	3.21876	-0.35032
C	-2.34237	4.59303	-0.36240
C	-1.35156	5.57750	-0.37238
C	-0.01726	5.14951	-0.37386
C	0.34613	3.79641	-0.36238
C	-2.77827	0.82399	-0.34182
C	-3.81049	-0.15452	-0.35982

C	-5.14323	0.27703	-0.36946
C	-5.50316	1.63159	-0.36839
C	-4.46935	2.57068	-0.36043
C	-3.11213	2.20374	-0.34938
C	-5.29802	-4.98287	-0.47484
C	-4.77349	-6.43011	-0.48274
C	-6.12938	-4.76144	-1.76032
C	-6.20439	-4.80251	0.76547
C	1.73209	-7.05883	-0.38300
C	2.56684	-7.37738	0.87965
C	2.57478	-7.34856	-1.64747
C	0.50562	-7.98879	-0.39784
C	6.96208	-2.08875	-0.38088
C	7.95459	-0.91248	-0.38710
C	7.20882	-2.93738	-1.65045
C	7.23577	-2.94668	0.87669
C	5.29006	4.99149	-0.47307
C	6.19463	4.81180	0.76864
C	4.76628	6.43899	-0.48304
C	6.12321	4.76838	-1.75710
C	-1.67089	7.08517	-0.38603
C	-3.18517	7.36172	-0.37859
C	-1.05088	7.74886	0.86614
C	-1.06807	7.72102	-1.66093
C	-6.99204	2.03014	-0.38101
C	-7.68739	1.44646	0.87132
C	-7.65970	1.46308	-1.65600

C	-7.18663	3.55690	-0.37291
C	1.07780	0.56014	3.28812
C	0.85371	-0.85488	3.28991
C	-0.56142	-1.07861	3.28809
C	-1.21191	0.19782	3.28658
C	-0.19869	1.21086	3.28649
H	-2.55709	-5.36882	-0.42306
H	-5.49986	-2.28271	-0.42741
H	3.36788	-4.90014	-0.35673
H	-0.77899	-5.89356	-0.38533
H	5.92796	0.47990	-0.37919
H	4.72305	-3.61063	-0.35743
H	2.54880	5.37859	-0.42700
H	5.49056	2.29145	-0.42150
H	-3.38158	4.90591	-0.36583
H	0.76291	5.90696	-0.38519
H	-5.93922	-0.46381	-0.37904
H	-4.72756	3.62471	-0.36471
H	-5.62114	-7.13108	-0.51560
H	-4.19097	-6.66362	0.42232
H	-4.14499	-6.63670	-1.36306
H	-6.95225	-5.49211	-1.81279
H	-5.50814	-4.88477	-2.66144
H	-6.57781	-3.75679	-1.79642
H	-7.02613	-5.53591	0.74622
H	-5.63756	-4.95333	1.69794
H	-6.65845	-3.80052	0.80587

H	2.86281	-8.43853	0.88264
H	3.48875	-6.77820	0.92985
H	1.98906	-7.18444	1.79754
H	2.86745	-8.41030	-1.67463
H	3.49882	-6.75131	-1.67674
H	2.00430	-7.13037	-2.56404
H	0.83674	-9.03815	-0.40813
H	-0.12581	-7.85373	0.49428
H	-0.11825	-7.83405	-1.29192
H	8.98534	-1.29766	-0.39707
H	7.85038	-0.27977	0.50835
H	7.83472	-0.27661	-1.27816
H	8.25345	-3.28626	-1.67786
H	7.02329	-2.34996	-2.56350
H	6.56307	-3.82807	-1.68735
H	8.28016	-3.29726	0.87837
H	7.07234	-2.36543	1.79811
H	6.59006	-3.83704	0.92142
H	7.01672	5.54482	0.74991
H	6.64814	3.80964	0.81026
H	5.62657	4.96369	1.70021
H	5.61431	7.13953	-0.51524
H	4.13934	6.64515	-1.36463
H	4.18264	6.67357	0.42109
H	6.94641	5.49872	-1.80919
H	6.57127	3.76353	-1.79117
H	5.50333	4.89089	-2.65929

H	-3.36322	8.44764	-0.38749
H	-3.68674	6.94201	-1.26462
H	-3.67516	6.95817	0.52149
H	-1.26486	8.82942	0.86962
H	0.04285	7.62959	0.90061
H	-1.46600	7.31832	1.79128
H	-1.28362	8.80099	-1.68592
H	0.02519	7.60170	-1.70693
H	-1.49412	7.26860	-2.57029
H	-8.75467	1.71934	0.87617
H	-7.23377	1.83670	1.79626
H	-7.62837	0.34777	0.90508
H	-8.72624	1.73771	-1.68152
H	-7.18409	1.86357	-2.56515
H	-7.60076	0.36485	-1.70206
H	-8.26128	3.79382	-0.38075
H	-6.75618	4.02394	0.52688
H	-6.74112	4.03524	-1.25918
H	-2.28773	0.36779	3.28012
H	-0.36859	2.28672	3.28097
H	2.04810	1.05500	3.28268
H	1.62370	-1.62511	3.28770
H	-1.05659	-2.04875	3.28281

Cartesian coordinates of **2a'''** at the B3LYP/def2-SVP level

Ru	-0.90232	-0.00104	0.00085
C	0.89380	0.03033	1.44015
C	0.89236	1.26338	0.69350

C	0.89268	1.23355	-0.74761
C	0.89554	-0.02923	-1.44229
C	0.89638	-1.26222	-0.69586
C	0.89504	-1.23256	0.74526
C	0.90563	0.06029	2.89663
C	0.92165	1.30855	3.57938
C	0.94845	1.30877	4.98403
C	0.96120	0.11824	5.70159
C	0.94949	-1.10091	5.03380
C	0.92299	-1.15858	3.63033
C	0.89712	2.53958	1.39583
C	0.90534	3.75512	0.65616
C	0.91815	4.97186	1.35853
C	0.92641	4.99794	2.74832
C	0.92590	3.81000	3.47020
C	0.91382	2.56548	2.81836
C	0.89675	2.47965	-1.50167
C	0.91236	2.44700	-2.92413
C	0.92255	3.66347	-3.62692
C	0.92233	4.88020	-2.95469
C	0.91535	4.91149	-1.56497
C	0.90449	3.72485	-0.81286
C	0.90801	-0.05937	-2.89841
C	0.92981	-1.30759	-3.58121
C	0.95655	-1.30769	-4.98583
C	0.96450	-0.11718	-5.70346
C	0.94832	1.10197	-5.03579

C	0.92142	1.15962	-3.63234
C	0.90875	-2.53860	-1.39784
C	0.92152	-3.75399	-0.65808
C	0.94383	-4.97063	-1.36030
C	0.95665	-4.99685	-2.75006
C	0.95065	-3.80903	-3.47212
C	0.92887	-2.56458	-2.82037
C	0.90365	-2.47887	1.49970
C	0.91800	-2.44605	2.92204
C	0.93037	-3.66245	3.62492
C	0.93381	-4.87924	2.95279
C	0.92922	-4.91056	1.56306
C	0.91664	-3.72388	0.81096
C	-2.72981	0.53071	-1.09010
C	-2.72543	1.20541	0.17368
C	-2.72144	0.21199	1.20587
C	-2.72252	-1.07662	0.57982
C	-2.72899	-0.87960	-0.83912
H	0.96287	2.24591	5.53702
H	0.92417	5.91941	0.82354
H	0.93655	3.86509	4.55694
H	0.93241	3.67333	-4.71500
H	0.92059	5.88049	-1.06976
H	0.97467	-2.24478	-5.53878
H	0.95437	-5.91806	-0.82520
H	0.96512	-3.86415	-4.55882
H	0.93863	-3.67220	4.71301



H	0.93744	-5.87952	1.06784
H	0.97485	-5.95368	-3.27621
H	0.98691	-0.13981	-6.79510
H	0.96045	2.01560	-5.62683
H	0.93102	5.81449	-3.52013
H	0.93666	5.95479	3.27467
H	0.98357	0.14086	6.79323
H	0.96481	-2.01452	5.62477
H	0.94363	-5.81349	3.51829
H	-2.73005	1.00631	-2.06999
H	-2.72976	-1.66458	-1.59420
H	-2.71547	-2.03743	1.09296
H	-2.71525	0.40269	2.27826
H	-2.72196	2.28424	0.32376

Cartesian coordinates of **2b'** at the B3LYP/def2-SVP level

Ru	-1.91498	-0.00394	0.51018
C	-0.23680	0.71484	-0.98398
C	-0.23211	-0.72386	-0.98115
C	0.98371	-1.43721	-0.68981
C	2.17275	-0.71620	-0.42576
C	2.16751	0.72511	-0.42601
C	0.97385	1.43734	-0.69288
C	-1.45866	1.43486	-1.30379
C	-2.66113	0.71752	-1.64938
C	-3.82373	1.45517	-2.00722
C	-3.80182	2.83152	-2.03570
C	-2.63694	3.53491	-1.68807

C	-1.46949	2.87744	-1.31041
C	-1.45012	-1.45299	-1.29490
C	-1.45257	-2.89558	-1.29273
C	-2.61814	-3.56211	-1.66031
C	-3.78847	-2.86769	-2.00769
C	-3.81749	-1.49132	-1.99021
C	-2.65739	-0.74473	-1.64267
C	0.97448	-2.88251	-0.66970
C	2.17363	-3.59631	-0.37234
C	2.13453	-5.00174	-0.30938
C	0.95767	-5.70098	-0.53862
C	-0.21008	-5.01227	-0.85293
C	-0.22666	-3.61171	-0.93441
C	3.40304	-1.43250	-0.15830
C	4.61518	-0.71934	0.08441
C	5.79508	-1.44107	0.31817
C	5.80163	-2.83265	0.32247
C	4.62502	-3.53338	0.09947
C	3.41328	-2.85975	-0.13951
C	3.39143	1.45049	-0.15356
C	3.38991	2.87770	-0.12935
C	4.59385	3.56013	0.12387
C	5.77421	2.86811	0.35405
C	5.77987	1.47659	0.34009
C	4.60843	0.74627	0.09104
C	0.95447	2.88252	-0.67538
C	-0.25016	3.60280	-0.94834

C	-0.24385	5.00359	-0.86982
C	0.91728	5.70107	-0.55026
C	2.09748	5.01046	-0.31222
C	2.14670	3.60518	-0.37161
C	-1.37848	-0.69305	2.49930
C	-2.69784	-1.17654	2.17234
C	-3.55126	-0.03309	1.94591
C	-2.76072	1.15917	2.14709
C	-1.41732	0.75461	2.48435
C	-0.20194	-1.53251	2.89329
C	-3.13184	-2.61056	2.15910
C	-5.02278	-0.07533	1.66338
C	-3.27198	2.56659	2.09721
C	-0.28970	1.66510	2.86357
H	-4.73645	0.93433	-2.28846
H	-2.66250	4.62202	-1.73712
H	-2.63801	-4.64966	-1.70147
H	-4.73435	-0.97744	-2.27071
H	3.03399	-5.56633	-0.07183
H	-1.11727	-5.58697	-1.03209
H	6.73367	-0.92078	0.49885
H	4.66072	-4.62101	0.10520
H	4.62027	4.64797	0.13663
H	6.72101	0.96325	0.52724
H	-1.15407	5.57154	-1.05501
H	2.99166	5.58193	-0.07123
H	-0.19914	-1.69597	3.98510

H	-0.22219	-2.51884	2.40983
H	0.74945	-1.05018	2.62942
H	-3.52200	-2.89612	3.15162
H	-2.29924	-3.28763	1.92439
H	-3.93057	-2.79110	1.42605
H	-5.59420	-0.08817	2.60792
H	-5.30311	-0.97416	1.09644
H	-5.35257	0.80310	1.09108
H	-3.70181	2.84847	3.07423
H	-4.06068	2.68870	1.34151
H	-2.47195	3.28383	1.86851
H	-0.29278	1.84149	3.95336
H	0.68756	1.23649	2.60172
H	-0.36955	2.64262	2.36868
H	0.90034	6.79139	-0.49127
H	6.69996	3.41499	0.54553
H	6.73394	-3.37276	0.50094
H	0.94852	-6.79125	-0.47694
H	-4.67880	-3.42788	-2.30180
H	-4.69365	3.38462	-2.33854

Cartesian coordinates of **2b''** at the B3LYP/def2-SVP level

Ru	-2.19952	-0.07336	1.37241
C	-0.87193	0.69753	-0.38894
C	-0.82227	-0.73930	-0.39134
C	0.44668	-1.41411	-0.32977
C	1.63734	-0.65670	-0.29099
C	1.58806	0.78266	-0.29139

C	0.34778	1.45719	-0.32805
C	-2.15222	1.37588	-0.46269
C	-3.37695	0.62586	-0.57011
C	-4.61050	1.32957	-0.67584
C	-4.67114	2.71020	-0.69964
C	-3.45361	3.42691	-0.58488
C	-2.21360	2.81800	-0.45456
C	-2.05304	-1.50347	-0.47107
C	-2.01530	-2.94651	-0.47215
C	-3.20832	-3.63858	-0.62223
C	-4.47106	-3.00687	-0.74756
C	-4.50659	-1.62586	-0.70613
C	-3.32619	-0.83939	-0.57969
C	0.48459	-2.85569	-0.30774
C	1.73319	-3.53421	-0.23221
C	1.74493	-4.94069	-0.16226
C	0.58064	-5.70770	-0.17148
C	-0.63792	-5.01988	-0.27141
C	-0.71815	-3.62553	-0.34797
C	2.91376	-1.33199	-0.24888
C	4.12717	-0.58753	-0.23073
C	5.34941	-1.27577	-0.20427
C	5.43269	-2.67196	-0.19228
C	4.23025	-3.38500	-0.20108
C	2.97475	-2.75761	-0.22574
C	2.81433	1.54374	-0.25271
C	2.77882	2.96733	-0.23443

C	3.99068	3.68405	-0.21333
C	5.23454	3.05568	-0.20505
C	5.24556	1.65255	-0.21251
C	4.07842	0.88159	-0.23383
C	0.28803	2.89710	-0.30761
C	-0.96458	3.58409	-0.34264
C	-0.97729	4.98088	-0.27438
C	0.19331	5.74983	-0.18832
C	1.40643	5.06324	-0.18101
C	1.48896	3.65824	-0.24126
C	-5.99239	3.48694	-0.84724
C	-7.20618	2.55044	-0.98029
C	-5.92274	4.37379	-2.11301
C	-6.19985	4.37822	0.39999
C	-5.73175	-3.87151	-0.93019
C	-5.89350	-4.80185	0.29507
C	-5.58047	-4.72394	-2.21249
C	-7.00682	-3.02028	-1.06375
C	0.58853	-7.24615	-0.08231
C	2.01359	-7.81557	0.03869
C	-0.06169	-7.83431	-1.35668
C	-0.21679	-7.69001	1.16147
C	6.77624	-3.42727	-0.17189
C	6.84582	-4.31309	1.09406
C	7.98269	-2.47086	-0.15736
C	6.87912	-4.31768	-1.43242
C	6.56442	3.83443	-0.18853

C	6.34667	5.35820	-0.18317
C	7.36298	3.45460	1.08046
C	7.38624	3.46699	-1.44625
C	0.09966	7.28619	-0.11255
C	-0.73055	7.68788	1.12920
C	-0.59071	7.81835	-1.39040
C	1.48436	7.94915	-0.00101
C	-1.19140	-0.62482	3.21157
C	-2.45631	-1.29301	3.15387
C	-3.48715	-0.29536	3.11709
C	-2.85525	0.99018	3.15290
C	-1.43717	0.79070	3.20961
H	-5.52785	0.75721	-0.76370
H	-3.50233	4.51302	-0.61253
H	-3.18072	-4.72506	-0.66034
H	-5.45974	-1.11664	-0.80184
H	2.69970	-5.45160	-0.09047
H	-1.55584	-5.60386	-0.28314
H	6.27228	-0.70503	-0.19357
H	4.27837	-4.47140	-0.19478
H	3.95819	4.76863	-0.20900
H	6.20992	1.15008	-0.20214
H	-1.93190	5.50283	-0.28371
H	2.32536	5.63714	-0.12034
H	-8.12476	3.14719	-1.08449
H	-7.33311	1.90890	-0.09401
H	-7.13352	1.90474	-1.86936

H	-6.86300	4.93450	-2.23425
H	-5.77240	3.76384	-3.01761
H	-5.10605	5.10989	-2.06351
H	-7.13898	4.94639	0.30823
H	-6.26143	3.77096	1.31727
H	-5.38586	5.10745	0.53180
H	-6.78870	-5.43262	0.17702
H	-5.03194	-5.47463	0.42407
H	-6.01021	-4.22061	1.22370
H	-6.47776	-5.34504	-2.36183
H	-4.71554	-5.40290	-2.16353
H	-5.45784	-4.08581	-3.10168
H	-7.87947	-3.67806	-1.19244
H	-7.19068	-2.40658	-0.16777
H	-6.96832	-2.35368	-1.93945
H	1.96950	-8.91331	0.10389
H	2.52680	-7.45412	0.94361
H	2.63452	-7.56562	-0.83579
H	-0.06471	-8.93502	-1.30989
H	0.49267	-7.53452	-2.25995
H	-1.10546	-7.50650	-1.47900
H	-0.22038	-8.78873	1.24134
H	0.22423	-7.28440	2.08585
H	-1.26643	-7.36064	1.11628
H	7.80019	-4.86277	1.12308
H	6.03529	-5.05717	1.12301
H	6.77677	-3.70434	2.00953



H	8.91673	-3.05280	-0.14268
H	8.01168	-1.82892	-1.05177
H	7.98650	-1.82406	0.73411
H	7.83410	-4.86710	-1.43449
H	6.06944	-5.06177	-1.47986
H	6.83352	-3.71236	-2.35151
H	7.32016	5.87144	-0.17206
H	5.80647	5.70124	-1.07948
H	5.79034	5.69304	0.70643
H	8.31866	4.00209	1.10699
H	7.59762	2.37979	1.11654
H	6.80143	3.70726	1.99381
H	8.34296	4.01336	-1.44914
H	7.61987	2.39225	-1.48934
H	6.84208	3.72996	-2.36709
H	-0.80561	8.78474	1.19857
H	-0.26219	7.32094	2.05628
H	-1.75656	7.29040	1.08986
H	-0.66723	8.91681	-1.35337
H	-0.01912	7.54840	-2.29234
H	-1.61049	7.42045	-1.50734
H	1.36838	9.04218	0.05418
H	2.02290	7.63037	0.90521
H	2.11810	7.73215	-0.87501
H	-3.36303	1.95355	3.12720
H	-4.55882	-0.48281	3.06995
H	-2.60822	-2.37133	3.12872

H	-0.68064	1.57334	3.24636
H	-0.21441	-1.10550	3.24100

Cartesian coordinates of **2b'''** at the B3LYP/def2-SVP level

Ru	2.12692	0.00013	0.92440
C	0.55839	-0.71995	-0.66409
C	0.55836	0.71998	-0.66412
C	-0.67383	1.43827	-0.46340
C	-1.88244	0.72095	-0.29970
C	-1.88242	-0.72099	-0.29974
C	-0.67378	-1.43829	-0.46339
C	1.79896	-1.44462	-0.88865
C	3.02599	-0.73162	-1.15092
C	4.21211	-1.47457	-1.40812
C	4.18760	-2.85063	-1.42612
C	2.99801	-3.54962	-1.16202
C	1.80711	-2.88869	-0.87656
C	1.79887	1.44469	-0.88886
C	1.80693	2.88876	-0.87696
C	2.99770	3.54973	-1.16290
C	4.18726	2.85079	-1.42721
C	4.21189	1.47473	-1.40889
C	3.02592	0.73175	-1.15117
C	-0.65882	2.88295	-0.43423
C	-1.87410	3.60026	-0.22545
C	-1.83191	5.00441	-0.13961
C	-0.63657	5.69862	-0.26567
C	0.54800	5.00669	-0.49998

C	0.56236	3.60767	-0.59968
C	-3.12749	1.44146	-0.13493
C	-4.35943	0.73272	-0.00502
C	-5.55182	1.45910	0.12813
C	-5.55214	2.85082	0.14092
C	-4.35737	3.54712	0.02832
C	-3.13233	2.86863	-0.10653
C	-3.12746	-1.44154	-0.13504
C	-3.13228	-2.86872	-0.10680
C	-4.35731	-3.54724	0.02794
C	-5.55210	-2.85097	0.14056
C	-5.55180	-1.45925	0.12792
C	-4.35941	-0.73284	-0.00511
C	-0.65874	-2.88296	-0.43428
C	0.54811	-5.00669	-0.50011
C	-0.63649	-5.69865	-0.26610
C	-1.83185	-5.00447	-0.14007
C	-1.87403	-3.60031	-0.22571
C	1.47800	0.71828	2.86553
C	2.82001	1.15873	2.62850
C	3.65133	-0.00001	2.47987
C	2.82019	-1.15892	2.62805
C	1.47810	-0.71875	2.86525
H	5.14574	-0.95765	-1.61893
H	3.02513	-4.63717	-1.19884
H	3.02471	4.63728	-1.19995
H	5.14550	0.95785	-1.61991

H	-2.74375	5.57174	0.03633
H	1.46992	5.57749	-0.59884
H	-6.50511	0.94294	0.22318
H	-4.38849	4.63487	0.03703
H	-4.38842	-4.63499	0.03655
H	-6.50510	-0.94311	0.22298
H	1.47004	-5.57747	-0.59896
H	-2.74370	-5.57184	0.03565
H	-0.62562	-6.78767	-0.18610
H	-6.49410	-3.39467	0.23930
H	-6.49414	3.39449	0.23975
H	-0.62569	6.78762	-0.18548
H	5.09871	3.40831	-1.65358
H	5.09918	-3.40813	-1.65204
H	3.14982	-2.19493	2.55897
H	0.61080	-1.35988	3.01718
H	0.61061	1.35923	3.01773
H	3.14951	2.19482	2.55982
H	4.72356	0.00012	2.28914
C	0.56249	-3.60765	-0.59960

Cartesian coordinates of **2c'** at the B3LYP/def2-SVP level

Ru	-3.12032	-0.00133	0.09195
C	0.13988	-0.00038	-0.94105
C	0.81849	-1.23573	-0.75585
C	2.18616	-1.23671	-0.35372
C	2.86568	0.00036	-0.13978
C	2.18537	1.23730	-0.35367

C	0.81715	1.23572	-0.75414
C	-1.26609	-0.00069	-1.31447
C	-1.97145	-1.24689	-1.49206
C	-3.37041	-1.21983	-1.77865
C	-4.06192	-0.00177	-1.94722
C	-3.37197	1.21681	-1.77833
C	-1.97352	1.24539	-1.48824
C	0.12913	-2.49318	-0.98409
C	0.82429	-3.72926	-0.84291
C	0.14573	-4.92960	-1.12720
C	-1.18235	-4.93537	-1.53119
C	-1.87568	-3.73401	-1.64567
C	-1.24472	-2.51302	-1.36663
C	2.88321	-2.49141	-0.15955
C	4.24078	-2.49819	0.27763
C	4.89609	-3.72945	0.44930
C	4.24525	-4.93274	0.20628
C	2.92104	-4.93355	-0.21551
C	2.22062	-3.73114	-0.40627
C	4.24355	0.00079	0.30484
C	4.92694	1.23340	0.52931
C	6.25016	1.20527	0.99968
C	6.90271	0.00179	1.23846
C	6.24940	-1.20217	1.00449
C	4.92599	-1.23138	0.53457
C	2.88331	2.49233	-0.16439
C	2.22038	3.73160	-0.41246

C	2.92372	4.93404	-0.23263
C	4.25047	4.93368	0.18102
C	4.90075	3.73088	0.42799
C	4.24271	2.49968	0.26701
C	0.12623	2.49291	-0.97987
C	-1.24866	2.51199	-1.35801
C	-1.88322	3.73337	-1.62706
C	-1.19152	4.93540	-1.50964
C	0.13922	4.92984	-1.11446
C	0.82107	3.72937	-0.83952
C	-2.41465	-0.38991	2.14607
C	-3.55521	-1.22924	1.86998
C	-4.68203	-0.37026	1.59272
C	-4.23618	0.99952	1.70382
C	-2.83646	0.98688	2.04799
C	-1.05177	-0.86327	2.55188
C	-3.58526	-2.72525	1.96213
C	-6.09463	-0.81707	1.36047
C	-5.10451	2.21895	1.60825
C	-1.99358	2.19021	2.34229
H	-3.92717	-2.14916	-1.86633
H	-3.93006	2.14540	-1.86616
H	0.66312	-5.88342	-1.04318
H	-2.91365	-3.76457	-1.97307
H	5.93420	-3.76003	0.77449
H	2.43607	-5.89174	-0.39274
H	6.78796	2.13193	1.19075

H	6.78686	-2.12837	1.19871
H	2.43951	5.89191	-0.41350
H	5.94080	3.76172	0.74693
H	-2.92273	3.76394	-1.94970
H	0.65529	5.88416	-1.02850
H	-0.97594	-0.90956	3.65197
H	-0.83769	-1.86732	2.16127
H	-0.26234	-0.18862	2.19242
H	-3.76871	-3.03875	3.00441
H	-2.63367	-3.17444	1.64492
H	-4.38462	-3.15683	1.34380
H	-6.62563	-0.91570	2.32310
H	-6.13947	-1.79465	0.86014
H	-6.65643	-0.09689	0.74937
H	-5.53061	2.45917	2.59781
H	-5.94658	2.07252	0.91728
H	-4.53775	3.09913	1.27397
H	-2.10304	2.48144	3.40136
H	-0.92774	1.99561	2.16172
H	-2.28535	3.05439	1.72915
H	4.78205	5.87871	0.31180
H	7.93026	0.00220	1.60861
H	4.77439	-5.87778	0.34654
H	-1.68065	-5.87935	-1.76145
H	-5.13168	-0.00271	-2.16167
H	-1.69290	5.87974	-1.73172

Cartesian coordinates of  $2c''$  at the B3LYP/def2-SVP level

Ru	-3.79008	-0.03987	1.17405
C	-0.75306	0.00493	-0.41442
C	-0.03942	-1.22117	-0.36765
C	1.37970	-1.20590	-0.26003
C	2.07355	0.03727	-0.19851
C	1.35031	1.26501	-0.25553
C	-0.06811	1.24796	-0.36304
C	-2.19924	-0.01162	-0.52023
C	-2.91411	-1.26326	-0.55916
C	-4.34251	-1.24418	-0.61505
C	-5.10011	-0.04573	-0.68315
C	-4.37178	1.17028	-0.60157
C	-2.94454	1.22250	-0.55016
C	-0.74657	-2.48393	-0.43271
C	-0.03009	-3.71516	-0.40760
C	-0.74819	-4.91810	-0.49315
C	-2.14196	-4.97657	-0.60343
C	-2.82844	-3.75963	-0.61836
C	-2.16512	-2.52551	-0.52955
C	2.11525	-2.44969	-0.21547
C	3.53286	-2.44497	-0.09776
C	4.22169	-3.67044	-0.07307
C	3.57339	-4.90394	-0.15197
C	2.17680	-4.88673	-0.25745
C	1.43330	-3.69983	-0.29292
C	3.51234	0.05439	-0.07134
C	4.21786	1.28895	-0.00108



C	5.61482	1.27214	0.15052
C	6.35044	0.08790	0.22877
C	5.63951	-1.11515	0.14139
C	4.24700	-1.16694	-0.00792
C	2.05541	2.52458	-0.20828
C	1.34599	3.75638	-0.28735
C	2.06204	4.96588	-0.25699
C	3.45300	5.01319	-0.14746
C	4.13066	3.79066	-0.06197
C	3.47610	2.55155	-0.08805
C	-0.80239	2.49385	-0.42509
C	-2.22477	2.50292	-0.52163
C	-2.90984	3.71920	-0.61462
C	-2.24986	4.95642	-0.59802
C	-0.86024	4.93138	-0.48369
C	-0.11526	3.73855	-0.39987
C	-6.62495	-0.06020	-0.89399
C	-7.26990	-1.34247	-0.33166
C	-6.85531	-0.00745	-2.42524
C	-7.30558	1.15838	-0.23891
C	-2.85204	-6.34057	-0.70739
C	-2.52758	-7.18427	0.54753
C	-2.35247	-7.07986	-1.97084
C	-4.38118	-6.19488	-0.80766
C	4.32777	-6.24827	-0.12580
C	5.85215	-6.05837	-0.02807
C	4.02101	-7.03364	-1.42233

C	3.86246	-7.07024	1.09893
C	7.88136	0.06406	0.40555
C	8.23101	-0.68222	1.71446
C	8.48260	1.47920	0.48269
C	8.52382	-0.66931	-0.79508
C	4.24573	6.33470	-0.12062
C	3.33019	7.56635	-0.24013
C	5.02397	6.43715	1.21203
C	5.24194	6.35676	-1.30368
C	-3.05982	6.26288	-0.71093
C	-4.07477	6.34044	0.45355
C	-3.81769	6.27622	-2.05922
C	-2.16177	7.51143	-0.65000
C	-2.82036	-0.67162	3.05302
C	-4.12754	-1.24758	2.98603
C	-5.07985	-0.17649	2.95111
C	-4.35672	1.06054	3.00099
C	-2.96199	0.75355	3.06437
H	-4.87583	-2.18853	-0.60599
H	-4.92733	2.10173	-0.58237
H	-0.19919	-5.85682	-0.47922
H	-3.91021	-3.77870	-0.70791
H	5.30381	-3.65964	0.00708
H	1.65763	-5.84081	-0.31536
H	6.14672	2.21595	0.21385
H	6.19980	-2.04544	0.19740
H	1.51769	5.90248	-0.32355

H	5.21467	3.81186	0.02163
H	-3.99363	3.71985	-0.71008
H	-0.32809	5.87701	-0.46440
H	-8.36241	-1.28883	-0.44833
H	-7.05082	-1.47231	0.73970
H	-6.94062	-2.24807	-0.86294
H	-7.93409	-0.01824	-2.64650
H	-6.39737	-0.87168	-2.93121
H	-6.42864	0.90728	-2.86558
H	-8.39588	1.08540	-0.36592
H	-7.09330	1.21101	0.84012
H	-6.99939	2.11086	-0.69680
H	-3.02716	-8.16441	0.48820
H	-1.44818	-7.37089	0.65375
H	-2.87343	-6.68232	1.46526
H	-2.84549	-8.06114	-2.05893
H	-1.26660	-7.25704	-1.94366
H	-2.57561	-6.50404	-2.88289
H	-4.84512	-7.19019	-0.87963
H	-4.80849	-5.69978	0.07909
H	-4.68475	-5.62904	-1.70269
H	6.34840	-7.04071	-0.01518
H	6.14467	-5.53234	0.89416
H	6.25393	-5.49972	-0.88792
H	4.55613	-7.99676	-1.42053
H	4.33983	-6.46963	-2.31308
H	2.94776	-7.25349	-1.53053

H	4.38710	-8.03863	1.13098
H	4.07570	-6.53719	2.03901
H	2.78222	-7.28057	1.06975
H	9.32304	-0.70998	1.85827
H	7.87237	-1.72289	1.70588
H	7.78555	-0.18070	2.58819
H	9.57387	1.41179	0.60930
H	8.29561	2.05870	-0.43507
H	8.08857	2.04908	1.33882
H	9.61976	-0.69532	-0.68404
H	8.17580	-1.71008	-0.87915
H	8.29023	-0.15933	-1.74305
H	3.93770	8.48386	-0.21949
H	2.76419	7.56961	-1.18497
H	2.61343	7.63056	0.59371
H	5.60316	7.37389	1.24504
H	5.73316	5.60542	1.34198
H	4.33814	6.43128	2.07407
H	5.81504	7.29782	-1.30265
H	5.96651	5.52989	-1.25123
H	4.71500	6.28062	-2.26797
H	-4.65929	7.27204	0.38956
H	-3.56210	6.32874	1.42854
H	-4.79016	5.50338	0.43737
H	-4.40543	7.20280	-2.15821
H	-3.11811	6.22581	-2.90831
H	-4.51709	5.43061	-2.15010

H	-2.78095	8.41760	-0.73145
H	-1.60820	7.57651	0.29977
H	-1.43516	7.53734	-1.47683
H	-1.87986	-1.22056	3.08217
H	-2.14838	1.47664	3.10593
H	-4.35780	-2.31186	2.97112
H	-6.16277	-0.28421	2.92087
H	-4.79215	2.05878	3.00073

Cartesian coordinates of  $2c'''$  at the B3LYP/def2-SVP level

Ru	-3.51624	-0.00060	0.55958
C	-0.31482	-0.00065	-0.66832
C	0.37539	-1.23690	-0.53512
C	1.77251	-1.23730	-0.25136
C	2.46843	0.00065	-0.10098
C	1.77136	1.23794	-0.25138
C	0.37435	1.23624	-0.53564
C	-1.74226	-0.00132	-0.94340
C	-2.45974	-1.24872	-1.06753
C	-3.87372	-1.22076	-1.27566
C	-4.57322	-0.00252	-1.40857
C	-3.87447	1.21636	-1.27761
C	-2.46050	1.24546	-1.06954
C	-0.33170	-2.49420	-0.69648
C	0.36918	-3.73082	-0.59481
C	-0.33630	-4.93245	-0.79441
C	-1.69382	-4.94028	-1.08492
C	-2.38872	-3.73814	-1.17061

C	-1.73157	-2.51556	-0.96985
C	2.48359	-2.49166	-0.11587
C	3.87719	-2.49780	0.18761
C	4.54388	-3.72901	0.30766
C	3.87140	-4.93294	0.13841
C	2.51316	-4.93441	-0.15574
C	1.79938	-3.73206	-0.28820
C	3.88280	0.00132	0.20867
C	4.58469	1.23402	0.36654
C	5.95186	1.20590	0.68773
C	6.62788	0.00257	0.84843
C	5.95322	-1.20137	0.68659
C	4.58613	-1.23073	0.36524
C	2.48107	2.49298	-0.11494
C	1.79574	3.73274	-0.28746
C	2.50775	4.93582	-0.15213
C	3.86547	4.93566	0.14442
C	4.53925	3.73234	0.31290
C	3.87431	2.50045	0.19015
C	-0.33360	2.49286	-0.69848
C	-1.73317	2.51289	-0.97350
C	-2.39078	3.73471	-1.17730
C	-1.69669	4.93742	-1.09286
C	-0.33967	4.93095	-0.80004
C	0.36619	3.73010	-0.59707
C	-2.86849	-0.71499	2.54501
C	-4.20635	-1.15871	2.30184

C	-5.03535	0.00034	2.14661
C	-4.20688	1.16003	2.29996
C	-2.86881	0.71730	2.54387
H	-4.43698	-2.14919	-1.32517
H	-4.43827	2.14439	-1.32847
H	0.18188	-5.88733	-0.73103
H	-3.45064	-3.77140	-1.40856
H	5.60760	-3.75922	0.53521
H	2.01316	-5.89311	-0.28059
H	6.50740	2.13238	0.81887
H	6.50977	-2.12734	0.81707
H	2.00665	5.89404	-0.27618
H	5.60255	3.76359	0.54227
H	-3.45236	3.76689	-1.41692
H	0.17792	5.88623	-0.73784
H	4.40277	5.88113	0.24475
H	7.69043	0.00306	1.10106
H	4.41011	-5.87787	0.23626
H	-2.21363	-5.88646	-1.24855
H	-5.65417	-0.00298	-1.55692
H	-2.21677	5.88298	-1.25925
H	-4.53865	2.19613	2.24858
H	-2.00048	1.35714	2.69581
H	-1.99985	-1.35418	2.69788
H	-4.53772	-2.19502	2.25209
H	-6.10966	-0.00002	1.96661

Cartesian coordinates of hexabenzocoronene at the B3LYP/def2-SVP level

C	0.00000	1.42593	0.00000
C	1.23489	0.71296	0.00000
C	1.23489	-0.71296	0.00000
C	0.00000	-1.42593	0.00000
C	-1.23489	-0.71296	0.00000
C	-1.23489	0.71296	0.00000
C	0.00000	-2.87552	0.00000
C	-1.23154	-3.59657	0.00000
C	1.23154	-3.59657	0.00000
C	-1.20283	-5.00153	0.00000
C	1.20283	-5.00153	0.00000
C	0.00000	-5.69685	0.00000
H	-2.13011	-5.57157	0.00000
H	2.13011	-5.57157	0.00000
H	0.00000	-6.78949	0.00000
C	2.49027	-1.43776	0.00000
C	3.73049	-0.73174	0.00000
C	2.49896	-2.86483	0.00000
C	4.93287	-1.45909	0.00000
C	3.73004	-3.54245	0.00000
C	4.93361	-2.84842	0.00000
H	5.89017	-0.94105	0.00000
H	3.76006	-4.63051	0.00000
H	5.87987	-3.39474	0.00000
C	2.49027	1.43776	0.00000
C	2.49896	2.86483	0.00000
C	3.73049	0.73174	0.00000



C	3.73004	3.54245	0.00000
C	4.93287	1.45909	0.00000
C	4.93361	2.84842	0.00000
H	3.76006	4.63051	0.00000
H	5.89017	0.94105	0.00000
H	5.87987	3.39474	0.00000
C	0.00000	2.87552	0.00000
C	-1.23154	3.59657	0.00000
C	1.23154	3.59657	0.00000
C	-1.20283	5.00153	0.00000
C	1.20283	5.00153	0.00000
C	0.00000	5.69685	0.00000
H	-2.13011	5.57157	0.00000
H	2.13011	5.57157	0.00000
H	0.00000	6.78949	0.00000
C	-2.49027	1.43776	0.00000
C	-3.73049	0.73174	0.00000
C	-2.49896	2.86483	0.00000
C	-4.93287	1.45909	0.00000
C	-3.73004	3.54245	0.00000
C	-4.93361	2.84842	0.00000
H	-5.89017	0.94105	0.00000
H	-3.76006	4.63051	0.00000
H	-5.87987	3.39474	0.00000
C	-2.49027	-1.43776	0.00000
C	-2.49896	-2.86483	0.00000
C	-3.73049	-0.73174	0.00000

C	-3.73004	-3.54245	0.00000
C	-4.93287	-1.45909	0.00000
C	-4.93361	-2.84842	0.00000
H	-3.76006	-4.63051	0.00000
H	-5.89017	-0.94105	0.00000
H	-5.87987	-3.39474	0.00000

Cartesian coordinates of benzene at the B3LYP/def2-SVP level (including the positions of the NICS calculations)

C	0.000000	1.399200	0.000000
C	1.211743	0.699600	0.000000
C	1.211743	-0.699600	0.000000
C	0.000000	-1.399200	0.000000
C	-1.211743	-0.699600	0.000000
C	-1.211743	0.699600	0.000000
H	0.000000	2.492300	0.000000
H	2.158395	1.246150	0.000000
H	2.158395	-1.246150	0.000000
H	0.000000	-2.492300	0.000000
H	-2.158395	-1.246150	0.000000
H	-2.158395	1.246150	0.000000
Bq	0.0	0.0	0.0
Bq	0.0	0.0	0.25
Bq	0.0	0.0	0.5
Bq	0.0	0.0	1.0
Bq	0.0	0.0	1.5
Bq	0.0	0.0	2.0
Bq	0.0	0.0	3.0

Bq	0.0	0.0	4.0
Bq	0.0	0.0	5.0

Cartesian coordinates of the cyclopentadiene anion ( $\text{Cp}^-$ ) at the B3LYP/def2-SVP level (including the positions of the NICS calculations)

C	0.466574	1.111337	0.000000
H	0.890976	2.122374	0.000000
C	1.201123	-0.100316	0.000000
H	2.293824	-0.191519	0.000000
C	0.275761	-1.173336	0.000000
H	0.526685	-2.240739	0.000000
C	-0.912765	0.787160	0.000000
H	-1.743171	1.503218	0.000000
C	-1.030694	-0.624845	0.000000
H	-1.968315	-1.193334	0.000000
Bq	0.0	0.0	0.0
Bq	0.0	0.0	0.25
Bq	0.0	0.0	0.5
Bq	0.0	0.0	1.0
Bq	0.0	0.0	1.5
Bq	0.0	0.0	2.0
Bq	0.0	0.0	3.0
Bq	0.0	0.0	4.0
Bq	0.0	0.0	5.0

Cartesian coordinates of the pentamethylcyclopentadiene anion ( $\text{Cp}^{*-}$ ) at the B3LYP/def2-SVP level (including the positions of the NICS calculations)

C	0.000000	1.209978	-0.028520
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C	-1.150758	0.373904	-0.028520
C	-0.711207	-0.978893	-0.028520
C	1.150758	0.373904	-0.028520
C	0.711207	-0.978893	-0.028520
C	0.000000	2.714041	-0.014065
H	-0.886385	3.135929	-0.525171
H	0.000000	3.163783	1.005218
H	0.886385	3.135929	-0.525171
C	-2.581206	0.838685	-0.014065
H	-3.008936	0.977663	1.005218
H	-2.708538	1.812058	-0.525171
H	-3.256354	0.126053	-0.525171
C	-1.595273	-2.195705	-0.014065
H	-1.859625	-2.559554	1.005218
H	-2.560353	-2.016016	-0.525171
H	-1.126152	-3.058024	-0.525171
C	2.581206	0.838685	-0.014065
H	3.008936	0.977663	1.005218
H	3.256354	0.126053	-0.525171
H	2.708538	1.812058	-0.525171
C	1.595273	-2.195705	-0.014065
H	2.560353	-2.016016	-0.525171
H	1.859625	-2.559554	1.005218
H	1.126152	-3.058024	-0.525171
Bq	0.0	0.0	0.0
Bq	0.0	0.0	0.25
Bq	0.0	0.0	0.5

Bq	0.0	0.0	1.0
Bq	0.0	0.0	1.5
Bq	0.0	0.0	2.0
Bq	0.0	0.0	3.0
Bq	0.0	0.0	4.0
Bq	0.0	0.0	5.0

Cartesian coordinates of ruthenocene, Ru(Cp)<sub>2</sub> at the B3LYP/def2-SVP level

H	-0.16399	2.30225	1.85281
C	-0.08656	1.21612	1.83712
C	-1.18335	0.29348	1.83712
C	1.12985	0.45813	1.83712
C	-0.64479	-1.03474	1.83712
H	-2.24024	0.55547	1.85281
C	0.78485	-0.93298	1.83712
H	2.13889	0.86740	1.85281
H	-1.22056	-1.95895	1.85281
H	1.48590	-1.76617	1.85281
C	0.64479	-1.03474	-1.83712
C	1.18335	0.29348	-1.83712
C	-0.78485	-0.93298	-1.83712
H	1.22056	-1.95895	-1.85281
C	0.08656	1.21612	-1.83712
H	2.24024	0.55547	-1.85281
C	-1.12985	0.45813	-1.83712
H	-1.48590	-1.76617	-1.85281
H	0.16399	2.30225	-1.85281
H	-2.13889	0.86740	-1.85281

Ru	0.00000	0.00000	0.00000
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Cartesian coordinates of [CpRu-Bz<sup>+</sup> at the B3LYP/def2-SVP level

C	1.91480	-0.13429	1.21004
C	1.91291	1.10884	0.50138
C	1.91441	-1.19312	0.24662
H	1.92806	-0.25360	2.29303
C	1.91196	0.81919	-0.90055
H	1.92504	2.10179	0.95024
C	1.91308	-0.60376	-1.05782
H	1.92745	-2.26002	0.46733
H	1.92320	1.55248	-1.70635
H	1.92492	-1.14366	-2.00437
Ru	0.06886	-0.00088	0.00107
C	-1.67175	-0.37442	-1.37065
C	-1.67698	-1.37276	-0.36037
C	-1.66864	1.00003	-1.01153
H	-1.63341	-0.66351	-2.42258
C	-1.67913	-0.99712	1.00908
H	-1.64111	-2.42824	-0.63648
C	-1.66949	1.37601	0.35840
H	-1.62913	1.76720	-1.78700
C	-1.67514	0.37715	1.36859
H	-1.64449	-1.76473	1.78441
H	-1.62846	2.43118	0.63474
H	-1.63787	0.66518	2.42087