

**Versatile reactivity of amines towards the ruthenocenylmethylium cation**



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Geometry optimization and transition state search were performed without constraints using PBE and BPBE exchange-correlation functional,<sup>1</sup> the scalar-relativistic Hamiltonian,<sup>2</sup> atomic basis sets of generally-contracted Gaussian functions,<sup>3</sup> and a density-fitting technique<sup>4</sup> as implemented in a recent version of Priroda code.<sup>5</sup> The all-electron triple- $\zeta$  basis set L2 (close to cc-pVTZ)<sup>6</sup> augmented by two polarization functions was used.<sup>7</sup> Frequency calculations were performed at the same level of theory. The ChemCraft software<sup>8</sup> was used for molecular modeling and visualization.

**References**

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- <sup>8</sup> G. A. Zhurko, *ChemCraft 1.6*, <http://www.chemcraftprog.com>, 2011.

## Cartesian coordinates and energies for structures optimized at PBE/L2

### [Cp\*Ru(C<sub>5</sub>Me<sub>4</sub>CH<sub>2</sub>)]<sup>+</sup> (1)

PBE/L2				BPBE/L2			
E = -5310.328443 a.u. E <sub>0</sub> = -5309.906138 a.u.				E = -5310.781807 a.u. E <sub>0</sub> = -5310.359506 a.u.			
ZPVE = 0.422305 a.u. = 265.0006 kcal/mol				ZPVE = 0.422301 a.u. = 264.9979 kcal/mol			
T = 298.150 K: G = 231.6391 kcal/mol				T = 298.150 K: G = 231.3815 kcal/mol			
44	-0.06351082	-0.18135886	-0.00000065	44	-0.00555389	0.19013392	-0.00000023
6	1.74174530	1.12687020	0.00000049	6	1.33705832	-1.60398163	0.00000032
6	-1.94249475	-1.05828542	0.00000062	6	2.06273905	0.48444086	0.73297571
6	1.81447736	-1.07850841	-0.73145787	6	1.62529709	-0.81054869	-1.17484690
6	1.78087724	0.28519597	1.17276506	6	2.06273869	0.48444059	-0.73297457
6	1.81447670	-1.07850981	0.73145728	6	1.62529757	-0.81054836	1.17484769
6	-1.80007491	1.13728608	-0.72607629	6	0.96005077	-3.05621034	0.00000107
6	1.78087917	0.28519761	-1.17276461	1	1.87364983	-3.67246258	0.00000025
6	-1.91960996	-0.20289240	-1.19743170	1	0.38298931	-3.33576674	-0.88965600
6	1.79131637	2.62146842	0.00000179	1	0.38299087	-3.33576572	0.88965943
1	2.84037577	2.95735912	0.00000266	6	1.59255132	-1.29337771	-2.59416103
1	1.31557829	3.05122530	0.89014288	1	2.56726567	-1.73266242	-2.86171014
1	1.31557975	3.05122678	-0.89013943	1	1.39810129	-0.47721806	-3.30056249
6	1.86976829	0.75442876	2.58898825	1	0.83349336	-2.06963117	-2.74985769
1	2.92458024	0.89125916	2.87574658	6	2.61093340	1.56982321	1.61124843
1	1.43363492	0.02927075	3.28713210	1	3.68394435	1.39571661	1.79288138
1	1.36636480	1.71812482	2.73579036	1	2.11516310	1.59834236	2.58966027
6	-1.80007500	1.13728631	0.72607487	1	2.51702952	2.56129096	1.15197314
6	-1.10346076	-2.19489194	0.00000194	6	1.59255224	-1.29337896	2.59416142
1	-0.93784017	-2.74733589	-0.92453416	1	2.56726739	-1.73266276	2.86170862
1	-0.93784050	-2.74733400	0.92453920	1	0.83349572	-2.06963383	2.74985811
6	1.99436168	-2.27639290	-1.60746882	1	1.39810117	-0.47722058	3.30056383
1	3.06609317	-2.44403381	-1.79960307	6	2.61093236	1.56982247	-1.61124778
1	1.50453129	-2.14996602	-2.58131589	1	3.68394378	1.39571758	-1.79288084
1	1.60169619	-3.18927281	-1.14317476	1	2.51702851	2.56128994	-1.15197226
6	1.86977216	0.75443038	-2.58898788	1	2.11516259	1.59834225	-2.58965991
1	2.92458211	0.89126394	-2.87575208	6	-1.53674576	1.59572285	-0.00000021
1	1.36636486	1.71812488	-2.73578736	6	-2.07737170	-0.53991724	0.72757778
1	1.43363612	0.02927526	-3.28713304	6	-1.77835214	0.77412215	1.19993113
6	-1.91960952	-0.20289130	1.19743206	6	-2.07737138	-0.53991723	-0.72757872
6	1.99436013	-2.27639516	1.60746720	6	-0.39644951	2.43256165	-0.00000111
1	3.06609154	-2.44403751	1.79960083	1	-0.07445302	2.91174286	0.92385006
1	1.60169825	-3.18927953	1.14317887	1	-0.07445244	2.91173996	-0.92385351
1	1.50452820	-2.14997324	2.58131416	6	-1.77835255	0.77412248	-1.19993171
6	-1.78456968	2.36043909	1.58372808	6	-2.46046516	-1.70675923	-1.58698186
1	-2.81389640	2.72569718	1.72770983	1	-3.55464316	-1.72287111	-1.71818144
1	-1.21286883	3.17919980	1.13028120	1	-2.17551123	-2.66652759	-1.13991025
1	-1.37073536	2.15581638	2.57871367	1	-2.01470956	-1.64301977	-2.58684663
6	-2.08555824	-0.65618215	-2.60969665	6	-1.82271871	1.26677262	2.61338336
1	-3.14794766	-0.61350259	-2.89805392	1	-2.85439507	1.54986453	2.87842173
1	-1.75743991	-1.69441235	-2.74561012	1	-1.19897070	2.15815349	2.75563400
1	-1.52734195	-0.02443004	-3.31226654	1	-1.49628267	0.50146513	3.32857388
6	-1.78456942	2.36043815	-1.58373045	6	-2.46046685	-1.70675852	1.58698089
1	-2.81389589	2.72569600	-1.72771464	1	-3.55464500	-1.72286959	1.71818007
1	-1.37073654	2.15581105	-2.57871576	1	-2.01471275	-1.64302005	2.58684647
1	-1.21286876	3.17920049	-1.13028624	1	-2.17551418	-2.66652808	1.13991108
6	-2.08555599	-0.65617976	2.60969766	6	-1.82271985	1.26677348	-2.61338362
1	-3.14794473	-0.61350297	2.89805786	1	-2.85439644	1.54986534	-2.87842134
1	-1.52733798	-0.02442853	3.31226696	1	-1.49628552	0.50146618	-3.32857508
1	-1.75743668	-1.69440980	2.74560951	1	-1.19897249	2.15815464	-2.75563482

### [Cp\*Ru(C<sub>5</sub>Me<sub>4</sub>CH<sub>2</sub>NMe<sub>3</sub>)]<sup>+</sup> (analogue of 3)

PBE/L2				BPBE/L2			
E = -5484.718335 E <sub>0</sub> = -5484.174238				E = -5485.252215 a.u. E <sub>0</sub> = -5484.708131 a.u.			
ZPVE = 0.544097 a.u. = 341.4263 kcal/mol				ZPVE = 0.544084 a.u. = 341.4178 kcal/mol			
T = 298.150 K: G = 305.9881 kcal/mol				T = 298.150 K: G = 305.9683 kcal/mol			
44	-0.07734728	0.12014716	-0.00055290	44	0.64860867	0.02308717	0.00001682
6	1.70684422	-0.25920930	1.19312776	6	-0.90742249	1.00349242	-1.18453116
6	1.75278876	1.11016345	0.74827697	6	0.00463098	2.02205964	-0.72309370
6	1.76505110	1.12622757	-0.69545791	6	0.00467630	2.02203957	0.72315898
6	1.73548062	-0.70390253	2.62476455	6	-1.24089687	0.73313499	-2.62629128
6	1.87177995	2.31149444	1.63347579	6	0.73341823	3.00366217	-1.59562685
6	1.89882881	2.34684990	-1.55169580	6	0.73347984	3.00365048	1.59566408
6	-1.92809169	-0.13816702	1.16373789	1	-2.00792717	1.42518837	-3.01348183
6	-1.84654549	1.21913702	0.67995139	1	-0.35559599	0.85760669	-3.26219855
6	-1.83616709	1.17938779	-0.76492556	1	-1.60011877	-0.29341319	-2.78550055
6	-2.08179017	-0.55069966	2.59440520	1	0.11963379	3.90373568	-1.76560916
6	-1.89733162	2.45509207	1.52230478	1	1.67506464	3.33363973	-1.13952128
6	-1.87522460	2.36696613	-1.67482362	1	0.97238599	2.58008560	-2.57934650

1	2.76084994	-0.75181725	3.02867583	1	0.11971163	3.90372932	1.76566782
1	1.17815417	-0.00508577	3.26135287	1	1.67512322	3.33361881	1.13954232
1	1.27173682	-1.69142083	2.76147037	6	-0.90738435	1.00348696	1.18461722
1	2.92921385	2.55735053	1.82283022	6	-2.46373040	-0.73992342	0.00005131
1	1.40765471	3.19658829	1.18033512	6	-1.24083499	0.73315811	2.62638886
1	1.39334098	2.14935974	2.60795264	1	-2.36980700	-1.36970670	0.89335065
1	2.95929995	2.58757407	-1.73041482	1	-2.36978935	-1.36974962	-0.89321594
1	1.44084176	3.22501806	-1.07925741	1	-2.00782374	1.42525436	3.01358644
1	-3.14518123	-0.57283874	2.88272971	1	-0.35551368	0.85763954	3.26226794
1	-1.67420319	-1.55392895	2.77775373	1	-1.60007524	-0.29337530	2.78564258
1	-1.57545223	0.14589783	3.27545982	1	0.97248815	2.58008136	2.57937898
1	-2.94075568	2.76528076	1.69329482	7	-4.02273942	-0.34422807	-0.00001153
1	-1.38178812	3.29691998	1.04225807	6	-4.82055978	-1.61713776	0.00008315
1	-1.43764676	2.29817311	2.50684295	1	-4.57195501	-2.19637896	-0.89606724
1	-2.91582962	2.67365976	-1.86791409	1	-4.57204787	-2.19618963	0.89638122
1	-1.35599172	3.23107380	-1.24059877	1	-5.88982550	-1.37519797	0.00000291
6	1.71646861	-1.10237097	0.00132440	6	-4.35662997	0.46054668	1.22233382
6	1.72704487	-0.23290106	-1.17136114	1	-5.42198612	0.71824173	1.19855669
6	1.62518024	-2.57447280	-0.01621018	1	-4.13670324	-0.13420333	2.11460194
6	1.78057545	-0.64524212	-2.61192944	1	-3.74707517	1.36881524	1.21894918
1	1.12588159	-2.94994809	-0.91891507	6	-4.35653041	0.46032206	-1.22253331
1	1.10838575	-2.97066935	0.86759565	1	-4.13655973	-0.13460307	-2.11467496
1	2.81313289	-0.68863675	-2.99764366	1	-5.42188070	0.71805142	-1.19887720
1	1.23884325	0.07117942	-3.24242213	1	-3.74695105	1.36857387	-1.21927921
1	1.31490859	-1.62694588	-2.78014439	6	-1.50229605	0.38365887	0.00004839
1	1.42329466	2.21243736	-2.53179701	6	1.78592241	-1.46710723	-1.17164731
6	-1.96610226	-1.01418680	0.01821371	6	2.67806242	-0.42103233	-0.72414550
6	-1.90985817	-0.20263423	-1.17414022	6	2.67806293	-0.42105338	0.72412904
6	-2.17110853	-2.49713703	0.05829651	6	1.59561548	-1.91001933	-2.59411511
6	-2.04495996	-0.69363583	-2.58183476	6	3.56854676	0.41022321	-1.60210795
1	-3.24584551	-2.74118741	0.05640843	6	3.56853604	0.41017620	1.60211036
1	-1.74157594	-2.94482784	0.96498367	1	2.35462747	-2.66025519	-2.87089916
1	-1.72733835	-2.99524254	-0.81460091	1	0.61132492	-2.36980696	-2.75429615
1	-3.10350678	-0.71931730	-2.88721012	1	1.69333019	-1.07474654	-3.29960797
1	-1.51811476	-0.04328201	-3.29244219	1	4.52964687	-0.10309823	-1.76995781
1	-1.64770936	-1.71066949	-2.70077507	1	3.79460828	1.38491545	-1.15133063
1	-1.41259487	2.15199395	-2.64700419	1	3.12001866	0.59264474	-2.58716138
7	3.01451303	-3.35330509	-0.01188867	1	4.52965887	-0.10309981	1.76997724
6	2.72375257	-4.82100194	-0.03002809	1	3.79459716	1.38489839	1.15139106
1	2.15373388	-5.06164210	-0.93414261	6	1.23596962	-2.11102954	-0.00004273
1	3.66797546	-5.37763799	-0.02754453	6	1.78593507	-1.46716367	1.17159127
1	2.13751262	-5.08064671	0.85830454	6	0.37391871	-3.34169849	-0.00004324
6	3.79376347	-3.00819895	1.21784694	6	1.59564232	-1.91013473	2.59404000
1	3.21527771	-3.29798161	2.10105057	1	0.99930328	-4.24976097	-0.00006140
1	4.74619469	-3.55029035	1.19861995	1	-0.26808674	-3.39410365	-0.88976786
1	3.96989589	-1.92834136	1.22609138	1	-0.26807161	-3.39411024	0.88969012
6	3.81541011	-2.98225422	-1.21995509	1	2.35464145	-2.66038000	2.87083266
1	4.76756728	-3.52460950	-1.19534679	1	1.69336694	-1.07488453	3.29956330
1	3.25281699	-3.25312610	-2.11929314	1	0.61134494	-2.36989938	2.75425725
1	3.99134251	-1.90247408	-1.20214331	1	3.12001444	0.59259135	2.58717082

[Cp\**Ru*(C<sub>5</sub>Me<sub>4</sub>CH<sub>2</sub>···NMe<sub>3</sub>)]<sup>+</sup> (TS-N-1)

PBE/L2 $\nu = 117.84i \text{ cm}^{-1}$				BPBE/L2 $\nu = 113.32i \text{ cm}^{-1}$			
E = -5484.708288 a.u. E <sub>0</sub> = -5484.168237 a.u.				E = -5485.245125 a.u. E <sub>0</sub> = -5484.704713 a.u.			
ZPVE = 0.540051 a.u. = 338.8873 kcal/mol				ZPVE = 0.540413 a.u. = 339.1141 kcal/mol			
T = 298.150 K; G = 298.7711 kcal/mol				T = 298.150 K; G = 301.9946 kcal/mol			
44	-0.08066386	0.04866951	-0.05661739	44	-0.11283456	0.04536789	-0.07235107
6	1.70063928	0.68066976	1.05511854	6	1.68749619	0.66745482	1.02817508
6	1.24918922	1.82622929	0.32820989	6	1.26656449	1.80138349	0.25937228
6	1.27517796	1.52666289	-1.08801278	6	1.28914233	1.45131329	-1.14735390
6	1.92207409	0.59839371	2.53166619	6	1.91091767	0.64129328	2.51213268
6	0.90482984	3.15456900	0.92285740	6	0.97296189	3.16746731	0.80697139
6	0.96205437	2.49794296	-2.18115353	6	1.02255807	2.39930638	-2.27981666
6	-1.62841072	-1.08725085	1.00931905	6	-1.66715861	-1.12745110	0.96403471
6	-2.00067499	0.30109135	1.00628216	6	-2.02137481	0.26488473	1.04575647
6	-2.15822896	0.71496529	-0.36965211	6	-2.19324306	0.75901141	-0.30416096
6	-1.48527470	-1.95406292	2.22084434	6	-1.53190838	-2.06822882	2.12671751
6	-2.27961307	1.13995875	2.21264520	6	-2.29043597	1.03525809	2.30516880
6	-2.63179127	2.05772778	-0.82841889	6	-2.67942917	2.12882546	-0.67836445
1	2.92686185	0.96306533	2.79958238	1	2.91782111	1.01135150	2.76557870
1	1.19630087	1.21129928	3.08114939	1	1.18981167	1.27981816	3.03753534
1	1.83608574	-0.43098451	2.90354743	1	1.81633257	-0.37074403	2.92669476
1	1.80140364	3.79271828	0.97314069	1	1.89449096	3.77168237	0.83039748
1	0.15842284	3.69140525	0.32448943	1	0.24503092	3.71040811	0.19210890
1	0.51704453	3.05600401	1.94437429	1	0.58615111	3.12348203	1.83247928
1	1.86349656	3.07140910	-2.44978674	1	1.94899326	2.92882635	-2.55584610
1	0.19487142	3.22201180	-1.88077287	1	0.28063309	3.16169210	-2.01337837
1	-2.46252492	-2.36821196	2.51696921	1	-2.51741083	-2.47813849	2.40276719

1	-0.81524129	-2.80414572	2.03824559	1	-0.88111003	-2.92022077	1.89208072
1	-1.09524561	-1.39290353	3.07978544	1	-1.12767948	-1.56660968	3.01527814
1	-3.33989275	1.05562355	2.49992223	1	-3.35143892	0.94065344	2.58867336
1	-2.07658908	2.20256564	2.02905117	1	-2.08078886	2.10551117	2.18549275
1	-1.68164304	0.82306494	3.07664143	1	-1.69382691	0.66445955	3.14814298
1	-3.73206465	2.07384712	-0.88001209	1	-3.78122148	2.14311221	-0.70309324
1	-2.32814517	2.85705697	-0.14060697	1	-2.36155525	2.89061461	0.04423383
6	2.01115936	-0.35657176	0.06365598	6	1.99062759	-0.40984590	0.07414038
6	1.74174965	0.18825159	-1.27279299	6	1.72434200	0.09251644	-1.28210308
6	1.91359634	-1.72823738	0.35350827	6	2.00883264	-1.77864764	0.41523203
6	2.00989553	-0.48385716	-2.58134732	6	1.99136988	-0.62447453	-2.57336542
1	1.75308640	-2.44785414	-0.44502991	1	1.83058045	-2.52511049	-0.35518356
1	1.72387661	-2.06109363	1.37069177	1	1.80239525	-2.07804156	1.44006724
1	3.01908180	-0.23889109	-2.95003210	1	3.00785804	-0.40864525	-2.94107134
1	1.29562432	-0.16467393	-3.35100582	1	1.29049804	-0.31240860	-3.35767745
1	1.94574072	-1.57696142	-2.50216838	1	1.90209872	-1.71346980	-2.46766437
1	0.61566247	1.99058827	-3.09026511	1	0.66651011	1.87702658	-3.17632199
6	-1.58052478	-1.53825084	-0.37522598	6	-1.64108155	-1.50277850	-0.44651681
6	-1.91449278	-0.42701255	-1.21947372	6	-1.97816965	-0.33914595	-1.22241917
6	-1.37064431	-2.94805700	-0.83047680	6	-1.47254752	-2.89546269	-0.98233311
6	-2.07831934	-0.46608869	-2.70551821	6	-2.19339271	-0.29915423	-2.70702529
1	-2.33682375	-3.47343056	-0.89981937	1	-2.45171465	-3.39690534	-1.05482005
1	-0.74264545	-3.51544049	-0.13195333	1	-0.84028431	-3.51244057	-0.33120835
1	-0.90490081	-2.99249182	-1.82353872	1	-1.03075133	-2.89793387	-1.98703737
1	-3.11603466	-0.72452308	-2.97057951	1	-3.24456595	-0.53061686	-2.94477281
1	-1.85772688	0.50507024	-3.16661292	1	-1.97601124	0.69062545	-3.12756231
1	-1.42641507	-1.21791026	-3.16833405	1	-1.57115724	-1.03509701	-3.23166352
1	-2.25632298	2.30576387	-1.82914199	1	-2.32885051	2.43331888	-1.67227775
7	4.00339096	-2.63250350	0.58028313	7	4.06192389	-2.57529556	0.64582734
6	3.82001901	-4.04796304	0.90085005	6	3.90476053	-3.99587756	0.99592176
1	3.25035321	-4.14733798	1.83452096	1	3.33567924	-4.08792744	1.93034804
1	3.26538948	-4.54368418	0.09287915	1	3.36338809	-4.51834940	0.19628470
1	4.78619179	-4.56965060	1.02800177	1	4.88286648	-4.48936508	1.13403544
6	4.68687792	-2.43677095	-0.69777010	6	4.75692382	-2.39835946	-0.63850428
1	5.72816575	-2.80612013	-0.66426421	1	5.79884437	-2.76028887	-0.58398837
1	4.15441416	-2.97548265	-1.49235065	1	4.23498095	-2.95779200	-1.42486164
1	4.70512390	-1.36671597	-0.94355429	1	4.76927861	-1.33376260	-0.90372760
6	4.66205943	-1.89882988	1.66035771	6	4.71915251	-1.81330709	1.71880527
1	4.11234319	-2.04357790	2.59942065	1	4.16943707	-1.94400044	2.65927469
1	5.70280012	-2.23986255	1.80976983	1	5.75944160	-2.15105797	1.87139717
1	4.67820347	-0.82768319	1.41893484	1	4.73165067	-0.74817223	1.45577071

[Cp\*Ru(C<sub>5</sub>Me<sub>4</sub>CH<sub>2</sub>NMe<sub>2</sub>Ph)]<sup>+</sup>

PBE/L2				BPBE/L2			
E = -5676.358529 a.u. E <sub>0</sub> = -5675.763330 a.u. ZPVE = 0.595199 a.u. = 373.4932 kcal/mol T = 298.150 K: G = 335.0055 kcal/mol				E = -5676.979169 a.u. E <sub>0</sub> = -5676.384190 a.u. ZPVE = 0.594979 a.u. = 373.3549 kcal/mol T = 298.150 K: G = 334.7803 kcal/mol			
44	-1.93399748	-0.06292982	0.03608594	44	-1.94025318	-0.06527475	0.07482969
6	-0.85809861	1.45961557	1.16575359	6	-0.83154259	1.43487764	1.21859600
6	-2.10310968	2.03259411	0.72336538	6	-2.08626821	2.02372458	0.81910337
6	-2.13602890	2.00564343	-0.71993289	6	-2.15382788	2.03211387	-0.62554035
6	-2.40085276	-1.83440252	1.25686721	6	-2.54657144	-1.79996617	1.31142476
6	-3.62653398	-1.22744163	0.79586048	6	-3.71440880	-1.21155368	0.69454236
6	-3.62991681	-1.26806638	-0.64916383	6	-3.56078567	-1.30936830	-0.74212583
6	-0.09871772	1.09560917	-0.02737934	6	-0.09789161	1.10007354	-0.00322836
6	-0.911190694	1.41577313	-1.19721797	6	-0.94185539	1.44899508	-1.14722837
6	1.20602313	0.41341283	-0.04199471	6	1.21227260	0.42503996	-0.06857047
1	1.35685576	-0.21079748	-0.93080025	1	1.34837593	-0.16797760	-0.97983765
1	1.37299520	-0.19486635	0.85248591	1	1.40938767	-0.20505705	0.80339665
6	-1.64898992	-2.24807812	0.09715426	6	-1.67078787	-2.25472774	0.25755619
6	-2.40581342	-1.89901461	-1.08107531	6	-2.29441138	-1.95163871	-1.01332421
7	2.50658744	1.38441083	-0.07665195	7	2.53266225	1.40483532	-0.10888592
6	3.72810470	0.51955677	-0.09368228	6	3.74994633	0.53014398	-0.20337624
6	3.99390498	-0.28102755	1.02233599	6	4.05686967	-0.31086325	0.87547981
6	4.57281643	0.48007172	-1.20333045	6	4.55169417	0.52072639	-1.34898036
6	5.10995358	-1.11558352	1.02488346	6	5.16834243	-1.15309465	0.80533221
6	5.68969365	-0.36047611	-1.18831219	6	5.66430118	-0.32780022	-1.40688561
6	5.96205654	-1.15824208	-0.07981051	6	5.97674092	-1.16482391	-0.33535739
1	3.34714162	-0.26776868	1.89864160	1	3.44761703	-0.32492808	1.77804943
1	4.39494412	1.09229144	-2.08354064	1	4.34517808	1.16188874	-2.20194920
1	5.31156372	-1.73348162	1.89952924	1	5.40004445	-1.80062623	1.65114323
1	6.34785882	-0.38135573	-2.05653443	1	6.28657068	-0.32326526	-2.30194305
1	6.83523102	-1.80986540	-0.07361613	1	6.84523487	-1.82142089	-0.38578753
6	-3.14375702	2.64718495	1.60666314	6	-3.09707746	2.64019099	1.74339439
1	-2.94289977	3.71938936	1.76324457	1	-2.87849738	3.70930693	1.90136006
1	-4.14700267	2.56406289	1.16990447	1	-4.11471035	2.57230114	1.33919343
1	-3.17272308	2.17131886	2.59536218	1	-3.09893451	2.15786719	2.72916894
6	-0.41606987	1.35351281	2.59441722	6	-0.35334395	1.30488420	2.63881982

1	0.04488107	2.28629542	2.96039795	1	0.10070234	2.23838869	3.01202156
1	-1.26882556	1.14284089	3.25226058	1	-1.18619600	1.06762206	3.31243701
1	0.30598862	0.53801977	2.74418686	1	0.38534309	0.49947194	2.75554890
6	-0.53549891	1.25624725	-2.63956128	6	-0.59823066	1.33694540	-2.60732399
1	-0.09056364	2.17438335	-3.05892441	1	-0.17156874	2.27299249	-3.00599039
1	0.17750780	0.43361619	-2.79274570	1	0.11728169	0.52664877	-2.80535333
1	-1.41804019	1.02597211	-3.24982715	1	-1.49326786	1.12023849	-3.20383599
6	-3.21658984	2.58728852	-1.57722639	6	-3.24644173	2.65850568	-1.44404410
1	-3.29601457	2.06909971	-2.54157031	1	-3.35634187	2.17345254	-2.42219206
1	-4.19732380	2.52915832	-1.08838879	1	-4.21748314	2.60491772	-0.93608214
1	-3.01978558	3.65052071	-1.79007914	1	-3.03240597	3.72443493	-1.62778494
6	2.39570228	2.26509153	-1.27983669	6	2.38722551	2.33717255	-1.27447484
1	3.26269690	2.93296471	-1.32331944	1	3.25727563	3.00127132	-1.32124198
1	2.33483174	1.65268637	-2.18331909	1	2.29104947	1.76374184	-2.19971440
1	1.47484046	2.84615354	-1.17489076	1	1.47623496	2.92094712	-1.11476284
6	2.51240425	2.28038821	1.12973616	6	2.58919904	2.25631300	1.13356174
1	1.59348378	2.87484005	1.11462353	1	1.67932910	2.86300494	1.17137352
1	2.54606591	1.67967054	2.04065592	1	2.64553723	1.62259459	2.02035687
1	3.39495641	2.92735992	1.07759604	1	3.47765730	2.89535825	1.07745646
6	-2.04094316	-2.10692218	2.68406916	6	-2.35347442	-2.03267498	2.78242716
1	-2.44199165	-3.08034943	3.00975065	1	-2.78712664	-3.00135779	3.08106712
1	-0.95325278	-2.13675467	2.83328079	1	-1.29141708	-2.05224145	3.06027103
1	-2.45066987	-1.34466323	3.35981419	1	-2.84360215	-1.25823914	3.38670099
6	-0.37047696	-3.02750889	0.11595537	6	-0.41077044	-3.05040941	0.44882346
1	0.23922208	-2.79205018	0.99887051	1	0.10378754	-2.78605071	1.38243073
1	-0.57649141	-4.10983278	0.14503865	1	-0.64080094	-4.12756734	0.50041137
1	0.23740176	-2.83909627	-0.77924819	1	0.29458523	-2.91124325	-0.38118557
6	-2.05188101	-2.25171910	-2.49216885	6	-1.79860212	-2.38275177	-2.36422836
1	-0.96483975	-2.29206598	-2.64345486	1	-0.70236347	-2.43744660	-2.40125772
1	-2.45590700	-3.24105974	-2.76130589	1	-2.18335106	-3.38455672	-2.61726971
1	-2.46270024	-1.52767034	-3.20804958	1	-2.12645239	-1.69920391	-3.15805321
6	-4.76121189	-0.85006565	-1.53527126	6	-4.60121186	-0.94995575	-1.76353039
1	-4.40850057	-0.53047981	-2.52462520	1	-4.15264561	-0.67976338	-2.72834430
1	-5.46131795	-1.68654178	-1.69145890	1	-5.27426401	-1.80434536	-1.94368485
1	-5.33514610	-0.02138645	-1.10079101	1	-5.22424037	-0.10797920	-1.43619098
6	-4.75381556	-0.76010829	1.66223156	6	-4.94057769	-0.73040543	1.41553100
1	-5.33178570	0.04043243	1.18264476	1	-5.47378091	0.04161588	0.84611028
1	-5.45139723	-1.58713597	1.87110188	1	-5.64452220	-1.56383274	1.57436744
1	-4.39662416	-0.38190517	2.62902892	1	-4.70043944	-0.31343246	2.40197201

[Cp\*Ru(C<sub>5</sub>Me<sub>4</sub>CH<sub>2</sub>···NMe<sub>2</sub>Ph)]<sup>+</sup> (TS-N-1)

PBE/L2	$\nu = 142.45i \text{ cm}^{-1}$			BPBE/L2	$\nu = 151.22i \text{ cm}^{-1}$		
E = -5676.354797 a.u.	E <sub>0</sub> = -5675.762134 a.u.			E = -5676.977041 a.u.	E <sub>0</sub> = -5676.384206 a.u.		
ZPVE = 0.592663 a.u.	= 371.9018 kcal/mol			ZPVE = 0.592835 a.u.	= 372.0097 kcal/mol		
T = 298.150 K:	G = 330.2438 kcal/mol			T = 298.150 K:	G = 332.7316 kcal/mol		
44	-1.79796836	-0.00463521	0.11504874	44	-1.81989930	-0.02300081	0.15122681
6	-0.83127892	1.56596159	1.29622531	6	-0.77678011	1.50224173	1.33605014
6	-2.13416049	2.04596496	0.94520999	6	-2.07698103	2.02641558	1.02427570
6	-2.24118015	2.09829225	-0.49638447	6	-2.21514021	2.10838526	-0.41500052
6	-2.49455478	-1.72271467	1.33384274	6	-2.66936493	-1.68731364	1.35819169
6	-3.58496855	-1.20355068	0.54194902	6	-3.66996239	-1.18953074	0.43925620
6	-3.23810670	-1.34722553	-0.85518721	6	-3.18875881	-1.39654866	-0.91093022
6	-0.10445606	1.33431306	0.04317593	6	-0.07984143	1.28052968	0.06165111
6	-1.00527041	1.65378867	-1.06937790	6	-1.00237818	1.63776972	-1.02462533
6	1.06529606	0.54279890	-0.07327901	6	1.13302774	0.54349581	-0.09689005
1	1.28471267	0.07237822	-1.03178791	1	1.32060164	0.07662328	-1.06440930
1	1.40591089	-0.01477018	0.79804491	1	1.47925803	-0.04555199	0.75163208
6	-1.47067319	-2.16866686	0.43051002	6	-1.56134470	-2.17649576	0.58066943
6	-1.92292638	-1.93005553	-0.92823122	6	-1.87909338	-1.99361366	-0.82854311
7	2.78499437	1.65556579	-0.14807022	7	2.77129504	1.65636882	-0.18068437
6	3.85814482	0.69789769	-0.32650203	6	3.87401050	0.72804706	-0.43211972
6	4.16105763	-0.19874798	0.71129143	6	4.23268970	-0.19886805	0.56282334
6	4.56474079	0.60472354	-1.53310247	6	4.54946661	0.70483991	-1.66185302
6	5.15393007	-1.16095046	0.54315860	6	5.25183527	-1.12354038	0.33007642
6	5.55811290	-0.36436681	-1.69131482	6	5.56978207	-0.22675600	-1.88476694
6	5.85820455	-1.25026953	-0.65901767	6	5.92625186	-1.14340062	-0.89480965
1	3.63077911	-0.15526888	1.66198911	1	3.72910239	-0.21115150	1.52860950
1	4.37098972	1.29074382	-2.35441432	1	4.31243407	1.41259696	-2.45267226
1	5.37805292	-1.84455792	1.36211755	1	5.51897009	-1.83104693	1.11562927
1	6.10443150	-0.41413225	-2.63325259	1	6.09025570	-0.22268179	-2.84292366
1	6.63711296	-2.00142898	-0.78603651	1	6.72431123	-1.86424240	-1.07224532
6	-3.17896460	2.51515163	1.90752917	6	-3.08158746	2.52423355	2.02274915
1	-3.07203148	3.59570252	2.09411200	1	-2.92060833	3.59572025	2.22573106
1	-4.19339433	2.35028886	1.52392209	1	-4.11072675	2.41351590	1.65999085
1	-3.09769962	2.00690030	2.87672160	1	-3.00331664	1.99556712	2.98096115
6	-0.28861729	1.43922980	2.68546679	6	-0.20741642	1.34517147	2.71750088
1	0.11672001	2.39751385	3.04924815	1	0.22081844	2.29119723	3.08801275
1	-1.07065299	1.13101729	3.39111892	1	-0.98165976	1.04216244	3.43344435

1	0.51561099	0.69362982	2.74576924	1	0.58269930	0.58336589	2.75447991
6	-0.67261512	1.63344958	-2.52859872	6	-0.70660306	1.64459122	-2.49761271
1	-0.28406575	2.60797596	-2.86663525	1	-0.33264971	2.62741906	-2.82907790
1	0.08101438	0.87142653	-2.76900057	1	0.04235588	0.89007435	-2.77293104
1	-1.56134488	1.41410189	-3.13393918	1	-1.60960931	1.43209303	-3.08350102
6	-3.41447309	2.62952727	-1.25751349	6	-3.38561679	2.70449435	-1.14218095
1	-3.49844661	2.17110967	-2.25082804	1	-3.50266410	2.28101587	-2.14738788
1	-4.35836569	2.45748687	-0.72525742	1	-4.32673802	2.55080286	-0.60003889
1	-3.31692133	3.71699172	-1.40497214	1	-3.25026161	3.79231778	-1.25851282
6	2.56622738	2.58382892	-1.26875494	6	2.51891066	2.63873934	-1.25954050
1	3.42825115	3.25504655	-1.40078905	1	3.37644443	3.31691079	-1.37740318
1	2.38950125	2.02920043	-2.19580066	1	2.32277420	2.12464892	-2.20494215
1	1.67672786	3.18320401	-1.04303320	1	1.63337792	3.22170660	-0.98408664
6	2.84682867	2.41610699	1.11815821	6	2.88966859	2.38188322	1.11309827
1	1.91835564	2.98973281	1.22382432	1	1.97690755	2.96849567	1.26539826
1	2.94685787	1.74351310	1.97339479	1	3.00610946	1.68109026	1.94277237
1	3.70399689	3.10582137	1.10445804	1	3.75984306	3.05353053	1.08577939
6	-2.48349667	-1.86761318	2.82278799	6	-2.81865408	-1.79150584	2.84820581
1	-2.91447939	-2.83696535	3.12060618	1	-3.29586464	-2.74762494	3.11909463
1	-1.46512464	-1.82417853	3.23016520	1	-1.84930511	-1.75457588	3.36153743
1	-3.07664135	-1.08438751	3.31236399	1	-3.44702921	-0.98872175	3.25446397
6	-0.21052826	-2.87576391	0.82021288	6	-0.36145405	-2.89915983	1.12277712
1	0.15468479	-2.54871731	1.80253079	1	-0.08001354	-2.53606637	2.11982191
1	-0.38832471	-3.96153999	0.88449510	1	-0.57587562	-3.97659228	1.21705179
1	0.59160064	-2.72093049	0.08731825	1	0.51093463	-2.79899749	0.46437478
6	-1.22200895	-2.36498294	-2.17744487	6	-1.07093086	-2.50634615	-1.98636089
1	-0.13103748	-2.36546707	-2.05372518	1	0.00423272	-2.51436384	-1.76469196
1	-1.51904126	-3.38932498	-2.45467804	1	-1.36073736	-3.54176516	-2.23035482
1	-1.46427020	-1.71393804	-3.02737545	1	-1.22415932	-1.90387077	-2.89086367
6	-4.13421459	-1.05362342	-2.01641790	6	-3.97163626	-1.15773710	-2.16922227
1	-3.56261489	-0.79275725	-2.91654205	1	-3.31779365	-0.94699214	-3.02512252
1	-4.74571679	-1.93667214	-2.26193299	1	-4.56547612	-2.05088026	-2.42397354
1	-4.82550825	-0.22859814	-1.80281066	1	-4.67300514	-0.32047531	-2.06457427
6	-4.90263624	-0.73380278	1.07215324	6	-5.03821661	-0.70010800	0.81611914
1	-5.37845810	-0.00808745	0.40011876	1	-5.43939955	0.00629676	0.07849206
1	-5.59652908	-1.58289113	1.17851668	1	-5.74180716	-1.54669850	0.87299594
1	-4.80417367	-0.26735174	2.06064555	1	-5.04310095	-0.20668233	1.79610159

[Cp\**Ru*(C<sub>5</sub>Me<sub>4</sub>CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>NHMe<sub>2</sub>)]<sup>+</sup> (analogue of 5)

PBE/L2				BPBE/L2			
E = -5676.361260 a.u. E <sub>0</sub> = -5675.766597 a.u.				E = -5676.985587 E <sub>0</sub> = -5676.391021			
ZPVE = 0.594663 a.u. = 373.1569 kcal/mol				ZPVE = 0.594566 a.u. = 373.0958 kcal/mol			
T = 298.150 K: G = 330.3506 kcal/mol				T = 298.150 K: G = 330.0610 kcal/mol			
44	1.83767959	0.06894081	0.03215051	44	1.84528666	0.06176396	0.03984700
6	0.07073972	0.27795957	-1.21204970	6	0.06449748	0.28250342	-1.20055638
6	0.00426182	-0.99084074	-0.51577336	6	0.00695442	-0.99989760	-0.52242181
6	-0.02566946	-0.71113938	0.90077011	6	-0.02194183	-0.74172735	0.90084429
6	0.01800789	0.72239253	1.07950962	6	0.01533534	0.69142070	1.10221184
6	0.07512364	1.33874536	-0.22528614	6	0.06772042	1.32973288	-0.19507184
6	0.01727310	0.46507509	-2.69721504	6	-0.00034132	0.49335554	-2.68749311
1	0.52591781	-0.37228298	-3.20356056	1	0.51280994	-0.33085316	-3.20958992
1	0.59003049	1.36146203	-2.98813042	1	0.56259393	1.39902500	-2.96675510
6	-0.12304938	-2.34316474	-1.14884229	6	-0.13236113	-2.34664812	-1.17656877
1	-1.17920541	-2.62203465	-1.30531849	1	-1.19237351	-2.62467822	-1.30907616
1	0.32694474	-3.12316294	-0.52072366	1	0.33499451	-3.13675650	-0.57468824
1	0.37871917	-2.38516263	-2.12563753	1	0.34205647	-2.37192240	-2.16726416
6	-0.18330368	-1.72743266	1.98962568	6	-0.19877765	-1.77556548	1.97704228
1	-1.24696010	-1.94196420	2.18641487	1	-1.26795337	-1.95537821	2.18200038
1	0.25900240	-1.38031524	2.93257221	1	0.26532868	-1.46306035	2.92140301
1	0.30112285	-2.67830413	1.73050357	1	0.24637880	-2.73848623	1.69430991
6	-0.08321361	1.44986110	2.38483580	6	-0.11625836	1.39632499	2.42284815
1	-1.13352812	1.65968117	2.64747720	1	-1.17629830	1.56789928	2.67654472
1	0.44554866	2.41146178	2.35024742	1	0.38029350	2.37544258	2.41359979
1	0.34945481	0.86644000	3.20811666	1	0.32356797	0.81194460	3.24133162
6	0.03365757	2.81004013	-0.50688290	6	0.00190845	2.80979282	-0.45221588
1	-1.00269755	3.18383342	-0.56971932	1	-1.04163683	3.16665966	-0.49856338
1	0.53269361	3.05764569	-1.45417056	1	0.48680422	3.08299060	-1.39955313
1	0.53656099	3.38390712	0.28253252	1	0.50185612	3.37893330	0.34219338
6	-1.37716252	0.58968744	-3.28616442	6	-1.39971776	0.61641528	-3.27954955
6	-2.52484558	0.52424896	-2.48279581	6	-2.55499470	0.52978707	-2.48506410
1	-2.40625655	0.38028961	-1.40845130	1	-2.44666784	0.37037859	-1.41221286
6	-3.80270280	0.63975663	-3.03012817	6	-3.83288665	0.64351576	-3.03985713
1	-4.67574457	0.58519441	-2.37778097	1	-4.70814791	0.57120018	-2.39246891
6	-3.92312940	0.82303147	-4.40346139	6	-3.94743049	0.84730688	-4.41339177
6	-2.80879454	0.89293267	-5.23458556	6	-2.82527492	0.93910283	-5.23678939
1	-2.91585269	1.03737405	-6.31334770	1	-2.92406064	1.09927898	-6.31425815
6	-1.54164024	0.77540466	-4.66811712	6	-1.55881562	0.82277067	-4.66236594
1	-0.66367173	0.82967638	-5.31396665	1	-0.67850419	0.89411106	-5.30368341

6	-6.01841638	2.17541540	-4.56621654	6	-6.06081119	2.19389088	-4.58240832
1	-6.95266885	2.25756548	-5.13311317	1	-6.98498275	2.27888083	-5.16569233
1	-6.23278278	2.06728159	-3.49902981	1	-6.29407168	2.07189921	-3.52079044
6	-6.10293251	-0.29773058	-4.89117216	6	-6.12413385	-0.28719027	-4.94522542
1	-6.31829223	-0.45483235	-3.83029206	1	-6.35868129	-0.46271944	-3.89142228
1	-7.03585929	-0.16768913	-5.45124785	1	-7.04716907	-0.15542614	-5.52158051
7	-5.27129009	0.95147636	-5.03026236	7	-5.29671787	0.97521678	-5.05216198
1	-5.09017075	1.07753542	-6.03562468	1	-5.10654678	1.11665872	-6.05313917
1	-5.38356952	3.05124053	-4.73219425	1	-5.42695595	3.07440457	-4.72737238
1	-5.52706695	-1.14154986	-5.28361261	1	-5.53405075	-1.11988738	-5.34084233
6	3.70346376	1.21978325	-0.08626162	6	3.71572712	1.21714332	-0.11702264
6	3.63277724	0.55558704	1.19372099	6	3.65300226	0.58578998	1.18281862
6	3.59126871	-0.86840971	0.95617445	6	3.61554611	-0.84677326	0.98305737
6	3.70384075	0.20621528	-1.11431850	6	3.71604278	0.17446434	-1.11944988
6	3.63560555	-1.08440959	-0.47070635	6	3.65505817	-1.10109225	-0.44027407
6	3.87306794	2.69178285	-0.30221120	6	3.90476191	2.68553504	-0.37250749
1	3.39350768	3.27615585	0.49434788	1	3.42915571	3.29928113	0.40379320
1	4.94016893	2.96847189	-0.31409217	1	4.97661332	2.94547790	-0.38403738
1	3.44064557	3.01566517	-1.25854352	1	3.48493469	2.99006790	-1.34057587
6	3.87989369	0.44643881	-2.58213974	6	3.90922039	0.37529138	-2.59608170
1	3.45533910	1.41228073	-2.88882876	1	3.48764652	1.33073100	-2.93689461
1	4.94800539	0.45863303	-2.85508438	1	4.98187669	0.38279332	-2.85296023
1	3.40012332	-0.33863936	-3.18262976	1	3.44119383	-0.42737193	-3.18209999
6	3.72536006	-2.41372782	-1.15416976	6	3.77021711	-2.45139863	-1.08880078
1	3.29575799	-2.38141825	-2.16462009	1	3.34254796	-2.45758676	-2.10033708
1	4.77495084	-2.73578591	-1.25445463	1	4.82731342	-2.75323863	-1.17824351
1	3.19625459	-3.19534466	-0.59286783	1	3.25777850	-3.22862261	-0.50667199
6	3.71580159	1.21950700	2.53311986	6	3.76342496	1.28617081	2.50720175
1	4.76487034	1.32977447	2.85318482	1	4.82005824	1.39288063	2.80468252
1	3.27106268	2.22346956	2.51804427	1	3.33004396	2.29442198	2.47401707
1	3.19749104	0.63800987	3.30703369	1	3.25399631	0.73167224	3.30611046
6	3.62427689	-1.93470990	2.00669611	6	3.68030793	-1.88725579	2.06470032
1	4.66242575	-2.19399680	2.27161374	1	4.72789511	-2.12514906	2.31432209
1	3.12215349	-1.61272520	2.92857001	1	3.19401903	-1.54700391	2.98827430
1	3.13405493	-2.85637077	1.66569411	1	3.19622466	-2.82445342	1.76005063

[Cp\*Ru(C<sub>5</sub>Me<sub>4</sub>CH<sub>2</sub>···C<sub>6</sub>H<sub>5</sub>NMe<sub>2</sub>)]<sup>+</sup> (TS-C-1)

PBE/L2	$\nu = 273.86i \text{ cm}^{-1}$			BPBE/L2	$\nu = 279.44i \text{ cm}^{-1}$		
E = -5676.350098 a.u.	E <sub>0</sub> = -5675.759093 a.u.			E = -5676.975066	E <sub>0</sub> = -5676.384342		
ZPVE = 0.591006 a.u.	= 370.8616 kcal/mol			ZPVE = 0.590725 a.u.	= 370.6855 kcal/mol		
T = 298.150 K:	G = 330.0733 kcal/mol			T = 298.150 K:	G = 329.7641 kcal/mol		
44	1.72829622	-0.29888163	-0.11061405	44	1.75761362	-0.32816421	-0.18087600
6	0.31002822	0.79909565	-1.37869698	6	0.27997790	0.67624491	-1.46926574
6	1.59687797	1.41334757	-1.53214090	6	1.55427899	1.29827018	-1.70489899
6	2.03417528	1.90327796	-0.24242741	6	2.02547922	1.87614501	-0.46207864
6	2.28241374	-2.28434774	-0.92469155	6	2.59025985	-2.21386905	-1.00952711
6	3.47142683	-1.49838680	-0.69085209	6	3.66410572	-1.40499218	-0.47281611
6	3.54651863	-1.20157673	0.72343203	6	3.43801742	-1.23388877	0.94732118
6	-0.05917975	0.91747711	0.02857764	6	-0.04896817	0.88166849	-0.05910937
6	1.02557368	1.59799829	0.73040022	6	1.05235051	1.61721755	0.56305410
6	-1.14868041	0.25641511	0.66503758	6	-1.13844279	0.28160770	0.64903521
1	-1.05212197	0.06682003	1.73371009	1	-1.00324065	0.14237700	1.72109721
1	-1.67996299	-0.51855619	0.11309116	1	-1.68674210	-0.52300615	0.15993796
6	1.62003640	-2.46219824	0.33835175	6	1.68669747	-2.51965679	0.06893304
6	2.39334099	-1.78441999	1.36142831	6	2.21181814	-1.91059849	1.28438431
6	-2.76914041	1.53180340	0.88185336	6	-2.72376206	1.57756743	0.85636475
6	-3.23442640	1.71961915	-0.45619543	6	-3.26939484	1.71667781	-0.46262114
6	-3.62920992	0.80096318	1.75849627	6	-3.56060031	0.92133886	1.81955721
6	-4.36217302	1.09296837	-0.92606471	6	-4.44421086	1.10662593	-0.83336536
6	-4.75438869	0.15953936	1.30240467	6	-4.73221849	0.29725911	1.46308040
6	-5.15717060	0.27161970	-0.06573125	6	-5.21381836	0.35240610	0.11312125
1	-2.65968187	2.35604266	-1.13028406	1	-2.72193600	2.30542409	-1.19984090
1	-3.37052676	0.72604440	2.81616614	1	-3.24521234	0.89258644	2.86438258
1	-4.66058159	1.24533079	-1.96086350	1	-4.79954619	1.22314257	-1.85475665
1	-5.36048178	-0.40984615	2.00344662	1	-5.31294557	-0.21195712	2.22896273
1	-2.12267264	2.29545003	1.31523204	1	-2.05700158	2.36221050	1.21582128
7	-6.26422171	-0.36238933	-0.52567826	7	-6.36667527	-0.26890143	-0.24991808
6	1.87874478	-2.89808514	-2.22817637	6	2.50584788	-2.74574756	-2.41072212
1	2.20241143	-2.28834740	-3.08175459	1	2.96501960	-2.06301900	-3.13683558
1	2.33474664	-3.89420058	-2.34697147	1	3.03670648	-3.70893076	-2.48751184
1	0.79071845	-3.02555917	-2.29907570	1	1.46752103	-2.92015994	-2.72055376
6	0.40291634	-3.30032185	0.57509751	6	0.50238789	-3.43996327	-0.01153290
1	-0.26165772	-3.31083012	-0.29851264	1	0.02289363	-3.40362949	-0.99823362
1	0.69268741	-4.34431321	0.77819170	1	0.81440567	-4.48315956	0.16296128
1	-0.17447802	-2.94814613	1.43938063	1	-0.25699924	-3.19646920	0.74259840
6	2.12933071	-1.82240538	2.83454984	6	1.66487977	-2.10034954	2.67042181
1	1.05659271	-1.90485645	3.05355540	1	0.57705334	-2.24710922	2.66440756
1	2.62557745	-2.69010648	3.29867761	1	2.11206026	-2.99116485	3.14202743

1	2.50604478	-0.92265465	3.33799092	1	1.88639831	-1.24272812	3.31860276
6	4.51812958	-1.17422522	-1.70935559	6	4.88765896	-0.96494919	-1.22321325
1	5.25987260	-1.98675862	-1.76847795	1	5.66653553	-1.74309436	-1.16914691
1	4.08974225	-1.04966645	-2.71209403	1	4.67727338	-0.78912010	-2.28561196
1	5.06278397	-0.25517978	-1.45726857	1	5.31744620	-0.04587248	-0.80543420
6	4.68213618	-0.51938194	1.41810860	6	4.38158173	-0.58230452	1.91598010
1	5.44850905	-1.25358262	1.71434461	1	5.10757207	-1.31925736	2.29714014
1	5.17245858	0.22058480	0.77290590	1	4.95579936	0.22714778	1.44795836
1	4.35178860	-0.00628235	2.33062111	1	3.85438730	-0.16520573	2.78345779
6	-0.54027532	0.24787811	-2.47967364	6	-0.60358612	0.05520742	-2.51241351
1	0.06880414	-0.23933851	-3.25229707	1	-0.01527265	-0.45661662	-3.28472608
1	-1.25871089	-0.49443412	-2.10788566	1	-1.29335144	-0.68131373	-2.08029380
1	-1.11646786	1.04661439	-2.97512742	1	-1.21192434	0.82051876	-3.02242146
6	1.01976871	2.02291782	2.16508573	6	1.08278587	2.14776134	1.96753509
1	0.46103340	1.32228101	2.80021291	1	0.53311980	1.50206994	2.66535222
1	2.03847126	2.08774197	2.56834580	1	2.11004952	2.23439286	2.34342872
1	0.56080958	3.01866530	2.28257093	1	0.63336902	3.15385916	2.01955734
6	2.31722818	1.61609350	-2.82732421	6	2.22341263	1.44238193	-3.04095921
1	3.40629649	1.62332649	-2.69492635	1	3.31538121	1.49408405	-2.95070025
1	2.07106096	0.83296613	-3.55594880	1	1.97866595	0.60974869	-3.71242680
1	2.03633094	2.58208154	-3.27681799	1	1.89287661	2.37033045	-3.53595809
6	3.27847738	2.69474064	0.00860050	6	3.25933540	2.71669113	-0.30518711
1	3.64988080	2.55700341	1.03196949	1	3.66081102	2.66727685	0.71470478
1	4.08472357	2.41883797	-0.68280450	1	4.05471695	2.41201090	-0.99648769
1	3.08474993	3.77064678	-0.12858104	1	3.03077950	3.77421957	-0.51642700
6	-6.69919586	-0.19214859	-1.90969655	6	-6.88148040	-0.15479054	-1.61806043
1	-5.91319507	-0.50145518	-2.61434739	1	-6.14633712	-0.52005255	-2.35019641
1	-7.57861740	-0.81730590	-2.08635968	1	-7.78416235	-0.76497959	-1.71094988
1	-6.97149362	0.85304811	-2.12284468	1	-7.14263905	0.88560253	-1.86624292
6	-7.09016390	-1.16637278	0.37183257	6	-7.16689172	-1.00259312	0.73575886
1	-7.88371621	-1.64570768	-0.20784237	1	-8.00212592	-1.48963059	0.22479819
1	-6.49684133	-1.95581028	0.85574087	1	-6.56872785	-1.78226830	1.22933971
1	-7.55930242	-0.54911689	1.15365497	1	-7.57833828	-0.33051504	1.50489812

[CpRu(C<sub>5</sub>H<sub>4</sub>CH<sub>2</sub>)]<sup>+</sup> (1')

PBE/L2	BPBE/L2
E = -4956.674149 a.u. E <sub>0</sub> = -4956.492509 a.u. ZPVE = 0.181641 a.u. = 113.9814 kcal/mol T = 298.150 K: G = 91.6655 kcal/mol	E = -4956.951685 E <sub>0</sub> = -4956.770248 ZPVE = 0.181437 a.u. = 113.8537 kcal/mol T = 298.150 K: G = 91.4989 kcal/mol
44 -0.03486431 0.01034604 0.00000000	44 0.03614226 -0.00671595 -0.00000026
6 1.71293789 -1.11422803 0.00000000	6 1.75929700 -1.16362339 -0.72034074
6 1.78473086 -0.25383540 -1.18411598	6 1.75929759 -1.16362215 0.72034258
6 1.81375157 1.08435641 -0.72011470	6 1.91990915 0.18970304 1.16848829
6 1.81375157 1.08435641 0.72011470	6 2.02213085 1.01539572 -0.00000124
6 1.78473086 -0.25383540 1.18411598	6 1.91990858 0.18970106 -1.16848925
6 0.74171631 -2.14115177 0.00000000	1 1.66468060 -2.03760268 -1.35876809
6 -1.66842330 1.28238472 -0.71904383	1 1.66468180 -2.03760022 1.35877170
6 -1.66842330 1.28238472 0.71904383	1 1.97994664 0.52342281 2.19988637
6 -1.92236247 -0.05416933 1.16644407	1 2.14579686 2.09501546 -0.00000221
6 -2.08102447 -0.86939661 0.00000000	1 1.97994494 0.52341909 -2.19988795
6 -1.92236247 -0.05416933 -1.16644407	6 -1.79297004 0.99042518 -0.00000021
1 1.77674459 -0.59071936 -2.21622978	6 -1.80255421 0.12508108 -1.18634961
1 1.82362520 1.97367857 -1.34425649	6 -1.73618872 -1.21374860 -0.72140366
1 1.82362520 1.97367857 1.34425649	6 -1.73618906 -1.21374898 0.72140197
1 1.77674459 -0.59071936 2.21622978	6 -1.80255432 0.12508034 1.18634882
1 0.50048543 -2.65758864 0.92897726	6 -0.90277031 2.09108598 0.00000121
1 0.50048543 -2.65758864 -0.92897726	1 -1.82148361 0.46076555 -2.21897902
1 -1.51173911 2.14711093 -1.35736787	1 -1.68425067 -2.10190170 -1.34562740
1 -1.51173911 2.14711093 1.35736787	1 -1.68425164 -2.10190253 1.34562516
1 -2.00419532 -0.38299256 2.19756880	1 -1.82148397 0.46076392 2.21897850
1 -2.27665543 -1.93812856 0.00000000	1 -0.70136182 2.62493956 0.92885525
1 -2.00419532 -0.38299256 -2.19756880	1 -0.70135951 2.62494308 -0.92885022

[CpRu(C<sub>5</sub>H<sub>4</sub>CH<sub>2</sub>NMe<sub>3</sub>)]<sup>+</sup> (analogue of 3)

PBE/L2	BPBE/L2
E = -5131.087854 a.u. E <sub>0</sub> = -5130.784569 a.u. ZPVE = 0.303285 a.u. = 190.3143 kcal/mol T = 298.150 K: G = 162.9176 kcal/mol	E = -5131.447357 E <sub>0</sub> = -5131.144334 ZPVE = 0.303023 a.u. = 190.1497 kcal/mol T = 298.150 K: G = 162.7255 kcal/mol
44 1.08182062 -0.13926248 0.00001265	44 1.09212289 -0.13872780 0.00001853
6 -0.54564044 -0.97784141 1.16878261	6 -0.53618750 -0.98518250 1.17074776
6 0.28452694 -2.05323260 0.71726585	6 0.29914715 -2.05934095 0.71851149
6 0.28455972 -2.05323920 -0.71720549	6 0.29913779 -2.05939628 -0.71833762
6 2.33993934 1.23645143 1.16124095	6 2.35235698 1.24162843 1.16335648
6 3.12928788 0.12497087 0.71737027	6 3.14367822 0.12855667 0.71868780
6 3.12920111 0.12505334 -0.71751398	6 3.14360667 0.12860590 -0.71883966

6	-1.07555808	-0.30247799	-0.00000362	6	-1.07253514	-0.31156038	0.00002927
6	-0.54562048	-0.97787488	-1.16876182	6	-0.53618996	-0.98526281	-1.17064571
6	-1.98139324	0.86808279	-0.00003342	6	-1.98314106	0.86042716	-0.00000217
1	-1.84766131	1.49011698	-0.89455130	1	-1.85063044	1.48248314	-0.89434222
1	-1.84765256	1.49017536	0.89444211	1	-1.85065842	1.48249710	0.89433236
6	1.85334904	1.92192663	0.00011085	6	1.86487562	1.92807784	0.00005088
6	2.33981015	1.23659484	-1.16116074	6	2.35223624	1.24170495	-1.16335231
7	-3.51408230	0.51198388	-0.00001281	7	-3.52834595	0.51048927	-0.00002334
6	-4.28983954	1.79459531	-0.00004103	6	-4.29725378	1.80438705	0.00001516
1	-4.03157299	2.36839146	-0.89679698	1	-4.03499705	2.37663935	-0.89667632
1	-5.36168702	1.56675303	-0.00003571	1	-5.37103811	1.58511119	-0.00003060
1	-4.03156332	2.36844503	0.89667673	1	-4.03503295	2.37657948	0.89675348
6	-3.85761038	-0.28253161	1.22422488	6	-3.88104488	-0.28368878	1.22858592
1	-3.61518842	0.31144145	2.11241393	1	-3.63231766	0.30681703	2.11734220
1	-4.92932399	-0.51012003	1.20852601	1	-4.95530364	-0.49997534	1.21372722
1	-3.27178676	-1.20669917	1.22141151	1	-3.30659050	-1.21472630	1.22510009
6	-3.85757849	-0.28260303	-1.22421642	6	-3.88102672	-0.28361144	-1.22868686
1	-4.92929105	-0.51019396	-1.20852857	1	-4.95528533	-0.49989813	-1.21386696
1	-3.61514420	0.31133746	-2.11242459	1	-3.63229639	0.30696467	-2.11739721
1	-3.27173326	-1.20675659	-1.22134741	1	-3.30655789	-1.21463939	-1.22526888
1	3.64760777	-0.58476229	1.35495858	1	3.66378402	-0.58027998	1.35649948
1	3.64750893	-0.58455818	-1.35524752	1	3.66363660	-0.58019662	-1.35675117
1	2.16253019	1.52053779	-2.19403075	1	2.17583373	1.52653377	-2.19657099
1	1.24533147	2.82205223	0.00020103	1	1.25731043	2.82893863	0.00011334
1	2.16273855	1.52024224	2.19416643	1	2.17605421	1.52638309	2.19661268
1	-0.75153896	-0.72302213	2.20536516	1	-0.74212846	-0.73241139	2.20798200
1	-0.75149858	-0.72305679	-2.20534901	1	-0.74214404	-0.73256201	-2.20789446
1	0.82357067	-2.74942791	-1.35253024	1	0.83965860	-2.75466385	-1.35406988
1	0.82357394	-2.74936523	1.35262184	1	0.83965768	-2.75457413	1.35429022

[CpRu(C<sub>5</sub>H<sub>4</sub>CH<sub>2</sub>NMe<sub>2</sub>Ph)]<sup>+</sup>

PBE/L2				BPBE/L2			
E = -5322.728350 a.u. E <sub>0</sub> = -5322.373923 a.u.				E = -5323.174668 E <sub>0</sub> = -5322.820714			
ZPVE = 0.354427 a.u. = 222.4066 kcal/mol				ZPVE = 0.353954 a.u. = 222.1098 kcal/mol			
T = 298.150 K: G = 191.8984 kcal/mol				T = 298.150 K: G = 191.4835 kcal/mol			
44	2.07636353	-0.14466901	0.14931973	44	2.08617616	-0.14983905	0.14836471
6	1.01445333	1.27887667	-1.10093111	6	1.02638100	1.28101008	-1.10319594
6	2.18822800	1.91820428	-0.58844999	6	2.20570867	1.91657627	-0.59230438
6	2.10421034	1.93640473	0.84355314	6	2.12410886	1.93612385	0.84219591
6	2.71639383	-1.93056105	-0.95675247	6	2.72307607	-1.94211526	-0.95973939
6	3.86811861	-1.24277095	-0.45054950	6	3.87855456	-1.25460242	-0.45450154
6	3.78245885	-1.22749876	0.98177228	6	3.79473886	-1.23849706	0.98056814
6	0.18400853	0.89877081	0.02529031	6	0.19220315	0.90699630	0.02643815
6	0.87777641	1.30815737	1.23126863	6	0.89353418	1.31264337	1.23310860
6	-1.11672008	0.19696045	-0.03955683	6	-1.11445540	0.20792617	-0.03614386
1	-1.29196374	-0.42513629	0.84391761	1	-1.29105456	-0.41248052	0.84778648
1	-1.21779172	-0.42236016	-0.93900081	1	-1.21979045	-0.41050053	-0.93536748
6	1.92083286	-2.33970312	0.16329451	6	1.92733094	-2.35038354	0.16369275
6	2.57770974	-1.90593155	1.36142616	6	2.58735713	-1.91612442	1.36291870
7	-2.38789697	1.15558651	-0.10362492	7	-2.39905026	1.16877312	-0.09940183
6	-3.61641097	0.29202985	-0.16674352	6	-3.62711659	0.29432821	-0.16577423
6	-4.43192888	0.27725736	-1.29781004	6	-4.43708400	0.26759494	-1.30426996
6	-3.91328642	-0.52223829	0.93060203	6	-3.92835346	-0.51842822	0.93520370
6	-5.55450659	-0.55573228	-1.32274156	6	-5.55664846	-0.57363227	-1.33266747
6	-5.03484057	-1.34867184	0.89268101	6	-5.04708982	-1.35307984	0.89372587
6	-5.85932428	-1.36795451	-0.23343616	6	-5.86545405	-1.38348785	-0.23953024
1	-4.22816205	0.89998525	-2.16484965	1	-4.23281229	0.88595248	-2.17436438
1	-3.28838096	-0.52819951	1.82285489	1	-3.31092979	-0.51817543	1.83258958
1	-6.19061143	-0.55938117	-2.20742499	1	-6.18628375	-0.58517517	-2.22241019
1	-5.26196105	-1.97855466	1.75232601	1	-5.27599820	-1.97974667	1.75577216
1	-6.73651080	-2.01364897	-0.25900046	1	-6.73904490	-2.03457573	-0.26772062
6	-2.43359932	2.03765611	1.11664055	6	-2.45274274	2.05311533	1.12556356
1	-3.32725513	2.66748902	1.05337622	1	-3.35377611	2.67290246	1.06427241
1	-2.47913454	1.42054239	2.01709360	1	-2.48900123	1.43666064	2.02672090
1	-1.52638223	2.64972632	1.13355698	1	-1.55364641	2.67678846	1.14069400
6	-2.24277543	2.04943036	-1.29772480	6	-2.25785276	2.06934509	-1.29566739
1	-1.33411463	2.64219019	-1.15991646	1	-1.35584932	2.67100490	-1.15392106
1	-2.14619327	1.44190868	-2.20263832	1	-2.15264617	1.46550770	-2.20190941
1	-3.11605444	2.70614632	-1.36603828	1	-3.13652215	2.71894690	-1.36535417
1	0.52419957	1.17501346	2.25055602	1	0.54257941	1.18289919	2.25389805
1	0.78178874	1.11897921	-2.15066456	1	0.79276371	1.12230727	-2.15305620
1	3.00359308	2.32010049	-1.18220632	1	3.02186487	2.31491810	-1.18809831
1	2.84500009	2.35459009	1.51825563	1	2.86776521	2.35215350	1.51572362
1	0.99369028	-2.90346224	0.11331001	1	0.99963675	-2.91403758	0.11525346
1	2.23729327	-2.07961682	2.37769791	1	2.24849833	-2.09003123	2.38012590
1	4.50965882	-0.79073572	1.65949897	1	4.52444060	-0.80339345	1.65731811
1	4.67138667	-0.81933397	-1.04583248	1	4.68251839	-0.83350565	-1.05123605
1	2.49863657	-2.12561211	-2.00239899	1	2.50396162	-2.13842950	-2.00530070

[CpRu(C<sub>5</sub>H<sub>4</sub>CH<sub>2</sub>...NMe<sub>2</sub>Ph)]<sup>+</sup> (TS-N-1')

PBE/L2 $\nu = 35.13i \text{ cm}^{-1}$				BPBE/L2 $\nu = 66.49i \text{ cm}^{-1}$			
E = -5322.713775 a.u. E <sub>0</sub> = -5322.363242 a.u. ZPVE = 0.350533 a.u. = 219.9629 kcal/mol T = 298.150 K: G = 187.1612 kcal/mol				E = -5323.163101 E <sub>0</sub> = -5322.812884 ZPVE = 0.350217 a.u. = 219.7645 kcal/mol T = 298.150 K: G = 187.0308 kcal/mol			
44	1.91807824	-0.16340300	0.10086252	44	2.00295408	-0.18263804	0.08518382
6	1.37593387	1.61174894	-1.04413054	6	1.29718653	1.50437179	-1.11042787
6	2.67499712	1.84489484	-0.52124596	6	2.59918371	1.84099884	-0.64645668
6	2.61495603	1.79749419	0.91475707	6	2.59182263	1.85157869	0.79369759
6	2.14836135	-1.99701014	-1.11613881	6	2.31066969	-2.04944123	-1.06825805
6	3.42128336	-1.58483714	-0.60301626	6	3.57276892	-1.53486022	-0.61711525
6	3.36118906	-1.63223429	0.83264326	6	3.56370543	-1.52630064	0.82333667
6	0.48423743	1.38428371	0.09199034	6	0.45561833	1.28159641	0.06673397
6	1.27746068	1.53401546	1.31101164	6	1.28511755	1.52170263	1.24916653
6	-0.54159607	0.42494676	0.01744127	6	-0.59889783	0.34886470	0.06811456
1	-0.98595502	0.00793662	0.91719030	1	-0.97629963	-0.06236511	0.99982249
1	-0.90820606	0.06926282	-0.94171612	1	-0.97015557	-0.07452556	-0.86101422
6	1.31190080	-2.30350765	0.00482896	6	1.53225808	-2.36295269	0.09506676
6	2.05101468	-2.07378358	1.20945422	6	2.29591753	-2.03556619	1.26447939
7	-2.80148118	1.56045817	-0.03952860	7	-2.78725886	1.49890105	0.03211321
6	-3.63566821	0.41435305	-0.11089203	6	-3.70434691	0.40711161	-0.11325312
6	-3.98720942	-0.15049958	-1.35342665	6	-4.33020533	0.12981745	-1.34476880
6	-4.08710706	-0.22805039	1.05960170	6	-3.95508927	-0.46034962	0.97153248
6	-4.74436787	-1.31973684	-1.41471895	6	-5.17273458	-0.97823145	-1.48134619
6	-4.84363517	-1.39679964	0.98308813	6	-4.80027830	-1.56047421	0.82429193
6	-5.17513476	-1.95614582	-0.25080885	6	-5.41445721	-1.83089657	-0.40303411
1	-3.69458979	0.32570162	-2.28692715	1	-4.19103612	0.78245855	-2.20384876
1	-3.87384188	0.18656186	2.04267399	1	-3.49874890	-0.28498052	1.94499617
1	-5.00968090	-1.72666758	-2.39103673	1	-5.65255087	-1.16176574	-2.44356798
1	-5.18758076	-1.86476971	1.90606478	1	-4.98155651	-2.20937455	1.68218992
1	-5.77422011	-2.86443316	-0.30480181	1	-6.07789346	-2.68863238	-0.51255550
6	-2.82556525	2.33188696	1.20422426	6	-2.85530220	2.25055748	1.29911276
1	-3.82044919	2.76500683	1.40558079	1	-3.79165014	2.82983424	1.37028391
1	-2.54119029	1.70917544	2.06061677	1	-2.79706388	1.58252619	2.16310456
1	-2.09753503	3.14798860	1.12615345	1	-2.00751582	2.94582328	1.34461140
6	-2.72501139	2.41018403	-1.22895582	6	-2.65442651	2.40923984	-1.11289140
1	-2.00812536	3.21770810	-1.03889477	1	-1.85564821	3.12888887	-0.89550941
1	-2.36928998	1.84298651	-2.09717053	1	-2.38221749	1.85611034	-2.01942251
1	-3.70107709	2.85790300	-1.48346346	1	-3.58477669	2.97068140	-1.30707353
1	0.90714839	1.43567529	2.32689626	1	0.95793197	1.44927613	2.28221892
1	1.09189607	1.58152166	-2.09161976	1	0.98067799	1.41611051	-2.14553267
1	3.57310605	2.02237387	-1.10566838	1	3.46239912	2.05081002	-1.27175291
1	3.46071189	1.93364429	1.58244551	1	3.44856743	2.07073174	1.42466816
1	0.27952208	-2.63783039	-0.04942031	1	0.52366370	-2.76751156	0.09067488
1	1.69393584	-2.23165403	2.22217844	1	1.98477948	-2.17563163	2.29522631
1	4.17091905	-1.38735537	1.51354454	1	4.37923008	-1.20441730	1.46459399
1	4.28434986	-1.29788887	-1.19633928	1	4.39628049	-1.22035199	-1.25180077
1	1.87751158	-2.08687253	-2.16332737	1	2.01206672	-2.20128135	-2.10104653

[CpRu(C<sub>5</sub>H<sub>4</sub>CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>NHMe<sub>2</sub>)]<sup>+</sup> (analogue of 5)

PBE/L2				BPBE/L2			
E = -5322.734202 a.u. E <sub>0</sub> = -5322.380003 a.u. ZPVE = 0.354199 a.u. = 222.2630 kcal/mol T = 298.150 K: G = 190.1203 kcal/mol				E = -5323.182969 E <sub>0</sub> = -5322.829126 ZPVE = 0.353842 a.u. = 222.0394 kcal/mol T = 298.150 K: G = 189.9286 kcal/mol			
44	1.83602848	0.06373631	0.02923933	44	1.85328569	0.06185465	0.03887099
6	0.07835050	0.28307060	-1.22733742	6	0.07974799	0.28090268	-1.20941905
6	0.00968423	-0.98104603	-0.53386979	6	0.01962915	-0.98592288	-0.51394949
6	-0.02048292	-0.71986947	0.87689457	6	-0.00121905	-0.72493397	0.89950046
6	0.02105004	0.70241851	1.06707338	6	0.04039536	0.69967488	1.09033318
6	0.07698224	1.32260371	-0.22583895	6	0.08705283	1.32153318	-0.20484424
6	0.02017348	0.48335011	-2.71171769	6	0.01236319	0.48235914	-2.69833206
1	0.53210882	-0.34923429	-3.22151795	1	0.52276231	-0.34979125	-3.21046468
1	0.58513129	1.38823546	-2.98938193	1	0.57533497	1.38797156	-2.97784992
6	-1.37903336	0.60339835	-3.29160368	6	-1.39121251	0.60283640	-3.28168848
6	-2.52451675	0.52627311	-2.48642595	6	-2.54324359	0.52664459	-2.48152768
1	-2.40949850	0.37623212	-1.41297218	1	-2.43682116	0.37682071	-1.40743113
6	-3.80356488	0.63782045	-3.03206147	6	-3.82255634	0.63895146	-3.03350000
1	-4.67482284	0.57355434	-2.37856985	1	-4.69514760	0.57501638	-2.38186358
6	-3.92724608	0.82914394	-4.40377104	6	-3.94175818	0.83033910	-4.40821798
6	-2.81453695	0.91101657	-5.23583411	6	-2.82238991	0.91134605	-5.23636781
1	-2.92326653	1.06181567	-6.31342129	1	-2.92398002	1.06176469	-6.31484148
6	-1.54587263	0.79722193	-4.67191936	6	-1.55405672	0.79677786	-4.66556165
1	-0.66951026	0.86060510	-5.31896426	1	-0.67624090	0.85980326	-5.31102911
6	-6.03006808	2.17115923	-4.55478337	6	-6.05210960	2.18121580	-4.58000725
1	-6.96554503	2.25120462	-5.11991623	1	-6.97819993	2.26336936	-5.16059697

1	-6.24231637	2.05589990	-3.48791342	1	-6.28174569	2.06923469	-3.51650078
6	-6.10188695	-0.30115239	-4.89286772	6	-6.12377609	-0.30332289	-4.91964764
1	-6.31560482	-0.46437305	-3.83257213	1	-6.35492422	-0.46782739	-3.86332116
1	-7.03593750	-0.17322898	-5.45151190	1	-7.04850358	-0.17421493	-5.49382896
7	-5.27727495	0.95357136	-5.02713962	7	-5.29332990	0.95601377	-5.04233481
1	-5.09958741	1.08585606	-6.03232592	1	-5.10804886	1.08781806	-6.04554399
1	-5.40031604	3.05137676	-4.71706663	1	-5.41663041	3.05877207	-4.73554257
1	-5.52204733	-1.13998255	-5.29017795	1	-5.53777624	-1.14151436	-5.30973592
6	3.70472288	1.20007331	-0.10800799	6	3.72500719	1.20149289	-0.10914013
6	3.62360671	0.57921278	1.18249707	6	3.65086145	0.57961081	1.18417055
6	3.58228481	-0.84154614	0.98947760	6	3.60938295	-0.84380570	0.99121528
6	3.71395942	0.16238794	-1.09840924	6	3.72984004	0.16171745	-1.10112125
6	3.63789218	-1.09949464	-0.42043789	6	3.65787368	-1.10243171	-0.42145997
1	3.79199682	0.30600892	-2.17215179	1	3.80350615	0.30522591	-2.17554841
1	3.64188013	-2.07885246	-0.88940656	1	3.66133215	-2.08228428	-0.89044178
1	3.76787324	2.26714388	-0.29895484	1	3.78807426	2.26893629	-0.30059046
1	3.60863225	1.09390333	2.13843240	1	3.64243502	1.09454604	2.14055308
1	3.53058457	-1.59073054	1.77369141	1	3.56414095	-1.59323622	1.77620131
1	-0.02059142	-1.96114918	-1.00314342	1	-0.01393054	-1.96669339	-0.98234881
1	0.10647302	2.39158853	-0.42112478	1	0.11336207	2.39121287	-0.39855711
1	0.00960892	1.21863845	2.02244547	1	0.03317099	1.21593631	2.04622854
1	-0.06892849	-1.46724794	1.66329635	1	-0.04538940	-1.47310626	1.68601216

[CpRu(C<sub>5</sub>H<sub>4</sub>CH<sub>2</sub>...C<sub>6</sub>H<sub>5</sub>NMe<sub>2</sub>)]<sup>+</sup> (TS-C-1')

PBE/L2 $\nu = 128.06i \text{ cm}^{-1}$				BPBE/L2 $\nu = 153.10i \text{ cm}^{-1}$			
E = -5322.712686 a.u. E <sub>0</sub> = -5322.362699 a.u.				E = -5323.162970 E <sub>0</sub> = -5322.813321			
ZPVE = 0.349987 a.u. = 219.6201 kcal/mol				ZPVE = 0.349648 a.u. = 219.4077 kcal/mol			
T = 298.150 K: G = 186.9480 kcal/mol				T = 298.150 K: G = 186.7224 kcal/mol			
44	1.71985625	-0.26735969	-0.04181874	44	1.78256362	-0.27801711	-0.03320283
6	0.43190223	0.99072863	-1.27393579	6	0.45769429	0.93740617	-1.27726612
6	1.74111475	1.54901451	-1.30064128	6	1.74930110	1.54292299	-1.28871904
6	2.11526450	1.90538467	0.04051961	6	2.09535973	1.90995912	0.05947814
6	1.98874786	-2.31449270	-0.81850544	6	2.12908972	-2.31810937	-0.80942712
6	3.23015086	-1.59965747	-0.87882822	6	3.34863345	-1.56072317	-0.85715736
6	3.60465037	-1.24193687	0.46219023	6	3.69803467	-1.19096332	0.49008214
6	-0.02332364	0.99454069	0.10888752	6	-0.01857864	0.92706014	0.10100416
6	1.04384013	1.57051103	0.91549856	6	1.02349196	1.53407280	0.92204108
6	-1.07998620	0.20817028	0.61506588	6	-1.10380308	0.15918413	0.59289204
1	-1.11951974	-0.00117822	1.68157867	1	-1.14519223	-0.06257830	1.65717206
1	-1.62790859	-0.45943204	-0.04567108	1	-1.62456747	-0.52598261	-0.07230110
6	1.60663804	-2.40201631	0.55902609	6	1.73547519	-2.41977827	0.56667470
6	2.59497796	-1.73493506	1.35269697	6	2.69474573	-1.71932865	1.37176963
1	2.35848917	1.68285739	-2.18384613	1	2.37077180	1.70146925	-2.16535306
1	3.06025558	2.35253328	0.33395851	1	3.01970697	2.39125548	0.36561700
1	1.01569981	1.72411773	1.99031089	1	0.97758635	1.68784069	1.99659112
1	-0.13508913	0.62992320	-2.12689871	1	-0.08543489	0.56126505	-2.13943430
1	4.50229721	-0.70395109	0.75168129	1	4.57531292	-0.62456249	0.78899525
1	3.79579614	-1.37922238	-1.77907850	1	3.91661569	-1.32198660	-1.75168039
1	1.45237475	-2.73788379	-1.66177581	1	1.61613116	-2.75982896	-1.65839023
1	0.70779089	-2.88035049	0.93790997	1	0.85027552	-2.93026666	0.93660779
1	2.59573014	-1.64419931	2.43431527	1	2.68225180	-1.63042496	2.45388338
6	-2.98461024	1.54608204	0.81147236	6	-2.96557080	1.48931829	0.76925238
6	-3.29544590	1.72820606	-0.55915928	6	-3.30101279	1.68468511	-0.59951516
6	-3.81152214	0.67641688	1.56432255	6	-3.81755827	0.64878909	1.53806759
6	-4.30646440	1.01685079	-1.16787824	6	-4.34486402	1.00516358	-1.19118334
6	-4.82213694	-0.04841409	0.97062144	6	-4.86116614	-0.04381822	0.96120859
6	-5.10442760	0.09617492	-0.42191987	6	-5.16127313	0.10610264	-0.43129971
1	-2.71841345	2.44187391	-1.14900905	1	-2.71568321	2.38364583	-1.19890511
1	-3.64676288	0.57240036	2.63803290	1	-3.64264644	0.54308324	2.61036538
1	-4.50721281	1.18069006	-2.22424468	1	-4.55747459	1.17860245	-2.24369179
1	-5.42733843	-0.71237999	1.58363997	1	-5.47827032	-0.68435766	1.58718014
1	-2.34684953	2.26549228	1.32266948	1	-2.32822618	2.21371677	1.27446530
7	-6.10630983	-0.60671061	-1.01330056	7	-6.19372542	-0.56877755	-1.00753544
6	-6.42196839	-0.40579817	-2.42407146	6	-6.52773225	-0.36173833	-2.41927520
1	-5.55648397	-0.63471729	-3.06410913	1	-5.67802904	-0.61442468	-3.07122207
1	-7.23847711	-1.07612664	-2.70607237	1	-7.36476792	-1.01262267	-2.68675460
1	-6.74204011	0.62859177	-2.62417647	1	-6.82653215	0.67976154	-2.61516573
6	-6.93707305	-1.51740800	-0.23147712	6	-7.04341953	-1.45916724	-0.21189352
1	-7.64430976	-2.01723671	-0.89901982	1	-7.76756326	-1.94466907	-0.87206584
1	-6.32762876	-2.29056243	0.25971209	1	-6.44811505	-2.24498406	0.27623458
1	-7.51204123	-0.98148610	0.53988616	1	-7.59960205	-0.90508939	0.56041528

NMe<sub>3</sub>

PBE/L2		BPBE/L2	
E = -174.376721 a.u. E <sub>0</sub> = -174.260320 a.u.		E = -174.467497 E <sub>0</sub> = -174.351197	
ZPVE = 0.116401 a.u. = 73.0426 kcal/mol		ZPVE = 0.116300 a.u. = 72.9793 kcal/mol	
T = 298.150 K: G = 55.8626 kcal/mol		T = 298.150 K: G = 55.7716 kcal/mol	

7	-0.00000033	0.00000026	-0.35430631	7	-0.00000320	-0.00000503	-0.34792476
6	1.38572619	0.00000001	0.08770743	6	0.69618771	-1.20582362	0.08981038
1	1.49057873	0.00000012	1.19759839	1	0.75354572	-1.30520161	1.19857467
1	1.90166272	-0.88975954	-0.30007318	1	0.18272043	-2.09548218	-0.30279372
1	1.90166310	0.88975926	-0.30007339	1	1.72340080	-1.20594251	-0.30276352
6	-0.69286383	-1.20007385	0.08770731	6	-1.39236560	0.00000415	0.08982248
1	-1.72138610	-1.20201190	-0.30007431	1	-1.90608103	0.88952087	-0.30278099
1	-0.18027785	-2.09176773	-0.30007354	1	-1.90609620	-0.88951396	-0.30275416
1	-0.74528777	-1.29087980	1.19759828	1	-1.50710719	0.00002521	1.19858569
6	-0.69286331	1.20007477	0.08770703	6	0.69617643	1.20581678	0.08981699
1	-1.72138582	1.20201086	-0.30007398	1	0.18269586	2.09547142	-0.30277761
1	-0.74528822	1.29087879	1.19759811	1	0.75354260	1.30518870	1.19858019
1	-0.18027752	2.09176876	-0.30007384	1	1.72338367	1.20594178	-0.30276963

### NMe<sub>2</sub>Ph

PBE/L2				BPBE/L2			
E = -366.030988 a.u. E <sub>0</sub> = -365.862805 a.u.				E = -366.208659 E <sub>0</sub> = -366.040689			
ZPVE = 0.168183 a.u. = 105.5365 kcal/mol				ZPVE = 0.167971 a.u. = 105.4033 kcal/mol			
T = 298.150 K: G = 84.3168 kcal/mol				T = 298.150 K: G = 84.1561 kcal/mol			
7	-1.61540919	-0.17155752	-0.00000010	7	1.56388942	0.44913789	-0.00001355
6	-0.23382469	-0.05616079	-0.00000018	6	0.21937368	0.09353084	-0.00001416
6	0.49931077	0.00119901	-1.20960082	6	-0.49575459	-0.08994388	-1.21130375
6	0.49931054	0.00119961	1.20960055	6	-0.49573947	-0.08990885	1.21128783
6	1.88947938	0.08419242	-1.19917411	6	-1.85317047	-0.41282638	-1.20095344
6	1.88947914	0.08419300	1.19917408	6	-1.85315655	-0.41278839	1.20096385
6	2.60307832	0.12350919	0.00000004	6	-2.55095320	-0.57560890	0.00001224
1	-0.01809824	-0.01819286	-2.16694238	1	0.00811991	0.01867437	-2.17002886
1	-0.01809872	-0.01819175	2.16694199	1	0.00814858	0.01874141	2.17000324
1	2.42091922	0.12373492	-2.15169098	1	-2.36945895	-0.54338796	-2.15427023
1	2.42091879	0.12373596	2.15169103	1	-2.36943493	-0.54331567	2.15429067
1	3.69073929	0.19099563	0.00000013	1	-3.61099715	-0.83049854	0.00002280
6	-2.34451494	-0.03445278	1.24531935	6	2.31017648	0.44293456	1.24833910
1	-2.21456056	0.95940260	1.71469381	1	2.36109535	-0.55869974	1.71678437
1	-3.41288524	-0.18405249	1.05323612	1	3.33482259	0.78061075	1.05479464
1	-2.03057473	-0.79550374	1.97674600	1	1.86774848	1.13692665	1.98027495
6	-2.34451512	-0.03445283	-1.24532002	6	2.31020873	0.44299235	-1.24835057
1	-2.03057463	-0.79550349	-1.97674630	1	1.86777495	1.13698867	-1.98027372
1	-3.41288560	-0.18404856	-1.05323487	1	3.33483729	0.78070283	-1.05476177
1	-2.21456041	0.95940315	-1.71469333	1	2.36121128	-0.55863416	-1.71680362