

Cartesian Coordinates of optimized geometries at the M06/6-31G,SDD(Ru,Rh,Ir) Level of Theory. Descriptors such as 'for' and 'rev' represent the optimized geometries from the end point of intrinsic reaction coordinate computations respectively in the 'forward' and 'reverse' directions from the transition state.**

Gas Phase Calculations (Schemes 2-3 and Schemes S2-S3)

CH4

Number of imaginary frequencies : 0
The smallest frequencies are : 1319.2532 1320.2232 1320.5501 cm(-1)

Electronic energy : =-40.4779528
Zero-point correction= 0.044686
Thermal correction to Energy= 0.047558
Thermal correction to Enthalpy= 0.048502
Thermal correction to Gibbs Free Energy= 0.025019
Sum of electronic and zero-point Energies= -40.433267
Sum of electronic and thermal Energies= -40.430395
Sum of electronic and thermal Enthalpies= -40.429451
Sum of electronic and thermal Free Energies= -40.452934

Cartesian Coordinates

6	0.000084	-0.000033	-0.000186
1	0.569382	0.890331	-0.274913
1	0.642001	-0.880157	-0.075558
1	-0.851860	-0.110873	-0.674252
1	-0.360026	0.100897	1.025840

CO2

Number of imaginary frequencies : 0
The smallest frequencies are : 677.5866 677.5866 1403.4508 cm(-1)

Electronic energy : =-188.4980684
Zero-point correction= 0.012011
Thermal correction to Energy= 0.014623
Thermal correction to Enthalpy= 0.015567
Thermal correction to Gibbs Free Energy= -0.009340
Sum of electronic and zero-point Energies= -188.486058
Sum of electronic and thermal Energies= -188.483446
Sum of electronic and thermal Enthalpies= -188.482502
Sum of electronic and thermal Free Energies= -188.507409

Cartesian Coordinates

8	0.000000	0.000000	1.164686
6	0.000000	0.000000	-0.000007
8	0.000000	0.000000	-1.164681

Bn-Ru-OO

Number of imaginary frequencies : 0
The smallest frequencies are : 58.4269 70.1998 124.4968 cm(-1)

Electronic energy : =-555.8869437
Zero-point correction= 0.165579
Thermal correction to Energy= 0.175544
Thermal correction to Enthalpy= 0.176488
Thermal correction to Gibbs Free Energy= 0.129373
Sum of electronic and zero-point Energies= -555.721365
Sum of electronic and thermal Energies= -555.711400
Sum of electronic and thermal Enthalpies= -555.710455
Sum of electronic and thermal Free Energies= -555.757571

Cartesian Coordinates

8	1.462309	-1.288418	0.151304
6	2.709435	-0.724055	-0.201877
6	2.709672	0.723874	0.201737
8	1.462386	1.288516	-0.151026
44	0.006167	0.000171	-0.000039
1	3.523034	-1.287594	0.282583
1	2.853353	-0.809821	-1.295766
1	3.523074	1.287334	-0.283087
1	2.853834	0.809773	1.295555
6	-1.624844	-0.463565	1.330972
6	-1.698093	-1.404270	0.273342
6	-1.646865	-0.944970	-1.058802

6	-1.625153	0.463224	-1.330907
6	-1.698653	1.403951	-0.273298
6	-1.647059	0.944624	1.058845
1	-1.598821	2.464180	-0.484944
1	-1.506600	-0.810726	2.353324
1	-1.597598	-2.464447	0.484956
1	-1.541223	-1.653473	-1.874945
1	-1.506854	0.810407	-2.353250
1	-1.541765	1.653184	1.874990

Bn-Ru-OO-TS1_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 7.6541 61.0217 77.7058 cm(-1)

Electronic energy : =-596.3700029
Zero-point correction= 0.212242
Thermal correction to Energy= 0.226221
Thermal correction to Enthalpy= 0.227165
Thermal correction to Gibbs Free Energy= 0.169487
Sum of electronic and zero-point Energies= -596.157761
Sum of electronic and thermal Energies= -596.143782
Sum of electronic and thermal Enthalpies= -596.142838
Sum of electronic and thermal Free Energies= -596.200516

Cartesian Coordinates

8	1.301885	-0.374163	-1.313608
6	2.545993	-0.629590	-0.693924
6	2.306799	-1.452152	0.542682
8	1.178521	-0.934153	1.218921
44	-0.155751	-0.233873	-0.022638
1	3.217436	-1.137717	-1.404418
1	3.023389	0.331628	-0.420709
1	3.178877	-1.445630	1.216195
1	2.113275	-2.505212	0.262691
6	-2.036741	-0.834919	-0.882538
6	-1.752071	0.447901	-1.414857
6	-1.388183	1.489420	-0.537285
6	-1.409216	1.273657	0.880382
6	-1.832478	0.031568	1.414762
6	-2.097834	-1.039508	0.535834
1	-1.763889	-0.148390	2.483239
1	-2.163353	-1.680586	-1.552179
1	-1.625617	0.572202	-2.486065
1	-1.008437	2.427804	-0.931805
1	-1.051224	2.054013	1.546533
1	-2.268385	-2.036967	0.929803
6	1.933355	2.861740	0.303938
1	2.948301	3.258515	0.223902
1	1.230221	3.694169	0.403431
1	1.864118	2.208778	1.178949
1	1.697326	2.275633	-0.589952

Bn-Ru-OO-TS1

Number of imaginary frequencies : 1
The smallest frequencies are : -1501.6215 41.7416 106.3507 cm(-1)

Electronic energy : =-596.3259476
Zero-point correction= 0.208442
Thermal correction to Energy= 0.220452
Thermal correction to Enthalpy= 0.221396
Thermal correction to Gibbs Free Energy= 0.170696
Sum of electronic and zero-point Energies= -596.117505
Sum of electronic and thermal Energies= -596.105496
Sum of electronic and thermal Enthalpies= -596.104552
Sum of electronic and thermal Free Energies= -596.155252

Cartesian Coordinates

8	1.334570	-0.650005	-1.228502
6	2.612051	-0.470524	-0.711986
6	2.561331	-0.619900	0.796749
8	1.537622	0.213783	1.300492
44	-0.108377	0.104217	-0.048119
1	3.301553	-1.210479	-1.152984
1	3.024510	0.530759	-0.953075
1	3.520493	-0.354797	1.269029
1	2.328272	-1.669611	1.048539
6	-1.295407	-1.683259	0.345293
6	-1.522929	-1.248902	-0.984683
6	-1.928160	0.084656	-1.258356
6	-2.106087	0.989781	-0.168804
6	-1.916650	0.572935	1.169725
6	-1.449270	-0.745739	1.412002
1	-1.979930	1.289788	1.982341
1	-0.892621	-2.672674	0.537603
1	-1.247998	-1.899911	-1.810525
1	-2.018692	0.432113	-2.282389
1	-2.310531	2.037827	-0.376796

1	-1.139434	-1.025475	2.415524
6	0.892511	2.209465	-0.301516
1	1.931187	2.561297	-0.357646
1	0.296254	2.957484	0.228827
1	1.328390	1.265862	0.546258
1	0.565268	2.130979	-1.343923

 Bn-Ru-OO-TS1_for

Number of imaginary frequencies : 0
 The smallest frequencies are : 23.7358 102.8213 143.2089 cm(-1)

Electronic energy : =-596.3576566
 Zero-point correction= 0.213838
 Thermal correction to Energy= 0.226249
 Thermal correction to Enthalpy= 0.227193
 Thermal correction to Gibbs Free Energy= 0.175333
 Sum of electronic and zero-point Energies= -596.143819
 Sum of electronic and thermal Energies= -596.131407
 Sum of electronic and thermal Enthalpies= -596.130463
 Sum of electronic and thermal Free Energies= -596.182324

 Cartesian Coordinates

8	-1.380079	-0.073797	1.358875
6	-2.634257	-0.048723	0.800936
6	-2.660639	-0.877184	-0.465855
8	-1.624885	-0.380022	-1.349271
44	0.112453	0.166839	-0.026047
1	-3.387213	-0.446815	1.506416
1	-2.978978	0.978105	0.534089
1	-3.623045	-0.860553	-0.995337
1	-2.377180	-1.915178	-0.257531
6	1.404936	-1.382697	1.045550
6	1.681209	-0.019840	1.409557
6	2.067309	0.922735	0.419364
6	2.057213	0.557576	-0.958194
6	1.615696	-0.744883	-1.303626
6	1.379462	-1.745174	-0.299439
1	1.468986	-0.998004	-2.350743
1	1.075305	-2.082980	1.807720
1	1.581912	0.293104	2.444904
1	2.266583	1.952039	0.707239
1	2.258602	1.296545	-1.728074
1	1.053013	-2.739014	-0.593660
6	-0.598545	2.138095	-0.236878
1	-1.155603	2.403416	0.669842
1	-1.277065	2.258325	-1.100844
1	-1.905743	0.493089	-1.661808
1	0.217916	2.858119	-0.381470

 Bn-Ru-OO-TS2_rev

Number of imaginary frequencies : 0
 The smallest frequencies are : 24.9326 60.1615 79.8813 cm(-1)

Electronic energy : =-784.8650163
 Zero-point correction= 0.228163
 Thermal correction to Energy= 0.244194
 Thermal correction to Enthalpy= 0.245138
 Thermal correction to Gibbs Free Energy= 0.184305
 Sum of electronic and zero-point Energies= -784.636854
 Sum of electronic and thermal Energies= -784.620822
 Sum of electronic and thermal Enthalpies= -784.619878
 Sum of electronic and thermal Free Energies= -784.680711

 Cartesian Coordinates

8	1.751515	1.452209	-0.563675
6	1.175651	2.680836	-0.350423
6	0.423597	2.679082	0.962606
8	-0.528720	1.587419	0.934819
44	0.476676	-0.102048	-0.147689
1	1.944804	3.474969	-0.321766
1	0.457743	2.975898	-1.149888
1	-0.109496	3.614488	1.180296
1	1.098964	2.442046	1.792765
6	2.005758	-1.535408	-0.539584
6	0.772559	-2.021166	-1.046893
6	-0.357091	-2.129092	-0.181269
6	-0.222182	-1.709764	1.164534
6	1.057849	-1.347401	1.705012
6	2.165486	-1.266663	0.862789
1	1.132105	-1.022875	2.739599
1	2.828437	-1.336731	-1.220842
1	0.663076	-2.211066	-2.111655
1	-1.329079	-2.415276	-0.571637
1	-1.101663	-1.677840	1.803889
1	3.104923	-0.861355	1.227092
6	-0.589413	0.540248	-1.849541
1	0.139078	0.964357	-2.551267

1	-1.330750	1.325646	-1.628168
1	-1.261981	1.844188	0.354834
1	-1.120410	-0.287203	-2.343272
6	-3.374253	-0.092266	0.085887
8	-3.452794	-1.252178	0.034279
8	-3.324660	1.071353	0.147030

Bn-Ru-OO-TS2

Number of imaginary frequencies : 1
The smallest frequencies are : -367.4869 59.6500 77.6590 cm(-1)

Electronic energy : =-784.8251215
Zero-point correction= 0.227960
Thermal correction to Energy= 0.242597
Thermal correction to Enthalpy= 0.243541
Thermal correction to Gibbs Free Energy= 0.187208
Sum of electronic and zero-point Energies= -784.597161
Sum of electronic and thermal Energies= -784.582524
Sum of electronic and thermal Enthalpies= -784.581580
Sum of electronic and thermal Free Energies= -784.637913

Cartesian Coordinates

8	0.692733	-1.744098	-1.069352
6	2.037338	-1.798415	-0.741104
6	2.181946	-1.749228	0.762191
8	1.439270	-0.613107	1.231397
44	-0.270597	-0.238435	-0.099592
1	2.485877	-2.723322	-1.141259
1	2.618176	-0.951400	-1.166690
1	3.221821	-1.671130	1.103378
1	1.716360	-2.628035	1.225196
6	-1.846773	-1.430349	0.833787
6	-2.126137	-1.242455	-0.545015
6	-2.155930	0.063379	-1.107566
6	-1.921155	1.194855	-0.267297
6	-1.655338	1.031139	1.107882
6	-1.561031	-0.286016	1.634508
1	-1.368772	1.890577	1.705686
1	-1.722537	-2.430204	1.237927
1	-2.171826	-2.107473	-1.201865
1	-2.270080	0.194279	-2.179567
1	-1.803552	2.183609	-0.703349
1	-1.186884	-0.428021	2.645374
6	0.923069	1.165111	-1.579315
1	1.010703	0.161305	-2.019342
1	1.915150	1.594351	-1.772025
1	1.952413	0.229613	1.106676
1	0.183811	1.748408	-2.132742
8	0.394933	3.121525	-0.026179
6	1.156330	2.198407	0.059547
8	2.114526	1.804432	0.705251

Bn-Ru-OO-TS2_for

Number of imaginary frequencies : 0
The smallest frequencies are : 26.0332 39.4586 70.7245 cm(-1)

Electronic energy : =-784.8804898
Zero-point correction= 0.229249
Thermal correction to Energy= 0.245145
Thermal correction to Enthalpy= 0.246089
Thermal correction to Gibbs Free Energy= 0.183611
Sum of electronic and zero-point Energies= -784.651241
Sum of electronic and thermal Energies= -784.635345
Sum of electronic and thermal Enthalpies= -784.634401
Sum of electronic and thermal Free Energies= -784.696879

Cartesian Coordinates

8	1.622468	1.810247	-0.641123
6	0.645009	2.829831	-0.602529
6	-0.268913	2.589174	0.568421
8	-0.564308	1.204215	0.617320
44	0.982591	0.102711	0.036138
1	1.138866	3.812124	-0.537271
1	0.066173	2.811639	-1.544596
1	-1.205471	3.165335	0.487704
1	0.229626	2.890278	1.507228
6	2.528780	-1.154990	0.850752
6	2.696187	-1.157604	-0.556655
6	1.577193	-1.422334	-1.377403
6	0.321563	-1.778836	-0.787888
6	0.196689	-1.901755	0.617249
6	1.283963	-1.551749	1.440393
1	-0.794347	-2.063233	1.030011
1	3.334311	-0.800048	1.487529
1	3.614737	-0.778487	-0.994156
1	1.645885	-1.271439	-2.450909
1	-0.573910	-1.876757	-1.394123

1	1.155765	-1.488162	2.516832
6	-4.918098	-0.587344	-0.304933
1	-5.452125	-0.393698	0.630584
1	-5.260953	0.160263	-1.027227
1	-5.148148	-1.589842	-0.667749
6	-3.439217	-0.440800	-0.087020
8	-2.633742	-1.327349	-0.312135
8	-3.124084	0.753954	0.375404
1	-2.126008	0.832662	0.488011

 Bn-Ru-OO-2-mol-CF3COOH

Number of imaginary frequencies : 0
 The smallest frequencies are : 10.7910 24.8062 27.0814 cm⁻¹)

Electronic energy : =-1609.1440215
 Zero-point correction= 0.248151
 Thermal correction to Energy= 0.273301
 Thermal correction to Enthalpy= 0.274245
 Thermal correction to Gibbs Free Energy= 0.187364
 Sum of electronic and zero-point Energies= -1608.895871
 Sum of electronic and thermal Energies= -1608.870721
 Sum of electronic and thermal Enthalpies= -1608.869777
 Sum of electronic and thermal Free Energies= -1608.956657

 Cartesian Coordinates

8	1.044492	-0.617209	1.426153
6	0.433514	-0.011187	2.558988
6	-0.782924	-0.820744	2.909760
8	-1.493117	-1.104461	1.711461
44	-0.260242	-1.422584	0.173301
1	1.154747	0.031184	3.388661
1	0.143831	1.023858	2.304560
1	-1.442066	-0.282694	3.608662
1	-0.486412	-1.768967	3.386965
6	0.440284	-3.072238	-1.033094
6	1.064740	-1.908114	-1.541416
6	0.272928	-0.779230	-1.836487
6	-1.149347	-0.850701	-1.704304
6	-1.781696	-2.057159	-1.308369
6	-0.985824	-3.157362	-0.936495
1	-2.849393	-2.044367	-1.110007
1	1.049483	-3.886852	-0.651052
1	2.144652	-1.799658	-1.531256
1	0.766672	0.161818	-2.059537
1	-1.754482	0.041418	-1.845244
1	-1.443873	-4.030781	-0.482114
6	-4.060526	2.239900	-0.394065
8	-3.969289	-0.147675	-0.456342
6	-3.645122	0.858279	0.132536
8	-2.863846	0.967205	1.171176
6	3.615503	0.730949	-0.188647
8	3.303198	0.501254	1.053639
8	3.011071	0.399428	-1.184600
1	-2.431034	0.064991	1.394284
6	4.936029	1.515591	-0.271167
9	5.247954	1.787659	-1.528573
9	5.924231	0.800400	0.266883
9	4.835892	2.661257	0.400528
1	2.407310	0.008842	1.127721
9	-3.043931	2.706990	-1.134952
9	-5.131417	2.152864	-1.166368
9	-4.300974	3.108460	0.578902

 Bn-Ru-OO.2TFA-Presence-TS1_rev

Number of imaginary frequencies : 0
 The smallest frequencies are : 15.5010 28.4591 31.9164 cm⁻¹)

Electronic energy : =-1649.6323445
 Zero-point correction= 0.295116
 Thermal correction to Energy= 0.323932
 Thermal correction to Enthalpy= 0.324876
 Thermal correction to Gibbs Free Energy= 0.230787
 Sum of electronic and zero-point Energies= -1649.337228
 Sum of electronic and thermal Energies= -1649.308413
 Sum of electronic and thermal Enthalpies= -1649.307468
 Sum of electronic and thermal Free Energies= -1649.401558

 Cartesian Coordinates

8	1.062573	-0.892061	1.576820
6	0.307286	-0.237397	2.589673
6	-0.971175	-1.002409	2.780293
8	-1.508594	-1.299282	1.498315
44	-0.074704	-1.738462	0.182012
1	0.899093	-0.186445	3.515462
1	0.087608	0.798334	2.268576
1	-1.706787	-0.425249	3.362204
1	-0.777879	-1.944085	3.319789

6	0.701164	-3.517185	-0.756660
6	1.479113	-2.436863	-1.241638
6	0.823416	-1.303713	-1.762646
6	-0.601700	-1.280806	-1.859038
6	-1.371424	-2.408106	-1.476318
6	-0.724040	-3.517234	-0.897061
1	-2.453993	-2.322366	-1.463304
1	1.181675	-4.326141	-0.213208
1	2.546872	-2.381761	-1.052375
1	1.408471	-0.415295	-1.981546
1	-1.121021	-0.371020	-2.147070
1	-1.306693	-4.321150	-0.457198
6	0.122591	2.127929	-0.387050
1	-0.688426	2.851560	-0.278647
1	0.498183	2.153747	-1.414554
1	-0.252689	1.123233	-0.156402
1	0.934486	2.376603	0.301088
6	-3.364933	0.891376	-0.192136
8	-3.109479	0.194531	-1.148398
8	-3.054357	0.681683	1.055943
6	-4.143070	2.210102	-0.336055
9	-5.264511	2.162707	0.380465
9	-4.456381	2.439258	-1.601130
9	-3.405851	3.229013	0.110302
1	-2.502982	-0.173729	1.149945
6	3.498105	0.751759	-0.003896
8	3.424423	-0.115612	-0.845961
8	2.892682	0.807051	1.147057
6	4.352127	2.011848	-0.221955
9	5.180918	2.210010	0.799572
9	3.549603	3.074943	-0.322527
9	5.063381	1.915571	-1.334128
1	2.233910	0.026260	1.262457

 Bn-Ru-OO.2TFA-Presence-TS1

Number of imaginary frequencies : 1

The smallest frequencies are : -1427.0600 14.1377 19.4422 cm(-1)

Electronic energy : =-1649.5930234
 Zero-point correction= 0.289833
 Thermal correction to Energy= 0.316652
 Thermal correction to Enthalpy= 0.317596
 Thermal correction to Gibbs Free Energy= 0.228977
 Sum of electronic and zero-point Energies= -1649.303191
 Sum of electronic and thermal Energies= -1649.276372
 Sum of electronic and thermal Enthalpies= -1649.275427
 Sum of electronic and thermal Free Energies= -1649.364047

 Cartesian Coordinates

8	-1.241463	-0.598135	-1.560473
6	-0.622599	0.074740	-2.629563
6	0.652176	-0.658247	-2.956982
8	1.413556	-0.817001	-1.753756
44	0.116714	-1.055435	-0.022321
1	-1.296138	0.090563	-3.499778
1	-0.393747	1.123673	-2.367986
1	1.259494	-0.134146	-3.704550
1	0.426084	-1.667750	-3.322953
6	-0.485243	-3.167119	0.101986
6	-1.356523	-2.358151	0.887281
6	-0.839832	-1.486898	1.876391
6	0.571854	-1.415222	2.081497
6	1.447864	-2.198044	1.300203
6	0.911768	-3.056713	0.293953
1	2.519796	-2.044396	1.377166
1	-0.880917	-3.753897	-0.721216
1	-2.414747	-2.278953	0.648947
1	-1.520472	-0.804199	2.376386
1	0.987575	-0.665203	2.749851
1	1.590009	-3.549431	-0.398186
6	0.150101	1.233195	0.325266
1	0.585688	1.974837	-0.356191
1	0.143109	1.634587	1.345182
1	1.336924	0.627049	0.477883
1	-0.894508	1.124967	0.022382
6	3.389060	1.047488	-0.080869
8	2.618242	0.681120	0.857393
8	3.178928	1.017219	-1.299285
6	4.740498	1.584439	0.424097
9	5.551302	1.916129	-0.569362
9	5.345110	0.652479	1.166576
9	4.546226	2.659503	1.188451
1	2.062954	-0.055462	-1.639859
6	-3.714275	0.565599	0.116536
8	-3.445424	-0.264863	0.968215
8	-3.148148	0.758700	-1.022900
6	-4.853691	1.574875	0.348499
9	-5.469396	1.358651	1.503085
9	-5.756183	1.496289	-0.629900
9	-4.364019	2.817556	0.361139

1 -2.276357 0.055487 -1.228166

Bn-Ru-OO.2TFA-Presence-TS1_for

Number of imaginary frequencies : 0

The smallest frequencies are : 14.8767 28.0979 32.8802 cm(-1)

Electronic energy : =-1649.612952
Zero-point correction= 0.296384
Thermal correction to Energy= 0.323520
Thermal correction to Enthalpy= 0.324464
Thermal correction to Gibbs Free Energy= 0.235960
Sum of electronic and zero-point Energies= -1649.316568
Sum of electronic and thermal Energies= -1649.289432
Sum of electronic and thermal Enthalpies= -1649.288488
Sum of electronic and thermal Free Energies= -1649.376992

Cartesian Coordinates

8 -1.382850 0.624822 1.697542
6 -0.940042 -0.184306 2.747584
6 0.502113 0.136660 3.032437
8 1.268077 -0.042141 1.816405
44 0.006402 0.740017 0.086285
1 -1.540370 -0.005827 3.653845
1 -1.031556 -1.260312 2.505165
1 0.931683 -0.483757 3.827769
1 0.618210 1.194987 3.289954
6 -0.035101 3.044140 -0.101710
6 -1.107536 2.369845 -0.760946
6 -0.864883 1.383416 -1.755835
6 0.477997 0.981085 -2.018515
6 1.532410 1.549421 -1.270414
6 1.271464 2.600658 -0.329728
1 2.546841 1.180185 -1.395135
1 -0.243467 3.783780 0.665109
1 -2.141876 2.548256 -0.477024
1 -1.713138 0.883879 -2.213833
1 0.682204 0.165209 -2.706568
1 2.095423 3.001531 0.257428
6 -0.454001 -1.282375 -0.261407
1 0.397700 -1.922416 0.020348
1 -0.665836 -1.469339 -1.321372
1 2.934219 0.399514 1.338276
1 -1.335866 -1.583660 0.316254
6 3.758466 -0.960800 0.352411
8 3.739661 0.288401 0.776856
8 2.997064 -1.844345 0.663864
6 4.890926 -1.159071 -0.664913
9 4.972148 -2.421694 -1.033460
9 6.053411 -0.774780 -0.151818
9 4.635708 -0.408837 -1.741150
1 1.409962 -0.991590 1.628168
6 -3.909011 -0.154666 -0.097868
8 -3.659216 0.790331 -0.827858
8 -3.427500 -0.433303 1.059430
6 -4.880772 -1.249523 -0.574133
9 -5.797059 -1.534792 0.351039
9 -4.185093 -2.367691 -0.822455
9 -5.510903 -0.902444 -1.689825
1 -2.473829 0.173902 1.332387

Bn-Ru-OO.2TFA-AlCl3-Presence-CO2-insertion-TS2_rev

Number of imaginary frequencies : 0

The smallest frequencies are : 14.0724 19.2521 22.0575 cm(-1)

Electronic energy : =-3461.2446039
Zero-point correction= 0.318716
Thermal correction to Energy= 0.355947
Thermal correction to Enthalpy= 0.356891
Thermal correction to Gibbs Free Energy= 0.243422
Sum of electronic and zero-point Energies= -3460.925888
Sum of electronic and thermal Energies= -3460.888657
Sum of electronic and thermal Enthalpies= -3460.887713
Sum of electronic and thermal Free Energies= -3461.001182

Cartesian Coordinates

8 2.137401 -1.438206 0.822192
6 1.964177 -2.009674 2.090765
6 0.565520 -2.542805 2.168496
8 -0.236004 -1.398531 1.847035
1 2.706053 -2.810812 2.228176
1 2.115224 -1.265161 2.893745
1 0.290084 -2.903601 3.166466
1 0.399791 -3.336778 1.425124
6 1.415763 1.089969 1.367693
1 0.980697 1.040976 2.371865
1 1.275836 2.087287 0.948052
1 2.475828 0.830368 1.410940

8	-2.053208	0.311668	1.361790
6	-1.146531	0.932983	0.841117
8	-1.045721	2.164282	0.595359
6	-3.433333	-2.410087	0.401724
8	-3.973521	-1.231557	0.277449
8	-2.436192	-2.721548	1.020171
6	-4.169789	-3.440010	-0.468596
9	-3.803201	-3.213441	-1.739690
9	-5.481708	-3.320901	-0.378795
9	-3.814063	-4.668544	-0.142391
1	-3.435534	-0.543893	0.747169
6	5.049667	-0.328084	-0.305042
8	4.561510	-0.614365	0.870482
8	4.476708	-0.380171	-1.371212
6	6.518358	0.111408	-0.189760
9	7.013162	0.414915	-1.377751
9	7.244980	-0.870636	0.340387
9	6.611771	1.178398	0.600750
1	3.586759	-0.907974	0.783281
13	-2.344945	3.390996	0.097947
17	-1.296621	4.402172	-1.465258
17	-3.895441	2.137117	-0.709603
17	-2.894722	4.538466	1.776720
6	0.321004	0.981039	-1.641491
6	-0.892471	0.237149	-1.646352
6	-0.874984	-1.173618	-1.685262
6	0.349396	-1.859550	-1.770735
6	1.545735	-1.114265	-1.819319
6	1.553250	0.299436	-1.744032
1	2.510679	-1.615301	-1.786800
1	0.281275	2.064911	-1.543539
1	-1.848157	0.761709	-1.588713
1	-1.812418	-1.723232	-1.640654
1	0.380942	-2.944784	-1.762955
1	2.504288	0.823346	-1.732555
44	0.516832	-0.367205	0.117553
1	-1.173151	-1.658907	1.699210

Bn-Ru-OO.2TFA-AICl3-Presence-CO2-insertion-TS2

Number of imaginary frequencies : 1

The smallest frequencies are : -153.0013 13.6466 16.8940 cm(-1)

Electronic energy : =-3461.2327295
Zero-point correction= 0.316342
Thermal correction to Energy= 0.353720
Thermal correction to Enthalpy= 0.354664
Thermal correction to Gibbs Free Energy= 0.239581
Sum of electronic and zero-point Energies= -3460.916388
Sum of electronic and thermal Energies= -3460.879010
Sum of electronic and thermal Enthalpies= -3460.878065
Sum of electronic and thermal Free Energies= -3460.993149

Cartesian Coordinates

8	1.933449	-1.559676	0.978161
6	1.576999	-1.865158	2.293187
6	0.141865	-2.310106	2.299374
8	-0.602314	-1.232696	1.696572
1	2.222151	-2.671274	2.676386
1	1.693263	-0.998753	2.969393
1	-0.243495	-2.489632	3.310609
1	0.020608	-3.215559	1.686904
6	1.269470	1.091518	1.323529
1	0.723967	1.062844	2.275378
1	1.197227	2.097268	0.896691
1	2.323092	0.858273	1.511659
8	-2.525881	0.453144	0.810188
6	-1.681877	1.267434	0.745961
8	-1.257662	2.382299	0.864814
6	-3.793774	-2.606073	0.203331
8	-4.510686	-1.507807	0.156367
8	-2.638740	-2.707991	0.548974
6	-4.622029	-3.809521	-0.275548
9	-4.998993	-3.609043	-1.534002
9	-5.702886	-3.940512	0.482289
9	-3.903115	-4.913764	-0.207510
1	-3.970084	-0.748613	0.450179
6	4.907419	-1.018874	-0.192872
8	4.317809	-0.858610	0.953330
8	4.420754	-1.394007	-1.238902
6	6.395395	-0.641250	-0.093756
9	7.009162	-0.808855	-1.255062
9	7.005126	-1.393994	0.821421
9	6.516931	0.636635	0.269242
1	3.308125	-1.148507	0.910250
13	-1.754046	4.110006	0.025305
17	0.036692	4.594071	-0.975514
17	-3.299099	3.352337	-1.223072
17	-2.332101	5.269714	1.669041
6	0.735516	1.016375	-1.684116
6	-0.624593	0.620884	-1.678857

6	-0.937816	-0.768092	-1.650977
6	0.059495	-1.760992	-1.819999
6	1.401044	-1.348104	-1.828581
6	1.754623	0.033437	-1.739098
1	2.213790	-2.069729	-1.777617
1	0.990644	2.070568	-1.594784
1	-1.418719	1.365962	-1.700310
1	-1.976570	-1.067363	-1.529499
1	-0.201382	-2.814742	-1.813320
1	2.804451	0.305735	-1.693370
44	0.539428	-0.381261	-0.000035
1	-1.432934	-1.605468	1.343417

 Bn-Ru-OO.2TFA-AlCl3-Presence-CO2-insertion-TS2_for

Number of imaginary frequencies : 0
 The smallest frequencies are : 7.8710 14.7560 20.2977 cm(-1)

Electronic energy : =-3461.2393657
 Zero-point correction= 0.315987
 Thermal correction to Energy= 0.354251
 Thermal correction to Enthalpy= 0.355195
 Thermal correction to Gibbs Free Energy= 0.237683
 Sum of electronic and zero-point Energies= -3460.923379
 Sum of electronic and thermal Energies= -3460.885115
 Sum of electronic and thermal Enthalpies= -3460.884171
 Sum of electronic and thermal Free Energies= -3461.001683

 Cartesian Coordinates

8	-2.205792	0.856117	1.287305
6	-1.891800	0.884902	2.649358
6	-0.589430	1.617689	2.809766
8	0.386538	0.937814	1.989832
1	-2.679022	1.412841	3.209539
1	-1.805640	-0.129288	3.075953
1	-0.243033	1.624776	3.850854
1	-0.693732	2.650060	2.446588
6	-0.791746	-1.584789	1.071971
1	-0.299083	-1.540779	2.052748
1	-0.375603	-2.423625	0.500870
1	-1.862821	-1.769949	1.225222
8	2.980704	0.137824	1.221339
6	2.619491	-0.958697	1.161948
8	2.316711	-2.092936	1.130246
6	2.639114	3.484020	0.415777
8	3.749432	2.854713	0.080243
8	1.865852	3.164955	1.284037
6	2.409123	4.690993	-0.507441
9	2.219529	4.240186	-1.746912
9	3.460869	5.495119	-0.496832
9	1.337331	5.357050	-0.123657
1	3.846655	2.066567	0.642242
6	-4.850051	-0.091285	-0.129342
8	-4.222895	-0.387526	0.952956
8	-4.521865	0.678171	-1.017367
6	-6.163749	-0.887022	-0.248788
9	-6.851783	-0.540906	-1.329534
9	-6.939663	-0.693179	0.819342
9	-5.895581	-2.195329	-0.329338
1	-3.250021	0.227472	1.079014
13	3.039820	-3.569833	-0.253517
17	1.270617	-4.143960	-1.202218
17	4.234631	-2.151379	-1.275571
17	3.981838	-4.833234	1.110905
6	-0.496993	-0.850710	-1.790915
6	0.770812	-0.251748	-1.585664
6	0.828739	1.151983	-1.350082
6	-0.318564	1.988055	-1.453380
6	-1.567023	1.365581	-1.600273
6	-1.668003	-0.053523	-1.766476
1	-2.496970	1.918848	-1.489092
1	-0.574429	-1.932813	-1.868492
1	1.678472	-0.852262	-1.586284
1	1.800141	1.593256	-1.129776
1	-0.245418	3.057975	-1.283161
1	-2.655934	-0.499317	-1.824665
44	-0.599082	0.259163	0.073346
1	1.072604	1.594424	1.778861

 Bn-Ru-OO.2TFA-AlCl3-Presence-C-C_bond formation-TS3_rev

Number of imaginary frequencies : 0
 The smallest frequencies are : 19.1686 23.7961 29.7431 cm(-1)

Electronic energy : =-5084.4909217
 Zero-point correction= 0.328332
 Thermal correction to Energy= 0.371571
 Thermal correction to Enthalpy= 0.372515
 Thermal correction to Gibbs Free Energy= 0.247451
 Sum of electronic and zero-point Energies= -5084.162589

Sum of electronic and thermal Energies= -5084.119351
Sum of electronic and thermal Enthalpies= -5084.118407
Sum of electronic and thermal Free Energies= -5084.243471

.....
Cartesian Coordinates

.....
8 0.258104 -0.892829 1.105634
6 -0.494506 -0.465049 2.217452
6 -1.931996 -0.265682 1.810876
8 -1.924934 0.576170 0.625911
44 -0.276372 -0.087499 -0.674986
1 -0.430003 -1.225963 3.012246
1 -0.093354 0.477211 2.629600
1 -2.540542 0.226752 2.579406
1 -2.392799 -1.209444 1.502095
6 -1.266560 -1.611021 -1.814432
6 0.112973 -1.942971 -1.736391
6 1.095541 -0.995583 -2.114891
6 0.692737 0.275609 -2.608390
6 -0.676929 0.589788 -2.769604
6 -1.649111 -0.341655 -2.345158
1 -0.975349 1.590242 -3.067172
1 -2.012715 -2.280580 -1.393873
1 0.430300 -2.867846 -1.258482
1 2.150714 -1.206365 -1.958544
1 1.450448 1.039100 -2.773010
1 -2.691714 -0.042435 -2.304167
6 2.525981 1.673872 2.046207
1 1.797277 2.232865 2.636232
1 3.488915 2.195630 2.023278
1 2.706504 0.694210 2.511755
8 2.785785 0.815901 -0.162977
6 2.066990 1.409641 0.660038
8 0.869171 1.769147 0.283394
1 -1.852213 1.497481 0.949244
13 0.131793 3.472376 0.489942
17 -1.111893 3.268731 2.215929
17 1.764136 4.789232 0.643331
17 -1.075967 3.730941 -1.268419
13 4.360146 -0.205560 -0.183316
17 4.689272 -0.354724 -2.278620
17 5.800924 0.882584 0.919467
17 3.667095 -2.009840 0.699210
6 -4.237600 1.715061 -0.156052
8 -3.834550 1.954771 -1.399835
8 -4.101187 2.437731 0.791185
6 -4.956599 0.359207 -0.076281
9 -4.285674 -0.590577 -0.739624
9 -6.165337 0.462526 -0.616424
9 -5.070543 -0.018439 1.184541
1 -3.327249 2.791237 -1.389865
6 -0.747987 -3.940393 0.896459
8 0.437432 -3.449796 1.132627
8 -1.796539 -3.339502 0.806390
6 -0.661063 -5.447365 0.610600
9 0.102213 -6.078211 1.490736
9 -0.118051 -5.594586 -0.606325
9 -1.861932 -6.000195 0.603740
1 0.402724 -2.426628 1.158222

.....
Bn-Ru-OO.2TFA-AlCl3-Presence-C-C_bond formation-TS3

.....
Number of imaginary frequencies : 1
The smallest frequencies are : -244.3700 19.4139 25.0616 cm(-1)

Electronic energy : =-5084.3994024
Zero-point correction= 0.325703
Thermal correction to Energy= 0.368431
Thermal correction to Enthalpy= 0.369375
Thermal correction to Gibbs Free Energy= 0.246207
Sum of electronic and zero-point Energies= -5084.073700
Sum of electronic and thermal Energies= -5084.030972
Sum of electronic and thermal Enthalpies= -5084.030027
Sum of electronic and thermal Free Energies= -5084.153195

.....
Cartesian Coordinates

.....
8 -1.517749 -1.095337 1.654926
6 -1.465866 0.023136 2.507606
6 -1.645593 1.257390 1.671194
8 -0.644844 1.157701 0.618528
44 -0.344972 -0.875670 -0.013842
1 -2.264470 -0.069219 3.260145
1 -0.499201 0.061595 3.042914
1 -1.483550 2.204601 2.197825
1 -2.619786 1.254841 1.171238
6 -2.085125 -0.737814 -1.536040
6 -2.024010 -2.091024 -1.154226
6 -0.787807 -2.772495 -1.169047
6 0.358446 -2.134504 -1.715461
6 0.269107 -0.817358 -2.233466
6 -0.933170 -0.105775 -2.091527

1	1.160594	-0.322853	-2.612220
1	-3.002297	-0.174224	-1.390482
1	-2.896011	-2.571517	-0.714889
1	-0.703546	-3.778485	-0.766293
1	1.317010	-2.653929	-1.705778
1	-0.970919	0.955769	-2.335766
6	0.974381	-2.072958	1.379294
1	1.770034	-1.663795	2.010938
1	1.365586	-2.913787	0.802877
1	0.126334	-2.329359	2.013872
8	2.574484	-0.910845	-0.398873
6	1.677715	-0.434490	0.336699
8	1.861989	0.573375	1.093277
1	0.200406	1.490023	0.991237
13	2.845573	2.129660	0.798710
17	1.653841	3.370230	2.055665
17	4.882171	1.919039	1.202896
17	2.364105	2.482997	-1.294283
13	4.138913	-1.922000	-0.365841
17	5.391812	-1.014824	-1.791626
17	4.675276	-1.935799	1.683167
17	3.381256	-3.842566	-1.001702
6	-1.407070	3.628656	-0.794395
8	-0.667329	3.191198	-1.805097
8	-1.026256	4.127516	0.225710
6	-2.891184	3.380518	-1.101555
9	-3.086722	2.059634	-1.284708
9	-3.262937	4.004020	-2.210287
9	-3.648603	3.771569	-0.097692
1	0.284267	3.281144	-1.569841
6	-4.645282	-1.310351	0.867901
8	-3.827633	-2.154398	1.447049
8	-4.437427	-0.149264	0.601943
6	-5.925849	-2.029710	0.420082
9	-6.426666	-2.797886	1.375191
9	-5.591975	-2.810988	-0.621147
9	-6.843755	-1.169773	0.023282
1	-2.915946	-1.713297	1.582142

Bn-Ru-OO_2TFA-AlCl3-Presence-C-C_bond formation-TS3_for

Number of imaginary frequencies : 0
The smallest frequencies are : 21.2517 23.6841 33.4141 cm(-1)

Electronic energy : =-5084.4044944
Zero-point correction= 0.326646
Thermal correction to Energy= 0.369882
Thermal correction to Enthalpy= 0.370826
Thermal correction to Gibbs Free Energy= 0.246653
Sum of electronic and zero-point Energies= -5084.077848
Sum of electronic and thermal Energies= -5084.034613
Sum of electronic and thermal Enthalpies= -5084.033668
Sum of electronic and thermal Free Energies= -5084.157841

Cartesian Coordinates

8	-1.439485	-0.971329	1.691686
6	-1.335310	0.187902	2.481776
6	-1.567578	1.375872	1.593826
8	-0.645490	1.197023	0.474354
44	-0.438097	-0.860216	-0.085624
1	-2.090099	0.132585	3.281372
1	-0.342202	0.249234	2.959306
1	-1.343350	2.347421	2.049336
1	-2.572181	1.364080	1.160491
6	-2.279351	-0.635550	-1.687078
6	-2.302199	-1.973709	-1.293402
6	-1.091593	-2.705495	-1.272790
6	0.100555	-2.162487	-1.827598
6	0.087804	-0.847619	-2.346777
6	-1.074281	-0.074504	-2.204820
1	1.000598	-0.409071	-2.741795
1	-3.165169	-0.016014	-1.582340
1	-3.210416	-2.423921	-0.901268
1	-1.072094	-3.712572	-0.864532
1	1.022835	-2.744998	-1.833572
1	-1.046891	0.985761	-2.452663
6	0.484924	-2.467061	1.094843
1	0.944281	-2.014685	1.976354
1	1.212575	-3.032207	0.507715
1	-0.374986	-3.065585	1.396134
8	2.404712	-1.011654	-0.496538
6	1.549147	-0.452611	0.221858
8	1.819798	0.434367	1.087485
1	0.227719	1.511156	0.793595
13	2.923686	1.939970	0.985076
17	1.706698	3.176852	2.222553
17	4.903762	1.583309	1.531627
17	2.624552	2.418466	-1.118482
13	4.001155	-1.978405	-0.402017
17	5.401163	-0.859880	-1.503168
17	4.276642	-2.248570	1.680523

17	3.336561	-3.780924	-1.381177
6	-1.051036	3.666749	-0.927798
8	-0.366374	3.135098	-1.933549
8	-0.608635	4.175163	0.062120
6	-2.558440	3.522951	-1.187557
9	-2.874790	2.212894	-1.245795
9	-2.903476	4.074441	-2.342182
9	-3.252732	4.066273	-0.209981
1	0.592044	3.166829	-1.707601
6	-4.588033	-1.162248	0.956748
8	-3.763536	-1.996467	1.535653
8	-4.371661	-0.019658	0.622396
6	-5.908142	-1.866044	0.606771
9	-6.366112	-2.599530	1.608411
9	-5.656892	-2.681557	-0.433877
9	-6.830642	-0.996821	0.242057
1	-2.840421	-1.564667	1.640714

Bn-Ru-OO.2TFA-AlCl3-Presence-C-C_bond formation-TS3_rev1

Number of imaginary frequencies : 0
The smallest frequencies are : 16.8168 18.8741 25.0045 cm(-1)

Electronic energy : =-3461.2528386
Zero-point correction= 0.319153
Thermal correction to Energy= 0.356124
Thermal correction to Enthalpy= 0.357068
Thermal correction to Gibbs Free Energy= 0.244745
Sum of electronic and zero-point Energies= -3460.933686
Sum of electronic and thermal Energies= -3460.896715
Sum of electronic and thermal Enthalpies= -3460.895771
Sum of electronic and thermal Free Energies= -3461.008094

Cartesian Coordinates

8	-2.093162	-1.307791	-0.017053
6	-1.354079	-2.445245	-0.376520
6	-0.418545	-2.734208	0.766049
8	0.251420	-1.492743	1.075298
44	-0.893056	0.240101	0.526081
1	-2.049665	-3.282168	-0.544839
1	-0.780205	-2.280568	-1.303420
1	0.344573	-3.488298	0.545514
1	-0.977740	-3.023484	1.664028
6	-1.329245	0.395606	2.877984
6	-2.508553	0.806420	2.266934
6	-2.433325	1.740355	1.201874
6	-1.218850	2.435181	0.928186
6	-0.058366	2.131830	1.665257
6	-0.090528	1.034514	2.535621
1	0.876117	2.648480	1.456021
1	-1.326909	-0.428742	3.586048
1	-3.456955	0.313197	2.459158
1	-3.333334	1.948788	0.631737
1	-1.173413	3.187975	0.145083
1	0.842792	0.677293	2.966534
6	-1.641380	0.791769	-1.444143
1	-1.400007	-0.018619	-2.134352
1	-1.234764	1.739712	-1.801016
1	-2.723671	0.848422	-1.308220
8	1.100701	1.629790	-0.999684
6	0.666377	0.433660	-0.843941
8	1.118691	-0.588532	-1.340332
6	3.646590	-2.135221	-0.233651
8	3.635460	-1.519097	-1.380048
8	2.715967	-2.325953	0.523602
1	1.172253	-1.549417	0.711296
6	5.055896	-2.658250	0.085617
9	5.920403	-1.654053	0.108463
9	5.430696	-3.525405	-0.853358
9	5.068798	-3.269215	1.258978
1	2.739380	-1.126568	-1.545037
6	-5.258359	-0.510774	-0.360023
8	-4.470526	-1.344336	-0.978743
8	-4.958102	0.286555	0.501840
6	-6.699829	-0.641275	-0.879416
9	-7.507349	0.185779	-0.236200
9	-7.137410	-1.886776	-0.709949
9	-6.737422	-0.354074	-2.179090
1	-3.523219	-1.268740	-0.612215
13	2.802388	2.217274	-0.682010
17	4.030556	1.944426	-2.374334
17	2.448943	4.228631	-0.049793
17	3.342755	0.984478	1.017340

Bn-Ru-OO.2TFA-AlCl3-Presence-C-C_bond formation-TS3

Number of imaginary frequencies : 1
The smallest frequencies are : -312.2152 14.5390 17.8468 cm(-1)

Electronic energy : =-3461.245371

Zero-point correction= 0.317972
 Thermal correction to Energy= 0.354576
 Thermal correction to Enthalpy= 0.355520
 Thermal correction to Gibbs Free Energy= 0.243541
 Sum of electronic and zero-point Energies= -3460.927399
 Sum of electronic and thermal Energies= -3460.890795
 Sum of electronic and thermal Enthalpies= -3460.889851
 Sum of electronic and thermal Free Energies= -3461.001830

 Cartesian Coordinates

 8 -2.088801 -1.463206 0.408855
 6 -1.314605 -2.588562 0.080606
 6 -0.257896 -2.733722 1.140868
 8 0.400833 -1.458313 1.247094
 44 -0.936908 0.182128 0.787544
 1 -1.969420 -3.472905 0.043588
 1 -0.829718 -2.482290 -0.906139
 1 0.495509 -3.497122 0.919231
 1 -0.713385 -2.938897 2.117505
 6 -1.404557 0.366277 2.977881
 6 -2.558134 0.787876 2.288723
 6 -2.454605 1.756011 1.263634
 6 -1.202240 2.381040 1.005739
 6 -0.071671 2.072939 1.798119
 6 -0.159469 1.023321 2.725845
 1 0.886887 2.544273 1.593813
 1 -1.449703 -0.467498 3.672545
 1 -3.501207 0.257459 2.399509
 1 -3.330400 1.969449 0.658266
 1 -1.092532 3.080917 0.180435
 1 0.748509 0.665016 3.205639
 6 -1.418158 0.397081 -1.435969
 1 -1.420382 -0.605469 -1.860574
 1 -1.026237 1.124098 -2.149772
 1 -2.433296 0.713331 -1.183212
 8 0.886291 1.697934 -0.955869
 6 0.495517 0.483526 -0.844800
 8 1.063008 -0.530116 -1.223403
 6 3.685068 -2.097173 -0.351418
 8 3.609809 -1.402758 -1.451272
 8 2.794371 -2.345701 0.434886
 1 1.245368 -1.507478 0.735053
 6 5.119795 -2.598889 -0.127568
 9 5.925793 -1.561212 0.057269
 9 5.537765 -3.281996 -1.189945
 9 5.176547 -3.385682 0.935040
 1 2.703657 -1.012831 -1.534110
 6 -5.113852 -0.550545 -0.470782
 8 -4.309128 -1.502161 -0.847643
 8 -4.891437 0.327196 0.335793
 6 -6.460533 -0.654363 -1.205967
 9 -7.277618 0.315558 -0.829980
 9 -7.034550 -1.825949 -0.941700
 9 -6.267021 -0.566627 -2.520644
 1 -3.421950 -1.437210 -0.340517
 13 2.603025 2.308045 -0.735030
 17 3.682526 2.063030 -2.532262
 17 2.241192 4.308074 -0.078086
 17 3.306703 1.096554 0.910634

 Bn-Ru-OO_2TFA-AlCl3-Presence-C-C_bond formation-TS3_rev

Number of imaginary frequencies : 0
 The smallest frequencies are : 22.2048 25.4984 30.2350 cm(-1)

Electronic energy : =-3461.3314762
 Zero-point correction= 0.319413
 Thermal correction to Energy= 0.355970
 Thermal correction to Enthalpy= 0.356914
 Thermal correction to Gibbs Free Energy= 0.246753
 Sum of electronic and zero-point Energies= -3461.012063
 Sum of electronic and thermal Energies= -3460.975507
 Sum of electronic and thermal Enthalpies= -3460.974562
 Sum of electronic and thermal Free Energies= -3461.084723

 Cartesian Coordinates

 8 -0.965423 -0.350220 -0.827259
 6 -0.564287 -1.559402 -1.464965
 6 -0.603582 -2.682817 -0.464342
 8 0.100384 -2.240646 0.722574
 44 -0.663484 -0.264287 1.232795
 1 -1.259177 -1.764240 -2.293415
 1 0.446685 -1.430341 -1.869852
 1 -0.122198 -3.593223 -0.838763
 1 -1.632036 -2.895459 -0.155349
 6 -1.672166 -1.116891 2.930285
 6 -2.657778 -0.673711 2.003042
 6 -2.619839 0.672232 1.548157
 6 -1.608325 1.555344 1.997213
 6 -0.649777 1.099109 2.945679

6	-0.686487	-0.226157	3.435523
1	0.190080	1.747453	3.187503
1	-1.611069	-2.174524	3.175399
1	-3.358362	-1.376079	1.556907
1	-3.288629	0.984635	0.749640
1	-1.496285	2.543697	1.558788
1	0.104318	-0.592893	4.082373
6	-0.421972	1.375439	-3.506598
1	-0.261541	0.614813	-4.272417
1	-0.465285	2.368389	-3.964404
1	-1.383452	1.210486	-3.007594
8	0.592503	2.262092	-1.573229
6	0.676599	1.334504	-2.491381
8	1.575061	0.496669	-2.540726
6	3.510037	-1.685398	-0.824940
8	3.743645	-0.647066	-1.563246
8	2.453793	-2.262196	-0.652835
1	1.049802	-2.199670	0.466984
6	4.787076	-2.124213	-0.089772
9	5.089413	-1.203325	0.823788
9	5.808476	-2.245501	-0.927788
9	4.594655	-3.282917	0.523918
1	2.906652	-0.236703	-1.931670
6	-4.012574	-0.824520	-1.100245
8	-3.222740	0.129546	-1.440367
8	-3.727305	-1.950907	-0.720711
6	-5.480443	-0.368482	-1.047243
9	-6.323618	-1.388313	-1.026027
9	-5.810719	0.439418	-2.045612
9	-5.630650	0.317018	0.107372
1	-2.081343	-0.119762	-1.140182
13	1.723455	2.446972	-0.220129
17	3.726525	2.838778	-0.735268
17	0.863233	3.820384	1.172970
17	1.711653	0.449989	0.842169

 Bn-Ru-NTs-AA

Number of imaginary frequencies : 0

The smallest frequencies are : 14.9571 25.5358 33.3269 cm(-1)

Electronic energy : =-1563.8004874

Zero-point correction= 0.373514

Thermal correction to Energy= 0.399106

Thermal correction to Enthalpy= 0.400050

Thermal correction to Gibbs Free Energy= 0.314732

Sum of electronic and zero-point Energies= -1563.426973

Sum of electronic and thermal Energies= -1563.401381

Sum of electronic and thermal Enthalpies= -1563.400437

Sum of electronic and thermal Free Energies= -1563.485755

 Cartesian Coordinates

6	0.612790	0.449585	2.044302
6	-0.800219	0.725243	2.499486
44	-1.105257	-0.695992	-0.080650
1	1.234170	0.092957	2.875761
1	1.078255	1.362568	1.635854
1	-0.857480	1.648812	3.090227
1	-1.148565	-0.103966	3.127387
6	-2.577352	-2.242745	-0.529717
6	-1.321799	-2.633717	-1.095644
6	-0.646011	-1.764164	-1.970973
6	-1.198274	-0.475842	-2.231294
6	-2.467143	-0.105755	-1.708611
6	-3.169273	-1.004927	-0.872465
1	-2.814634	0.923051	-1.790787
1	-3.048403	-2.873454	0.218920
1	-0.834746	-3.548527	-0.771036
1	0.353729	-2.019120	-2.307355
1	-0.621460	0.256073	-2.791097
1	-4.042465	-0.635756	-0.336048
7	-1.658273	0.784590	1.311621
1	-1.650627	1.685212	0.797239
7	0.532389	-0.575026	0.980541
16	1.972092	-1.419198	0.741079
6	3.080839	-0.166616	0.137384
6	4.020409	0.388681	0.997291
6	2.965383	0.269562	-1.180771
6	4.855052	1.395583	0.525071
1	4.095181	0.020770	2.017862
6	3.803743	1.275786	-1.634654
1	2.231613	-0.189869	-1.839993
6	4.759822	1.852382	-0.790183
1	5.596869	1.835779	1.189487
1	3.724644	1.623686	-2.663718
6	5.674860	2.921198	-1.304876
1	5.137927	3.637366	-1.936587
1	6.148611	3.474961	-0.488396
1	6.475906	2.489479	-1.918039
8	1.734852	-2.377466	-0.332634
8	2.472015	-1.869229	2.035592

6	-4.122297	2.177411	0.211360
8	-4.305596	1.168415	0.956809
8	-3.016463	2.571465	-0.245764
6	-5.370861	2.956307	-0.173918
1	-2.691622	0.733871	1.483564
1	-5.937079	3.215648	0.726407
1	-5.121847	3.860528	-0.734590
1	-6.025422	2.320511	-0.781608

Bn-Ru-NNTs

Number of imaginary frequencies : 0
The smallest frequencies are : 19.1549 37.9711 56.3000 cm(-1)

Electronic energy : =-1334.8152968
Zero-point correction= 0.308893
Thermal correction to Energy= 0.328692
Thermal correction to Enthalpy= 0.329636
Thermal correction to Gibbs Free Energy= 0.259415
Sum of electronic and zero-point Energies= -1334.506404
Sum of electronic and thermal Energies= -1334.486605
Sum of electronic and thermal Enthalpies= -1334.485661
Sum of electronic and thermal Free Energies= -1334.555882

Cartesian Coordinates

6	-0.046700	2.142331	-1.154277
6	-1.364342	2.305012	-1.867233
44	-1.720245	-0.151548	-0.315622
1	0.379663	3.113293	-0.873450
1	0.669734	1.622195	-1.819422
1	-1.207874	2.624606	-2.908007
1	-1.968568	3.082910	-1.366419
6	-2.546685	-0.824646	1.601883
6	-1.353294	-1.563931	1.432311
6	-1.097688	-2.221704	0.215110
6	-2.089861	-2.219304	-0.816273
6	-3.348645	-1.602343	-0.598197
6	-3.552463	-0.851495	0.586967
1	-4.083352	-1.568679	-1.398170
1	-2.661394	-0.189049	2.474227
1	-0.564846	-1.441212	2.167526
1	-0.121648	-2.660115	0.025548
1	-1.869642	-2.674565	-1.777639
1	-4.452274	-0.253736	0.702606
7	-2.043075	1.019713	-1.801053
1	-2.843985	0.950888	-2.423515
7	-0.330207	1.327113	0.032810
16	0.821179	1.367558	1.194722
6	2.182125	0.400867	0.547889
6	3.099597	1.002643	-0.309920
6	2.288565	-0.952735	0.850864
6	4.109963	0.236192	-0.876988
1	3.028832	2.069991	-0.506382
6	3.306688	-1.706994	0.280998
1	1.590139	-1.397980	1.556041
6	4.228395	-1.126587	-0.593734
1	4.830238	0.704252	-1.547197
1	3.399689	-2.764626	0.526855
6	5.345055	-1.935148	-1.182535
1	5.094617	-3.000577	-1.221298
1	5.587432	-1.605154	-2.198631
1	6.260754	-1.837757	-0.585281
8	0.313809	0.654921	2.367712
8	1.327831	2.731551	1.334905

Bn-Ru-NNTs-TS1_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 11.0660 49.3233 52.5278 cm(-1)

Electronic energy : =-1375.3006893
Zero-point correction= 0.356268
Thermal correction to Energy= 0.379615
Thermal correction to Enthalpy= 0.380559
Thermal correction to Gibbs Free Energy= 0.303170
Sum of electronic and zero-point Energies= -1374.944421
Sum of electronic and thermal Energies= -1374.921075
Sum of electronic and thermal Enthalpies= -1374.920131
Sum of electronic and thermal Free Energies= -1374.997520

Cartesian Coordinates

6	0.079585	1.799653	1.595614
6	1.384915	1.765972	2.348818
44	1.786300	-0.171215	0.187661
1	-0.346084	2.810642	1.581640
1	-0.646614	1.120767	2.083739
1	1.206657	1.782757	3.434305
1	1.988099	2.656607	2.096214
6	2.649916	-0.307148	-1.825289

6	1.455354	-1.061605	-1.880251
6	1.178100	-2.019014	-0.886906
6	2.152203	-2.295793	0.124912
6	3.414481	-1.647515	0.100955
6	3.637120	-0.606737	-0.835810
1	4.135045	-1.830583	0.893530
1	2.780825	0.536959	-2.494655
1	0.680013	-0.743674	-2.569183
1	0.197663	-2.486427	-0.835944
1	1.911506	-2.984883	0.930014
1	4.537960	-0.002884	-0.772037
7	2.079669	0.553285	1.942747
1	2.876596	0.324221	2.530982
7	0.383116	1.334030	0.236953
16	-0.724517	1.729525	-0.900408
6	-2.132556	0.672790	-0.581279
6	-3.074983	1.052368	0.371455
6	-2.252475	-0.546814	-1.239935
6	-4.125944	0.195173	0.672479
1	-2.988891	2.025238	0.850227
6	-3.312099	-1.391891	-0.934539
1	-1.527790	-0.811338	-2.006203
6	-4.261241	-1.036805	0.027498
1	-4.865157	0.489445	1.416723
1	-3.415193	-2.342606	-1.456961
6	-5.419777	-1.936872	0.334475
1	-5.194983	-2.980394	0.089763
1	-5.697318	-1.887887	1.393095
1	-6.306972	-1.650405	-0.244787
8	-0.196762	1.342754	-2.209173
8	-1.191508	3.096714	-0.678020
6	-1.069243	-1.871551	2.272043
1	-0.875152	-2.946215	2.206483
1	-1.440109	-1.502122	1.311163
1	-1.823113	-1.687414	3.041920
1	-0.145388	-1.340952	2.523618

Bn-Ru-NNTs-TS1

Number of imaginary frequencies : 1
The smallest frequencies are : -1536.3597 22.3540 47.9835 cm(-1)

Electronic energy = -1375.2490182
Zero-point correction= 0.353493
Thermal correction to Energy= 0.374789
Thermal correction to Enthalpy= 0.375733
Thermal correction to Gibbs Free Energy= 0.304247
Sum of electronic and zero-point Energies= -1374.895525
Sum of electronic and thermal Energies= -1374.874229
Sum of electronic and thermal Enthalpies= -1374.873285
Sum of electronic and thermal Free Energies= -1374.944771

Cartesian Coordinates

6	0.130382	2.056305	1.365610
6	1.419273	1.905568	2.137243
44	1.536626	-0.376020	0.271189
1	-0.107282	3.110241	1.179269
1	-0.695262	1.621048	1.962892
1	1.310375	2.327389	3.148777
1	2.211079	2.472473	1.613258
6	2.381862	0.007785	-1.704962
6	1.606562	-1.183378	-1.816414
6	1.826707	-2.229284	-0.897268
6	2.860527	-2.142408	0.084066
6	3.629292	-0.958069	0.165472
6	3.412078	0.123748	-0.743065
1	4.349702	-0.842941	0.972573
1	2.089956	0.867222	-2.301204
1	0.771451	-1.203641	-2.508035
1	1.157420	-3.087209	-0.886922
1	2.989531	-2.933255	0.817090
1	3.957745	1.055718	-0.630177
7	1.703494	0.481998	2.191078
1	2.590687	0.264362	2.633683
7	0.333206	1.343269	0.105751
16	-0.804375	1.582537	-1.033120
6	-2.203595	0.564226	-0.580785
6	-3.058790	0.993070	0.432479
6	-2.386579	-0.679664	-1.176195
6	-4.077250	0.154395	0.866132
1	-2.932098	1.985838	0.858783
6	-3.415461	-1.505398	-0.737980
1	-1.731505	-0.978865	-1.991491
6	-4.268603	-1.106312	0.293516
1	-4.747450	0.484999	1.659118
1	-3.566805	-2.477171	-1.207395
6	-5.393472	-1.987863	0.745591
1	-5.184101	-3.043419	0.542270
1	-5.583155	-1.879149	1.819030
1	-6.326770	-1.735102	0.226126
8	-0.311972	1.049968	-2.307038

8	-1.271808	2.966435	-0.961054
6	-0.156954	-1.398734	1.563767
1	0.171232	-2.353395	1.987003
1	-0.650529	-1.565707	0.601081
1	-0.931552	-0.956353	2.204589
1	0.693263	-0.500830	1.980975

 Bn-Ru-NNTs-TS1_for

Number of imaginary frequencies : 0
 The smallest frequencies are : 30.1776 46.2578 54.6603 cm(-1)

Electronic energy : =-1375.3019843
 Zero-point correction= 0.359241
 Thermal correction to Energy= 0.381019
 Thermal correction to Enthalpy= 0.381963
 Thermal correction to Gibbs Free Energy= 0.309243
 Sum of electronic and zero-point Energies= -1374.942743
 Sum of electronic and thermal Energies= -1374.920965
 Sum of electronic and thermal Enthalpies= -1374.920021
 Sum of electronic and thermal Free Energies= -1374.992742

 Cartesian Coordinates

6	0.078424	2.107229	1.220099
6	1.384631	2.136575	1.974525
44	1.559248	-0.366190	0.311932
1	-0.235607	3.128808	0.970143
1	-0.703682	1.677901	1.881429
1	1.291611	2.671498	2.929841
1	2.151528	2.627177	1.363419
6	2.404938	-0.151577	-1.754678
6	1.568243	-1.310135	-1.660853
6	1.834280	-2.289074	-0.674029
6	2.898440	-2.112684	0.251636
6	3.664504	-0.915807	0.171316
6	3.493392	0.025871	-0.888464
1	4.418331	-0.724595	0.934990
1	2.115472	0.630471	-2.451046
1	0.701740	-1.383624	-2.309305
1	1.163171	-3.137905	-0.563947
1	3.068600	-2.830257	1.048649
1	4.101556	0.924179	-0.934432
7	1.815677	0.733426	2.179021
1	2.767731	0.696126	2.535084
7	0.300929	1.319019	0.020616
16	-0.841986	1.474982	-1.126997
6	-2.246125	0.497526	-0.605030
6	-3.110754	1.013036	0.358184
6	-2.427588	-0.791587	-1.093731
6	-4.136120	0.217715	0.852610
1	-2.985973	2.038456	0.699239
6	-3.463202	-1.573580	-0.597111
1	-1.763508	-1.163411	-1.870318
6	-4.324916	-1.086874	0.388090
1	-4.814002	0.616515	1.606877
1	-3.610998	-2.582241	-0.982242
6	-5.454324	-1.927263	0.903237
1	-5.236323	-2.996191	0.806432
1	-5.663746	-1.717387	1.957949
1	-6.379691	-1.732352	0.345855
8	-0.348972	0.860007	-2.361311
8	-1.309589	2.862992	-1.149765
6	-0.043368	-1.243405	1.386798
1	0.360184	-1.831916	2.226575
1	-0.628627	-1.919245	0.751577
1	-0.741549	-0.492767	1.780950
1	1.218164	0.286513	2.874774

 Bn-Ru-NNTs-TS2_rev

Number of imaginary frequencies : 0
 The smallest frequencies are : 28.2486 33.7983 42.2770 cm(-1)

Electronic energy : =-1563.8069939
 Zero-point correction= 0.373881
 Thermal correction to Energy= 0.399246
 Thermal correction to Enthalpy= 0.400190
 Thermal correction to Gibbs Free Energy= 0.318131
 Sum of electronic and zero-point Energies= -1563.433113
 Sum of electronic and thermal Energies= -1563.407748
 Sum of electronic and thermal Enthalpies= -1563.406804
 Sum of electronic and thermal Free Energies= -1563.488863

 Cartesian Coordinates

6	0.715789	1.441130	0.812281
6	-0.175638	1.390962	2.034637
44	-1.559741	-0.263041	-0.104747
1	1.761765	1.586165	1.121871
1	0.453297	2.313531	0.195121

1	-0.115776	2.310011	2.634864
1	0.117142	0.535512	2.653846
6	-1.370138	-2.533821	0.195955
6	-1.392632	-2.162170	-1.191631
6	-2.468521	-1.417960	-1.715385
6	-3.495890	-0.945215	-0.843536
6	-3.399536	-1.225399	0.542550
6	-2.372804	-2.086428	1.055763
1	-4.131723	-0.794937	1.224806
1	-0.509736	-3.073619	0.579157
1	-0.544035	-2.424907	-1.813625
1	-2.465001	-1.118612	-2.760110
1	-4.294269	-0.315039	-1.227846
1	-2.313520	-2.296577	2.120631
7	-1.557662	1.157596	1.553966
1	-2.149878	0.827190	2.312598
7	0.536619	0.240737	-0.005634
16	1.587951	-0.943049	0.398123
6	3.188778	-0.223052	0.049048
6	4.122245	-0.070850	1.064260
6	3.491512	0.141862	-1.261487
6	5.374785	0.457522	0.763140
1	3.858371	-0.372630	2.075066
6	4.742684	0.665669	-1.546019
1	2.744507	0.011585	-2.041458
6	5.702638	0.829333	-0.539917
1	6.113770	0.581670	1.553819
1	4.989264	0.954190	-2.567544
6	7.057254	1.378131	-0.872212
1	7.651944	0.648379	-1.436093
1	6.983236	2.277583	-1.494555
1	7.620883	1.635728	0.030288
8	1.419042	-2.059009	-0.537601
8	1.582965	-1.265123	1.837316
6	-1.581044	1.440015	-1.369308
1	-2.367424	1.363261	-2.133552
1	-0.609696	1.492013	-1.874643
1	-1.730678	2.390344	-0.829505
1	-1.976658	2.029403	1.229976
6	-4.608466	2.290074	-0.260426
8	-5.087736	2.084040	-1.299782
8	-4.152173	2.501991	0.792718

Bn-Ru-NNTs-TS2

Number of imaginary frequencies : 1
The smallest frequencies are : -424.3421 28.3892 36.7282 cm(-1)

Electronic energy : =-1563.7566428
Zero-point correction= 0.372764
Thermal correction to Energy= 0.397359
Thermal correction to Enthalpy= 0.398303
Thermal correction to Gibbs Free Energy= 0.318202
Sum of electronic and zero-point Energies= -1563.383879
Sum of electronic and thermal Energies= -1563.359284
Sum of electronic and thermal Enthalpies= -1563.358340
Sum of electronic and thermal Free Energies= -1563.438441

Cartesian Coordinates

6	0.667495	1.381593	0.812024
6	-0.080625	1.246453	2.118977
44	-1.689417	-0.208679	-0.051962
1	1.740009	1.545804	0.991093
1	0.304009	2.267285	0.270258
1	-0.017648	2.159207	2.726256
1	0.321060	0.401664	2.687327
6	-1.611128	-2.375252	0.281849
6	-1.565744	-2.145434	-1.128718
6	-2.551226	-1.359530	-1.746827
6	-3.609864	-0.794242	-0.972781
6	-3.678544	-1.026918	0.414691
6	-2.660040	-1.811016	1.043642
1	-4.442156	-0.527012	1.005189
1	-0.794913	-2.901674	0.767904
1	-0.691394	-2.476239	-1.678307
1	-2.453990	-1.095115	-2.795850
1	-4.283496	-0.069534	-1.421210
1	-2.648793	-1.920706	2.126030
7	-1.486086	0.959640	1.761304
1	-1.970065	0.518423	2.538892
7	0.423356	0.212040	-0.039068
16	1.444049	-1.034855	0.294154
6	3.066177	-0.349256	0.004269
6	3.975760	-0.255939	1.048944
6	3.412098	0.042353	-1.287179
6	5.250043	0.241620	0.794964
1	3.680649	-0.584576	2.042487
6	4.685101	0.537947	-1.522729
1	2.686236	-0.052680	-2.091634
6	5.620809	0.646646	-0.487067
1	5.973241	0.313409	1.606129

1	4.968834	0.843022	-2.529284
6	6.986040	1.203181	-0.755541
1	7.406011	0.802435	-1.684997
1	6.952896	2.294684	-0.863722
1	7.681429	0.974135	0.058183
8	1.235815	-2.082023	-0.709512
8	1.404034	-1.446236	1.708712
6	-1.781633	1.735067	-1.464607
1	-2.298021	1.462334	-2.387688
1	-0.762518	1.314100	-1.495831
1	-1.565986	2.811699	-1.482999
1	-1.977317	1.840355	1.543012
6	-3.278417	2.337005	-0.369233
8	-4.277736	2.068736	-0.980940
8	-2.889266	2.970908	0.592352

 Bn-Ru-NNTs-TS2_for

Number of imaginary frequencies : 0

The smallest frequencies are : 27.7569 46.6967 56.8528 cm(-1)

Electronic energy : =-1563.8068461
 Zero-point correction= 0.374240
 Thermal correction to Energy= 0.399113
 Thermal correction to Enthalpy= 0.400057
 Thermal correction to Gibbs Free Energy= 0.320251
 Sum of electronic and zero-point Energies= -1563.432606
 Sum of electronic and thermal Energies= -1563.407733
 Sum of electronic and thermal Enthalpies= -1563.406789
 Sum of electronic and thermal Free Energies= -1563.486595

 Cartesian Coordinates

6	0.118233	0.935131	2.226362
6	1.237272	0.169319	2.887821
44	1.862217	-0.118986	0.041714
1	-0.095393	1.871852	2.754605
1	-0.803989	0.326668	2.215619
1	0.867845	-0.335394	3.794545
1	2.033227	0.869071	3.196345
6	2.973679	0.891247	-1.549539
6	1.840105	0.326869	-2.176215
6	1.511155	-1.021506	-1.919912
6	2.386335	-1.853732	-1.155735
6	3.586750	-1.319231	-0.634049
6	3.851493	0.067634	-0.777776
1	4.214323	-1.923976	0.015241
1	3.128829	1.964997	-1.592148
1	1.131642	0.986609	-2.665790
1	0.553049	-1.432585	-2.225982
1	2.061297	-2.859114	-0.906002
1	4.692017	0.516841	-0.256253
7	1.732237	-0.790994	1.902826
1	2.469557	-1.381232	2.280368
7	0.562090	1.203508	0.846506
16	-0.403163	2.272530	0.039987
6	-1.905317	1.352384	-0.275980
6	-3.012529	1.542242	0.541817
6	-1.943825	0.427846	-1.318411
6	-4.168743	0.802738	0.306339
1	-2.964132	2.281348	1.338094
6	-3.100628	-0.302264	-1.541245
1	-1.073509	0.297855	-1.957135
6	-4.230598	-0.124661	-0.733421
1	-5.043353	0.954549	0.937280
1	-3.137059	-1.024850	-2.356474
6	-5.465522	-0.937097	-0.979485
1	-5.770553	-0.893098	-2.031458
1	-5.293535	-1.995596	-0.741982
1	-6.305589	-0.592359	-0.368433
8	0.212160	2.559501	-1.254161
8	-0.770662	3.372933	0.927982
6	-2.584714	-2.999220	0.646389
1	-2.909105	-3.407861	-0.312662
1	-3.152093	-2.088577	0.874993
1	-2.777311	-3.716016	1.450559
6	-1.125475	-2.658538	0.593990
8	-0.428058	-2.783651	-0.394910
8	-0.691118	-2.196302	1.760338
1	0.242024	-1.846641	1.676421

 Bn-Ru-NNTs-AA-Presence-TS1_rev

Number of imaginary frequencies : 0

The smallest frequencies are : 23.0988 27.3318 31.1479 cm(-1)

Electronic energy : =-1604.2864055
 Zero-point correction= 0.422500
 Thermal correction to Energy= 0.450675
 Thermal correction to Enthalpy= 0.451619
 Thermal correction to Gibbs Free Energy= 0.362219

Sum of electronic and zero-point Energies= -1603.863906
 Sum of electronic and thermal Energies= -1603.835731
 Sum of electronic and thermal Enthalpies= -1603.834787
 Sum of electronic and thermal Free Energies= -1603.924186

 Cartesian Coordinates

6	0.301667	-0.474280	2.399190
6	-1.129593	-0.812555	2.732896
44	-0.981643	-0.718622	-0.301217
1	0.972813	-0.872016	3.170480
1	0.422175	0.626491	2.378904
1	-1.453893	-0.357179	3.678049
1	-1.230453	-1.901749	2.807803
6	-2.115984	-2.639003	-0.900576
6	-0.770188	-2.794320	-1.232953
6	-0.097716	-1.789886	-2.006016
6	-0.794727	-0.662672	-2.482001
6	-2.165726	-0.477596	-2.135034
6	-2.788679	-1.434688	-1.292426
1	-2.708376	0.405283	-2.461630
1	-2.614025	-3.362354	-0.260247
1	-0.182787	-3.611890	-0.825396
1	0.968605	-1.897626	-2.169680
1	-0.262758	0.109364	-3.033444
1	-3.808207	-1.251531	-0.954440
6	-0.361859	1.317563	-0.203588
1	-0.804615	1.880278	0.632896
1	-0.584474	1.861138	-1.134718
1	-2.628740	1.371313	-0.453440
1	0.724790	1.334691	-0.067626
6	-3.821883	2.515421	0.502054
8	-3.406908	1.948640	-0.633273
8	-3.355970	2.250676	1.591877
6	-4.916237	3.505889	0.262162
1	-2.193836	0.645840	1.721485
7	-1.978348	-0.350688	1.608380
7	0.566806	-1.086340	1.107274
16	2.113643	-1.480828	0.807974
6	2.926770	0.000327	0.220402
6	3.332211	0.959857	1.145411
6	3.059753	0.238824	-1.143303
6	3.847317	2.168212	0.695912
1	3.252923	0.745962	2.209191
6	3.580113	1.451378	-1.579959
1	2.767426	-0.534008	-1.850264
6	3.974213	2.434834	-0.670439
1	4.164369	2.922012	1.416003
1	3.689961	1.639815	-2.647576
6	4.559048	3.731731	-1.143433
1	4.238018	3.970183	-2.162951
1	4.269257	4.563782	-0.492274
1	5.656043	3.693168	-1.147833
8	2.151077	-2.430829	-0.307212
8	2.775921	-1.828813	2.067106
1	-2.878865	-0.824706	1.641565
1	-5.715498	3.050369	-0.329714
1	-4.523893	4.345554	-0.320520
1	-5.305144	3.868021	1.213997

 Bn-Ru-NNTs-AA-Presence-TS1

Number of imaginary frequencies : 1
 The smallest frequencies are : -1637.5529 18.3039 24.4696 cm(-1)

Electronic energy : =-1604.2520514
 Zero-point correction= 0.416740
 Thermal correction to Energy= 0.444415
 Thermal correction to Enthalpy= 0.445359
 Thermal correction to Gibbs Free Energy= 0.356871
 Sum of electronic and zero-point Energies= -1603.835312
 Sum of electronic and thermal Energies= -1603.807636
 Sum of electronic and thermal Enthalpies= -1603.806692
 Sum of electronic and thermal Free Energies= -1603.895180

 Cartesian Coordinates

6	0.148925	-0.428813	2.396920
6	-1.306345	-0.690072	2.694428
44	-1.068104	-0.678379	-0.334342
1	0.785812	-0.836182	3.191168
1	0.317423	0.664454	2.349682
1	-1.640993	-0.171458	3.602284
1	-1.462026	-1.769059	2.816580
6	-2.320901	-2.404234	-0.797171
6	-0.984548	-2.720925	-1.116350
6	-0.241636	-1.877286	-2.001668
6	-0.834671	-0.716740	-2.528331
6	-2.189114	-0.385606	-2.209222
6	-2.922822	-1.225323	-1.348108
1	-2.612009	0.567687	-2.511010
1	-2.860956	-3.004655	-0.068714

1	-0.467811	-3.533669	-0.614942
1	0.812027	-2.087648	-2.148778
1	-0.230438	-0.015044	-3.098913
1	-3.912060	-0.910604	-1.023583
6	-0.286686	1.542029	-0.306113
1	-0.330131	2.231421	0.545837
1	-0.187381	2.106246	-1.241202
1	-1.587680	1.438440	-0.363028
1	0.637020	0.969653	-0.190430
6	-3.213464	2.657519	0.499549
8	-2.842436	1.995472	-0.537837
8	-2.795812	2.451472	1.652470
6	-4.223373	3.751529	0.244478
1	-2.235744	0.804015	1.592777
7	-2.077494	-0.227591	1.521970
7	0.415678	-1.087342	1.125595
16	1.941582	-1.591998	0.867994
6	2.837833	-0.172793	0.252338
6	3.218374	0.824266	1.149700
6	3.043319	-0.006498	-1.112762
6	3.779057	1.997798	0.667458
1	3.082781	0.667165	2.217707
6	3.610415	1.173582	-1.581986
1	2.773643	-0.810082	-1.794030
6	3.976685	2.194335	-0.703563
1	4.076320	2.780755	1.364337
1	3.779552	1.304570	-2.650216
6	4.600727	3.461907	-1.204045
1	4.485532	3.568378	-2.287447
1	4.154621	4.342121	-0.727287
1	5.675102	3.487811	-0.982275
8	1.930543	-2.571313	-0.222254
8	2.554561	-1.944296	2.148197
1	-3.007706	-0.641433	1.528225
1	-5.070388	3.354579	-0.324125
1	-3.764883	4.531093	-0.373269
1	-4.571139	4.187865	1.182929

 Bn-Ru-NNTs-AA-Presence-TS1_for

Number of imaginary frequencies : 0
 The smallest frequencies are : 20.4279 24.0732 33.7160 cm(-1)

Electronic energy : =-1604.2884862
 Zero-point correction= 0.420392
 Thermal correction to Energy= 0.449637
 Thermal correction to Enthalpy= 0.450581
 Thermal correction to Gibbs Free Energy= 0.358612
 Sum of electronic and zero-point Energies= -1603.868094
 Sum of electronic and thermal Energies= -1603.838849
 Sum of electronic and thermal Enthalpies= -1603.837905
 Sum of electronic and thermal Free Energies= -1603.929874

 Cartesian Coordinates

6	0.494053	-0.345578	2.301505
6	-0.945401	-0.193633	2.728111
44	-1.077596	-0.830905	-0.159357
1	1.072674	-0.913912	3.039453
1	0.967305	0.645681	2.181844
1	-1.043756	0.525441	3.551908
1	-1.329630	-1.162335	3.070714
6	-2.636421	-2.029027	-1.127675
6	-1.356961	-2.426539	-1.632697
6	-0.495261	-1.472290	-2.207613
6	-0.873084	-0.101089	-2.183430
6	-2.153370	0.295089	-1.701640
6	-3.051073	-0.681626	-1.207399
1	-2.384013	1.350139	-1.560479
1	-3.262551	-2.754615	-0.616620
1	-1.008581	-3.446568	-1.496946
1	0.506051	-1.770602	-2.500037
1	-0.157257	0.663664	-2.477209
1	-3.949813	-0.348691	-0.688424
6	0.562698	2.746048	-0.170210
1	1.134270	3.260145	0.607982
1	0.901691	3.095891	-1.150507
1	-0.506135	2.949284	-0.045446
1	0.745740	1.666608	-0.095687
6	-3.922049	2.063296	0.556576
8	-4.278975	0.954379	1.046767
8	-2.737730	2.490012	0.461327
6	-5.017320	2.928861	-0.046498
1	-1.648046	1.227650	1.305414
7	-1.718775	0.217946	1.552686
7	0.486662	-1.046433	0.999572
16	1.967684	-1.746918	0.588361
6	2.952575	-0.341950	0.121680
6	3.643344	0.365044	1.101327
6	2.962879	0.078005	-1.205344
6	4.322385	1.523455	0.744959
1	3.659285	-0.004211	2.124206

6	3.650117	1.233795	-1.545041
1	2.450778	-0.514845	-1.959768
6	4.321402	1.983230	-0.573938
1	4.865876	2.084106	1.503842
1	3.669039	1.567504	-2.581728
6	4.998633	3.267619	-0.940475
1	5.428776	3.224539	-1.946726
1	4.279560	4.097379	-0.930818
1	5.797710	3.520128	-0.236223
8	1.744885	-2.560979	-0.601190
8	2.552334	-2.331030	1.789969
1	-2.757099	0.179829	1.645465
1	-5.969512	2.771875	0.467182
1	-5.155444	2.634909	-1.096127
1	-4.737846	3.985613	-0.031315

 Bn-Ru-NNTs.AA-ALCl3-Presence-CO2-insertion-TS2_rev

Number of imaginary frequencies : 0
 The smallest frequencies are : 18.2642 24.1514 34.0645 cm(-1)

Electronic energy : =-3415.9298483
 Zero-point correction= 0.442701
 Thermal correction to Energy= 0.480738
 Thermal correction to Enthalpy= 0.481682
 Thermal correction to Gibbs Free Energy= 0.370333
 Sum of electronic and zero-point Energies= -3415.487147
 Sum of electronic and thermal Energies= -3415.449110
 Sum of electronic and thermal Enthalpies= -3415.448166
 Sum of electronic and thermal Free Energies= -3415.559515

 Cartesian Coordinates

6	2.567920	0.701906	1.781301
6	2.351427	-0.473126	2.701009
44	1.619385	-1.556566	0.008693
1	3.431474	1.294251	2.113440
1	1.674402	1.360749	1.850386
1	2.128990	-0.142600	3.726523
1	3.247516	-1.105500	2.717044
6	3.223054	-3.195897	-0.215919
6	3.218726	-2.310796	-1.315913
6	2.032460	-2.067100	-2.070434
6	0.818470	-2.688532	-1.672873
6	0.776222	-3.526490	-0.530774
6	1.977112	-3.718924	0.216592
1	-0.165388	-3.950463	-0.191366
1	4.124711	-3.352749	0.367804
1	4.104940	-1.731373	-1.560239
1	2.056179	-1.347844	-2.882812
1	-0.109163	-2.447723	-2.189324
1	1.931687	-4.287892	1.145077
6	-0.046425	-0.285254	-0.243696
1	-0.949304	-0.826625	0.079770
1	-0.190419	-0.030221	-1.301054
1	0.031515	0.653738	0.318515
8	-3.332306	-0.818708	1.261397
6	-2.500568	-1.464764	1.796306
8	-1.761979	-2.166088	2.331909
1	0.368413	-0.749305	2.267473
13	-4.040579	-0.662161	-0.657059
17	-6.093252	-0.817861	-0.289733
17	-3.287368	1.252322	-1.135346
17	-3.059943	-2.342716	-1.468041
1	1.134425	-2.148421	2.638766
16	3.300094	1.283568	-0.633006
6	1.928638	2.387311	-0.949644
6	1.631824	3.387084	-0.021545
6	1.101801	2.181594	-2.046521
6	0.474865	4.137972	-0.173485
1	2.325099	3.582289	0.794870
6	-0.049399	2.948749	-2.192236
1	1.367674	1.417497	-2.773653
6	-0.391457	3.919544	-1.250361
1	0.230781	4.914832	0.552272
1	-0.702594	2.785089	-3.048869
6	-1.653092	4.719095	-1.375852
1	-1.445008	5.795620	-1.405504
1	-2.208743	4.458416	-2.282592
1	-2.314297	4.545256	-0.516662
8	3.589645	0.600863	-1.895134
8	4.332747	2.107260	0.000580
7	2.770197	0.180053	0.441634
7	1.239949	-1.268985	2.138323
6	-1.149201	1.801228	2.515302
8	-1.737329	2.458619	1.526622
8	-1.215293	0.590139	2.656933
6	-0.388705	2.720227	3.413367
1	-2.131682	1.834168	0.887436
1	0.408172	3.196393	2.829367
1	-1.042015	3.518902	3.777368
1	0.038384	2.166632	4.250461

Bn-Ru-NNTs.AA-AICl3-Presence-CO2-insertion-TS2

Number of imaginary frequencies : 1

The smallest frequencies are : -155.2182 14.6272 20.2881 cm(-1)

Electronic energy : =-3415.9112088
Zero-point correction= 0.443140
Thermal correction to Energy= 0.480550
Thermal correction to Enthalpy= 0.481494
Thermal correction to Gibbs Free Energy= 0.370951
Sum of electronic and zero-point Energies= -3415.468069
Sum of electronic and thermal Energies= -3415.430659
Sum of electronic and thermal Enthalpies= -3415.429715
Sum of electronic and thermal Free Energies= -3415.540258

Cartesian Coordinates

6	2.393284	-1.459497	1.618057
6	1.351830	-1.637222	2.689838
44	-0.364609	-1.440180	0.280875
1	3.226177	-2.158775	1.773038
1	2.795427	-0.431568	1.694546
1	1.723993	-1.295072	3.664981
1	1.047179	-2.688036	2.771902
6	-0.847303	-3.709473	0.392646
6	-0.281654	-3.382957	-0.856826
6	-0.828193	-2.370444	-1.689809
6	-1.975967	-1.677492	-1.251820
6	-2.576450	-1.999465	-0.006240
6	-1.952827	-2.955349	0.842378
1	-3.525802	-1.548990	0.279066
1	-0.378749	-4.451254	1.031922
1	0.654259	-3.841738	-1.163151
1	-0.316251	-2.100911	-2.606389
1	-2.392318	-0.869367	-1.852642
1	-2.360411	-3.121323	1.838141
6	0.055746	0.553319	-0.316409
1	-0.147469	1.284433	0.478848
1	-0.540749	0.830209	-1.193608
1	1.117560	0.583667	-0.573409
8	-2.704562	0.968018	0.282143
6	-2.376510	0.272383	1.218030
8	-2.451947	0.001728	2.360412
1	0.459226	0.140678	2.269378
13	-4.348274	1.579782	-0.528422
17	-4.547106	3.558015	0.153264
17	-3.898381	1.306350	-2.577834
17	-5.685215	0.145966	0.293389
1	-0.595787	-0.945204	2.921045
16	2.797275	-1.775073	-0.921112
6	3.562487	-0.167253	-1.100018
6	4.596293	0.202278	-0.243712
6	3.092436	0.722931	-2.064320
6	5.121448	1.488161	-0.323055
1	5.006093	-0.524778	0.453514
6	3.629241	2.000272	-2.133367
1	2.312978	0.399194	-2.750604
6	4.630983	2.410662	-1.248102
1	5.938014	1.778396	0.338598
1	3.262440	2.700627	-2.882801
6	5.129288	3.822076	-1.271499
1	6.071723	3.930876	-0.724213
1	5.284912	4.181633	-2.294724
1	4.391663	4.488680	-0.804332
8	2.034689	-2.018074	-2.146943
8	3.882135	-2.685337	-0.551838
7	1.746161	-1.697120	0.329214
7	0.178652	-0.847854	2.267468
6	2.370326	2.544148	1.900399
8	2.154063	2.916245	0.640688
8	1.736365	1.672126	2.464334
6	3.491046	3.316693	2.516718
1	1.477430	2.327860	0.255009
1	4.420677	3.054276	1.997160
1	3.334277	4.390141	2.376467
1	3.576760	3.077196	3.576676

Bn-Ru-NNTs.AA-AICl3-Presence-CO2-insertion-TS2_for

Number of imaginary frequencies : 0

The smallest frequencies are : 16.3598 17.2287 25.7880 cm(-1)

Electronic energy : =-3415.9162694
Zero-point correction= 0.444490
Thermal correction to Energy= 0.482208
Thermal correction to Enthalpy= 0.483153
Thermal correction to Gibbs Free Energy= 0.371690
Sum of electronic and zero-point Energies= -3415.471779
Sum of electronic and thermal Energies= -3415.434061
Sum of electronic and thermal Enthalpies= -3415.433117

Sum of electronic and thermal Free Energies= -3415.544579

Cartesian Coordinates

```
6 2.213073 -1.537607 1.685916
6 1.134487 -1.479754 2.736041
44 -0.522309 -1.231525 0.317071
1 2.876996 -2.396347 1.852778
1 2.818136 -0.617232 1.760517
1 1.530852 -1.117704 3.693921
1 0.671398 -2.461184 2.895628
6 -0.987664 -3.567584 0.554745
6 -0.442207 -3.327199 -0.723275
6 -0.999528 -2.378607 -1.610911
6 -2.151355 -1.676835 -1.211899
6 -2.736384 -1.942371 0.055535
6 -2.126060 -2.845919 0.954118
1 -3.652201 -1.426442 0.346345
1 -0.497179 -4.260243 1.231936
1 0.489232 -3.810027 -1.006400
1 -0.501780 -2.170026 -2.550987
1 -2.591927 -0.911319 -1.849867
1 -2.545808 -2.970725 1.949455
6 0.092805 0.621161 -0.526124
1 -0.088450 1.471876 0.143470
1 -0.471961 0.786298 -1.448221
1 1.158132 0.532695 -0.739367
8 -2.591713 0.942831 -0.087778
6 -2.089683 0.344354 0.904048
8 -2.312563 0.424656 2.087312
1 0.539385 0.365963 2.111976
13 -4.276962 1.583259 -0.462818
17 -4.371053 3.629214 0.060446
17 -4.360473 1.155579 -2.559698
17 -5.578003 0.289008 0.647244
1 -0.706083 -0.454804 2.818374
16 2.598324 -1.840795 -0.871689
6 3.602719 -0.370906 -1.021094
6 4.653389 -0.159930 -0.132379
6 3.317575 0.563048 -2.016802
6 5.381010 1.023877 -0.208131
1 4.920373 -0.930225 0.587150
6 4.060050 1.732088 -2.085013
1 2.524030 0.355539 -2.730931
6 5.082913 1.992736 -1.167426
1 6.208287 1.191744 0.481525
1 3.840607 2.466143 -2.859100
6 5.812856 3.299312 -1.205837
1 6.710723 3.283992 -0.579102
1 6.113372 3.564688 -2.225540
1 5.163353 4.107615 -0.843237
8 1.815020 -1.948270 -2.102316
8 3.513587 -2.920076 -0.500680
7 1.551917 -1.633742 0.380020
7 0.110574 -0.563581 2.213911
6 2.641734 2.521305 1.641494
8 2.408495 2.905259 0.388533
8 2.002449 1.654493 2.207187
6 3.788645 3.263347 2.245195
1 1.701610 2.343055 0.021883
1 4.712136 2.916876 1.764681
1 3.698705 4.335118 2.048114
1 3.839091 3.070550 3.316910
```

Bn-Ru-NNTs-AlCl3-Presence-C-C_bond formation-TS3_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 16.6963 19.7513 26.0138 cm(-1)

```
Electronic energy : =-3415.9264523
Zero-point correction= 0.444455
Thermal correction to Energy= 0.482202
Thermal correction to Enthalpy= 0.483146
Thermal correction to Gibbs Free Energy= 0.370459
Sum of electronic and zero-point Energies= -3415.481998
Sum of electronic and thermal Energies= -3415.444251
Sum of electronic and thermal Enthalpies= -3415.443306
Sum of electronic and thermal Free Energies= -3415.555994
```

Cartesian Coordinates

```
6 -1.480724 -1.077321 -2.044631
6 -0.107257 -1.649179 -2.266341
44 -0.094927 -0.508551 0.553267
1 -2.228518 -1.648475 -2.606054
1 -1.505397 -0.023486 -2.373941
1 0.228550 -1.572359 -3.308372
1 -0.086079 -2.701340 -1.957685
6 1.067215 -2.475880 1.256882
6 -0.191108 -2.575884 1.839904
6 -0.713493 -1.456124 2.538956
6 0.114613 -0.343159 2.834590
```


6	1.430616	-0.290920	2.345923
6	1.854733	-1.292966	1.460174
1	2.066826	0.570709	2.525163
1	1.453762	-3.254741	0.602736
1	-0.840766	-3.424432	1.646068
1	-1.749028	-1.476939	2.860091
1	-0.282270	0.485924	3.414566
1	2.821452	-1.198057	0.969522
6	-1.570392	1.032760	0.986646
1	-2.029473	1.344721	0.048334
1	-1.133122	1.892116	1.504881
1	-2.306489	0.540732	1.627215
8	1.383090	1.946407	0.606601
6	0.484290	1.399466	-0.162756
8	0.100890	1.817720	-1.229486
13	3.035307	2.414785	0.049237
17	3.382668	1.217986	-1.755783
17	4.316008	1.577080	1.564252
17	3.254134	4.484752	-0.274404
7	0.798337	-0.879821	-1.390355
7	-1.714057	-1.188425	-0.607479
16	-3.205098	-1.685469	-0.149960
6	-4.336164	-0.305339	-0.247693
6	-4.606228	0.267015	-1.489603
6	-4.927929	0.196463	0.904734
6	-5.446798	1.367450	-1.563315
1	-4.176908	-0.155938	-2.394984
6	-5.775247	1.295189	0.813757
1	-4.727174	-0.283143	1.859492
6	-6.037256	1.903675	-0.414046
1	-5.659497	1.819411	-2.531195
1	-6.245727	1.687839	1.714080
6	-6.922860	3.108620	-0.509315
1	-7.612798	3.032005	-1.357158
1	-7.516126	3.246580	0.400151
1	-6.331494	4.020656	-0.658966
8	-3.146439	-2.068990	1.263608
8	-3.671349	-2.657924	-1.137425
1	1.711625	-1.342748	-1.296536
1	0.971989	0.026401	-1.830362
6	4.454860	-2.452765	-1.037792
8	5.176344	-1.348252	-1.066781
8	3.231926	-2.471496	-1.024986
6	5.307672	-3.680140	-1.017807
1	4.599752	-0.554837	-1.137985
1	4.686976	-4.570516	-0.916326
1	5.885692	-3.734025	-1.945741
1	6.028941	-3.619173	-0.197596

 Bn-Ru-NNTs-AICl3-Presence-C-C_bond formation-TS3

Number of imaginary frequencies : 1

The smallest frequencies are : -302.3641 10.4218 18.1218 cm(-1)

Electronic energy : =-3415.9199222

Zero-point correction= 0.443925

Thermal correction to Energy= 0.481062

Thermal correction to Enthalpy= 0.482006

Thermal correction to Gibbs Free Energy= 0.370004

Sum of electronic and zero-point Energies= -3415.475998

Sum of electronic and thermal Energies= -3415.438860

Sum of electronic and thermal Enthalpies= -3415.437916

Sum of electronic and thermal Free Energies= -3415.549918

 Cartesian Coordinates

6	-1.469929	-1.477998	-1.907241
6	-0.061600	-1.968972	-2.110191
44	-0.041500	-0.577750	0.573966
1	-2.189691	-2.162732	-2.370552
1	-1.580301	-0.479674	-2.370251
1	0.231839	-1.983907	-3.167756
1	0.050376	-2.978589	-1.696710
6	0.950657	-2.420320	1.463575
6	-0.276950	-2.290156	2.124096
6	-0.644714	-1.042783	2.693544
6	0.290967	0.021790	2.715897
6	1.592785	-0.154595	2.190284
6	1.885052	-1.332501	1.493694
1	2.303423	0.668754	2.203058
1	1.197320	-3.324050	0.912302
1	-1.030287	-3.070166	2.062323
1	-1.654361	-0.917086	3.071081
1	0.009465	0.991679	3.119716
1	2.823530	-1.423483	0.953575
6	-1.421324	1.239263	0.484467
1	-2.004167	1.168435	-0.432527
1	-1.182562	2.282986	0.707389
1	-1.993636	0.869704	1.339189
8	1.150135	2.099490	0.517719
6	0.388415	1.417850	-0.287656
8	0.273472	1.587736	-1.483419

13	2.792415	2.651357	-0.023574
17	3.551553	0.966078	-1.216591
17	3.887199	2.708594	1.817486
17	2.767782	4.451507	-1.121464
7	0.807300	-1.050818	-1.352383
7	-1.665304	-1.428789	-0.460783
16	-3.165138	-1.799102	0.083210
6	-4.227643	-0.387461	-0.173351
6	-4.581280	-0.029439	-1.473100
6	-4.651400	0.373171	0.910047
6	-5.328607	1.120648	-1.681612
1	-4.289291	-0.657881	-2.311563
6	-5.407056	1.518097	0.685589
1	-4.394525	0.055075	1.917789
6	-5.742677	1.917602	-0.609148
1	-5.607147	1.406354	-2.695027
1	-5.747796	2.113378	1.531593
6	-6.523217	3.173077	-0.853513
1	-7.265918	3.035003	-1.646967
1	-7.046569	3.505066	0.048757
1	-5.863370	3.990576	-1.170224
8	-3.086957	-1.990629	1.534613
8	-3.698401	-2.867580	-0.759459
1	1.750780	-1.440354	-1.252569
1	0.882679	-0.163216	-1.858211
6	4.410662	-2.799923	-1.052018
8	5.228941	-1.763194	-0.967197
8	3.194327	-2.712501	-0.989479
6	5.151717	-4.085414	-1.229815
1	4.717537	-0.927497	-0.910168
1	4.459844	-4.926993	-1.192856
1	5.669000	-4.073261	-2.194508
1	5.920322	-4.185090	-0.457952

Bn-Ru-NNTs-AlCl3-Presence-C-C_bond formation-TS3_for

Number of imaginary frequencies : 1
The smallest frequencies are : -3.7754 19.8455 28.7816 cm(-1)

Electronic energy : =-3416.0018833
Zero-point correction= 0.444935
Thermal correction to Energy= 0.482349
Thermal correction to Enthalpy= 0.483293
Thermal correction to Gibbs Free Energy= 0.371600
Sum of electronic and zero-point Energies= -3415.556949
Sum of electronic and thermal Energies= -3415.519535
Sum of electronic and thermal Enthalpies= -3415.518591
Sum of electronic and thermal Free Energies= -3415.630283

Cartesian Coordinates

6	-1.200237	-1.257959	-2.096440
6	0.253450	-1.565216	-2.355623
44	0.015024	-1.359127	0.596585
1	-1.849064	-1.863462	-2.739183
1	-1.396250	-0.190481	-2.283279
1	0.579045	-1.149102	-3.317566
1	0.410910	-2.650628	-2.364521
6	1.232105	-2.677072	1.831170
6	-0.138230	-2.769858	2.231967
6	-0.845859	-1.611666	2.627091
6	-0.206692	-0.350097	2.528122
6	1.164217	-0.255601	2.163103
6	1.884364	-1.423174	1.838563
1	1.632169	0.721042	2.059086
1	1.752434	-3.550491	1.448804
1	-0.669117	-3.714400	2.152529
1	-1.906134	-1.687480	2.841488
1	-0.771808	0.566119	2.685097
1	2.883505	-1.334106	1.419578
6	-1.684479	2.603926	-0.716771
1	-2.211319	2.410774	-1.654063
1	-1.799962	3.649831	-0.417339
1	-2.131581	1.989359	0.075979
8	0.497641	2.637206	0.170541
6	-0.230374	2.251996	-0.844580
8	0.205747	1.624747	-1.805748
13	2.270646	2.911380	0.207393
17	3.349201	1.042623	-0.228054
17	2.651617	3.300682	2.277190
17	2.813025	4.426789	-1.169857
7	1.033468	-0.997392	-1.240693
7	-1.452337	-1.567178	-0.669277
16	-3.041163	-2.051261	-0.330669
6	-3.927508	-0.512510	-0.277625
6	-4.457778	0.011414	-1.452603
6	-4.050050	0.166081	0.931813
6	-5.095448	1.244922	-1.411882
1	-4.386111	-0.554657	-2.378445
6	-4.695778	1.394320	0.955089
1	-3.662431	-0.282915	1.843561
6	-5.211699	1.958569	-0.216206

1	-5.515480	1.663968	-2.324840
1	-4.804543	1.930313	1.896784
6	-5.844704	3.315333	-0.192379
1	-6.577910	3.434321	-0.996397
1	-6.344919	3.511608	0.761572
1	-5.084269	4.096068	-0.326432
8	-3.043692	-2.621156	1.011920
8	-3.540112	-2.824095	-1.461981
1	1.985524	-1.373338	-1.194810
1	1.098644	0.024473	-1.366252
6	4.726768	-2.334289	-1.135030
8	5.323471	-1.191067	-1.439167
8	3.573544	-2.416782	-0.745085
6	5.637895	-3.504232	-1.326444
1	4.720885	-0.442192	-1.252831
1	5.110154	-4.432125	-1.105583
1	6.011218	-3.516820	-2.354894
1	6.509755	-3.401603	-0.672985

 Bn-Ru-NNTs-2.AICl3-Presence-C-C_bond formation-TS3_rev

Number of imaginary frequencies : 0
 The smallest frequencies are : 19.9563 21.2791 28.3035 cm(-1)

Electronic energy : =-5039.1871219
 Zero-point correction= 0.452416
 Thermal correction to Energy= 0.496920
 Thermal correction to Enthalpy= 0.497864
 Thermal correction to Gibbs Free Energy= 0.369497
 Sum of electronic and zero-point Energies= -5038.734706
 Sum of electronic and thermal Energies= -5038.690202
 Sum of electronic and thermal Enthalpies= -5038.689258
 Sum of electronic and thermal Free Energies= -5038.817625

 Cartesian Coordinates

6	-0.897208	-2.384501	-1.977469
6	0.577082	-2.694273	-2.007659
44	0.004974	-1.860390	0.788164
1	-1.468435	-3.129490	-2.542461
1	-1.089447	-1.392038	-2.422777
1	1.016807	-2.505872	-2.995942
1	0.745712	-3.742319	-1.736016
6	1.216575	-2.764358	2.365034
6	-0.172603	-2.956853	2.643891
6	-1.038791	-1.843600	2.758365
6	-0.535823	-0.551199	2.483629
6	0.845042	-0.353069	2.199935
6	1.721167	-1.457870	2.181831
1	1.211917	0.637313	1.933116
1	1.870462	-3.617758	2.208623
1	-0.584726	-3.960804	2.701344
1	-2.101888	-2.006014	2.897211
1	-1.216004	0.299531	2.431213
1	2.745856	-1.326536	1.843042
6	-1.407920	1.544548	-1.415875
1	-1.951555	2.490567	-1.318336
1	-1.917881	0.822860	-0.759556
1	-1.440023	1.187865	-2.446725
8	0.295236	2.352677	0.078037
6	-0.000152	1.707353	-0.960950
8	0.916039	1.143141	-1.647471
1	1.228530	-0.886466	-1.331597
13	2.738811	1.485992	-1.581099
17	3.378045	-0.077503	-2.947396
17	3.034337	3.453662	-2.252735
17	3.487704	1.016760	0.366879
13	-0.527745	3.441161	1.331148
17	0.782707	3.288511	2.988096
17	-0.784328	5.299810	0.362675
17	-2.414854	2.486256	1.757852
6	4.961917	-2.049895	0.071455
8	5.535165	-1.408664	-0.931777
8	3.819625	-2.483100	0.041961
6	5.856609	-2.150922	1.262573
1	4.873535	-1.224172	-1.630191
1	5.845927	-1.180073	1.773376
1	6.888850	-2.349501	0.964728
1	5.493318	-2.920749	1.945095
16	-2.921320	-2.865889	-0.305447
8	-3.240203	-3.897052	-1.285710
8	-3.069096	-3.127827	1.119902
6	-3.832615	-1.401035	-0.714507
6	-4.070008	-0.445374	0.271778
6	-4.243349	-1.199472	-2.028744
6	-4.721803	0.728609	-0.073025
1	-3.752351	-0.627337	1.296778
6	-4.883274	-0.009816	-2.357816
1	-4.076761	-1.974425	-2.773401
6	-5.124194	0.969985	-1.391672
1	-4.905376	1.484622	0.688218
1	-5.207370	0.160992	-3.383046

7	-1.308067	-2.381149	-0.555843
7	1.206312	-1.845793	-0.978012
1	2.182400	-2.109917	-0.786624
6	-5.794057	2.263140	-1.740102
1	-5.971550	2.353489	-2.815902
1	-6.760362	2.356988	-1.230353
1	-5.183983	3.117028	-1.420406

Bn-Ru-NNTs-2.AICl3-Presence-C-C_bond formation-TS3

Number of imaginary frequencies : 1

The smallest frequencies are : -167.0635 16.8446 19.1342 cm(-1)

Electronic energy : =-5039.0834817

Zero-point correction= 0.451111

Thermal correction to Energy= 0.494492

Thermal correction to Enthalpy= 0.495436

Thermal correction to Gibbs Free Energy= 0.371120

Sum of electronic and zero-point Energies= -5038.632371

Sum of electronic and thermal Energies= -5038.588990

Sum of electronic and thermal Enthalpies= -5038.588045

Sum of electronic and thermal Free Energies= -5038.712362

Cartesian Coordinates

6	-1.189727	-1.643965	-2.431831
6	-0.321696	-2.707251	-1.814806
44	-0.667773	-0.424790	0.221259
1	-1.838048	-2.033035	-3.222741
1	-0.566372	-0.848943	-2.868620
1	0.400120	-3.151788	-2.513013
1	-0.938657	-3.503646	-1.382678
6	-1.113367	-1.825411	2.009320
6	-2.269099	-1.046606	1.882581
6	-2.173867	0.362796	1.762490
6	-0.928858	0.994818	1.994413
6	0.213081	0.214589	2.292915
6	0.147681	-1.184427	2.204491
1	1.176822	0.698019	2.434982
1	-1.176535	-2.908970	1.945099
1	-3.216641	-1.547317	1.725116
1	-3.058385	0.951423	1.528169
1	-0.831056	2.078091	1.916309
1	1.054526	-1.782238	2.274983
6	-0.883583	1.385569	-1.131540
1	-0.141559	1.654210	-1.891445
1	-1.061612	2.241459	-0.477428
1	-1.777829	1.023980	-1.631394
8	1.325227	1.714357	0.280333
6	0.996488	0.709021	-0.397207
8	1.793844	0.215489	-1.267430
1	1.210466	-1.553373	-1.173816
13	3.573660	-0.190328	-0.944310
17	3.626355	-2.105241	-1.977544
17	4.887035	1.263331	-1.667120
17	3.607959	-0.593894	1.171049
13	1.761157	3.508039	0.247121
17	3.415710	3.666194	1.547376
17	1.990588	3.945159	-1.811969
17	-0.026795	4.380298	1.085974
6	2.892926	-4.020960	1.509595
8	3.884990	-4.028767	0.640465
8	1.762449	-3.627087	1.255962
6	3.316618	-4.517292	2.852115
1	3.624239	-3.570544	-0.185252
1	3.858319	-3.707709	3.355632
1	4.006305	-5.359108	2.756711
1	2.445714	-4.792603	3.447927
16	-3.421574	-1.845620	-1.106404
8	-3.897228	-2.293825	-2.413339
8	-3.370350	-2.846184	-0.027091
6	-4.489624	-0.534932	-0.540361
6	-5.361588	-0.772945	0.516826
6	-4.512349	0.683253	-1.217414
6	-6.219785	0.239449	0.934552
1	-5.367497	-1.747669	1.000567
6	-5.369474	1.684884	-0.787362
1	-3.859747	0.838726	-2.073148
6	-6.230945	1.482049	0.298139
1	-6.899317	0.059868	1.766100
1	-5.380627	2.643277	-1.304225
7	-1.985075	-1.050863	-1.349818
7	0.412632	-2.013715	-0.733022
1	0.810805	-2.676402	-0.053338
6	-7.162673	2.569757	0.736468
1	-7.978543	2.698117	0.014560
1	-7.613655	2.349618	1.708824
1	-6.646422	3.533401	0.809007

Bn-Ru-NNTs-2.AICl3-Presence-C-C_bond formation-TS3_for

Number of imaginary frequencies : 0
The smallest frequencies are : 19.3048 22.7564 28.5143 cm(-1)

Electronic energy : =-5039.093611
Zero-point correction= 0.452362
Thermal correction to Energy= 0.496036
Thermal correction to Enthalpy= 0.496980
Thermal correction to Gibbs Free Energy= 0.372854
Sum of electronic and zero-point Energies= -5038.641249
Sum of electronic and thermal Energies= -5038.597575
Sum of electronic and thermal Enthalpies= -5038.596631
Sum of electronic and thermal Free Energies= -5038.720757

.....
Cartesian Coordinates

.....
6 -1.043439 -0.846049 -2.620220
6 -0.196888 -2.036667 -2.201513
44 -0.754365 -0.171811 0.210906
1 -1.617114 -1.051326 -3.530169
1 -0.409412 0.025742 -2.818095
1 0.812586 -2.014529 -2.617160
1 -0.680292 -2.977413 -2.492859
6 -0.973304 -1.595604 2.110935
6 -2.237371 -1.019718 1.953742
6 -2.343051 0.385118 1.829333
6 -1.207159 1.201585 2.056518
6 0.056657 0.619410 2.252030
6 0.192627 -0.784532 2.189105
1 0.931006 1.259242 2.352810
1 -0.847337 -2.676858 2.085669
1 -3.108069 -1.651442 1.818728
1 -3.306216 0.839734 1.604938
1 -1.279460 2.286328 2.014292
1 1.176102 -1.249489 2.229143
6 -1.199578 1.775670 -0.681814
1 -0.888110 1.763699 -1.726407
1 -0.680882 2.565043 -0.137955
1 -2.284286 1.869251 -0.612503
8 1.541554 1.603683 -0.108166
6 1.073252 0.512534 -0.498856
8 1.784655 -0.292084 -1.182162
1 0.799402 -2.325911 -0.371637
13 3.566420 -0.672766 -0.932724
17 3.561253 -2.695824 -1.722166
17 4.796977 0.665787 -1.975497
17 3.743415 -0.728560 1.211624
13 2.109946 3.331876 0.174424
17 4.063116 3.195703 0.951963
17 1.793715 4.281736 -1.691425
17 0.725622 4.029666 1.689939
6 2.469298 -3.786382 1.774419
8 3.555414 -4.158102 1.126314
8 1.458598 -3.366676 1.227618
6 2.624099 -3.902130 3.255600
1 3.472968 -3.911259 0.180094
1 3.256373 -3.071412 3.592312
1 3.135165 -4.829014 3.527350
1 1.650511 -3.839767 3.746108
16 -3.230183 -1.525335 -1.384736
8 -3.650198 -1.900429 -2.731720
8 -2.976556 -2.621979 -0.424704
6 -4.476395 -0.486330 -0.655869
6 -5.286881 -0.993145 0.354527
6 -4.684765 0.794101 -1.165274
6 -6.283141 -0.186445 0.894383
1 -5.136258 -2.012183 0.704867
6 -5.679793 1.587761 -0.613103
1 -4.058472 1.159552 -1.976136
6 -6.490527 1.113093 0.425235
1 -6.918189 -0.573697 1.689593
1 -5.840100 2.594418 -0.996077
7 -1.942525 -0.490374 -1.517506
7 -0.114611 -2.009513 -0.711982
1 -0.813681 -2.671016 -0.362003
6 -7.579906 1.972296 0.989370
1 -8.466406 1.947748 0.343442
1 -7.889893 1.633761 1.982860
1 -7.267598 3.019277 1.064837

.....
Bn-Ru-PP

.....
Number of imaginary frequencies : 0
The smallest frequencies are : 47.1402 84.6848 115.4536 cm(-1)

Electronic energy : =-1089.3611328
Zero-point correction= 0.175782
Thermal correction to Energy= 0.187498
Thermal correction to Enthalpy= 0.188442
Thermal correction to Gibbs Free Energy= 0.137621
Sum of electronic and zero-point Energies= -1089.185350
Sum of electronic and thermal Energies= -1089.173635
Sum of electronic and thermal Enthalpies= -1089.172691

Sum of electronic and thermal Free Energies= -1089.223512

Cartesian Coordinates

```
6 3.031547 -0.685179 0.159205
6 2.943933 0.693075 -0.458338
44 -0.271284 -0.073993 -0.106474
1 2.831424 0.605879 -1.547024
1 3.848434 1.283789 -0.259239
6 -1.677386 0.712790 1.321519
6 -1.822930 -0.711445 1.270837
6 -2.169145 -1.348662 0.054710
6 -2.200354 -0.569686 -1.121762
6 -2.107045 0.859649 -1.078019
6 -1.886604 1.497103 0.151972
1 -2.149500 1.434366 -1.997674
1 -1.382777 1.194023 2.249392
1 -1.656618 -1.298583 2.169634
1 -2.243764 -2.430563 0.000453
1 -2.311234 -1.060554 -2.085155
1 -1.736966 2.573124 0.192294
15 1.446659 1.554817 0.294275
15 1.411464 -1.636929 0.057629
1 3.840805 -1.294640 -0.263483
1 3.231245 -0.608923 1.241494
1 0.964054 -1.009594 -1.278245
1 1.157433 2.413188 -0.816900
```

Bn-Ru-PP-TS1_rev

Number of imaginary frequencies : 0

The smallest frequencies are : 24.8925 61.0845 116.1658 cm(-1)

Electronic energy : =-1129.8452856
Zero-point correction= 0.223660
Thermal correction to Energy= 0.238754
Thermal correction to Enthalpy= 0.239698
Thermal correction to Gibbs Free Energy= 0.181554
Sum of electronic and zero-point Energies= -1129.621626
Sum of electronic and thermal Energies= -1129.606532
Sum of electronic and thermal Enthalpies= -1129.605587
Sum of electronic and thermal Free Energies= -1129.663732

Cartesian Coordinates

```
6 -2.907330 -0.597051 -0.762967
6 -2.987564 0.661244 0.075100
44 0.352973 -0.000462 0.163496
1 -3.094348 0.396341 1.136274
1 -3.845384 1.291980 -0.201084
6 1.295502 0.653989 -1.646124
6 1.378267 -0.764945 -1.572740
6 2.049954 -1.395459 -0.484531
6 2.533331 -0.589850 0.559213
6 2.473700 0.838698 0.485977
6 1.883701 1.462617 -0.623403
1 2.839101 1.435454 -1.317416
1 0.754080 1.124505 -2.462653
1 0.899119 -1.371900 -2.337085
1 2.081910 -2.478670 -0.413147
1 2.940359 -1.056394 1.453849
1 1.791646 2.544782 -0.667468
6 -0.227603 -0.253244 2.744109
1 -1.168560 -0.505062 3.241765
1 0.392724 0.385119 3.375898
1 -0.565170 0.355547 1.864436
1 0.292698 -1.181278 2.502975
15 -1.403146 1.626747 -0.237824
15 -1.395535 -1.623320 -0.310412
1 -3.799032 -1.230029 -0.660320
1 -2.819358 -0.343243 -1.829918
1 -1.826635 -1.822097 1.045887
1 -1.375510 2.327875 1.015089
```

Bn-Ru-PP-TS1

Number of imaginary frequencies : 1

The smallest frequencies are : -520.8059 31.2774 66.9679 cm(-1)

Electronic energy : =-1129.8240172
Zero-point correction= 0.220507
Thermal correction to Energy= 0.234470
Thermal correction to Enthalpy= 0.235414
Thermal correction to Gibbs Free Energy= 0.180074
Sum of electronic and zero-point Energies= -1129.603511
Sum of electronic and thermal Energies= -1129.589547
Sum of electronic and thermal Enthalpies= -1129.588603
Sum of electronic and thermal Free Energies= -1129.643943

Cartesian Coordinates

6	-2.823780	-0.578876	-0.861157
6	-3.036192	0.629632	0.026962
44	0.339649	0.001060	0.222559
1	-3.271316	0.307482	1.050057
1	-3.860964	1.267952	-0.322118
6	1.361679	0.664802	-1.716560
6	1.444001	-0.735015	-1.611712
6	2.029488	-1.335785	-0.459404
6	2.510284	-0.506561	0.578060
6	2.444452	0.908561	0.481632
6	1.829588	1.483933	-0.650039
1	2.796141	1.532811	1.297519
1	0.853365	1.119893	-2.562245
1	1.013792	-1.365720	-2.385095
1	2.050319	-2.416684	-0.359652
1	2.891807	-0.961748	1.489816
1	1.694120	2.561234	-0.707272
6	-0.063828	-0.525594	2.315689
1	-1.069274	-0.438084	2.747883
1	0.629277	0.044280	2.944661
1	-0.715836	0.592611	1.304362
1	0.195158	-1.589737	2.339206
15	-1.459283	1.652819	-0.019537
15	-1.368195	-1.632164	-0.293407
1	-3.715193	-1.219842	-0.896751
1	-2.615870	-0.264957	-1.894970
1	-1.932167	-1.878931	1.001477
1	-1.649915	2.322414	1.233887

 Bn-Ru-PP-TS1_for

Number of imaginary frequencies : 0
 The smallest frequencies are : 47.1135 59.0150 110.0566 cm(-1)

Electronic energy : =-1129.8271101
 Zero-point correction= 0.221912
 Thermal correction to Energy= 0.236102
 Thermal correction to Enthalpy= 0.237046
 Thermal correction to Gibbs Free Energy= 0.181463
 Sum of electronic and zero-point Energies= -1129.605198
 Sum of electronic and thermal Energies= -1129.591008
 Sum of electronic and thermal Enthalpies= -1129.590064
 Sum of electronic and thermal Free Energies= -1129.645647

 Cartesian Coordinates

6	-2.848655	-0.448897	-0.887907
6	-3.048543	0.594293	0.191788
44	0.345061	-0.025235	0.246000
1	-3.225156	0.112264	1.161794
1	-3.898119	1.262122	-0.015372
6	1.349813	0.955832	-1.617094
6	1.428040	-0.441485	-1.721335
6	1.995432	-1.208268	-0.662911
6	2.518852	-0.541919	0.476002
6	2.447398	0.862790	0.596530
6	1.789476	1.593016	-0.424615
1	2.815726	1.362388	1.487100
1	0.848942	1.536369	-2.386887
1	1.003104	-0.951083	-2.582324
1	2.007875	-2.292821	-0.721486
1	2.921081	-1.131527	1.297086
1	1.639624	2.664274	-0.310856
6	0.084199	-1.145778	2.059807
1	-0.930080	-1.131148	2.472575
1	0.767682	-0.732963	2.813514
1	-0.668682	0.702411	1.344970
1	0.352817	-2.192600	1.864527
15	-1.506045	1.652409	0.233547
15	-1.363233	-1.556589	-0.542805
1	-3.729201	-1.096449	-0.994857
1	-2.687842	0.034340	-1.862841
1	-1.912129	-2.056169	0.680371
1	-1.745228	2.266143	1.505970

 Bn-Ru-PP-TS2_rev

Number of imaginary frequencies : 0
 The smallest frequencies are : 31.9366 53.0378 63.7461 cm(-1)

Electronic energy : =-1318.368597
 Zero-point correction= 0.236587
 Thermal correction to Energy= 0.254601
 Thermal correction to Enthalpy= 0.255545
 Thermal correction to Gibbs Free Energy= 0.189915
 Sum of electronic and zero-point Energies= -1318.132010
 Sum of electronic and thermal Energies= -1318.113996
 Sum of electronic and thermal Enthalpies= -1318.113052
 Sum of electronic and thermal Free Energies= -1318.178682

 Cartesian Coordinates

6	2.835796	1.711283	-0.475294
6	2.237987	2.177679	0.840605
44	0.173258	-0.424746	-0.050326
1	3.926638	1.827309	-0.481338
1	2.450539	2.318074	-1.306666
1	2.340344	3.256333	1.021192
1	2.702932	1.640964	1.678634
6	0.451015	-2.043738	1.539553
6	0.759153	-2.553440	0.254838
6	-0.183947	-2.489916	-0.805318
6	-1.451558	-1.884241	-0.570901
6	-1.783770	-1.377065	0.701427
6	-0.792983	-1.389716	1.725072
1	-2.755912	-0.926804	0.876605
1	1.189992	-2.067345	2.334503
1	1.746982	-2.968468	0.063449
1	0.084851	-2.840913	-1.796922
1	-2.157402	-1.775706	-1.391872
1	-1.009816	-0.917714	2.681330
6	-0.269473	0.605607	-1.882555
1	0.345918	1.490019	-2.097239
1	-1.322313	0.924984	-1.891661
1	-0.120664	-0.099254	-2.710779
8	-3.802309	0.747509	-0.842492
6	-3.284224	1.566929	-0.195860
8	-2.787060	2.390049	0.462097
15	0.460281	1.670953	0.795407
1	-0.014943	2.042231	2.081713
1	-0.100781	2.749985	0.061625
15	2.442499	-0.099622	-0.859680
1	3.135546	-0.575605	0.309641

Bn-Ru-PP-TS2

Number of imaginary frequencies : 1

The smallest frequencies are : -371.7120 28.2948 64.4265 cm(-1)

Electronic energy : =-1318.3068735
 Zero-point correction= 0.236126
 Thermal correction to Energy= 0.253023
 Thermal correction to Enthalpy= 0.253967
 Thermal correction to Gibbs Free Energy= 0.191801
 Sum of electronic and zero-point Energies= -1318.070748
 Sum of electronic and thermal Energies= -1318.053851
 Sum of electronic and thermal Enthalpies= -1318.052906
 Sum of electronic and thermal Free Energies= -1318.115073

Cartesian Coordinates

6	3.203597	0.469631	-0.524160
6	2.971612	0.648398	0.968869
44	-0.155657	-0.331561	-0.071367
1	4.194243	0.049560	-0.735451
1	3.159364	1.443690	-1.031706
1	3.631666	1.394624	1.430933
1	3.098396	-0.305932	1.497894
6	-0.099373	-2.118695	1.176949
6	-0.333758	-2.534663	-0.161015
6	-1.430093	-2.017436	-0.892570
6	-2.285632	-1.068355	-0.274047
6	-2.116925	-0.688637	1.077073
6	-0.988592	-1.174756	1.777951
1	-2.757626	0.076287	1.503125
1	0.769593	-2.483049	1.718846
1	0.370648	-3.206845	-0.645848
1	-1.562354	-2.278695	-1.937622
1	-3.036010	-0.545557	-0.860420
1	-0.782485	-0.814447	2.783827
6	-0.512979	1.544928	-1.615368
1	0.498496	1.962531	-1.616527
1	-1.119589	2.226408	-2.223513
1	-0.567769	0.631367	-2.229306
8	-2.786973	1.736471	-0.571624
6	-1.652301	2.083787	-0.298765
8	-1.084798	2.783811	0.524291
15	1.202947	1.150056	1.069977
1	0.944206	1.409127	2.435919
1	1.251438	2.459500	0.558681
15	1.917877	-0.659508	-1.331378
1	2.385190	-1.815582	-0.618474

Bn-Ru-PP-TS2_for

Number of imaginary frequencies : 0

The smallest frequencies are : 20.4560 33.9373 42.4885 cm(-1)

Electronic energy : =-1318.3524516
 Zero-point correction= 0.240146
 Thermal correction to Energy= 0.258065
 Thermal correction to Enthalpy= 0.259009

Thermal correction to Gibbs Free Energy= 0.191970
Sum of electronic and zero-point Energies= -1318.112306
Sum of electronic and thermal Energies= -1318.094387
Sum of electronic and thermal Enthalpies= -1318.093442
Sum of electronic and thermal Free Energies= -1318.160482

Cartesian Coordinates

6 -1.531891 2.718745 0.629122
6 -2.007390 2.553667 -0.799935
44 -0.496128 -0.506418 -0.101070
1 -2.213878 3.350399 1.212334
1 -0.548261 3.208099 0.642899
1 -1.856613 3.448162 -1.419180
1 -3.078162 2.300848 -0.829479
6 -1.480181 -2.431272 0.115677
6 -0.863942 -2.124279 1.359384
6 0.525811 -1.849126 1.423454
6 1.287176 -1.850605 0.233948
6 0.693545 -2.224413 -1.005339
6 -0.684152 -2.509270 -1.068858
1 1.290594 -2.188217 -1.911722
1 -2.552039 -2.596950 0.067164
1 -1.477395 -2.017656 2.250836
1 0.973668 -1.523879 2.357821
1 2.331756 -1.547621 0.254774
1 -1.155519 -2.725258 -2.023065
6 2.473975 2.033480 0.803856
1 2.178371 2.904305 0.208403
1 3.170167 2.333732 1.588243
1 1.565163 1.627039 1.271693
8 4.100202 0.355681 0.264967
6 3.110703 0.969335 -0.047459
8 2.489591 0.698066 -1.212187
15 -1.078591 1.097095 -1.470996
1 -1.405500 1.100151 -2.855754
15 -1.329241 1.079270 1.544135
1 -2.723092 0.741719 1.484052
1 1.587556 1.074472 -1.234367

Bn-Ru-PP-TS2_for

Number of imaginary frequencies : 0
The smallest frequencies are : 25.7407 39.4479 45.8210 cm(-1)

Electronic energy : =-2941.5798081
Zero-point correction= 0.246497
Thermal correction to Energy= 0.270136
Thermal correction to Enthalpy= 0.271080
Thermal correction to Gibbs Free Energy= 0.191624
Sum of electronic and zero-point Energies= -2941.333311
Sum of electronic and thermal Energies= -2941.309673
Sum of electronic and thermal Enthalpies= -2941.308728
Sum of electronic and thermal Free Energies= -2941.388185

Cartesian Coordinates

6 -2.959910 -2.681315 -0.151189
6 -2.528610 -2.581921 1.303970
44 -1.488066 0.390813 -0.096773
1 -3.841545 -3.325355 -0.253466
1 -2.154509 -3.122201 -0.754733
1 -2.258831 -3.545041 1.752259
1 -3.321303 -2.128143 1.914985
6 -2.804521 1.878938 0.796460
6 -2.710788 2.207529 -0.587907
6 -1.444063 2.371049 -1.174147
6 -0.256398 2.315586 -0.370339
6 -0.336554 2.077293 1.004180
6 -1.615747 1.780693 1.569305
1 0.569147 1.980408 1.599883
1 -3.771195 1.660160 1.241000
1 -3.607401 2.221881 -1.202488
1 -1.358361 2.507065 -2.248183
1 0.723788 2.402846 -0.837836
1 -1.684768 1.493312 2.616319
6 1.649402 -1.237895 -2.715533
1 1.013609 -1.488842 -3.565114
1 2.274552 -2.089805 -2.428478
1 2.335726 -0.427091 -2.991568
8 1.434982 -0.560572 -0.437594
6 0.839581 -0.788582 -1.543459
8 -0.398936 -0.642129 -1.657565
1 -0.042815 -2.273141 0.886228
13 3.026710 -0.080059 0.262101
17 2.545999 0.083422 2.345425
17 3.414501 1.819244 -0.658956
17 4.455731 -1.580872 -0.209879
15 -3.393682 -0.948180 -0.781355
15 -1.098327 -1.420481 1.280673
1 -2.984639 -1.182805 -2.129134
1 -0.742267 -1.205495 2.632432

Bn-Ru-PP-AlCl3-Presence-C-C_bond formation-TS3

Number of imaginary frequencies : 1

The smallest frequencies are : -342.6401 28.9251 39.3140 cm(-1)

Electronic energy : =-2941.4913789
 Zero-point correction= 0.244561
 Thermal correction to Energy= 0.267559
 Thermal correction to Enthalpy= 0.268503
 Thermal correction to Gibbs Free Energy= 0.191948
 Sum of electronic and zero-point Energies= -2941.246818
 Sum of electronic and thermal Energies= -2941.223820
 Sum of electronic and thermal Enthalpies= -2941.222875
 Sum of electronic and thermal Free Energies= -2941.299431

Cartesian Coordinates

6	-2.889946	-2.499696	-0.494859
6	-2.247669	-2.802399	0.851297
44	-1.282651	0.440908	-0.140777
1	-3.771927	-3.130350	-0.660683
1	-2.167930	-2.713040	-1.289699
1	-1.601748	-3.684575	0.813115
1	-2.997978	-2.957387	1.634734
6	-2.169435	1.881115	1.313253
6	-2.597074	2.341821	0.044165
6	-1.648284	2.595107	-0.960175
6	-0.261147	2.458544	-0.672739
6	0.180511	2.156407	0.629037
6	-0.774075	1.801617	1.600237
1	1.245096	2.076350	0.840059
1	-2.903898	1.602885	2.065199
1	-3.659995	2.401233	-0.177653
1	-1.974036	2.857781	-1.963097
1	0.477762	2.588160	-1.460607
1	-0.435977	1.461686	2.577402
6	-0.821289	-0.366143	-2.270650
1	-1.400974	-1.266508	-2.459325
1	0.101330	-0.408274	-2.856635
1	-1.342401	0.519913	-2.644582
8	1.439242	-0.072313	-1.006140
6	0.400271	-0.840211	-0.917820
8	0.374591	-2.042255	-0.731007
1	0.033011	-1.807945	1.769054
13	2.977844	-0.183984	-0.050236
17	2.335012	-0.438098	2.008320
17	3.735410	1.813506	-0.284108
17	4.250989	-1.724487	-0.741035
15	-3.415164	-0.694155	-0.516471
15	-1.222859	-1.340454	1.346767
1	-3.525109	-0.570215	-1.935598
1	-1.786065	-0.964853	2.593805

Bn-Ru-PP-AlCl3-Presence-C-C_bond formation-TS3_rev

Number of imaginary frequencies : 0

The smallest frequencies are : 28.7497 43.2035 50.3387 cm(-1)

Electronic energy : =-2941.5053178
 Zero-point correction= 0.245501
 Thermal correction to Energy= 0.268984
 Thermal correction to Enthalpy= 0.269928
 Thermal correction to Gibbs Free Energy= 0.192168
 Sum of electronic and zero-point Energies= -2941.259816
 Sum of electronic and thermal Energies= -2941.236334
 Sum of electronic and thermal Enthalpies= -2941.235390
 Sum of electronic and thermal Free Energies= -2941.313149

Cartesian Coordinates

6	-2.865927	-2.519380	-0.546694
6	-2.158014	-2.881551	0.752012
44	-1.255686	0.416188	-0.161946
1	-3.744168	-3.154833	-0.712644
1	-2.176329	-2.657994	-1.385668
1	-1.437606	-3.693481	0.621393
1	-2.863402	-3.158402	1.543237
6	-2.089896	1.896787	1.424374
6	-2.582608	2.373181	0.193832
6	-1.682951	2.608365	-0.860767
6	-0.283297	2.483581	-0.655180
6	0.213832	2.161833	0.621054
6	-0.686057	1.809191	1.639438
1	1.288396	2.084534	0.778915
1	-2.784181	1.612180	2.211530
1	-3.654050	2.450973	0.029246
1	-2.059874	2.873695	-1.844862
1	0.413768	2.634662	-1.475602
1	-0.297123	1.464276	2.595664
6	-1.281940	-0.006642	-2.303730

1	-1.406981	-1.061655	-2.552923
1	-0.339074	0.351448	-2.730880
1	-2.111016	0.566169	-2.732504
8	1.415657	-0.075465	-0.953065
6	0.375179	-0.812711	-0.721699
8	0.323839	-2.026940	-0.754887
1	0.008039	-1.778868	1.837281
13	3.003699	-0.193120	-0.089752
17	2.398586	-0.527219	1.974798
17	3.739744	1.817581	-0.278198
17	4.276799	-1.699501	-0.846850
15	-3.408368	-0.728467	-0.434257
15	-1.240685	-1.381643	1.325222
1	-3.712150	-0.562121	-1.816107
1	-1.909498	-1.021969	2.523886

 Bn-Ru-PP-2.AICI3-Presence-C-C_bond formation-TS3_rev

Number of imaginary frequencies : 0

The smallest frequencies are : 16.3097 31.4768 33.6234 cm(-1)

Electronic energy : =-4564.7360708
 Zero-point correction= 0.252830
 Thermal correction to Energy= 0.283167
 Thermal correction to Enthalpy= 0.284111
 Thermal correction to Gibbs Free Energy= 0.188389
 Sum of electronic and zero-point Energies= -4564.483241
 Sum of electronic and thermal Energies= -4564.452904
 Sum of electronic and thermal Enthalpies= -4564.451960
 Sum of electronic and thermal Free Energies= -4564.547681

 Cartesian Coordinates

6	-1.081350	-0.619765	3.040677
6	-2.557468	-0.945666	2.873423
44	-1.030391	-1.296933	-0.265878
1	-0.767266	-0.765350	4.081485
1	-0.898484	0.432423	2.782925
1	-3.221029	-0.262735	3.414964
1	-2.769788	-1.969626	3.207411
6	-2.071796	-1.840338	-2.251502
6	-2.065143	-2.894832	-1.287983
6	-0.846686	-3.392512	-0.747091
6	0.392342	-2.812992	-1.152137
6	0.371963	-1.708757	-2.015912
6	-0.858916	-1.218532	-2.561765
1	1.305345	-1.195134	-2.228515
1	-3.007573	-1.445029	-2.635461
1	-3.006024	-3.330200	-0.958645
1	-0.863882	-4.187373	-0.006674
1	1.336478	-3.142984	-0.722855
1	-0.852795	-0.326035	-3.182607
6	1.287890	2.278915	1.148083
1	0.441017	2.847042	1.536096
1	1.969012	2.939546	0.598273
1	1.863189	1.847428	1.979432
8	1.741559	0.358364	-0.179236
6	0.887411	1.150005	0.269001
8	-0.365312	0.936999	-0.015028
1	-3.555699	0.376588	0.888586
13	3.579192	0.074209	0.028150
17	3.816039	-1.771440	-1.010023
17	3.861137	-0.071111	2.132142
17	4.468235	1.767008	-0.879657
15	-0.110000	-1.805173	1.940714
15	-2.905057	-0.865956	1.058406
1	1.093289	-1.037896	1.891068
1	-4.010421	-1.725754	0.856890
13	-1.581551	2.346500	-0.407130
17	-3.047850	1.551405	-1.732823
17	-0.375805	3.821923	-1.326840
17	-2.381820	2.835850	1.511409

 Bn-Ru-PP-2.AICI3-Presence-C-C_bond formation-TS3

Number of imaginary frequencies : 1

The smallest frequencies are : -240.9136 18.1656 27.7516 cm(-1)

Electronic energy : =-4564.6605221
 Zero-point correction= 0.251660
 Thermal correction to Energy= 0.280826
 Thermal correction to Enthalpy= 0.281771
 Thermal correction to Gibbs Free Energy= 0.190913
 Sum of electronic and zero-point Energies= -4564.408862
 Sum of electronic and thermal Energies= -4564.379696
 Sum of electronic and thermal Enthalpies= -4564.378752
 Sum of electronic and thermal Free Energies= -4564.469610

 Cartesian Coordinates

6	-2.297744	2.730858	1.146894
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6	-2.081839	3.078879	-0.317931
44	-1.894705	-0.436266	0.032138
1	-2.840845	3.532599	1.662002
1	-1.325636	2.614805	1.637953
1	-1.235664	3.763027	-0.455787
1	-2.975185	3.524807	-0.769520
6	-3.648461	-1.205303	-1.143228
6	-3.834354	-1.765995	0.141903
6	-2.793159	-2.497558	0.731616
6	-1.600995	-2.753722	-0.000345
6	-1.477438	-2.340222	-1.341508
6	-2.475205	-1.519600	-1.892333
1	-0.560263	-2.566803	-1.880712
1	-4.414668	-0.561006	-1.567739
1	-4.735404	-1.537199	0.705282
1	-2.886044	-2.849130	1.756000
1	-0.771529	-3.292828	0.457593
1	-2.355452	-1.120147	-2.896997
6	-0.568106	-0.268592	1.901523
1	-0.860933	0.648316	2.405768
1	0.489785	-0.463964	2.136978
1	-1.064602	-1.156376	2.301073
8	0.996981	-0.743582	-0.159798
6	0.157069	0.094592	0.297084
8	0.418884	1.353602	0.333294
1	-0.546097	1.682385	-1.982367
13	2.278028	-2.035205	0.096019
17	1.503570	-3.774465	-0.927728
17	2.168038	-2.361434	2.214791
17	4.121121	-1.447084	-0.719085
15	-3.326755	1.166757	1.229037
15	-1.734583	1.512478	-1.239264
1	-3.021544	0.810174	2.577438
1	-2.698921	1.502528	-2.277277
13	1.939243	2.301271	-0.119108
17	2.104981	1.986105	-2.229117
17	3.453182	1.583204	1.163624
17	1.276170	4.297024	0.303386

Bn-Ru-PP-2.AICI3-Presence-C-C_bond formation-TS3_for

Number of imaginary frequencies : 0
The smallest frequencies are : 29.0173 32.2289 50.5735 cm(-1)

Electronic energy : =-4564.677339
Zero-point correction= 0.253050
Thermal correction to Energy= 0.282841
Thermal correction to Enthalpy= 0.283785
Thermal correction to Gibbs Free Energy= 0.191625
Sum of electronic and zero-point Energies= -4564.424289
Sum of electronic and thermal Energies= -4564.394498
Sum of electronic and thermal Enthalpies= -4564.393554
Sum of electronic and thermal Free Energies= -4564.485714

Cartesian Coordinates

6	-1.268509	3.428815	-0.165266
6	-0.735164	2.975235	-1.515848
44	-1.883160	0.096481	0.239757
1	-1.564124	4.484677	-0.195375
1	-0.487893	3.321419	0.594896
1	0.330273	3.207566	-1.635301
1	-1.283544	3.425719	-2.350503
6	-4.167267	-0.452401	0.490977
6	-3.439644	-1.146174	1.476184
6	-2.397533	-2.031819	1.112176
6	-2.129671	-2.268529	-0.249629
6	-2.804161	-1.527157	-1.231467
6	-3.809114	-0.596817	-0.865703
1	-2.528312	-1.661040	-2.275875
1	-4.944487	0.251573	0.776630
1	-3.658220	-0.976062	2.526841
1	-1.802132	-2.543485	1.866093
1	-1.349124	-2.969898	-0.532732
1	-4.307933	0.004399	-1.622202
6	-1.389470	0.792346	2.254438
1	-0.790464	1.702112	2.264656
1	-0.839926	-0.013389	2.756177
1	-2.333377	0.967582	2.778441
8	0.770136	-1.003921	0.658468
6	0.170143	0.094360	0.506254
8	0.794659	1.197773	0.495224
1	0.254787	0.593545	-2.128743
13	1.492134	-2.492419	-0.142738
17	0.697998	-2.325511	-2.152523
17	0.506918	-4.096942	0.900535
17	3.580283	-2.540682	0.009111
15	-2.775133	2.402692	0.235352
15	-0.954928	1.143825	-1.652627
1	-2.857196	2.739924	1.616090
1	-1.804358	0.950638	-2.766899
13	2.585594	1.668691	0.284655

17	2.946931	0.901062	-1.679629
17	3.696002	0.885133	1.894267
17	2.399486	3.801782	0.268857

 Bn-Ru-PP-AlCl3-Presence-CO2-insertion-TS2_rev

Number of imaginary frequencies : 0
 The smallest frequencies are : 24.1222 25.1417 41.4570 cm(-1)

Electronic energy : =-2941.4959025
 Zero-point correction= 0.243277
 Thermal correction to Energy= 0.268014
 Thermal correction to Enthalpy= 0.268958
 Thermal correction to Gibbs Free Energy= 0.185999
 Sum of electronic and zero-point Energies= -2941.252626
 Sum of electronic and thermal Energies= -2941.227889
 Sum of electronic and thermal Enthalpies= -2941.226944
 Sum of electronic and thermal Free Energies= -2941.309903

 Cartesian Coordinates

6	-3.861038	-2.103942	-0.986508
6	-3.588450	-2.449948	0.466212
44	-1.669300	0.365768	-0.029886
1	-4.871448	-2.414812	-1.277984
1	-3.152716	-2.632674	-1.638692
1	-3.606049	-3.525400	0.679423
1	-4.318593	-1.957593	1.124129
6	-2.336825	1.934696	1.538862
6	-2.638528	2.384259	0.241059
6	-1.623971	2.478489	-0.758251
6	-0.295634	2.114386	-0.431419
6	0.028983	1.648304	0.863382
6	-1.017177	1.483859	1.811758
1	1.059711	1.409301	1.118926
1	-3.119126	1.843137	2.285953
1	-3.667539	2.617456	-0.022257
1	-1.875223	2.801262	-1.764231
1	0.477681	2.144018	-1.196731
1	-0.790679	1.049081	2.783854
6	-0.713226	-0.633425	-1.659258
1	-1.118710	-1.621225	-1.915766
1	0.357934	-0.753017	-1.444384
1	-0.803721	-0.002045	-2.553037
8	2.128520	-1.223334	0.272801
6	1.548640	-1.274095	1.297880
8	1.013050	-1.371833	2.313447
1	-1.074413	-2.745069	0.400761
13	3.750835	-0.052851	-0.348298
17	5.146801	-1.568132	-0.696745
17	2.903817	0.963892	-1.969706
17	3.886443	1.008797	1.475206
1	-3.269991	-0.285497	-2.560274
1	-1.808205	-1.955452	2.250603
15	-3.713073	-0.225521	-1.202019
15	-1.940915	-1.707135	0.857448

 Bn-Ru-PP-AlCl3-Presence-CO2-insertion-TS2

Number of imaginary frequencies : 1
 The smallest frequencies are : -151.4323 28.8213 38.0984 cm(-1)

Electronic energy : =-2941.4899197
 Zero-point correction= 0.243050
 Thermal correction to Energy= 0.266859
 Thermal correction to Enthalpy= 0.267803
 Thermal correction to Gibbs Free Energy= 0.188248
 Sum of electronic and zero-point Energies= -2941.246869
 Sum of electronic and thermal Energies= -2941.223061
 Sum of electronic and thermal Enthalpies= -2941.222117
 Sum of electronic and thermal Free Energies= -2941.301672

 Cartesian Coordinates

6	-3.769975	-2.141377	-0.785543
6	-3.535068	-2.339400	0.699428
44	-1.437487	0.329786	-0.043013
1	-4.793453	-2.415883	-1.067569
1	-3.084356	-2.770754	-1.368245
1	-3.610303	-3.382562	1.027472
1	-4.240995	-1.739703	1.290379
6	-2.230053	2.085604	1.314344
6	-2.523332	2.354902	-0.032288
6	-1.503005	2.345855	-1.023530
6	-0.159774	2.122021	-0.636118
6	0.156136	1.886293	0.719665
6	-0.896877	1.772200	1.667657
1	1.194759	1.783872	1.030500
1	-3.023372	2.051598	2.054523
1	-3.556713	2.498410	-0.338050
1	-1.754851	2.506560	-2.068116

1	0.631505	2.097861	-1.383595
1	-0.659410	1.487615	2.689430
6	-0.599921	-0.735148	-1.688449
1	-0.883555	-1.794282	-1.749171
1	0.489161	-0.671509	-1.622456
1	-0.910773	-0.251708	-2.622127
8	1.692623	-0.934008	0.232043
6	0.943940	-0.705992	1.161347
8	0.736573	-0.722741	2.318297
1	-1.056658	-2.776729	0.591901
13	3.433010	-0.249232	-0.249250
17	4.605324	-1.979428	-0.462235
17	3.016975	0.850015	-2.013427
17	3.813235	0.982763	1.442404
1	-3.101237	-0.504569	-2.519525
1	-1.680140	-1.797972	2.406287
15	-3.519851	-0.312145	-1.169390
15	-1.844776	-1.668757	1.007041

 Bn-Ru-PP-AICI3-Presence-CO2-insertion-TS2_for

Number of imaginary frequencies : 0
 The smallest frequencies are : 35.7399 41.1216 45.4005 cm(-1)

Electronic energy : =-2941.495093
 Zero-point correction= 0.245081
 Thermal correction to Energy= 0.268958
 Thermal correction to Enthalpy= 0.269903
 Thermal correction to Gibbs Free Energy= 0.190814
 Sum of electronic and zero-point Energies= -2941.250012
 Sum of electronic and thermal Energies= -2941.226135
 Sum of electronic and thermal Enthalpies= -2941.225190
 Sum of electronic and thermal Free Energies= -2941.304279

 Cartesian Coordinates

6	-3.757622	-2.082845	-0.782512
6	-3.604220	-2.245105	0.716774
44	-1.284533	0.298432	-0.023091
1	-4.777396	-2.311156	-1.115257
1	-3.073851	-2.754556	-1.318058
1	-3.732472	-3.274763	1.069478
1	-4.314355	-1.604590	1.256516
6	-2.055523	2.157285	1.339672
6	-2.446758	2.373199	0.012386
6	-1.500355	2.317167	-1.045793
6	-0.125969	2.157884	-0.750743
6	0.274435	1.985821	0.588162
6	-0.696036	1.901635	1.616624
1	1.329698	1.853098	0.831587
1	-2.794263	2.146862	2.135424
1	-3.500222	2.491769	-0.226554
1	-1.831120	2.423024	-2.076115
1	0.621237	2.118401	-1.541789
1	-0.374056	1.655746	2.624063
6	-0.563981	-0.730987	-1.756597
1	-0.819244	-1.797824	-1.769329
1	0.519910	-0.627182	-1.762353
1	-0.970589	-0.260949	-2.657761
8	1.532231	-0.949491	0.086594
6	0.598890	-0.670142	0.892002
8	0.552788	-0.748199	2.096610
1	-1.140290	-2.780851	0.710825
13	3.242608	-0.344015	-0.167440
17	4.490034	-2.029637	-0.419539
17	3.043834	0.886357	-1.922878
17	3.654340	0.891731	1.533607
1	-3.015840	-0.494594	-2.527813
1	-1.773333	-1.679585	2.469948
15	-3.405558	-0.282925	-1.175624
15	-1.901449	-1.642892	1.068571

 AICI3

Number of imaginary frequencies : 0
 The smallest frequencies are : 146.3910 146.4533 201.6079 cm(-1)

Electronic energy : =-1623.1068631
 Zero-point correction= 0.004917
 Thermal correction to Energy= 0.010206
 Thermal correction to Enthalpy= 0.011150
 Thermal correction to Gibbs Free Energy= -0.024366
 Sum of electronic and zero-point Energies= -1623.101946
 Sum of electronic and thermal Energies= -1623.096657
 Sum of electronic and thermal Enthalpies= -1623.095713
 Sum of electronic and thermal Free Energies= -1623.131230

 Cartesian Coordinates

13	0.000000	0.000000	0.000000
17	-0.000000	2.074350	0.000000

17 1.796440 -1.037175 0.000000
17 -1.796440 -1.037175 0.000000

Bn-Ru-PP-AICl3-Presence-proton-transfer-TS4_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 29.7070 42.5897 49.1711 cm(-1)

Electronic energy : =-2941.5635554
Zero-point correction= 0.246382
Thermal correction to Energy= 0.270218
Thermal correction to Enthalpy= 0.271162
Thermal correction to Gibbs Free Energy= 0.191224
Sum of electronic and zero-point Energies= -2941.317173
Sum of electronic and thermal Energies= -2941.293338
Sum of electronic and thermal Enthalpies= -2941.292394
Sum of electronic and thermal Free Energies= -2941.372332

Cartesian Coordinates

6 -0.769579 -3.240357 0.464725
6 -0.339243 -2.474326 1.707422
44 -1.932235 -0.025503 -0.169455
1 -1.618366 -3.906703 0.668762
1 0.052368 -3.841725 0.062145
1 0.684566 -2.102392 1.570200
1 -0.372296 -3.087748 2.613559
6 -2.906149 1.072606 -1.854681
6 -1.552742 1.471739 -1.771164
6 -1.030425 1.978170 -0.548321
6 -1.874621 2.099482 0.576354
6 -3.236951 1.699320 0.495592
6 -3.750095 1.168564 -0.709770
1 -3.864752 1.731565 1.381045
1 -3.287420 0.631518 -2.770572
1 -0.874576 1.328188 -2.608930
1 0.029742 2.206646 -0.481395
1 -1.435576 2.395970 1.526412
1 -4.775186 0.814178 -0.756112
6 2.678855 2.460815 1.534895
1 2.499981 3.328657 2.171473
1 2.737239 2.778210 0.485366
1 3.646673 2.007752 1.775946
8 1.672706 0.337933 1.020216
6 1.573345 1.454879 1.712797
8 0.627662 1.668617 2.458025
13 2.634390 -0.116278 -0.420684
17 2.074517 -2.140012 -0.929598
17 4.725710 -0.005829 -0.012813
17 2.040541 1.230139 -2.008673
15 -1.295286 -1.993084 -0.802430
15 -1.366789 -0.950211 1.903271
1 -1.123388 -2.658151 -2.041083
1 -2.423807 -1.362175 2.752129
1 -0.623195 -0.111458 2.758772

Bn-Ru-PP-AICl3-Presence-proton-transfer-TS4

Number of imaginary frequencies : 1
The smallest frequencies are : -417.9687 18.6718 34.5860 cm(-1)

Electronic energy : =-2941.5435379
Zero-point correction= 0.243169
Thermal correction to Energy= 0.266600
Thermal correction to Enthalpy= 0.267544
Thermal correction to Gibbs Free Energy= 0.187581
Sum of electronic and zero-point Energies= -2941.300369
Sum of electronic and thermal Energies= -2941.276938
Sum of electronic and thermal Enthalpies= -2941.275994
Sum of electronic and thermal Free Energies= -2941.355957

Cartesian Coordinates

6 -1.113110 -3.267884 0.505771
6 -0.339930 -2.488583 1.554952
44 -2.010439 0.046176 -0.133329
1 -1.965458 -3.805010 0.945816
1 -0.486629 -4.001185 -0.017523
1 0.667634 -2.275811 1.176247
1 -0.238980 -3.049214 2.491633
6 -2.800238 1.223089 -1.875397
6 -1.463050 1.606739 -1.595937
6 -1.111028 2.097647 -0.308641
6 -2.090431 2.141551 0.709689
6 -3.412059 1.688306 0.465115
6 -3.760613 1.225023 -0.833689
1 -4.140836 1.664100 1.268718
1 -3.059710 0.828976 -2.853010
1 -0.687166 1.509257 -2.351135
1 -0.078228 2.371991 -0.111939
1 -1.801873 2.429425 1.717855

1	-4.760708	0.843516	-1.017626
6	2.961347	2.064468	1.843395
1	2.856778	2.730139	2.700115
1	2.885132	2.633891	0.907764
1	3.947986	1.588393	1.835104
8	1.878251	0.105798	0.969715
6	1.904470	1.017111	1.849698
8	1.017144	1.068131	2.756249
13	2.719231	-0.156632	-0.647530
17	1.939943	-1.983257	-1.404364
17	4.806014	-0.215520	-0.226565
17	2.148763	1.584721	-1.772142
15	-1.777718	-2.024359	-0.693429
15	-1.090419	-0.813835	1.911884
1	-2.060902	-2.787816	-1.857489
1	-2.173961	-1.198203	2.752512
1	0.202742	0.297621	2.575240

Bn-Ru-PP-AlCl3-Presence-proton-transfer-TS4_for

Number of imaginary frequencies : 0
The smallest frequencies are : 16.0098 34.3872 42.6498 cm(-1)

Electronic energy : =-2941.5438797
Zero-point correction= 0.246539
Thermal correction to Energy= 0.270339
Thermal correction to Enthalpy= 0.271283
Thermal correction to Gibbs Free Energy= 0.190768
Sum of electronic and zero-point Energies= -2941.297341
Sum of electronic and thermal Energies= -2941.273541
Sum of electronic and thermal Enthalpies= -2941.272597
Sum of electronic and thermal Free Energies= -2941.353112

Cartesian Coordinates

6	-1.123389	-3.265206	0.543512
6	-0.367769	-2.475930	1.596536
44	-2.001245	0.043952	-0.146061
1	-1.995357	-3.779477	0.973192
1	-0.497631	-4.018640	0.048072
1	0.645289	-2.263427	1.231883
1	-0.278453	-3.030382	2.538438
6	-2.834878	1.198508	-1.885711
6	-1.503125	1.608974	-1.623962
6	-1.143654	2.115433	-0.343437
6	-2.109657	2.144424	0.686445
6	-3.423505	1.657054	0.462109
6	-3.780107	1.180318	-0.829703
1	-4.139607	1.618245	1.276569
1	-3.098407	0.795354	-2.858544
1	-0.736803	1.522693	-2.389753
1	-0.115246	2.415868	-0.162496
1	-1.816257	2.443427	1.690020
1	-4.774032	0.776122	-0.997861
6	2.944316	2.166754	1.738051
1	2.831451	2.867989	2.564642
1	2.850761	2.690590	0.777654
1	3.939521	1.708763	1.742359
8	1.880302	0.149004	0.974493
6	1.911151	1.101723	1.795944
8	1.029177	1.195387	2.719657
13	2.732667	-0.186968	-0.641342
17	2.011988	-2.070636	-1.293586
17	4.813871	-0.163481	-0.190755
17	2.120774	1.491445	-1.831318
15	-1.741323	-2.028200	-0.686027
15	-1.128959	-0.798675	1.941703
1	-2.034716	-2.806791	-1.838305
1	-2.264477	-1.218496	2.695168
1	0.283399	0.455989	2.612238

Cp-Rh-PP

Number of imaginary frequencies : 0
The smallest frequencies are : 38.9335 59.1757 92.1557 cm(-1)

Electronic energy : =-1066.3425115
Zero-point correction= 0.157669
Thermal correction to Energy= 0.169252
Thermal correction to Enthalpy= 0.170196
Thermal correction to Gibbs Free Energy= 0.119010
Sum of electronic and zero-point Energies= -1066.184843
Sum of electronic and thermal Energies= -1066.173259
Sum of electronic and thermal Enthalpies= -1066.172315
Sum of electronic and thermal Free Energies= -1066.223502

Cartesian Coordinates

6	2.926191	-0.641584	0.364496
6	2.893885	0.700776	-0.332019
1	2.889180	0.558066	-1.420327

1	3.759885	1.327583	-0.076028
15	1.320719	1.565618	0.244321
15	1.353038	-1.624473	0.041526
1	3.791684	-1.252279	0.075795
1	2.984267	-0.509265	1.455602
1	1.422943	-1.484200	-1.403045
1	1.077812	2.363069	-0.922840
45	-0.333818	-0.017492	-0.240497
6	-1.686179	0.107210	1.348783
6	-2.086206	1.208243	0.495843
6	-2.514523	0.652934	-0.710572
6	-2.505783	-0.794593	-0.588506
6	-2.063002	-1.129609	0.691155
1	-1.320110	0.199307	2.365161
1	-1.970050	2.260068	0.725740
1	-2.800340	1.202096	-1.599789
1	-2.787660	-1.488953	-1.370714
1	-1.918433	-2.125789	1.090009

Cp-Rh-PP-TS1_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 48.8684 60.7170 100.6176 cm(-1)

Electronic energy : =-1106.8305524
Zero-point correction= 0.205259
Thermal correction to Energy= 0.220035
Thermal correction to Enthalpy= 0.220979
Thermal correction to Gibbs Free Energy= 0.163507
Sum of electronic and zero-point Energies= -1106.625294
Sum of electronic and thermal Energies= -1106.610518
Sum of electronic and thermal Enthalpies= -1106.609573
Sum of electronic and thermal Free Energies= -1106.667045

Cartesian Coordinates

6	-2.795703	0.351553	-0.982832
6	-2.891124	0.416798	0.526954
1	-3.020634	-0.593246	0.939205
1	-3.737218	1.031125	0.868600
6	-0.195985	-2.432330	1.399601
1	-1.150429	-2.952977	1.289139
1	0.296005	-2.699076	2.336978
1	-0.454771	-1.347209	1.482888
1	0.447804	-2.691057	0.556027
15	-1.292844	1.206774	1.124951
15	-1.289161	-0.635797	-1.525735
1	-3.685030	-0.096620	-1.445866
1	-2.691678	1.361412	-1.405965
1	-1.748800	-1.850072	-0.911658
1	-1.293698	0.635181	2.441141
45	0.375212	-0.162061	0.121987
6	1.456712	1.355631	-0.888165
6	1.945126	1.422993	0.472048
6	2.606936	0.219045	0.743418
6	2.621313	-0.575959	-0.465190
6	1.969292	0.138410	-1.475979
1	0.941604	2.150944	-1.415254
1	1.758623	2.232641	1.167133
1	3.036226	-0.073176	1.694422
1	3.058238	-1.563257	-0.562388
1	1.789906	-0.193395	-2.491203

Cp-Rh-PP-TS1

Number of imaginary frequencies : 1
The smallest frequencies are : -653.4552 27.5417 57.5359 cm(-1)

Electronic energy : =-1106.8051587
Zero-point correction= 0.202404
Thermal correction to Energy= 0.216022
Thermal correction to Enthalpy= 0.216966
Thermal correction to Gibbs Free Energy= 0.161674
Sum of electronic and zero-point Energies= -1106.602754
Sum of electronic and thermal Energies= -1106.589137
Sum of electronic and thermal Enthalpies= -1106.588193
Sum of electronic and thermal Free Energies= -1106.643485

Cartesian Coordinates

6	-2.725906	-0.538559	-0.947478
6	-2.938511	0.616799	0.008784
1	-3.151803	0.239687	1.017609
1	-3.776912	1.262134	-0.292031
6	-0.010235	-0.674403	2.265896
1	-1.031263	-0.670577	2.663174
1	0.651533	-0.145884	2.958978
1	-0.516522	0.631850	1.415301
1	0.307019	-1.717577	2.170354
15	-1.378851	1.660149	-0.021910
15	-1.255574	-1.598464	-0.448132

1	-3.605948	-1.193442	-1.005487
1	-2.535913	-0.167643	-1.965069
1	-1.825451	-1.945752	0.819867
1	-1.581737	2.300742	1.244152
45	0.364434	0.011649	0.247113
6	1.578477	-0.175626	-1.651721
6	1.825541	1.132052	-1.153999
6	2.481677	1.021736	0.103813
6	2.638894	-0.363101	0.383334
6	2.087784	-1.109840	-0.693435
1	1.102864	-0.425259	-2.592395
1	1.523050	2.056357	-1.632491
1	2.797378	1.843064	0.734722
1	3.075645	-0.782492	1.282998
1	2.058568	-2.189069	-0.780312

Cp-Rh-PP-TS1_for

Number of imaginary frequencies : 0
The smallest frequencies are : 38.4946 64.2054 105.3357 cm(-1)

Electronic energy : ==-1106.8100906
Zero-point correction= 0.203994
Thermal correction to Energy= 0.217601
Thermal correction to Enthalpy= 0.218546
Thermal correction to Gibbs Free Energy= 0.163802
Sum of electronic and zero-point Energies= -1106.606096
Sum of electronic and thermal Energies= -1106.592489
Sum of electronic and thermal Enthalpies= -1106.591545
Sum of electronic and thermal Free Energies= -1106.646289

Cartesian Coordinates

6	-2.723131	-0.445242	-0.973976
6	-2.963927	0.580801	0.115519
1	-3.155508	0.085553	1.075968
1	-3.822207	1.231902	-0.106424
6	0.157954	-1.164691	2.019230
1	-0.865241	-1.197592	2.404947
1	0.814183	-0.717240	2.774002
1	-0.616939	0.773372	1.336988
1	0.488736	-2.185218	1.793878
15	-1.449028	1.674378	0.203452
15	-1.234799	-1.542601	-0.622755
1	-3.590339	-1.106466	-1.105749
1	-2.551460	0.052709	-1.938900
1	-1.804920	-2.075781	0.576498
1	-1.748574	2.293888	1.459242
45	0.365861	-0.010816	0.262218
6	1.628860	-0.131098	-1.655006
6	1.762531	1.194821	-1.202611
6	2.399488	1.176216	0.084715
6	2.642245	-0.166997	0.427331
6	2.119745	-0.996936	-0.621121
1	1.177259	-0.452528	-2.585653
1	1.419912	2.081998	-1.722484
1	2.641769	2.044804	0.684674
1	3.090747	-0.522197	1.347737
1	2.173633	-2.078381	-0.669498

Cp-Rh-PP-TS2_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 34.1472 45.7902 50.0242 cm(-1)

Electronic energy : ==-1295.3519479
Zero-point correction= 0.218326
Thermal correction to Energy= 0.236081
Thermal correction to Enthalpy= 0.237026
Thermal correction to Gibbs Free Energy= 0.171071
Sum of electronic and zero-point Energies= -1295.133622
Sum of electronic and thermal Energies= -1295.115867
Sum of electronic and thermal Enthalpies= -1295.114922
Sum of electronic and thermal Free Energies= -1295.180877

Cartesian Coordinates

6	3.050054	1.210262	-0.401132
6	2.464743	1.854783	0.844514
1	4.145219	1.168538	-0.348511
1	2.801521	1.801669	-1.293256
1	2.721280	2.916330	0.958781
1	2.806232	1.320003	1.740882
6	-0.090244	0.504785	-1.938284
1	0.675767	1.252004	-2.181694
1	-1.074448	0.990424	-1.990354
1	-0.043179	-0.290206	-2.691225
8	-3.671243	0.939576	-0.805412
6	-3.071865	1.720720	-0.183742
8	-2.490665	2.512600	0.444219
15	0.635146	1.613437	0.743239

1	0.163305	2.069675	1.998196
1	0.245536	2.729487	-0.042556
15	2.421331	-0.551433	-0.685380
1	2.929433	-1.010309	0.579580
6	0.135978	-2.565284	0.722989
6	-0.584764	-1.805731	1.670442
6	-1.756196	-1.288265	1.019769
6	-1.745519	-1.727843	-0.322567
6	-0.557399	-2.496397	-0.528941
1	1.073437	-3.080865	0.898304
1	-0.316284	-1.658297	2.709333
1	-2.527703	-0.691333	1.492475
1	-2.484109	-1.482971	-1.077347
1	-0.260833	-2.984865	-1.449356
45	0.122760	-0.423087	-0.057331

Cp-Rh-PP-TS2

Number of imaginary frequencies : 1

The smallest frequencies are : -311.2475 55.6186 61.8829 cm(-1)

Electronic energy : =-1295.2847896
Zero-point correction= 0.218353
Thermal correction to Energy= 0.234571
Thermal correction to Enthalpy= 0.235515
Thermal correction to Gibbs Free Energy= 0.175056
Sum of electronic and zero-point Energies= -1295.066437
Sum of electronic and thermal Energies= -1295.050219
Sum of electronic and thermal Enthalpies= -1295.049274
Sum of electronic and thermal Free Energies= -1295.109733

Cartesian Coordinates

6	3.158695	0.301246	-0.487938
6	2.940229	0.436851	1.012902
1	4.121649	-0.172328	-0.715149
1	3.180493	1.295486	-0.956568
1	3.653394	1.115822	1.498411
1	3.003498	-0.544216	1.502498
6	-0.505736	1.654999	-1.577491
1	0.547608	1.943754	-1.500105
1	-1.000121	2.515308	-2.044460
1	-0.663707	0.848877	-2.303652
8	-2.772974	1.584485	-0.619065
6	-1.665109	1.930738	-0.247404
8	-1.169267	2.516789	0.710299
15	1.205843	1.038441	1.155205
1	0.936264	1.210475	2.528661
1	1.308987	2.373965	0.725499
15	1.811479	-0.702868	-1.359844
1	2.174391	-1.923255	-0.695509
6	-0.336297	-2.187429	0.936792
6	-1.305140	-1.347687	1.610236
6	-2.280434	-0.973777	0.683465
6	-1.945977	-1.588234	-0.581647
6	-0.806432	-2.401725	-0.404228
1	0.513629	-2.678385	1.398164
1	-1.241313	-1.010862	2.638581
1	-3.082393	-0.261825	0.831322
1	-2.498016	-1.443253	-1.503070
1	-0.323909	-3.010292	-1.160009
45	-0.175003	-0.290066	-0.079401

Cp-Rh-PP-TS2_for

Number of imaginary frequencies : 0

The smallest frequencies are : 24.2296 46.9578 53.5536 cm(-1)

Electronic energy : =-1295.3562115
Zero-point correction= 0.220864
Thermal correction to Energy= 0.237617
Thermal correction to Enthalpy= 0.238561
Thermal correction to Gibbs Free Energy= 0.174864
Sum of electronic and zero-point Energies= -1295.135348
Sum of electronic and thermal Energies= -1295.118595
Sum of electronic and thermal Enthalpies= -1295.117651
Sum of electronic and thermal Free Energies= -1295.181348

Cartesian Coordinates

6	2.859461	0.437524	-0.781477
6	3.153737	-0.433555	0.429011
1	3.698840	0.420871	-1.488429
1	2.703608	1.480523	-0.480299
1	3.987146	-0.071240	1.044428
1	3.386154	-1.458537	0.110638
6	-0.459772	3.920912	0.248931
1	0.152912	4.074553	1.142082
1	-1.341730	4.563950	0.280148
1	0.152024	4.195826	-0.617146
8	-2.030412	2.160458	-0.151414

6	-0.877141	2.468708	0.122718
8	0.116242	1.650705	0.319870
15	1.594774	-0.523799	1.415771
1	1.816513	-1.602445	2.304459
1	1.718508	0.556184	2.318521
15	1.305803	-0.084242	-1.708967
1	1.746927	-1.446090	-1.865362
6	-1.092277	-2.433813	0.099815
6	-1.848204	-1.712965	1.099403
6	-2.505499	-0.653687	0.458118
6	-2.202629	-0.712598	-0.949104
6	-1.384388	-1.851704	-1.170711
1	-0.499825	-3.325397	0.269111
1	-1.859410	-1.927416	2.161046
1	-3.079154	0.135906	0.924529
1	-2.558188	-0.010550	-1.691131
1	-0.988961	-2.180472	-2.125118
45	-0.246453	-0.421051	0.076058

Cp-Rh-PP-AlCl3-Presence-CO2-insertion-TS2_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 16.7026 22.5606 36.4051 cm(-1)

Electronic energy : =-2918.4784041
Zero-point correction= 0.224724
Thermal correction to Energy= 0.249249
Thermal correction to Enthalpy= 0.250194
Thermal correction to Gibbs Free Energy= 0.166333
Sum of electronic and zero-point Energies= -2918.253680
Sum of electronic and thermal Energies= -2918.229155
Sum of electronic and thermal Enthalpies= -2918.228211
Sum of electronic and thermal Free Energies= -2918.312071

Cartesian Coordinates

6	-4.054263	-1.774544	-0.937852
6	-3.789773	-2.186268	0.500132
45	-1.621283	0.366245	-0.023170
1	-5.099964	-1.964884	-1.208727
1	-3.427074	-2.362276	-1.621273
1	-3.925013	-3.258099	0.686492
1	-4.446152	-1.634062	1.187073
6	-0.793781	-0.644125	-1.673569
1	-1.295746	-1.582335	-1.940966
1	0.260733	-0.856993	-1.457240
1	-0.842648	0.030233	-2.536294
8	1.964578	-1.177609	0.343247
6	1.393893	-1.189480	1.374694
8	0.871995	-1.263934	2.399722
1	-1.308907	-2.760482	0.412341
13	3.611135	-0.093089	-0.364019
17	4.917432	-1.685134	-0.731181
17	2.745800	0.909873	-1.983774
17	3.879251	0.997217	1.424704
1	-3.322260	-0.001404	-2.495242
1	-1.937581	-1.885079	2.269334
15	-3.715002	0.081367	-1.122492
15	-2.063153	-1.645609	0.878274
6	-1.711360	2.591669	-0.334662
6	-0.336622	2.218318	-0.372976
6	0.030627	1.737100	0.910287
6	-1.134774	1.799685	1.740500
6	-2.197685	2.354969	0.990515
1	-2.279977	3.013322	-1.155180
1	0.317328	2.280039	-1.235896
1	1.034041	1.471885	1.227285
1	-1.184412	1.489889	2.778952
1	-3.209436	2.528170	1.335601

Cp-Rh-PP-AlCl3-Presence-CO2-insertion-TS2

Number of imaginary frequencies : 1
The smallest frequencies are : -123.9666 28.9537 34.7124 cm(-1)

Electronic energy : =-2918.470546
Zero-point correction= 0.225028
Thermal correction to Energy= 0.248111
Thermal correction to Enthalpy= 0.249055
Thermal correction to Gibbs Free Energy= 0.170821
Sum of electronic and zero-point Energies= -2918.245518
Sum of electronic and thermal Energies= -2918.222435
Sum of electronic and thermal Enthalpies= -2918.221491
Sum of electronic and thermal Free Energies= -2918.299725

Cartesian Coordinates

6	3.828045	-1.804374	0.902342
6	3.679157	-2.170175	-0.564844
45	1.375511	0.334624	0.010749
1	4.838546	-2.033934	1.262680

1	3.117157	-2.366756	1.520869
1	3.793521	-3.240472	-0.769032
1	4.414413	-1.628036	-1.174624
6	0.656536	-0.833572	1.619546
1	0.607557	-1.903127	1.381501
1	-0.357060	-0.471185	1.809505
1	1.266181	-0.693491	2.516193
8	-1.542660	-0.889779	-0.253341
6	-0.748836	-0.606819	-1.140876
8	-0.542959	-0.639295	-2.304245
1	1.200878	-2.720942	-0.823093
13	-3.282934	-0.282494	0.237219
17	-4.392059	-2.056170	0.469800
17	-2.907083	0.823087	2.013658
17	-3.760924	0.946802	-1.431547
1	3.212582	0.053510	2.430034
1	2.019002	-1.614815	-2.485650
15	3.555350	0.049055	1.044484
15	2.006273	-1.583054	-1.075291
6	1.620089	2.462157	0.665951
6	0.227455	2.178784	0.654606
6	-0.163954	1.952648	-0.695545
6	1.007608	2.084195	-1.516221
6	2.094065	2.426072	-0.692434
1	2.210721	2.711333	1.540280
1	-0.433004	2.139264	1.514289
1	-1.184912	1.839482	-1.049874
1	1.035787	1.939721	-2.589935
1	3.119534	2.579647	-1.005567

Cp-Rh-PP-AICl3-Presence-CO2-insertion-TS2_for

Number of imaginary frequencies : 0
The smallest frequencies are : 17.1103 27.6248 39.0749 cm(-1)

Electronic energy : =-2918.4729049
Zero-point correction= 0.226113
Thermal correction to Energy= 0.249623
Thermal correction to Enthalpy= 0.250567
Thermal correction to Gibbs Free Energy= 0.170730
Sum of electronic and zero-point Energies= -2918.246792
Sum of electronic and thermal Energies= -2918.223282
Sum of electronic and thermal Enthalpies= -2918.222337
Sum of electronic and thermal Free Energies= -2918.302175

Cartesian Coordinates

6	-2.816987	2.755229	0.227840
6	-1.607272	2.980734	-0.660332
1	-3.611554	3.479577	0.008092
1	-2.553230	2.867831	1.286853
1	-1.113359	3.945268	-0.499283
1	-1.883493	2.914801	-1.720973
6	-1.861320	0.002448	2.147369
1	-1.749609	1.064463	2.389969
1	-1.124777	-0.580906	2.700680
1	-2.875042	-0.324223	2.398034
8	1.409487	-0.477423	-0.109851
6	0.649267	-0.738313	0.869325
8	0.814091	-1.113908	1.986718
1	0.324334	2.072267	0.779447
13	3.175807	0.123241	-0.105296
17	4.412670	-1.526091	0.358334
17	3.287024	0.857873	-2.107670
17	3.124566	1.700033	1.336884
1	-4.145054	0.849625	1.095176
1	0.512739	1.615495	-1.342292
15	-3.483386	1.043424	-0.152254
15	-0.445328	1.597984	-0.307248
6	-2.979638	-2.032944	-0.434653
6	-1.944390	-2.613742	0.346740
6	-0.738952	-2.543988	-0.411853
6	-1.035716	-1.911065	-1.662937
6	-2.410073	-1.617479	-1.689692
1	-4.023257	-1.953041	-0.151443
1	-2.044559	-3.030983	1.341763
1	0.217358	-2.964059	-0.125352
1	-0.309952	-1.685727	-2.435683
1	-2.946360	-1.115162	-2.485510
45	-1.519101	-0.419421	0.102840

Cp-Rh-PP-AICl3-Presence-C-C_bond formation-TS3_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 10.3299 38.0656 44.8549 cm(-1)

Electronic energy : =-2918.4755943
Zero-point correction= 0.227067
Thermal correction to Energy= 0.250048
Thermal correction to Enthalpy= 0.250992
Thermal correction to Gibbs Free Energy= 0.172799

Sum of electronic and zero-point Energies= -2918.248527
Sum of electronic and thermal Energies= -2918.225547
Sum of electronic and thermal Enthalpies= -2918.224603
Sum of electronic and thermal Free Energies= -2918.302795

Cartesian Coordinates

6 -2.956554 -2.356467 -0.497794
6 -2.270644 -2.731146 0.809928
45 -1.268913 0.480612 -0.158280
1 -3.851159 -2.969237 -0.664242
1 -2.265660 -2.521265 -1.330742
1 -1.610374 -3.596006 0.697589
1 -2.992840 -2.946426 1.605026
6 -1.355840 0.234479 -2.315971
1 -1.527186 -0.798441 -2.620547
1 -0.403576 0.594376 -2.716772
1 -2.169704 0.877850 -2.661775
8 1.376151 -0.083651 -0.963098
6 0.324760 -0.793679 -0.811841
8 0.164515 -1.985209 -0.932515
1 0.010042 -1.767590 1.781155
13 2.966324 -0.183705 -0.066717
17 2.330839 -0.481629 1.986963
17 3.762334 1.779291 -0.331615
17 4.143585 -1.778927 -0.798051
15 -3.457804 -0.555451 -0.405569
15 -1.246973 -1.292607 1.367143
1 -3.757986 -0.399224 -1.788289
1 -1.813412 -0.905249 2.603082
6 -2.278349 2.542863 0.133426
6 -1.108037 2.684214 -0.685454
6 0.040306 2.393218 0.103486
6 -0.414484 1.965024 1.368785
6 -1.856732 2.069917 1.390484
1 -3.301891 2.710143 -0.180460
1 -1.094876 3.019997 -1.715905
1 1.072621 2.406916 -0.232057
1 0.221457 1.633970 2.184079
1 -2.501678 1.823549 2.226748

Cp-Rh-PP-AlCl3-Presence-C-C_bond formation-TS3

Number of imaginary frequencies : 1
The smallest frequencies are : -328.7524 29.4351 50.3141 cm(-1)

Electronic energy : =-2918.465943
Zero-point correction= 0.226516
Thermal correction to Energy= 0.248873
Thermal correction to Enthalpy= 0.249817
Thermal correction to Gibbs Free Energy= 0.174436
Sum of electronic and zero-point Energies= -2918.239427
Sum of electronic and thermal Energies= -2918.217070
Sum of electronic and thermal Enthalpies= -2918.216126
Sum of electronic and thermal Free Energies= -2918.291507

Cartesian Coordinates

6 -3.012550 -2.310368 -0.439019
6 -2.404404 -2.625902 0.920546
45 -1.279784 0.486940 -0.154458
1 -3.915343 -2.909055 -0.613549
1 -2.287600 -2.552714 -1.223239
1 -1.841980 -3.564647 0.915794
1 -3.170202 -2.689878 1.701870
6 -0.945546 -0.182818 -2.306432
1 -1.483223 -1.103243 -2.525335
1 -0.014685 -0.148990 -2.879232
1 -1.518879 0.692659 -2.626389
8 1.386533 -0.069282 -1.002465
6 0.347055 -0.816170 -0.954832
8 0.247482 -2.016871 -0.850072
1 -0.009684 -1.802541 1.722043
13 2.933333 -0.188924 -0.034480
17 2.256064 -0.415404 2.012671
17 3.765498 1.759345 -0.321447
17 4.118138 -1.807808 -0.702311
15 -3.471572 -0.490738 -0.478936
15 -1.254410 -1.248161 1.382913
1 -3.597699 -0.383874 -1.896441
1 -1.712405 -0.820117 2.650619
6 -2.267931 2.548565 -0.014099
6 -1.076423 2.696678 -0.766315
6 0.048164 2.416600 0.083377
6 -0.447586 2.022214 1.332723
6 -1.895263 2.049993 1.267684
1 -3.279815 2.705013 -0.368287
1 -1.012903 3.015237 -1.800850
1 1.092877 2.437047 -0.212296
1 0.154209 1.705351 2.178699
1 -2.576124 1.829159 2.082761

Cp-Rh-PP- AlCl_3 -Presence-C-C_bond formation-TS3_for

Number of imaginary frequencies : 0

The smallest frequencies are : 16.0746 34.0507 42.7908 cm^{-1}

Electronic energy : =-2918.5520189
 Zero-point correction= 0.228198
 Thermal correction to Energy= 0.251330
 Thermal correction to Enthalpy= 0.252274
 Thermal correction to Gibbs Free Energy= 0.172942
 Sum of electronic and zero-point Energies= -2918.323821
 Sum of electronic and thermal Energies= -2918.300689
 Sum of electronic and thermal Enthalpies= -2918.299745
 Sum of electronic and thermal Free Energies= -2918.379077

Cartesian Coordinates

6	-3.164355	-2.398144	0.070603
6	-2.770833	-2.183550	1.524922
1	-4.084329	-2.991579	0.000676
1	-2.374362	-2.942837	-0.462666
1	-2.584746	-3.114550	2.072067
1	-3.547526	-1.620510	2.060506
6	1.490967	-2.138165	-2.117512
1	0.800259	-2.717286	-2.731486
1	1.915186	-2.785027	-1.337841
1	2.334430	-1.770908	-2.709162
8	1.487431	-0.098906	-0.868575
6	0.790482	-1.000285	-1.446742
8	-0.461116	-0.966497	-1.452260
1	-0.224258	-2.061849	1.224776
13	2.955949	-0.002565	0.188455
17	2.384976	-1.192008	1.891668
17	3.117771	2.073742	0.653826
17	4.616378	-0.811933	-0.866342
15	-3.474556	-0.717599	-0.736645
15	-1.260884	-1.130675	1.459056
1	-3.080538	-1.116526	-2.048892
1	-0.970173	-0.755291	2.787510
6	-2.564346	2.373214	-0.345319
6	-1.491950	2.426987	-1.268316
6	-0.257953	2.429892	-0.515797
6	-0.562216	2.326501	0.843603
6	-2.001142	2.215990	0.962107
1	-3.620914	2.361183	-0.585095
1	-1.578395	2.513748	-2.344250
1	0.744517	2.441077	-0.927646
1	0.162649	2.266020	1.648189
1	-2.562889	2.165702	1.887686
45	-1.461605	0.464624	-0.178770

Cp-Rh-PP- AlCl_3 -Presence-proton-transfer-TS4_rev

Number of imaginary frequencies : 0

The smallest frequencies are : 25.0839 45.7642 50.2988 cm^{-1}

Electronic energy : =-2918.5327263
 Zero-point correction= 0.228135
 Thermal correction to Energy= 0.251356
 Thermal correction to Enthalpy= 0.252300
 Thermal correction to Gibbs Free Energy= 0.173231
 Sum of electronic and zero-point Energies= -2918.304591
 Sum of electronic and thermal Energies= -2918.281371
 Sum of electronic and thermal Enthalpies= -2918.280426
 Sum of electronic and thermal Free Energies= -2918.359495

Cartesian Coordinates

6	0.922764	3.203686	0.371049
6	0.506236	2.486736	1.647781
45	1.899172	-0.047772	-0.199187
1	1.829003	3.807030	0.517384
1	0.127934	3.859425	0.000199
1	-0.538246	2.160942	1.560542
1	0.603868	3.120218	2.535253
6	-2.582404	-2.363736	1.633474
1	-2.425192	-3.197048	2.319889
1	-2.563986	-2.727357	0.597783
1	-3.575136	-1.928088	1.792799
8	-1.585990	-0.246189	1.075085
6	-1.519240	-1.318799	1.841739
8	-0.641231	-1.457652	2.679254
13	-2.483421	0.102058	-0.432507
17	-1.894758	2.104532	-1.033126
17	-4.589488	0.041500	-0.106509
17	-1.832136	-1.326112	-1.914771
15	1.290965	1.899842	-0.888116
15	1.465367	0.918884	1.855087
1	1.170289	2.541897	-2.141778
1	2.580328	1.293042	2.641754
1	0.701298	0.117335	2.731657

6	3.084371	-1.380254	-1.558546
6	1.701793	-1.700419	-1.681313
6	1.237910	-2.167355	-0.412420
6	2.332026	-2.113315	0.494732
6	3.479677	-1.629357	-0.209097
1	3.721276	-0.993719	-2.344437
1	1.083893	-1.596246	-2.565748
1	0.220988	-2.462761	-0.186463
1	2.288982	-2.382979	1.543804
1	4.468944	-1.480635	0.204552

Cp-Rh-PP-AlCl3-Presence-proton-transfer-TS4

Number of imaginary frequencies : 1

The smallest frequencies are : -665.0248 26.0540 38.6040 cm(-1)

Electronic energy : =-2918.5182689
Zero-point correction= 0.224742
Thermal correction to Energy= 0.247609
Thermal correction to Enthalpy= 0.248553
Thermal correction to Gibbs Free Energy= 0.170273
Sum of electronic and zero-point Energies= -2918.293527
Sum of electronic and thermal Energies= -2918.270660
Sum of electronic and thermal Enthalpies= -2918.269716
Sum of electronic and thermal Free Energies= -2918.347996

Cartesian Coordinates

6	0.979126	3.213496	0.439820
6	0.389255	2.436495	1.605915
45	1.973050	-0.044047	-0.176679
1	1.849978	3.810295	0.745721
1	0.248302	3.889885	-0.019991
1	-0.656478	2.189124	1.384596
1	0.410156	3.014864	2.536542
6	-2.657204	-2.224861	1.776674
1	-2.504142	-2.934805	2.589615
1	-2.566479	-2.732971	0.807710
1	-3.667987	-1.803906	1.811690
8	-1.693564	-0.165482	0.999140
6	-1.654471	-1.124537	1.837862
8	-0.761304	-1.167460	2.728284
13	-2.563684	0.114579	-0.591200
17	-1.928932	2.045525	-1.252616
17	-4.650075	0.033990	-0.170283
17	-1.893707	-1.497333	-1.838590
15	1.552853	1.965737	-0.794881
15	1.222492	0.789148	1.889246
1	1.636855	2.671487	-2.020920
1	2.341305	1.170252	2.678230
1	0.071938	-0.316849	2.546101
6	3.252572	-1.369596	-1.474273
6	1.891594	-1.708166	-1.684007
6	1.349831	-2.172399	-0.442825
6	2.387415	-2.119061	0.530672
6	3.563629	-1.612896	-0.097305
1	3.935242	-0.977509	-2.217590
1	1.334793	-1.611295	-2.608270
1	0.327513	-2.499798	-0.295653
1	2.292008	-2.394388	1.574836
1	4.522084	-1.449489	0.378779

Cp-Rh-PP-AlCl3-Presence-proton-transfer-TS4_for

Number of imaginary frequencies : 0

The smallest frequencies are : 24.8350 37.9276 55.3144 cm(-1)

Electronic energy : =-2918.5202525
Zero-point correction= 0.228820
Thermal correction to Energy= 0.252086
Thermal correction to Enthalpy= 0.253031
Thermal correction to Gibbs Free Energy= 0.174088
Sum of electronic and zero-point Energies= -2918.291432
Sum of electronic and thermal Energies= -2918.268166
Sum of electronic and thermal Enthalpies= -2918.267222
Sum of electronic and thermal Free Energies= -2918.346164

Cartesian Coordinates

6	1.162120	3.238814	0.426866
6	0.555008	2.496597	1.604211
45	1.941427	-0.073662	-0.202829
1	2.090859	3.755480	0.710124
1	0.478906	3.981253	-0.004844
1	-0.504628	2.300842	1.399346
1	0.613711	3.081718	2.529833
6	-2.624578	-2.327532	1.639839
1	-2.440877	-3.087354	2.399148
1	-2.546748	-2.762359	0.634904
1	-3.641166	-1.926988	1.722330
8	-1.681227	-0.208250	0.999686

6	-1.650236	-1.213768	1.750499
8	-0.749780	-1.322533	2.660697
13	-2.592100	0.193441	-0.576596
17	-1.986320	2.159585	-1.103317
17	-4.651812	0.049798	-0.056097
17	-1.945735	-1.360735	-1.896219
15	1.594391	1.948091	-0.819860
15	1.329803	0.815330	1.912446
1	1.756512	2.654743	-2.039060
1	2.557694	1.244278	2.495773
1	-0.060682	-0.554338	2.598470
6	3.193397	-1.455389	-1.484880
6	1.829057	-1.776196	-1.681791
6	1.284316	-2.206170	-0.427345
6	2.322415	-2.147884	0.540835
6	3.501694	-1.662507	-0.100816
1	3.879119	-1.087935	-2.237828
1	1.271480	-1.692037	-2.606743
1	0.258368	-2.517049	-0.270369
1	2.228584	-2.395663	1.591957
1	4.463679	-1.502369	0.369397

Cp-Ir-PP

Number of imaginary frequencies : 0
The smallest frequencies are : 4.6069 49.5731 111.8857 cm(-1)

Electronic energy : =-1060.1688291
Zero-point correction= 0.159059
Thermal correction to Energy= 0.170344
Thermal correction to Enthalpy= 0.171289
Thermal correction to Gibbs Free Energy= 0.118481
Sum of electronic and zero-point Energies= -1060.009770
Sum of electronic and thermal Energies= -1059.998485
Sum of electronic and thermal Enthalpies= -1059.997541
Sum of electronic and thermal Free Energies= -1060.050348

Cartesian Coordinates

6	2.991032	0.769930	-0.387103
6	3.127358	-0.627669	0.187774
1	3.362658	-0.586345	1.261809
1	3.902423	-1.230038	-0.304113
15	1.461113	-1.403463	-0.004215
15	1.377493	1.628327	0.090574
1	3.821080	1.414062	-0.070065
1	3.006645	0.727568	-1.483886
1	1.654370	1.580475	1.499154
1	1.639762	-2.792672	0.212743
77	-0.275967	-0.117140	-0.024441
6	-1.958556	1.335489	0.270804
6	-2.089380	0.778918	-1.028940
6	-2.327197	-0.633116	-0.875441
6	-2.342230	-0.941893	0.505149
6	-2.064494	0.272410	1.224468
1	-1.747593	2.373053	0.499308
1	-2.032841	1.317679	-1.965416
1	-2.455653	-1.338688	-1.686656
1	-2.491153	-1.919907	0.943179
1	-2.008511	0.377236	2.300251

Cp-Ir-PP-TS1_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 41.0955 52.5116 90.3182 cm(-1)

Electronic energy : =-1100.6330489
Zero-point correction= 0.204922
Thermal correction to Energy= 0.219917
Thermal correction to Enthalpy= 0.220861
Thermal correction to Gibbs Free Energy= 0.161896
Sum of electronic and zero-point Energies= -1100.428126
Sum of electronic and thermal Energies= -1100.413132
Sum of electronic and thermal Enthalpies= -1100.412188
Sum of electronic and thermal Free Energies= -1100.471153

Cartesian Coordinates

6	-2.866495	0.375640	-1.000831
6	-2.962436	0.456755	0.508110
1	-3.099066	-0.548616	0.930100
1	-3.807395	1.077890	0.838417
6	-0.384943	-2.444085	1.402842
1	-1.374153	-2.881739	1.248021
1	0.032765	-2.728728	2.370972
1	-0.548796	-1.337470	1.462219
1	0.280349	-2.765051	0.599992
15	-1.364913	1.246603	1.113672
15	-1.364003	-0.614983	-1.555906
1	-3.757667	-0.075974	-1.456352
1	-2.765144	1.382032	-1.433244

1	-1.829519	-1.841542	-0.970803
1	-1.372538	0.688190	2.434788
77	0.305776	-0.106718	0.084297
6	1.923286	0.146957	-1.485718
6	1.452538	1.380409	-0.880543
6	1.944492	1.406340	0.485954
6	2.553938	0.168973	0.740463
6	2.542421	-0.610338	-0.481240
1	1.734586	-0.162465	-2.506429
1	0.992224	2.211428	-1.402592
1	1.787394	2.210485	1.194410
1	2.959978	-0.156857	1.690380
1	2.939158	-1.612480	-0.591449

Cp-Ir-PP-TS1

Number of imaginary frequencies : 1
The smallest frequencies are : -526.1690 42.2707 53.8224 cm(-1)

Electronic energy : =-1100.6199676
Zero-point correction= 0.203408
Thermal correction to Energy= 0.216943
Thermal correction to Enthalpy= 0.217887
Thermal correction to Gibbs Free Energy= 0.162499
Sum of electronic and zero-point Energies= -1100.416560
Sum of electronic and thermal Energies= -1100.403025
Sum of electronic and thermal Enthalpies= -1100.402081
Sum of electronic and thermal Free Energies= -1100.457469

Cartesian Coordinates

6	-2.802339	-0.357272	-1.080285
6	-3.006829	0.639734	0.038421
1	-3.236105	0.113273	0.974491
1	-3.831654	1.338100	-0.165467
6	-0.122480	-1.109970	2.142371
1	-1.159411	-1.091396	2.493015
1	0.549691	-0.897269	2.980532
1	-0.136733	0.283831	1.749949
1	0.097446	-2.115951	1.776478
15	-1.424978	1.642688	0.182382
15	-1.349729	-1.488300	-0.718856
1	-3.685668	-0.987108	-1.251522
1	-2.589444	0.160153	-2.027674
1	-1.941854	-2.030167	0.467728
1	-1.583946	1.993004	1.561974
77	0.308821	-0.022657	0.228219
6	1.894187	-0.863193	-1.245468
6	1.350118	0.387678	-1.702243
6	1.784483	1.404842	-0.788959
6	2.522933	0.782323	0.247556
6	2.586939	-0.621550	-0.039334
1	1.741378	-1.826689	-1.716032
1	0.798618	0.547881	-2.620992
1	1.541101	2.458306	-0.858808
1	2.966300	1.278608	1.101749
1	3.069637	-1.371397	0.576464

Cp-Ir-PP-TS1_for

Number of imaginary frequencies : 0
The smallest frequencies are : 15.7290 41.2946 60.9682 cm(-1)

Electronic energy : =-1100.6298973
Zero-point correction= 0.205266
Thermal correction to Energy= 0.218907
Thermal correction to Enthalpy= 0.219851
Thermal correction to Gibbs Free Energy= 0.163153
Sum of electronic and zero-point Energies= -1100.424632
Sum of electronic and thermal Energies= -1100.410990
Sum of electronic and thermal Enthalpies= -1100.410046
Sum of electronic and thermal Free Energies= -1100.466744

Cartesian Coordinates

6	-2.867650	-0.208605	-1.009527
6	-3.029851	0.620879	0.244143
1	-3.203510	-0.027707	1.112635
1	-3.864239	1.334600	0.176557
6	0.332684	-1.844608	1.441037
1	-0.602976	-2.027313	1.974045
1	1.141241	-1.754945	2.175012
1	-0.168579	0.213787	1.745241
1	0.537446	-2.696820	0.780622
15	-1.451325	1.603689	0.432342
15	-1.397585	-1.361942	-0.855746
1	-3.749116	-0.827335	-1.225096
1	-2.706227	0.437524	-1.884898
1	-1.963172	-2.077889	0.243946
1	-1.572456	1.864363	1.830528
77	0.303482	-0.063301	0.262875

6	1.842745	-0.566115	-1.379751
6	1.287811	0.714417	-1.679969
6	1.673813	1.608596	-0.637385
6	2.475887	0.893800	0.297850
6	2.571947	-0.447831	-0.159009
1	1.723434	-1.467822	-1.968273
1	0.678842	0.963124	-2.540964
1	1.386383	2.650667	-0.562841
1	2.917925	1.296348	1.200300
1	3.086222	-1.255820	0.348524

Cp-Ir-PP-TS2_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 32.3480 46.0845 56.4079 cm(-1)

Electronic energy : =-1289.1670469
Zero-point correction= 0.218659
Thermal correction to Energy= 0.236390
Thermal correction to Enthalpy= 0.237335
Thermal correction to Gibbs Free Energy= 0.170902
Sum of electronic and zero-point Energies= -1288.948388
Sum of electronic and thermal Energies= -1288.930656
Sum of electronic and thermal Enthalpies= -1288.929712
Sum of electronic and thermal Free Energies= -1288.996144

Cartesian Coordinates

6	3.036427	1.299233	-0.374397
6	2.439238	1.927857	0.873960
1	4.130847	1.259657	-0.313151
1	2.793279	1.901801	-1.260709
1	2.685486	2.990861	0.997043
1	2.778461	1.388559	1.768573
6	-0.128557	0.589964	-1.934193
1	0.671435	1.291845	-2.206984
1	-1.079557	1.140149	-1.983611
1	-0.147061	-0.192675	-2.703022
8	-3.692971	0.991677	-0.772315
6	-3.093899	1.794867	-0.178881
8	-2.513606	2.603626	0.427755
15	0.613547	1.680865	0.754539
1	0.122248	2.120993	2.006891
1	0.229422	2.799204	-0.032538
15	2.414878	-0.461040	-0.688077
1	2.949857	-0.947654	0.555600
77	0.103061	-0.354276	-0.049340
6	-0.583028	-2.441630	-0.521220
6	0.116836	-2.505219	0.731341
6	-0.605096	-1.751773	1.687035
6	-1.779090	-1.230853	1.038674
6	-1.770629	-1.667408	-0.307819
1	-0.295675	-2.938607	-1.439351
1	1.055751	-3.019078	0.903373
1	-0.334232	-1.609246	2.725505
1	-2.550561	-0.635822	1.512835
1	-2.512317	-1.420736	-1.058744

Cp-Ir-PP-TS2

Number of imaginary frequencies : 1
The smallest frequencies are : -326.6921 52.9344 56.2059 cm(-1)

Electronic energy : =-1289.0909886
Zero-point correction= 0.218224
Thermal correction to Energy= 0.234551
Thermal correction to Enthalpy= 0.235495
Thermal correction to Gibbs Free Energy= 0.174085
Sum of electronic and zero-point Energies= -1288.872765
Sum of electronic and thermal Energies= -1288.856437
Sum of electronic and thermal Enthalpies= -1288.855493
Sum of electronic and thermal Free Energies= -1288.916904

Cartesian Coordinates

6	3.192869	0.328287	-0.464446
6	2.958706	0.475671	1.033759
1	4.157535	-0.148620	-0.674894
1	3.226717	1.320573	-0.937148
1	3.671063	1.155895	1.518714
1	3.013465	-0.501363	1.532566
6	-0.475428	1.780097	-1.550082
1	0.566140	2.102246	-1.449186
1	-0.975827	2.575515	-2.115709
1	-0.576748	0.924153	-2.232498
8	-2.717573	1.703519	-0.609617
6	-1.594414	2.050553	-0.264805
8	-1.108569	2.625038	0.712311
15	1.230006	1.090709	1.168147
1	0.945748	1.251778	2.538754
1	1.335292	2.425819	0.740569

15	1.851917	-0.666605	-1.357572
1	2.210234	-1.907240	-0.728472
77	-0.135016	-0.273172	-0.063104
6	-0.839397	-2.365863	-0.375691
6	-0.366663	-2.140351	0.971135
6	-1.321911	-1.256251	1.619807
6	-2.280575	-0.869476	0.676131
6	-1.953445	-1.519476	-0.576082
1	-0.369731	-3.002159	-1.116507
1	0.451268	-2.664809	1.452316
1	-1.256123	-0.898697	2.640935
1	-3.048965	-0.115471	0.795985
1	-2.491970	-1.372551	-1.504909

Cp-Ir-PP-TS2_for

Number of imaginary frequencies : 0
The smallest frequencies are : 25.1608 51.9235 56.7516 cm(-1)

Electronic energy : =-1289.1677584
Zero-point correction= 0.221073
Thermal correction to Energy= 0.237737
Thermal correction to Enthalpy= 0.238681
Thermal correction to Gibbs Free Energy= 0.174990
Sum of electronic and zero-point Energies= -1288.946686
Sum of electronic and thermal Energies= -1288.930022
Sum of electronic and thermal Enthalpies= -1288.929078
Sum of electronic and thermal Free Energies= -1288.992768

Cartesian Coordinates

6	2.965872	0.083219	-0.779760
6	3.097127	-0.895823	0.376273
1	3.786334	-0.048169	-1.496114
1	3.011993	1.117929	-0.417437
1	3.983867	-0.727725	1.000934
1	3.135016	-1.926306	-0.001704
6	0.196353	4.001606	0.340435
1	0.726372	4.052662	1.296086
1	-0.565885	4.781544	0.289271
1	0.934971	4.169867	-0.450811
8	-1.593696	2.516980	-0.231949
6	-0.437419	2.640521	0.147604
8	0.392798	1.669258	0.416486
15	1.555368	-0.747236	1.378170
1	1.578388	-1.878400	2.226289
1	1.877207	0.264728	2.311951
15	1.339457	-0.086550	-1.720298
1	1.552129	-1.479686	-2.012450
77	-0.257214	-0.324896	0.065010
6	-1.562572	-1.593786	-1.179821
6	-1.428823	-2.183324	0.116603
6	-2.100391	-1.320542	1.065115
6	-2.552299	-0.186786	0.365782
6	-2.212061	-0.330696	-1.025459
1	-1.190142	-2.013102	-2.107569
1	-1.000566	-3.155126	0.330573
1	-2.194181	-1.497349	2.129095
1	-3.006118	0.697703	0.792454
1	-2.433830	0.388981	-1.801372

Cp-Ir-PP-AlCl3-Presence-CO2-insertion-TS2_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 17.7666 24.9807 35.5388 cm(-1)

Electronic energy : =-2912.294371
Zero-point correction= 0.225724
Thermal correction to Energy= 0.249896
Thermal correction to Enthalpy= 0.250840
Thermal correction to Gibbs Free Energy= 0.167852
Sum of electronic and zero-point Energies= -2912.068647
Sum of electronic and thermal Energies= -2912.044475
Sum of electronic and thermal Enthalpies= -2912.043531
Sum of electronic and thermal Free Energies= -2912.126519

Cartesian Coordinates

6	3.914247	1.681403	-1.111065
6	3.828601	2.090264	0.350518
77	1.439314	-0.296488	-0.001326
1	4.927610	1.836587	-1.499945
1	3.228286	2.293254	-1.714144
1	4.036323	3.152290	0.526040
1	4.523968	1.497794	0.961135
6	0.496791	0.818551	-1.541163
1	0.270849	1.864270	-1.274806
1	-0.455217	0.326252	-1.781847
1	1.090516	0.846143	-2.463314
8	-2.228055	1.230976	0.079620
6	-1.572216	1.487191	1.023423

8	-0.970304	1.796334	1.956519
1	1.398774	2.821662	0.519021
13	-3.903675	0.058147	-0.306380
17	-5.244378	1.559923	-0.873276
17	-3.137865	-1.233305	-1.767064
17	-4.051479	-0.695744	1.660960
1	3.009197	-0.066139	-2.603750
1	2.124735	1.830738	2.288605
15	3.473785	-0.156024	-1.253326
15	2.119066	1.649217	0.884009
6	1.513914	-2.580593	-0.124027
6	0.161736	-2.173455	-0.299863
6	-0.289222	-1.580677	0.922002
6	0.813070	-1.590111	1.827197
6	1.923223	-2.224250	1.198741
1	2.133248	-3.064673	-0.869748
1	-0.435344	-2.307619	-1.194332
1	-1.304861	-1.272992	1.146689
1	0.800617	-1.194312	2.837126
1	2.898403	-2.400799	1.633844

Cp-Ir-PP-AlCl3-Presence-CO2-insertion-TS2

Number of imaginary frequencies : 1

The smallest frequencies are : -150.1501 25.9915 35.5660 cm(-1)

Electronic energy : =-2912.2894689
Zero-point correction= 0.225201
Thermal correction to Energy= 0.248386
Thermal correction to Enthalpy= 0.249330
Thermal correction to Gibbs Free Energy= 0.170264
Sum of electronic and zero-point Energies= -2912.064267
Sum of electronic and thermal Energies= -2912.041083
Sum of electronic and thermal Enthalpies= -2912.040139
Sum of electronic and thermal Free Energies= -2912.119205

Cartesian Coordinates

6	3.740417	1.825806	-0.897865
6	3.598323	2.141056	0.581577
77	1.245969	-0.274196	-0.020464
1	4.760621	2.030488	-1.243892
1	3.055419	2.445453	-1.492071
1	3.764584	3.196092	0.826992
1	4.296948	1.537522	1.176993
6	0.449566	0.906504	-1.595239
1	0.311457	1.963402	-1.328378
1	-0.535830	0.496260	-1.841199
1	1.069996	0.865091	-2.496349
8	-1.800403	0.945527	0.239794
6	-1.027189	0.764006	1.156410
8	-0.763934	0.862253	2.297875
1	1.140749	2.792901	0.748004
13	-3.535697	0.258144	-0.254610
17	-4.678881	1.998600	-0.540212
17	-3.099615	-0.888873	-1.982981
17	-3.964172	-0.911821	1.466989
1	2.987197	0.099166	-2.505301
1	1.858901	1.674257	2.454486
15	3.381453	-0.007687	-1.137142
15	1.891787	1.626279	1.044649
6	1.430377	-2.462912	-0.578379
6	0.043076	-2.154415	-0.550840
6	-0.316261	-1.842878	0.795672
6	0.875136	-1.934108	1.592271
6	1.942673	-2.342466	0.762014
1	1.998037	-2.764040	-1.450991
1	-0.635521	-2.154750	-1.396933
1	-1.327049	-1.701422	1.165915
1	0.931989	-1.732890	2.655781
1	2.971693	-2.499404	1.060361

Cp-Ir-PP-AlCl3-Presence-CO2-insertion-TS2_for

Number of imaginary frequencies : 0

The smallest frequencies are : 21.2012 28.8328 43.3464 cm(-1)

Electronic energy : =-2912.2935422
Zero-point correction= 0.227003
Thermal correction to Energy= 0.250207
Thermal correction to Enthalpy= 0.251151
Thermal correction to Gibbs Free Energy= 0.172223
Sum of electronic and zero-point Energies= -2912.066539
Sum of electronic and thermal Energies= -2912.043335
Sum of electronic and thermal Enthalpies= -2912.042391
Sum of electronic and thermal Free Energies= -2912.121319

Cartesian Coordinates

6	3.732494	1.726458	-0.948818
6	3.651363	2.063746	0.530815

77	1.128679	-0.257288	0.002031
1	4.745303	1.894500	-1.334828
1	3.044196	2.351065	-1.532967
1	3.855478	3.116881	0.754301
1	4.356086	1.451788	1.109470
6	0.463117	0.893644	-1.668158
1	0.351942	1.956930	-1.424641
1	-0.524150	0.508256	-1.935298
1	1.130375	0.798740	-2.527970
8	-1.662649	0.925201	0.101278
6	-0.719748	0.756544	0.912723
8	-0.599103	0.990674	2.088702
1	1.215886	2.791486	0.791459
13	-3.370863	0.315961	-0.191587
17	-4.597565	2.010483	-0.482527
17	-3.133741	-0.912700	-1.936814
17	-3.803902	-0.872015	1.534633
1	2.940377	-0.051273	-2.495124
1	1.955968	1.614919	2.465515
15	3.329952	-0.096129	-1.125236
15	1.948628	1.615815	1.059855
6	1.337549	-2.422406	-0.624216
6	-0.052450	-2.142731	-0.522311
6	-0.340649	-1.877382	0.852173
6	0.878330	-1.983934	1.595633
6	1.910262	-2.332440	0.698508
1	1.867958	-2.694512	-1.529510
1	-0.780883	-2.123122	-1.327263
1	-1.327261	-1.678427	1.264273
1	0.977643	-1.806754	2.659628
1	2.956280	-2.476132	0.940013

Cp-Ir-PP-AlCl3-Presence-C-C_bond formation-TS3_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 24.9093 34.1471 40.3566 cm(-1)

Electronic energy : =-2912.2987324
Zero-point correction= 0.227454
Thermal correction to Energy= 0.250375
Thermal correction to Enthalpy= 0.251319
Thermal correction to Gibbs Free Energy= 0.173334
Sum of electronic and zero-point Energies= -2912.071279
Sum of electronic and thermal Energies= -2912.048358
Sum of electronic and thermal Enthalpies= -2912.047414
Sum of electronic and thermal Free Energies= -2912.125399

Cartesian Coordinates

6	-2.822938	-2.444539	-0.511053
6	-2.111073	-2.846093	0.774299
77	-1.122956	0.398262	-0.126219
1	-3.716571	-3.059624	-0.671162
1	-2.148169	-2.589048	-1.360626
1	-1.429913	-3.688440	0.624079
1	-2.816825	-3.103680	1.571683
6	-1.213493	0.151615	-2.281569
1	-1.334806	-0.889161	-2.586408
1	-0.276202	0.543633	-2.690104
1	-2.050372	0.747043	-2.657696
8	1.548781	-0.130901	-0.963961
6	0.498454	-0.840226	-0.753102
8	0.375598	-2.044212	-0.833478
1	0.147065	-1.847607	1.797215
13	3.136026	-0.195311	-0.077536
17	2.539229	-0.719588	1.946044
17	3.768509	1.848882	-0.145289
17	4.464094	-1.595978	-0.937051
15	-3.331603	-0.644778	-0.375599
15	-1.115531	-1.405712	1.365549
1	-3.624493	-0.454659	-1.754954
1	-1.722275	-1.038484	2.588044
6	-2.154644	2.458962	0.454448
6	-1.225228	2.641464	-0.614260
6	0.091902	2.354571	-0.130638
6	-0.030900	1.907995	1.207402
6	-1.431198	1.962438	1.562750
1	-3.228628	2.588440	0.397654
1	-1.466629	2.991363	-1.611139
1	1.017933	2.401013	-0.694208
1	0.787430	1.590696	1.846464
1	-1.852718	1.696148	2.525614

Cp-Ir-PP-AlCl3-Presence-C-C_bond formation-TS3

Number of imaginary frequencies : 1
The smallest frequencies are : -343.8621 29.8376 46.4926 cm(-1)

Electronic energy : =-2912.2772599
Zero-point correction= 0.226594
Thermal correction to Energy= 0.248942

Thermal correction to Enthalpy= 0.249886
 Thermal correction to Gibbs Free Energy= 0.173892
 Sum of electronic and zero-point Energies= -2912.050666
 Sum of electronic and thermal Energies= -2912.028318
 Sum of electronic and thermal Enthalpies= -2912.027374
 Sum of electronic and thermal Free Energies= -2912.103368

 Cartesian Coordinates

6	-2.869882	-2.410482	-0.388128
6	-2.307976	-2.665539	1.002334
77	-1.143856	0.401093	-0.119000
1	-3.769389	-3.014502	-0.558554
1	-2.123121	-2.691361	-1.140057
1	-1.826274	-3.644777	1.088393
1	-3.092434	-2.604736	1.766207
6	-0.679642	-0.362639	-2.279701
1	-1.332711	-1.212091	-2.466397
1	0.221639	-0.472687	-2.891732
1	-1.115670	0.576680	-2.633974
8	1.585117	-0.107630	-1.042963
6	0.563821	-0.889061	-0.996560
8	0.511442	-2.087382	-0.824692
1	0.173913	-1.962536	1.622788
13	3.101226	-0.189599	-0.031476
17	2.386930	-0.450360	2.001633
17	3.876584	1.791656	-0.271873
17	4.371580	-1.752448	-0.675736
15	-3.320233	-0.588378	-0.516859
15	-1.063755	-1.348024	1.383017
1	-3.382236	-0.535517	-1.942690
1	-1.402659	-0.907312	2.682984
6	-2.133677	2.466655	0.009511
6	-0.949832	2.636919	-0.746159
6	0.184081	2.357283	0.098221
6	-0.300198	1.956656	1.352577
6	-1.751388	1.958148	1.295205
1	-3.149528	2.609607	-0.339273
1	-0.895971	2.962921	-1.778687
1	1.227849	2.387794	-0.201947
1	0.312089	1.643292	2.192122
1	-2.425614	1.753916	2.119635

 Cp-Ir-PP-ALCl3-Presence-C-C_bond formation-TS3_for

Number of imaginary frequencies : 0
 The smallest frequencies are : 21.5834 40.7405 45.9900 cm⁻¹

Electronic energy : =-2912.3621674
 Zero-point correction= 0.228617
 Thermal correction to Energy= 0.251600
 Thermal correction to Enthalpy= 0.252544
 Thermal correction to Gibbs Free Energy= 0.173923
 Sum of electronic and zero-point Energies= -2912.133550
 Sum of electronic and thermal Energies= -2912.110567
 Sum of electronic and thermal Enthalpies= -2912.109623
 Sum of electronic and thermal Free Energies= -2912.188245

 Cartesian Coordinates

6	-3.058534	-2.447135	0.100123
6	-2.692246	-2.194183	1.555419
77	-1.269434	0.385158	-0.141813
1	-4.003255	-2.999565	0.031988
1	-2.283067	-3.054963	-0.384945
1	-2.558052	-3.112560	2.138351
1	-3.458192	-1.582002	2.051309
6	1.694371	-2.262650	-2.051159
1	0.979037	-2.903243	-2.567975
1	2.198641	-2.837167	-1.262707
1	2.477567	-1.916508	-2.731588
8	1.722289	-0.146253	-0.941793
6	1.012864	-1.096237	-1.413263
8	-0.240436	-1.089552	-1.352191
1	-0.137803	-2.188294	1.312020
13	3.137176	-0.013411	0.185553
17	2.446414	-1.092700	1.919726
17	3.326289	2.081813	0.533837
17	4.823433	-0.930890	-0.727550
15	-3.265093	-0.792135	-0.799748
15	-1.139023	-1.209062	1.500138
1	-2.818711	-1.273434	-2.067265
1	-0.864778	-0.804417	2.822597
6	-2.360702	2.288275	-0.215046
6	-1.370273	2.351050	-1.240066
6	-0.080507	2.363628	-0.592925
6	-0.259000	2.276878	0.794715
6	-1.681121	2.162000	1.041790
1	-3.434634	2.273724	-0.360099
1	-1.552886	2.453091	-2.301812
1	0.883395	2.367619	-1.089139
1	0.537965	2.233496	1.529058

1 -2.158575 2.126253 2.013876

Cp-Ir-PP-AlCl3-Presence-proton-transfer-TS4_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 23.1345 31.0061 47.0760 cm(-1)

Electronic energy : =-2912.3454527
Zero-point correction= 0.228452
Thermal correction to Energy= 0.251647
Thermal correction to Enthalpy= 0.252591
Thermal correction to Gibbs Free Energy= 0.172834
Sum of electronic and zero-point Energies= -2912.117000
Sum of electronic and thermal Energies= -2912.093806
Sum of electronic and thermal Enthalpies= -2912.092862
Sum of electronic and thermal Free Energies= -2912.172619

Cartesian Coordinates

6	0.671148	3.216898	0.430327
6	0.218719	2.475202	1.681888
77	1.692726	-0.029058	-0.149182
1	1.543928	3.854011	0.623833
1	-0.133328	3.843334	0.030527
1	-0.823471	2.154347	1.557714
1	0.290502	3.093814	2.582099
6	-2.861015	-2.402960	1.565801
1	-2.705009	-3.250945	2.234322
1	-2.827677	-2.743059	0.522385
1	-3.858441	-1.977600	1.722094
8	-1.883723	-0.257236	1.084789
6	-1.805979	-1.357136	1.807740
8	-0.920883	-1.523821	2.634445
13	-2.747076	0.118680	-0.438768
17	-2.186928	2.140971	-0.973368
17	-4.859969	-0.007887	-0.175350
17	-2.022072	-1.275242	-1.924730
15	1.133755	1.946993	-0.830419
15	1.160320	0.900730	1.899926
1	1.027994	2.565274	-2.093436
1	2.243183	1.244224	2.742555
1	0.353528	0.072908	2.711628
6	2.865123	-1.382864	-1.515993
6	1.481378	-1.692675	-1.637691
6	1.011624	-2.145328	-0.359807
6	2.116384	-2.120738	0.541843
6	3.264266	-1.639542	-0.160301
1	3.506004	-1.003996	-2.301971
1	0.860190	-1.580262	-2.518577
1	-0.005848	-2.435434	-0.131456
1	2.071577	-2.391805	1.590218
1	4.257264	-1.506002	0.248345

Cp-Ir-PP-AlCl3-Presence-proton-transfer-TS4

Number of imaginary frequencies : 1
The smallest frequencies are : -620.4808 24.7315 43.6114 cm(-1)

Electronic energy : =-2912.3309973
Zero-point correction= 0.224935
Thermal correction to Energy= 0.247789
Thermal correction to Enthalpy= 0.248733
Thermal correction to Gibbs Free Energy= 0.170002
Sum of electronic and zero-point Energies= -2912.106063
Sum of electronic and thermal Energies= -2912.083208
Sum of electronic and thermal Enthalpies= -2912.082264
Sum of electronic and thermal Free Energies= -2912.160995

Cartesian Coordinates

6	0.767734	3.225202	0.486385
6	0.121331	2.435775	1.614106
77	1.740684	-0.036682	-0.134637
1	1.627385	3.811525	0.838793
1	0.059121	3.912905	0.009187
1	-0.911367	2.190724	1.336380
1	0.095478	3.007509	2.548599
6	-2.936969	-2.237402	1.749004
1	-2.787546	-2.952978	2.557675
1	-2.831707	-2.736695	0.776954
1	-3.951071	-1.824046	1.775403
8	-1.982222	-0.161961	1.004637
6	-1.943401	-1.130439	1.829332
8	-1.055016	-1.179555	2.726690
13	-2.825736	0.129829	-0.599843
17	-2.198929	2.072006	-1.225973
17	-4.918000	0.014924	-0.216123
17	-2.116455	-1.469356	-1.844148
15	1.373708	1.996491	-0.750951
15	0.939288	0.787071	1.926326
1	1.519017	2.691559	-1.973062

1	2.043031	1.175211	2.733856
1	-0.235976	-0.330634	2.563885
6	3.019850	-1.380152	-1.429156
6	1.655986	-1.706427	-1.647509
6	1.099245	-2.167667	-0.406209
6	2.136634	-2.135505	0.571908
6	3.320273	-1.627966	-0.044446
1	3.712126	-0.996002	-2.167179
1	1.104686	-1.602646	-2.574049
1	0.075033	-2.492349	-0.268896
1	2.032036	-2.410581	1.615028
1	4.278025	-1.479300	0.436842

Cp-Ir-PP-AlCl3-Presence-proton-transfer-TS4_for

Number of imaginary frequencies : 0
The smallest frequencies are : 29.1086 41.1291 46.2959 cm(-1)

Electronic energy : =-2912.3324852
Zero-point correction= 0.229126
Thermal correction to Energy= 0.252274
Thermal correction to Enthalpy= 0.253218
Thermal correction to Gibbs Free Energy= 0.174322
Sum of electronic and zero-point Energies= -2912.103359
Sum of electronic and thermal Energies= -2912.080211
Sum of electronic and thermal Enthalpies= -2912.079267
Sum of electronic and thermal Free Energies= -2912.158163

Cartesian Coordinates

6	0.896995	3.239918	0.496987
6	0.220065	2.464250	1.614356
77	1.734247	-0.053810	-0.145010
1	1.790256	3.769775	0.857109
1	0.228523	3.975568	0.032591
1	-0.815183	2.242205	1.324202
1	0.193184	3.039948	2.547159
6	-2.961206	-2.291084	1.649655
1	-2.811784	-3.036151	2.430851
1	-2.858539	-2.750510	0.657924
1	-3.973469	-1.873916	1.691155
8	-1.975825	-0.193617	1.000513
6	-1.972215	-1.190437	1.764716
8	-1.088491	-1.301191	2.689444
13	-2.839169	0.193098	-0.604702
17	-2.196841	2.141483	-1.150383
17	-4.914699	0.075404	-0.143487
17	-2.170860	-1.392023	-1.878943
15	1.432237	1.990573	-0.751270
15	1.013452	0.800380	1.958855
1	1.617883	2.687327	-1.968075
1	2.197774	1.253839	2.610209
1	-0.383622	-0.539692	2.627174
6	2.959956	-1.449731	-1.448766
6	1.586642	-1.747058	-1.636874
6	1.042071	-2.176915	-0.377933
6	2.096381	-2.154174	0.580762
6	3.277914	-1.677513	-0.064402
1	3.646729	-1.091442	-2.204652
1	1.021953	-1.645400	-2.555486
1	0.014214	-2.478832	-0.218010
1	2.007540	-2.409120	1.630398
1	4.247059	-1.542530	0.397775

benzene

Number of imaginary frequencies : 0
The smallest frequencies are : 408.1683 408.3223 611.1845 cm(-1)

Electronic energy : =-232.0567884
Zero-point correction= 0.100059
Thermal correction to Energy= 0.104490
Thermal correction to Enthalpy= 0.105435
Thermal correction to Gibbs Free Energy= 0.072585
Sum of electronic and zero-point Energies= -231.956730
Sum of electronic and thermal Energies= -231.952298
Sum of electronic and thermal Enthalpies= -231.951354
Sum of electronic and thermal Free Energies= -231.984204

Cartesian Coordinates

6	-0.869439	1.086814	0.000001
6	-1.375961	-0.209551	0.000062
6	-0.506551	-1.296312	-0.000031
6	0.869478	-1.086782	0.000012
6	1.375968	0.209500	0.000033
6	0.506505	1.296331	-0.000045
1	-1.549061	1.936072	-0.000015
1	-2.451270	-0.373396	-0.000028
1	-0.902178	-2.309532	-0.000108
1	1.548987	-1.936129	-0.000044

1 2.451255 0.373481 0.000061
1 0.902265 2.309500 -0.000052

Bn-Ru-PP-TS1_Benzene-C-H-activation

Number of imaginary frequencies : 1
The smallest frequencies are : -449.4608 28.8259 55.3504 cm(-1)

Electronic energy : =-1321.4167933
Zero-point correction= 0.273711
Thermal correction to Energy= 0.290866
Thermal correction to Enthalpy= 0.291810
Thermal correction to Gibbs Free Energy= 0.228514
Sum of electronic and zero-point Energies= -1321.143082
Sum of electronic and thermal Energies= -1321.125928
Sum of electronic and thermal Enthalpies= -1321.124983
Sum of electronic and thermal Free Energies= -1321.188280

Cartesian Coordinates

6 2.179251 2.414560 -0.655929
6 1.657052 2.796149 0.715891
44 0.441222 -0.353265 0.013211
1 0.746889 3.400465 0.613937
1 2.389054 3.383909 1.287746
6 2.289973 -1.711231 0.237282
6 1.897747 -1.676448 -1.112398
6 0.573470 -2.050924 -1.486064
6 -0.338275 -2.426336 -0.478988
6 0.047911 -2.478638 0.888980
6 1.350353 -2.083965 1.240743
1 -0.677333 -2.743913 1.652152
1 3.278040 -1.363605 0.527340
1 2.589573 -1.321186 -1.871935
1 0.255546 -1.978789 -2.521806
1 -1.373987 -2.623063 -0.745953
1 1.641599 -2.033897 2.287009
1 -0.194139 0.997173 0.653568
15 1.311960 1.218794 1.686875
15 0.961563 1.345990 -1.617522
1 2.406135 3.304877 -1.258709
1 3.115690 1.841690 -0.570271
1 -0.122498 2.268187 -1.452745
1 0.211856 1.717736 2.458200
6 -1.591425 0.240094 0.039370
6 -2.286342 0.516537 -1.147373
6 -2.343049 0.119873 1.217827
6 -3.674653 0.629144 -1.157382
1 -1.743123 0.625360 -2.085949
6 -3.731840 0.239463 1.209888
1 -1.831662 -0.073611 2.162343
6 -4.404548 0.491707 0.019807
1 -4.188021 0.826956 -2.096881
1 -4.285895 0.137883 2.141472
1 -5.488101 0.585824 0.008997

Bn-Ru-PP-AlCl3-Presence-TS3_Benzene-C-C bond formation

Number of imaginary frequencies : 1
The smallest frequencies are : -167.7707 36.1155 44.6016 cm(-1)

Electronic energy : =-3133.0828607
Zero-point correction= 0.297551
Thermal correction to Energy= 0.323987
Thermal correction to Enthalpy= 0.324932
Thermal correction to Gibbs Free Energy= 0.240540
Sum of electronic and zero-point Energies= -3132.785310
Sum of electronic and thermal Energies= -3132.758873
Sum of electronic and thermal Enthalpies= -3132.757929
Sum of electronic and thermal Free Energies= -3132.842321

Cartesian Coordinates

6 -3.581340 -0.877968 -2.032464
6 -2.317563 -0.690516 -2.855676
44 -1.024417 -0.541672 0.354204
1 -3.870657 -1.937410 -2.027018
1 -4.428211 -0.320310 -2.448875
1 -2.082187 0.364573 -3.030695
1 -2.335292 -1.207399 -3.823244
6 -1.640139 -2.534358 1.362006
6 -2.038177 -1.566262 2.315503
6 -1.099504 -0.670124 2.828643
6 0.260086 -0.778861 2.446672
6 0.684209 -1.817559 1.607226
6 -0.272022 -2.671606 1.031138
1 1.734640 -1.904244 1.335394
1 -2.383615 -3.190852 0.915044
1 -3.089500 -1.464088 2.568595
1 -1.417532 0.125418 3.496491
1 1.001283 -0.065908 2.801231

1	0.050892	-3.436566	0.327583
8	1.503045	0.732173	0.144440
6	0.488771	0.664621	-0.656049
8	0.471004	0.869604	-1.852621
1	0.206315	-1.486961	-2.466144
13	3.159887	0.120462	-0.297614
17	2.756903	-1.770713	-1.294472
17	3.963767	-0.294030	1.654830
17	4.280470	1.482663	-1.458889
15	-3.392627	-0.321447	-0.227978
15	-1.011424	-1.376213	-1.774011
1	-3.522307	1.060813	-0.519587
1	-1.423242	-2.737023	-1.745804
6	-1.053760	1.640933	0.262690
6	-0.687836	2.297233	1.448696
6	-1.634360	2.427432	-0.742200
6	-0.977226	3.643441	1.653873
1	-0.130847	1.774522	2.220273
6	-1.918613	3.772299	-0.546739
1	-1.823145	1.992053	-1.719991
6	-1.607823	4.385519	0.663177
1	-0.683080	4.113882	2.589605
1	-2.364216	4.347776	-1.355067
1	-1.822689	5.440001	0.817508

 Bn-Ru-NNTs-AA-Presence-TS1_Benzene-C-H-activation

Number of imaginary frequencies : 1
 The smallest frequencies are : -1556.9575 28.3725 29.9402 cm(-1)

Electronic energy = -1795.840456
 Zero-point correction= 0.470995
 Thermal correction to Energy= 0.501395
 Thermal correction to Enthalpy= 0.502339
 Thermal correction to Gibbs Free Energy= 0.409816
 Sum of electronic and zero-point Energies= -1795.369461
 Sum of electronic and thermal Energies= -1795.339061
 Sum of electronic and thermal Enthalpies= -1795.338117
 Sum of electronic and thermal Free Energies= -1795.430640

 Cartesian Coordinates

6	0.002437	-1.119685	2.375648
6	-1.480289	-1.094715	2.647747
44	-1.380765	-0.748628	-0.341650
1	0.485669	-1.876845	3.004270
1	0.444677	-0.143785	2.649761
1	-1.703513	-0.717454	3.654754
1	-1.885864	-2.110763	2.552948
6	-2.891280	-2.310717	-0.602545
6	-1.657640	-2.794430	-1.081277
6	-0.948410	-2.073887	-2.093248
6	-1.461882	-0.863486	-2.575426
6	-2.689496	-0.335136	-2.065842
6	-3.398528	-1.061279	-1.087271
1	-3.036388	0.653847	-2.352149
1	-3.400225	-2.828149	0.208071
1	-1.186168	-3.661104	-0.627939
1	0.039878	-2.414830	-2.380619
1	-0.869252	-0.280171	-3.273628
1	-4.284683	-0.615818	-0.640436
1	-1.706287	1.511001	-0.178117
6	-3.008820	2.772102	1.036501
8	-2.944797	2.122896	-0.072756
8	-2.372316	2.474498	2.061853
6	-3.924340	3.973328	1.034819
1	-1.992813	0.767697	1.834045
7	-2.113816	-0.247495	1.618817
7	0.166407	-1.437202	0.963330
16	1.553428	-2.186439	0.567204
6	2.771409	-0.919701	0.256041
6	3.524493	-0.424887	1.318900
6	2.939719	-0.416091	-1.027819
6	4.444472	0.587545	1.085987
1	3.401134	-0.858555	2.308830
6	3.867357	0.595417	-1.245673
1	2.354137	-0.829058	-1.846636
6	4.625104	1.115600	-0.195975
1	5.041485	0.976674	1.910714
1	4.000483	0.998014	-2.249583
6	5.598890	2.233028	-0.420693
1	5.645466	2.522157	-1.475923
1	5.317197	3.123097	0.157741
1	6.611422	1.956377	-0.102911
8	1.369303	-2.887689	-0.706991
8	2.045237	-2.940017	1.723116
1	-3.124601	-0.374830	1.635800
6	-0.454268	1.387254	-0.430736
6	0.426648	1.771063	0.597555
6	-0.186750	1.922505	-1.709794
6	1.524614	2.588510	0.362575
1	0.228965	1.457447	1.618403

6	0.904566	2.740672	-1.960334
1	-0.890348	1.742881	-2.522039
6	1.772439	3.065435	-0.919976
1	2.191778	2.852374	1.180939
1	1.070553	3.142168	-2.958037
1	2.633277	3.705720	-1.107482
1	-3.483896	4.756976	0.408789
1	-4.889577	3.714686	0.588658
1	-4.063905	4.357601	2.047333

 Bn-Ru-NNTs.AA-AICl3-Presence-TS3_Benzene-C-C bond formation

Number of imaginary frequencies : 1
 The smallest frequencies are : -184.1731 21.1139 24.4510 cm(-1)

Electronic energy : =-3607.5160795
 Zero-point correction= 0.496949
 Thermal correction to Energy= 0.536957
 Thermal correction to Enthalpy= 0.537901
 Thermal correction to Gibbs Free Energy= 0.423295
 Sum of electronic and zero-point Energies= -3607.019130
 Sum of electronic and thermal Energies= -3606.979123
 Sum of electronic and thermal Enthalpies= -3606.978178
 Sum of electronic and thermal Free Energies= -3607.092784

 Cartesian Coordinates

6	1.876230	-2.784131	0.733717
6	1.044571	-2.436485	1.945132
44	-0.112713	-1.036220	-0.526379
1	1.451090	-3.666787	0.221310
1	2.896960	-3.066575	1.016793
1	1.593762	-1.720301	2.567590
1	0.810324	-3.314971	2.557834
6	-0.552527	-3.053297	-1.609944
6	0.317440	-2.300764	-2.425155
6	-0.010332	-0.984496	-2.824889
6	-1.247645	-0.443050	-2.425029
6	-2.153470	-1.213343	-1.648789
6	-1.794685	-2.500145	-1.217312
1	-3.098133	-0.782527	-1.319173
1	-0.262015	-4.043782	-1.272360
1	1.299747	-2.695110	-2.675079
1	0.716015	-0.399655	-3.378413
1	-1.519888	0.578408	-2.680678
1	-2.454379	-3.033369	-0.536422
8	-1.920448	1.319733	-0.371794
6	-1.323858	0.561845	0.460039
8	-1.568006	0.443876	1.655821
13	-3.581994	2.080059	-0.356859
17	-4.900408	0.425772	0.080792
17	-3.726858	2.630744	-2.419748
17	-3.688017	3.652312	1.051438
6	0.690557	0.896698	0.003187
6	0.814476	1.878668	-0.987721
6	1.342120	1.106230	1.221955
6	1.573731	3.021363	-0.768617
1	0.287618	1.780733	-1.933353
6	2.088880	2.256403	1.450243
1	1.254133	0.380661	2.027520
6	2.210876	3.216720	0.453294
1	1.650267	3.769663	-1.554221
1	2.577386	2.397078	2.412196
1	2.793944	4.117850	0.630090
7	-0.197158	-1.787244	1.472417
7	1.855072	-1.597878	-0.112697
6	-3.818350	-2.044396	2.332654
8	-3.690725	-0.859160	2.893709
8	-2.984429	-2.542227	1.585566
6	-5.106785	-2.706473	2.696310
1	-2.943848	-0.365391	2.485040
1	-5.318712	-2.576584	3.760729
1	-5.911974	-2.208102	2.144512
1	-5.082431	-3.763462	2.429160
1	-1.021613	-2.397100	1.512691
1	-0.468800	-0.982561	2.047190
16	3.198333	-1.300949	-1.018006
8	3.966055	-2.546891	-1.083133
8	2.805950	-0.641877	-2.263641
6	4.188234	-0.130252	-0.110572
6	4.552216	1.068518	-0.706819
6	4.636542	-0.457371	1.168004
6	5.364083	1.953986	-0.005356
1	4.193755	1.298705	-1.706452
6	5.435018	0.440521	1.858087
1	4.373323	-1.413438	1.617224
6	5.806897	1.661832	1.283856
1	5.652329	2.897612	-0.467186
1	5.789247	0.192140	2.857727
6	6.637029	2.644071	2.052996
1	6.003521	3.289328	2.675964
1	7.341443	2.140099	2.723402

1 7.208652 3.297795 1.386211

Bn-Ru-OO.2TFA-TS1_Benzene-C-H-activation

Number of imaginary frequencies : 1
The smallest frequencies are : -1415.5749 20.2427 28.9583 cm(-1)

Electronic energy : =-1841.1870407
Zero-point correction= 0.343980
Thermal correction to Energy= 0.373551
Thermal correction to Enthalpy= 0.374495
Thermal correction to Gibbs Free Energy= 0.282264
Sum of electronic and zero-point Energies= -1840.843061
Sum of electronic and thermal Energies= -1840.813489
Sum of electronic and thermal Enthalpies= -1840.812545
Sum of electronic and thermal Free Energies= -1840.904776

Cartesian Coordinates

8	1.108096	-1.104490	1.634063
6	0.640768	-0.580391	2.851150
6	-0.781488	-1.046106	3.060496
8	-1.528430	-0.872441	1.852943
44	-0.317321	-1.138017	0.079578
1	1.271274	-0.945735	3.676739
1	0.692507	0.520099	2.857634
1	-1.276582	-0.516784	3.883342
1	-0.797775	-2.123140	3.275097
6	-0.339705	-3.333056	-0.143262
6	0.802010	-2.785959	-0.782173
6	0.671794	-1.764126	-1.759372
6	-0.623156	-1.269337	-2.084532
6	-1.773513	-1.787205	-1.447816
6	-1.615373	-2.796049	-0.455518
1	-2.742666	-1.329351	-1.622039
1	-0.227107	-4.045749	0.668039
1	1.805299	-3.028083	-0.439786
1	1.578546	-1.319014	-2.157472
1	-0.729383	-0.411504	-2.745521
1	-2.476380	-3.086183	0.141875
1	-1.264447	0.954484	-0.465347
6	-3.378584	1.084219	-0.027544
8	-2.486396	1.119554	-0.926932
8	-3.259915	0.928876	1.192816
6	-4.800607	1.169768	-0.613438
9	-5.729433	1.278504	0.323462
9	-5.031233	0.033879	-1.297581
9	-4.927126	2.187499	-1.458118
1	-2.117919	-0.071570	1.802223
6	3.636648	-0.273387	-0.043893
8	3.386266	-1.251307	-0.733692
8	3.106371	0.089183	1.063324
6	4.731448	0.677972	-0.564087
9	5.907986	0.052710	-0.589606
9	4.864159	1.786937	0.156805
9	4.435672	1.042305	-1.820716
1	2.169386	-0.536596	1.319905
6	-0.024458	1.123704	-0.022254
6	-0.126809	1.959376	1.111264
6	0.971957	1.468980	-0.960647
6	0.737896	3.023605	1.325844
1	-0.945998	1.801983	1.813672
6	1.851447	2.522571	-0.751552
1	1.078943	0.897702	-1.881667
6	1.746115	3.290345	0.403600
1	0.623485	3.650402	2.207650
1	2.631782	2.733147	-1.478435
1	2.442673	4.107585	0.576695

Role of Acids (Table S3)

Bn-Ru-NNTs-AA

Number of imaginary frequencies : 0
The smallest frequencies are : 14.9571 25.5358 33.3269 cm(-1)

Electronic energy : =-1563.8004874
Zero-point correction= 0.373514
Thermal correction to Energy= 0.399106
Thermal correction to Enthalpy= 0.400050
Thermal correction to Gibbs Free Energy= 0.314732
Sum of electronic and zero-point Energies= -1563.426973
Sum of electronic and thermal Energies= -1563.401381
Sum of electronic and thermal Enthalpies= -1563.400437
Sum of electronic and thermal Free Energies= -1563.485755

Cartesian Coordinates

6	0.612790	0.449585	2.044302
6	-0.800219	0.725243	2.499486
44	-1.105257	-0.695992	-0.080650
1	1.234170	0.092957	2.875761
1	1.078255	1.362568	1.635854
1	-0.857480	1.648812	3.090227
1	-1.148565	-0.103966	3.127387
6	-2.577352	-2.242745	-0.529717
6	-1.321799	-2.633717	-1.095644
6	-0.646011	-1.764164	-1.970973
6	-1.198274	-0.475842	-2.231294
6	-2.467143	-0.105755	-1.708611
6	-3.169273	-1.004927	-0.872465
1	-2.814634	0.923051	-1.790787
1	-3.048403	-2.873454	0.218920
1	-0.834746	-3.548527	-0.771036
1	0.353729	-2.019120	-2.307355
1	-0.621460	0.256073	-2.791097
1	-4.042465	-0.635756	-0.336048
7	-1.658273	0.784590	1.311621
1	-1.650627	1.685212	0.797239
7	0.532389	-0.575026	0.980541
16	1.972092	-1.419198	0.741079
6	3.080839	-0.166616	0.137384
6	4.020409	0.388681	0.997291
6	2.965383	0.269562	-1.180771
6	4.855052	1.395583	0.525071
1	4.095181	0.020770	2.017862
6	3.803743	1.275786	-1.634654
1	2.231613	-0.189869	-1.839993
6	4.759822	1.852382	-0.790183
1	5.986869	1.835779	1.189487
1	3.724644	1.623686	-2.663718
6	5.674860	2.921198	-1.304876
1	5.137927	3.637366	-1.936587
1	6.148611	3.474961	-0.488396
1	6.475906	2.489479	-1.918039
8	1.734852	-2.377466	-0.332634
8	2.472015	-1.869229	2.035592
6	-4.122297	2.177411	0.211360
8	-4.305596	1.168415	0.956809
8	-3.016463	2.571465	-0.245764
6	-5.370861	2.956307	-0.173918
1	-2.691622	0.733871	1.483564
1	-5.937079	3.215648	0.726407
1	-5.121847	3.860528	-0.734590
1	-6.025422	2.320511	-0.781608

Bn-Ru-NNTs-Pivalic-acid

Number of imaginary frequencies : 0
The smallest frequencies are : 13.6797 18.1018 21.5550 cm(-1)

Electronic energy : =-1681.6545716
Zero-point correction= 0.457971
Thermal correction to Energy= 0.487305
Thermal correction to Enthalpy= 0.488249
Thermal correction to Gibbs Free Energy= 0.394493
Sum of electronic and zero-point Energies= -1681.196600
Sum of electronic and thermal Energies= -1681.167267
Sum of electronic and thermal Enthalpies= -1681.166323
Sum of electronic and thermal Free Energies= -1681.260079

Cartesian Coordinates

6	1.199740	0.161674	2.122717
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6	-0.220669	0.118693	2.632279
44	-0.359636	-1.055876	-0.083631
1	1.908019	-0.159045	2.897190
1	1.473344	1.183740	1.810493
1	-0.422897	0.946345	3.324611
1	-0.386640	-0.823682	3.168471
6	-1.537434	-2.799116	-0.662523
6	-0.251712	-2.891500	-1.284949
6	0.221068	-1.831203	-2.079632
6	-0.568359	-0.650493	-2.200319
6	-1.865494	-0.577738	-1.624258
6	-2.359938	-1.667643	-0.870732
1	-2.402527	0.369826	-1.608014
1	-1.858015	-3.576386	0.025336
1	0.407069	-3.725479	-1.061484
1	1.238416	-1.861854	-2.456150
1	-0.157666	0.226926	-2.693418
1	-3.271282	-1.525626	-0.290681
7	-1.120166	0.145511	1.474187
1	-1.293648	1.082771	1.063899
7	1.267244	-0.741590	0.953248
16	2.829109	-1.269676	0.594129
6	3.650788	0.222100	0.083303
6	4.490943	0.882503	0.971597
6	3.405599	0.732638	-1.189535
6	5.090906	2.072501	0.574474
1	4.673799	0.454455	1.954421
6	4.010009	1.920884	-1.568512
1	2.757140	0.189782	-1.874031
6	4.860134	2.607632	-0.693519
1	5.752866	2.596851	1.261733
1	3.827890	2.328658	-2.561897
6	5.523782	3.878627	-1.127698
1	4.828861	4.526455	-1.673307
1	5.915829	4.441128	-0.274707
1	6.365373	3.671459	-1.800584
8	2.727802	-2.155834	-0.559982
8	3.462524	-1.728792	1.825321
6	-3.819394	1.145123	0.475436
8	-3.808281	0.088788	1.175979
8	-2.807283	1.809099	0.126197
6	-5.205806	1.606152	-0.024500
1	-2.118193	-0.107224	1.662639
6	-6.143690	1.746744	1.172923
1	-7.156879	2.011310	0.839582
1	-6.188912	0.809494	1.736481
1	-5.798127	2.536405	1.852849
6	-5.115149	2.925861	-0.777092
1	-4.457502	2.839779	-1.649694
1	-6.111508	3.237912	-1.120468
1	-4.703889	3.716028	-0.139131
6	-5.740902	0.516901	-0.956288
1	-6.736682	0.785390	-1.335131
1	-5.083398	0.382805	-1.828599
1	-5.816771	-0.440444	-0.427891

Bn-Ru-NNTs-TCA

Number of imaginary frequencies : 1
The smallest frequencies are : -28.8264 9.6911 17.2684 cm(-1)

Electronic energy : ==-2942.4843087
Zero-point correction= 0.346009
Thermal correction to Energy= 0.373828
Thermal correction to Enthalpy= 0.374772
Thermal correction to Gibbs Free Energy= 0.283800
Sum of electronic and zero-point Energies= -2942.138300
Sum of electronic and thermal Energies= -2942.110481
Sum of electronic and thermal Enthalpies= -2942.109537
Sum of electronic and thermal Free Energies= -2942.200509

Cartesian Coordinates

6	1.735822	-0.058199	2.208105
6	0.337503	-0.270590	2.732899
44	0.236402	-1.171079	-0.091872
1	2.485518	-0.393348	2.935358
1	1.917245	1.009354	1.996813
1	0.086512	0.455478	3.516748
1	0.255304	-1.277872	3.158146
6	-0.848938	-2.922564	-0.828159
6	0.447052	-2.889491	-1.434534
6	0.865711	-1.744525	-2.138408
6	0.014143	-0.603714	-2.172392
6	-1.289114	-0.650448	-1.608109
6	-1.729871	-1.825347	-0.957493
1	-1.894695	0.251804	-1.549429
1	-1.135207	-3.772497	-0.215441
1	1.149751	-3.701563	-1.271911
1	1.885238	-1.690700	-2.506177
1	0.377527	0.331267	-2.591117
1	-2.666111	-1.796485	-0.402194

7	-0.586774	-0.184651	1.594669
1	-0.798094	0.779101	1.293791
7	1.849635	-0.833298	0.953857
16	3.446611	-1.192598	0.525387
6	4.108037	0.394119	0.074372
6	4.864833	1.109331	0.994723
6	3.824641	0.917426	-1.185712
6	5.338301	2.369273	0.644203
1	5.087357	0.669944	1.964314
6	4.303298	2.174517	-1.517943
1	3.250742	0.329293	-1.898697
6	5.064468	2.919197	-0.608539
1	5.935491	2.936480	1.356126
1	4.092974	2.591969	-2.501723
6	5.584657	4.270359	-0.992812
1	4.789429	4.899171	-1.409153
1	6.018978	4.795184	-0.136625
1	6.362557	4.187635	-1.761832
8	3.390291	-2.024256	-0.670804
8	4.151335	-1.652214	1.716277
6	-3.359415	0.698799	0.692772
8	-3.317872	-0.388196	1.303069
8	-2.454535	1.499947	0.407734
6	-4.781933	1.052141	0.093490
1	-1.549558	-0.524568	1.781502
17	-6.111784	0.451130	1.107849
17	-4.992093	2.794421	-0.183846
17	-4.841263	0.197455	-1.511709

Bn-Ru-NNTs-TFA

Number of imaginary frequencies : 1
The smallest frequencies are : -14.7483 15.6010 28.2791 cm(-1)

Electronic energy : =-1861.4529012
Zero-point correction= 0.352987
Thermal correction to Energy= 0.379133
Thermal correction to Enthalpy= 0.380077
Thermal correction to Gibbs Free Energy= 0.294834
Sum of electronic and zero-point Energies= -1861.099914
Sum of electronic and thermal Energies= -1861.073768
Sum of electronic and thermal Enthalpies= -1861.072824
Sum of electronic and thermal Free Energies= -1861.158067

Cartesian Coordinates

6	1.266621	0.090999	2.107462
6	-0.116983	0.058804	2.707177
44	-0.462635	-0.926061	-0.075080
1	2.010848	-0.296598	2.814485
1	1.554436	1.120709	1.836985
1	-0.245821	0.841716	3.465604
1	-0.284401	-0.913664	3.185321
6	-1.740944	-2.596663	-0.661244
6	-0.483953	-2.718068	-1.334350
6	-0.000274	-1.653268	-2.117801
6	-0.745000	-0.441015	-2.172173
6	-2.016319	-0.337793	-1.547851
6	-2.524938	-1.429694	-0.809364
1	-2.536349	0.615905	-1.518926
1	-2.070139	-3.383375	0.011438
1	0.148344	-3.584436	-1.163689
1	0.998985	-1.711805	-2.536289
1	-0.320888	0.433487	-2.658807
1	-3.422574	-1.287173	-0.210794
7	-1.086423	0.197529	1.613090
1	-1.231898	1.168940	1.290578
7	1.226700	-0.742517	0.885857
16	2.736097	-1.362685	0.445928
6	3.661238	0.093343	0.020141
6	4.617628	0.578100	0.903550
6	3.392786	0.745935	-1.181684
6	5.315580	1.734406	0.572923
1	4.812445	0.041663	1.829162
6	4.095163	1.898983	-1.493557
1	2.648204	0.340334	-1.864005
6	5.066445	2.408806	-0.623074
1	6.070280	2.121367	1.255548
1	3.896365	2.417588	-2.430398
6	5.832365	3.642880	-0.989833
1	5.171274	4.418136	-1.392902
1	6.362302	4.060917	-0.128548
1	6.579326	3.424770	-1.763300
8	2.539382	-2.154290	-0.762641
8	3.355343	-1.958024	1.624540
6	-3.772139	1.253416	0.735466
8	-3.818391	0.238261	1.468141
8	-2.817715	2.008109	0.462868
6	-5.063692	1.518367	-0.071177
9	-5.222971	2.793025	-0.413529
9	-6.169820	1.114790	0.545732
9	-4.968016	0.804987	-1.223605

1 -2.067500 -0.036796 1.866242

Bn-Ru-NNTs-TS1_AA

Number of imaginary frequencies : 1
The smallest frequencies are : -1637.5529 18.3039 24.4696 cm(-1)

Electronic energy : =-1604.2520514
Zero-point correction= 0.416740
Thermal correction to Energy= 0.444415
Thermal correction to Enthalpy= 0.445359
Thermal correction to Gibbs Free Energy= 0.356871
Sum of electronic and zero-point Energies= -1603.835312
Sum of electronic and thermal Energies= -1603.807636
Sum of electronic and thermal Enthalpies= -1603.806692
Sum of electronic and thermal Free Energies= -1603.895180

Cartesian Coordinates

6 0.148925 -0.428813 2.396920
6 -1.306345 -0.690072 2.694428
44 -1.068104 -0.678379 -0.334342
1 0.785812 -0.836182 3.191168
1 0.317423 0.664454 2.349682
1 -1.640993 -0.171458 3.602284
1 -1.462026 -1.769059 2.816580
6 -2.320901 -2.404234 -0.797171
6 -0.984548 -2.720925 -1.116350
6 -0.241636 -1.877286 -2.001668
6 -0.834671 -0.716740 -2.528331
6 -2.189114 -0.385606 -2.209222
6 -2.922822 -1.225323 -1.348108
1 -2.612009 0.567687 -2.511010
1 -2.860956 -3.004655 -0.068714
1 -0.467811 -3.533669 -0.614942
1 0.812027 -2.087648 -2.148778
1 -0.230438 -0.015044 -3.098913
1 -3.912060 -0.910604 -1.023583
6 -0.286686 1.542029 -0.306113
1 -0.330131 2.231421 0.545837
1 -0.187381 2.106246 -1.241202
1 -1.587680 1.438440 -0.363028
1 0.637020 0.969653 -0.190430
6 -3.213464 2.657519 0.499549
8 -2.842436 1.995472 -0.537837
8 -2.795812 2.451472 1.652470
6 -4.223373 3.751529 0.244478
1 -2.235744 0.804015 1.592777
7 -2.077494 -0.227591 1.521970
7 0.415678 -1.087342 1.125595
16 1.941582 -1.591998 0.867994
6 2.837833 -0.172793 0.252338
6 3.218374 0.824266 1.149700
6 3.043319 -0.006498 -1.112762
6 3.779057 1.997798 0.667458
1 3.082781 0.667165 2.217707
6 3.610415 1.173582 -1.581986
1 2.773643 -0.810082 -1.794030
6 3.976685 2.194335 -0.703563
1 4.076320 2.780755 1.364337
1 3.779552 1.304570 -2.650216
6 4.600727 3.461907 -1.204045
1 4.485532 3.568378 -2.287447
1 4.154621 4.342121 -0.727287
1 5.675102 3.487811 -0.982275
8 1.930543 -2.571313 -0.222254
8 2.554561 -1.944296 2.148197
1 -3.007706 -0.641433 1.528225
1 -5.070388 3.354579 -0.324125
1 -3.764883 4.531093 -0.373269
1 -4.571139 4.187865 1.182929

Bn-Ru-NNTs-TS1_Pivail-acid

Number of imaginary frequencies : 2
The smallest frequencies are : -1622.0871 -36.4481 15.8897 cm(-1)

Electronic energy : =-1722.1038959
Zero-point correction= 0.501226
Thermal correction to Energy= 0.531792
Thermal correction to Enthalpy= 0.532737
Thermal correction to Gibbs Free Energy= 0.438770
Sum of electronic and zero-point Energies= -1721.602670
Sum of electronic and thermal Energies= -1721.572103
Sum of electronic and thermal Enthalpies= -1721.571159
Sum of electronic and thermal Free Energies= -1721.665126

Cartesian Coordinates

6 0.769902 -0.472238 2.403084
6 -0.392715 -1.386831 2.698648

44	-0.120674	-1.314613	-0.329674
1	1.505788	-0.506064	3.215305
1	0.398490	0.567145	2.318687
1	-0.955854	-1.063315	3.583812
1	-0.019651	-2.405562	2.860040
6	-0.443762	-3.424566	-0.789267
6	0.902349	-3.106977	-1.063126
6	1.214637	-2.023651	-1.944712
6	0.180931	-1.260475	-2.514436
6	-1.187573	-1.573051	-2.236750
6	-1.494405	-2.649588	-1.381297
1	-1.984015	-0.915200	-2.571361
1	-0.679798	-4.199221	-0.063213
1	1.711251	-3.598736	-0.531515
1	2.254436	-1.734019	-2.053104
1	0.423442	-0.366096	-3.083847
1	-2.529455	-2.813260	-1.090686
6	-0.454820	1.016747	-0.350210
1	-0.834322	1.630417	0.476661
1	-0.625029	1.529744	-1.304793
1	-1.559782	0.306427	-0.394618
1	0.627069	0.954948	-0.213637
6	-3.514200	0.777882	0.439275
8	-2.917760	0.249415	-0.570885
8	-3.081416	0.723923	1.604759
6	-4.772678	1.592236	0.130250
1	-1.898556	-0.549910	1.548802
7	-1.263381	-1.379479	1.504342
7	1.345792	-0.957156	1.156407
16	2.939095	-0.710896	0.935174
6	3.100654	0.944580	0.278830
6	2.950313	2.027319	1.144357
6	3.252745	1.152422	-1.087718
6	2.924565	3.314727	0.628575
1	2.866099	1.852722	2.214958
6	3.228962	2.448826	-1.590715
1	3.406630	0.298479	-1.743366
6	3.055644	3.545612	-0.745016
1	2.805079	4.163769	1.300688
1	3.354491	2.615983	-2.659961
6	3.047035	4.944412	-1.283455
1	2.884077	4.959096	-2.365934
1	2.263280	5.549179	-0.813712
1	4.001831	5.448766	-1.087799
8	3.408725	-1.614272	-0.119173
8	3.610719	-0.707156	2.234235
1	-1.876076	-2.192387	1.510270
6	-5.611924	0.915295	-0.949005
1	-5.975084	-0.064824	-0.613685
1	-6.488405	1.532843	-1.186079
1	-5.032199	0.766896	-1.865105
6	-5.601822	1.802858	1.390194
1	-5.961217	0.847552	1.791899
1	-5.010797	2.287490	2.173117
1	-6.475616	2.429101	1.166669
6	-4.261572	2.943097	-0.385770
1	-5.105041	3.603181	-0.627578
1	-3.645257	3.440570	0.374521
1	-3.654319	2.810960	-1.289706

Bn-Ru-NNTs-TS1_TCA-Presence

Number of imaginary frequencies : 1
The smallest frequencies are : -1356.1170 14.6780 25.9211 cm(-1)

Electronic energy : =-2982.9259498
Zero-point correction= 0.389313
Thermal correction to Energy= 0.419944
Thermal correction to Enthalpy= 0.420888
Thermal correction to Gibbs Free Energy= 0.325314
Sum of electronic and zero-point Energies= -2982.536637
Sum of electronic and thermal Energies= -2982.506006
Sum of electronic and thermal Enthalpies= -2982.505062
Sum of electronic and thermal Free Energies= -2982.600636

Cartesian Coordinates

6	1.350665	-0.619219	2.410814
6	0.064982	-1.364810	2.664820
44	0.257499	-1.085042	-0.355109
1	2.092501	-0.854007	3.183137
1	1.151712	0.469897	2.451193
1	-0.405106	-1.073736	3.612895
1	0.266229	-2.442762	2.678040
6	-0.392236	-3.103166	-0.893923
6	0.981317	-2.983783	-1.185363
6	1.442464	-1.920662	-2.024291
6	0.529862	-0.985499	-2.542068
6	-0.866261	-1.107116	-2.258804
6	-1.321300	-2.155780	-1.436050
1	-1.563116	-0.336404	-2.572381
1	-0.733605	-3.863282	-0.194769

1	1.714543	-3.615057	-0.692517
1	2.512466	-1.788880	-2.142229
1	0.896329	-0.115679	-3.082391
1	-2.368559	-2.175824	-1.139678
6	0.269769	1.245281	-0.203632
1	-0.002682	1.811747	0.696105
1	0.160971	1.886396	-1.088082
1	-0.977321	0.761986	-0.356116
1	1.338512	1.033884	-0.120931
6	-2.984615	1.019913	0.443018
8	-2.269802	0.835364	-0.590418
8	-2.633511	1.133408	1.611084
6	-4.518750	0.958288	0.140947
1	-1.268079	-0.145575	1.667211
7	-0.832185	-1.069910	1.526036
7	1.807912	-1.053904	1.099740
16	3.415341	-1.008111	0.837261
6	3.779980	0.650059	0.279522
6	3.812472	1.682595	1.215736
6	3.906352	0.925676	-1.077697
6	3.944782	2.993257	0.780546
1	3.745670	1.449335	2.276396
6	4.041804	2.243997	-1.499292
1	3.915001	0.104340	-1.790494
6	4.053993	3.295199	-0.581052
1	3.969083	3.804014	1.507798
1	4.147625	2.463738	-2.561071
6	4.219218	4.714919	-1.031961
1	3.561388	5.390909	-0.474511
1	5.247557	5.062494	-0.870689
1	3.998267	4.828355	-2.098139
8	3.731101	-1.894892	-0.285742
8	4.113108	-1.181278	2.110643
1	-1.611200	-1.726837	1.505013
17	-4.886730	-0.820625	0.095037
17	-4.933222	1.679454	-1.428179
17	-5.474628	1.713733	1.420333

Bn-Ru-NNTs-TS1_TFA

Number of imaginary frequencies : 1
The smallest frequencies are : -1426.8478 19.1891 31.8585 cm(-1)

Electronic energy : =-1901.8954298
Zero-point correction= 0.395316
Thermal correction to Energy= 0.424607
Thermal correction to Enthalpy= 0.425551
Thermal correction to Gibbs Free Energy= 0.333650
Sum of electronic and zero-point Energies= -1901.500114
Sum of electronic and thermal Energies= -1901.470823
Sum of electronic and thermal Enthalpies= -1901.469879
Sum of electronic and thermal Free Energies= -1901.561779

Cartesian Coordinates

6	0.860115	-0.560011	2.405940
6	-0.401825	-1.332261	2.696770
44	-0.219331	-1.157161	-0.333695
1	1.609678	-0.737130	3.186322
1	0.627846	0.522755	2.395856
1	-0.882916	-1.006732	3.627923
1	-0.164640	-2.400602	2.767443
6	-0.791415	-3.211885	-0.828368
6	0.572392	-3.041083	-1.137206
6	0.981074	-1.976155	-2.001113
6	0.025423	-1.088259	-2.524595
6	-1.361448	-1.257230	-2.220086
6	-1.762788	-2.309667	-1.373823
1	-2.090155	-0.516590	-2.534356
1	-1.094237	-3.973919	-0.113834
1	1.336020	-3.632831	-0.641627
1	2.043649	-1.804824	-2.135641
1	0.350902	-0.214319	-3.084255
1	-2.803766	-2.370068	-1.064218
6	-0.262737	1.177238	-0.252211
1	-0.544075	1.767626	0.629020
1	-0.404920	1.777859	-1.159478
1	-1.480388	0.631133	-0.350754
1	0.812101	1.000467	-0.172306
6	-3.441717	1.098699	0.486615
8	-2.797856	0.716427	-0.545291
8	-3.069134	1.106767	1.658146
6	-4.872881	1.555573	0.146167
9	-5.521601	2.013427	1.207553
9	-5.563607	0.518918	-0.347976
9	-4.856735	2.513746	-0.781368
1	-1.801773	-0.223677	1.652772
7	-1.307792	-1.127693	1.544823
7	1.328600	-1.040727	1.114643
16	2.933728	-0.961549	0.845519
6	3.256439	0.692256	0.249884
6	3.268153	1.744765	1.164012

6	3.368189	0.942612	-1.113684
6	3.364130	3.049068	0.700951
1	3.213418	1.532484	2.229701
6	3.467492	2.254777	-1.563287
1	3.393539	0.107142	-1.809430
6	3.457554	3.325129	-0.667202
1	3.371528	3.875175	1.411076
1	3.561377	2.454892	-2.630066
6	3.583329	4.738513	-1.149681
1	3.335794	4.825651	-2.212522
1	2.924821	5.412484	-0.590724
1	4.607883	5.109668	-1.019805
8	3.266116	-1.865794	-0.258585
8	3.639136	-1.088843	2.119952
1	-2.041881	-1.833602	1.544751

Bn-Ru-OO_2-CCl3COOH

Number of imaginary frequencies : 0

The smallest frequencies are : 21.1977 24.9216 35.5505 cm(-1)

Electronic energy : =-3771.2331271

Zero-point correction= 0.237775

Thermal correction to Energy= 0.264424

Thermal correction to Enthalpy= 0.265368

Thermal correction to Gibbs Free Energy= 0.178577

Sum of electronic and zero-point Energies= -3770.995352

Sum of electronic and thermal Energies= -3770.968703

Sum of electronic and thermal Enthalpies= -3770.967759

Sum of electronic and thermal Free Energies= -3771.054551

Cartesian Coordinates

8	-1.030200	-1.304908	1.784501
6	-1.501356	-0.322963	2.667997
6	-2.994886	-0.194695	2.495149
8	-3.286757	0.001075	1.101264
44	-1.803050	-1.056346	-0.101039
1	-1.265709	-0.614090	3.703887
1	-1.017246	0.655314	2.485755
1	-3.421019	0.633690	3.074256
1	-3.493698	-1.128105	2.781975
6	-2.561909	-3.065737	-0.426901
6	-1.155975	-3.046685	-0.642238
6	-0.579202	-2.118828	-1.546213
6	-1.417920	-1.200870	-2.245862
6	-2.817149	-1.212926	-2.058982
6	-3.374702	-2.125173	-1.116904
1	-3.440583	-0.452611	-2.518750
1	-2.992949	-3.705484	0.336653
1	-0.488021	-3.626515	-0.009548
1	0.502271	-2.042436	-1.613786
1	-0.958545	-0.401889	-2.823889
1	-4.423617	-2.030701	-0.846796
6	-1.127468	1.908845	0.021433
8	-0.662079	0.742287	-0.125615
8	-2.263822	2.256630	0.353395
6	-0.063757	3.012295	-0.274169
1	-3.067116	0.948476	0.853985
6	2.029737	-1.579657	0.725748
8	1.665726	-2.675838	0.360493
8	1.420243	-0.766495	1.529296
6	3.312937	-0.946764	0.120754
1	0.445258	-1.083567	1.675733
17	0.383384	2.878109	-2.012101
17	1.363968	2.720982	0.746233
17	-0.699118	4.637230	0.032135
17	4.429164	-2.208297	-0.430238
17	4.145654	0.136845	1.252675
17	2.713429	-0.008157	-1.294546

Bn-Ru-OO-2-mol-CF3COOH

Number of imaginary frequencies : 0

The smallest frequencies are : 10.7910 24.8062 27.0814 cm(-1)

Electronic energy : =-1609.1440215

Zero-point correction= 0.248151

Thermal correction to Energy= 0.273301

Thermal correction to Enthalpy= 0.274245

Thermal correction to Gibbs Free Energy= 0.187364

Sum of electronic and zero-point Energies= -1608.895871

Sum of electronic and thermal Energies= -1608.870721

Sum of electronic and thermal Enthalpies= -1608.869777

Sum of electronic and thermal Free Energies= -1608.956657

Cartesian Coordinates

8	1.044492	-0.617209	1.426153
6	0.433514	-0.011187	2.558988
6	-0.782924	-0.820744	2.909760

8	-1.493117	-1.104461	1.711461
44	-0.260242	-1.422584	0.173301
1	1.154747	0.031184	3.388661
1	0.143831	1.023858	2.304560
1	-1.442066	-0.282694	3.608662
1	-0.486412	-1.768967	3.386965
6	0.440284	-3.072238	-1.033094
6	1.064740	-1.908114	-1.541416
6	0.272928	-0.779230	-1.836487
6	-1.149347	-0.850701	-1.704304
6	-1.781696	-2.057159	-1.308369
6	-0.985824	-3.157362	-0.936495
1	-2.849393	-2.044367	-1.110007
1	1.049483	-3.886852	-0.651052
1	2.144652	-1.799658	-1.531256
1	0.766672	0.161818	-2.059537
1	-1.754482	0.041418	-1.845244
1	-1.443873	-4.030781	-0.482114
6	-4.060526	2.239900	-0.394065
8	-3.969289	-0.147675	-0.456342
6	-3.645122	0.858279	0.132536
8	-2.863846	0.967205	1.171176
6	3.615503	0.730949	-0.188647
8	3.303198	0.501254	1.053639
8	3.011071	0.399428	-1.184600
1	-2.431034	0.064991	1.394284
6	4.936029	1.515591	-0.271167
9	5.247954	1.787659	-1.528573
9	5.924231	0.800400	0.266883
9	4.835892	2.661257	0.400528
1	2.407310	0.008842	1.127721
9	-3.043931	2.706990	-1.134952
9	-5.131417	2.152864	-1.166368
9	-4.300974	3.108460	0.578902

 Bn-Ru-OO-2-mol-CH3COOH

Number of imaginary frequencies : 0
 The smallest frequencies are : 13.9618 21.3613 32.7631 cm(-1)

Electronic energy : =-1013.872848
 Zero-point correction= 0.292500
 Thermal correction to Energy= 0.314562
 Thermal correction to Enthalpy= 0.315507
 Thermal correction to Gibbs Free Energy= 0.236450
 Sum of electronic and zero-point Energies= -1013.580348
 Sum of electronic and thermal Energies= -1013.558286
 Sum of electronic and thermal Enthalpies= -1013.557341
 Sum of electronic and thermal Free Energies= -1013.636398

 Cartesian Coordinates

8	1.260008	-0.909582	-1.066653
6	0.624743	-2.163730	-1.248938
6	-0.746370	-1.916609	-1.815608
8	-1.331653	-0.835753	-1.111391
44	-0.007509	0.524546	-0.550529
1	1.233363	-2.795170	-1.914871
1	0.546526	-2.679980	-0.274471
1	-1.391134	-2.806078	-1.728470
1	-0.672094	-1.659267	-2.886602
6	0.714336	2.512314	-1.005665
6	1.448210	2.058668	0.114701
6	0.753540	1.519121	1.219407
6	-0.676691	1.519065	1.237376
6	-1.410310	2.083161	0.164177
6	-0.718665	2.538203	-0.976013
1	-2.489372	1.964521	0.161373
1	1.234875	2.777553	-1.921666
1	2.525001	1.927394	0.070065
1	1.327417	1.010627	1.988623
1	-1.228387	1.008603	2.021606
1	-1.268719	2.821929	-1.868716
6	-5.230172	-1.355821	1.652533
8	-3.397850	0.174561	1.389471
6	-3.985819	-0.820912	1.005050
8	-3.609215	-1.554995	-0.026185
6	4.023402	-0.819222	0.952494
8	3.587387	-1.547938	-0.058380
8	3.474131	0.187938	1.363210
1	-2.762260	-1.183517	-0.418500
6	5.287378	-1.375124	1.542520
1	2.725696	-1.174089	-0.421481
1	-5.052037	-2.375384	2.008778
1	-5.526339	-0.716242	2.484738
1	-6.037102	-1.413094	0.915369
1	6.061904	-1.434005	0.771433
1	5.626083	-0.746335	2.366755
1	5.113035	-2.396043	1.896531

 Bn-Ru-OO-2-mol-Piv-OH

Number of imaginary frequencies : 0
The smallest frequencies are : 4.2797 6.5314 16.0446 cm(-1)

Electronic energy : =-1249.5757098
Zero-point correction= 0.461818
Thermal correction to Energy= 0.491500
Thermal correction to Enthalpy= 0.492444
Thermal correction to Gibbs Free Energy= 0.394748
Sum of electronic and zero-point Energies= -1249.113892
Sum of electronic and thermal Energies= -1249.084210
Sum of electronic and thermal Enthalpies= -1249.083265
Sum of electronic and thermal Free Energies= -1249.180962

Cartesian Coordinates

8 1.255099 -0.157436 1.531605
6 0.612772 0.843850 2.302013
6 -0.746750 0.333712 2.694717
8 -1.335876 -0.281255 1.562730
44 -0.010925 -1.184508 0.402864
1 1.226886 1.086297 3.183356
1 0.512925 1.763905 1.697333
1 -1.399652 1.144939 3.055437
1 -0.651876 -0.407825 3.507090
6 0.720653 -3.138767 -0.169475
6 1.442213 -2.193453 -0.934458
6 0.735719 -1.189333 -1.632373
6 -0.694609 -1.190294 -1.636949
6 -1.415857 -2.210698 -0.967860
6 -0.712339 -3.157667 -0.197645
1 -2.495094 -2.116622 -0.899095
1 1.251152 -3.811866 0.498256
1 2.519223 -2.094454 -0.839611
1 1.300397 -0.365595 -2.059427
1 -1.255798 -0.365992 -2.067926
1 -1.253006 -3.843460 0.448304
6 -5.290190 1.495400 -0.586529
8 -3.410289 0.058194 -1.111629
6 -4.013633 0.721161 -0.284335
8 -3.636082 0.836033 0.977038
6 4.028418 0.721170 -0.283458
8 3.611014 0.853325 0.963026
8 3.437386 0.068025 -1.127466
1 -2.780999 0.331167 1.129025
6 5.333012 1.462634 -0.545294
1 2.738210 0.371392 1.093145
6 -6.420981 0.916182 0.268847
1 -7.354127 1.455242 0.061207
1 -6.587987 -0.143995 0.040024
1 -6.197901 1.006988 1.336753
6 -5.079930 2.968445 -0.227858
1 -4.262286 3.407329 -0.813442
1 -5.992913 3.535801 -0.449415
1 -4.844998 3.089953 0.834181
6 -5.632425 1.360140 -2.063843
1 -5.777381 0.311088 -2.343409
1 -6.556139 1.910031 -2.283331
1 -4.832097 1.761792 -2.695150
6 5.729030 1.300965 -2.006315
1 5.863591 0.245579 -2.266738
1 4.961633 1.709456 -2.673025
1 6.671428 1.829534 -2.196840
6 6.416822 0.871039 0.360908
1 6.569513 -0.195472 0.152352
1 7.368875 1.387181 0.182967
1 6.154493 0.980970 1.418039
6 5.140888 2.944405 -0.212766
1 6.074392 3.489154 -0.403320
1 4.357651 3.393366 -0.836502
1 4.865688 3.084044 0.837340

Bn-Ru-OO-TS1_CF3COOH

Number of imaginary frequencies : 1
The smallest frequencies are : -1427.0600 14.1377 19.4422 cm(-1)

Electronic energy : =-1649.5930234
Zero-point correction= 0.289833
Thermal correction to Energy= 0.316652
Thermal correction to Enthalpy= 0.317596
Thermal correction to Gibbs Free Energy= 0.228977
Sum of electronic and zero-point Energies= -1649.303191
Sum of electronic and thermal Energies= -1649.276372
Sum of electronic and thermal Enthalpies= -1649.275427
Sum of electronic and thermal Free Energies= -1649.364047

Cartesian Coordinates

8 -1.241463 -0.598135 -1.560473
6 -0.622599 0.074740 -2.629563
6 0.652176 -0.658247 -2.956982

8	1.413556	-0.817001	-1.753756
44	0.116714	-1.055435	-0.022321
1	-1.296138	0.090563	-3.499778
1	-0.393747	1.123673	-2.367986
1	1.259494	-0.134146	-3.704550
1	0.426084	-1.667750	-3.322953
6	-0.485243	-3.167119	0.101986
6	-1.356523	-2.358151	0.887281
6	-0.839832	-1.486898	1.876391
6	0.571854	-1.415222	2.081497
6	1.447864	-2.198044	1.300203
6	0.911768	-3.056713	0.293953
1	2.519796	-2.044396	1.377166
1	-0.880917	-3.753897	-0.721216
1	-2.414747	-2.278953	0.648947
1	-1.520472	-0.804199	2.376386
1	0.987575	-0.665203	2.749851
1	1.590009	-3.549431	-0.398186
6	0.150101	1.233195	0.325266
1	0.585688	1.974837	-0.356191
1	0.143109	1.634587	1.345182
1	1.336924	0.627049	0.477883
1	-0.894508	1.124967	0.022382
6	3.389060	1.047488	-0.080869
8	2.618242	0.681120	0.857393
8	3.178928	1.017219	-1.299285
6	4.740498	1.584439	0.424097
9	5.551302	1.916129	-0.569362
9	5.345110	0.652479	1.166576
9	4.546226	2.659503	1.188451
1	2.062954	-0.055462	-1.639859
6	-3.714275	0.565599	0.116536
8	-3.445424	-0.264863	0.968215
8	-3.148148	0.758700	-1.022900
6	-4.853691	1.574875	0.348499
9	-5.469396	1.358651	1.503085
9	-5.756183	1.496289	-0.629900
9	-4.364019	2.817556	0.361139
1	-2.276357	0.055487	-1.228166

Bn-Ru-OO-TS1_CC13COOH

Number of imaginary frequencies : 1
The smallest frequencies are : -1424.5902 17.3399 20.6723 cm(-1)

Electronic energy : =-3811.6531422
Zero-point correction= 0.278614
Thermal correction to Energy= 0.307674
Thermal correction to Enthalpy= 0.308618
Thermal correction to Gibbs Free Energy= 0.215427
Sum of electronic and zero-point Energies= -3811.374529
Sum of electronic and thermal Energies= -3811.345468
Sum of electronic and thermal Enthalpies= -3811.344524
Sum of electronic and thermal Free Energies= -3811.437715

Cartesian Coordinates

8	1.268269	-1.640816	1.324043
6	0.642632	-1.628533	2.585619
6	-0.691196	-2.311719	2.427843
8	-1.381020	-1.733167	1.315029
44	-0.027432	-1.017484	-0.230856
1	1.265649	-2.165713	3.315634
1	0.505124	-0.598394	2.955446
1	-1.312816	-2.233083	3.326982
1	-0.543772	-3.372381	2.188487
6	0.093713	-2.803304	-1.514105
6	1.287128	-2.052904	-1.629673
6	1.251055	-0.666792	-1.957136
6	-0.002634	-0.037213	-2.180576
6	-1.209556	-0.771679	-2.079693
6	-1.151919	-2.138929	-1.699233
1	-2.165912	-0.261438	-2.142768
1	0.122555	-3.831115	-1.165834
1	2.243364	-2.469141	-1.320375
1	2.176227	-0.096948	-1.947947
1	-0.046279	1.041317	-2.318608
1	-2.078213	-2.657745	-1.461717
6	0.033889	1.037778	0.825207
1	-0.376107	1.177710	1.832721
1	0.053569	2.004656	0.306995
1	-1.145982	0.784258	0.254065
1	1.087621	0.761820	0.940967
6	-3.302500	0.733244	0.594820
8	-2.366334	1.153903	-0.141379
8	-3.234787	0.036659	1.610432
6	-4.725850	1.071293	0.051256
1	-2.043508	-1.033410	1.587255
6	3.876744	-0.242123	0.302495
8	3.904717	-1.098652	-0.563400
8	3.164994	-0.196038	1.363978
6	4.713580	1.061128	0.088760

1	2.275585	-0.992604	1.344494
17	-5.031317	-0.217154	-1.187175
17	-4.784795	2.662787	-0.729647
17	-5.958374	0.973907	1.313658
17	6.061926	0.791414	-1.025485
17	5.316109	1.746506	1.608895
17	3.540727	2.221064	-0.668554

 Bn-Ru-OO-TS1_CH3COOH

Number of imaginary frequencies : 1
 The smallest frequencies are : -1579.2215 25.7063 33.8807 cm(-1)

Electronic energy : =-1054.3154579
 Zero-point correction= 0.335407
 Thermal correction to Energy= 0.358839
 Thermal correction to Enthalpy= 0.359783
 Thermal correction to Gibbs Free Energy= 0.281048
 Sum of electronic and zero-point Energies= -1053.980051
 Sum of electronic and thermal Energies= -1053.956619
 Sum of electronic and thermal Enthalpies= -1053.955675
 Sum of electronic and thermal Free Energies= -1054.034410

 Cartesian Coordinates

8	-1.113031	-0.611780	1.347284
6	-0.404905	-1.676445	1.908231
6	0.863191	-1.136214	2.524897
8	1.531903	-0.335346	1.547635
44	0.109600	0.596589	0.204300
1	-1.022204	-2.177230	2.672656
1	-0.136489	-2.442320	1.153871
1	1.541530	-1.929850	2.864975
1	0.623563	-0.480361	3.372604
6	-0.538991	2.463298	1.136515
6	-1.462250	2.077471	0.122635
6	-1.018720	1.809635	-1.195072
6	0.371313	1.930992	-1.507679
6	1.299749	2.311602	-0.516925
6	0.840226	2.539988	0.813500
1	2.362755	2.272126	-0.731942
1	-0.867645	2.560679	2.166494
1	-2.491764	1.831991	0.369364
1	-1.727692	1.402753	-1.910079
1	0.738471	1.608300	-2.478881
1	1.568698	2.675305	1.609071
6	0.217495	-1.245805	-1.235879
1	0.707245	-2.210853	-1.056035
1	0.132740	-1.072155	-2.314676
1	1.364309	-0.601821	-1.073656
1	-0.796521	-1.344798	-0.838666
6	3.466056	-1.165938	-0.836596
8	2.655257	-0.393704	-1.450904
8	3.245437	-1.684037	0.281382
6	4.765800	-1.458598	-1.540218
1	2.208424	-0.913488	1.030904
6	-3.846740	-0.972093	-0.638836
8	-3.575236	0.185582	-0.907558
8	-3.190899	-1.705847	0.241444
6	-4.972801	-1.731100	-1.279401
1	-2.431754	-1.178053	0.657297
1	5.251103	-0.519460	-1.823674
1	4.561458	-2.002531	-2.468217
1	5.430030	-2.048565	-0.906178
1	-5.503188	-1.092793	-1.987059
1	-5.661359	-2.093053	-0.509558
1	-4.578087	-2.613435	-1.793114

 Bn-Ru-OO-TS1_Pivalicacid

Number of imaginary frequencies : 1
 The smallest frequencies are : -1561.0674 18.3766 21.0558 cm(-1)

Electronic energy : =-1290.0190569
 Zero-point correction= 0.504669
 Thermal correction to Energy= 0.535518
 Thermal correction to Enthalpy= 0.536462
 Thermal correction to Gibbs Free Energy= 0.442297
 Sum of electronic and zero-point Energies= -1289.514388
 Sum of electronic and thermal Energies= -1289.483539
 Sum of electronic and thermal Enthalpies= -1289.482595
 Sum of electronic and thermal Free Energies= -1289.576759

 Cartesian Coordinates

8	1.116400	-0.898128	1.615966
6	0.390907	-0.312974	2.656155
6	-0.893279	-1.085977	2.838676
8	-1.537287	-1.195543	1.566468
44	-0.075232	-1.240354	-0.035216
1	0.985021	-0.329625	3.585052

1	0.143338	0.746774	2.446455
1	-1.579778	-0.605738	3.548466
1	-0.677049	-2.106583	3.181354
6	0.570409	-3.311696	-0.290249
6	1.505485	-2.428751	-0.904244
6	1.076475	-1.472393	-1.856262
6	-0.309019	-1.396281	-2.203451
6	-1.247836	-2.260194	-1.603246
6	-0.803683	-3.193319	-0.620205
1	-2.308428	-2.104708	-1.773361
1	0.886020	-3.965187	0.517020
1	2.529502	-2.362304	-0.545698
1	1.791525	-0.736752	-2.214256
1	-0.665674	-0.587117	-2.836077
1	-1.541318	-3.747259	-0.044894
6	-0.147839	1.096753	-0.222328
1	-0.655064	1.822260	0.427494
1	-0.028918	1.526307	-1.224139
1	-1.302607	0.474564	-0.448536
1	0.850449	0.968854	0.204333
6	-3.350030	0.954854	0.057383
8	-2.581652	0.543029	-0.878041
8	-3.153302	0.727475	1.273201
6	-4.512620	1.856321	-0.352896
1	-2.186960	-0.408243	1.450532
6	3.710844	0.655881	0.091496
8	3.601336	-0.290043	-0.672119
8	3.070750	0.747912	1.243647
6	4.536735	1.893125	-0.232879
1	2.403307	-0.010192	1.352443
6	-5.106825	1.404162	-1.683315
1	-5.534858	0.396672	-1.605320
1	-5.911528	2.087606	-1.984065
1	-4.347921	1.390075	-2.471332
6	-3.900685	3.254501	-0.509827
1	-4.673907	3.974411	-0.807973
1	-3.462556	3.596303	0.436779
1	-3.114936	3.253793	-1.275328
6	-5.587726	1.881988	0.725971
1	-6.021163	0.885965	0.877492
1	-5.177854	2.213915	1.684555
1	-6.396188	2.564308	0.432838
6	5.547347	1.563998	-1.324075
1	6.260963	0.802883	-0.987121
1	5.050696	1.178179	-2.219768
1	6.110649	2.465746	-1.594807
6	5.248526	2.429929	1.006483
1	5.947571	1.690364	1.415845
1	5.824603	3.325584	0.740874
1	4.537092	2.695710	1.793828
6	3.536278	2.936172	-0.749244
1	4.066486	3.853984	-1.033709
1	3.004065	2.562487	-1.634337
1	2.794886	3.188333	0.018233

 Bn-Ru-PP_2-TFA

Number of imaginary frequencies : 0
 The smallest frequencies are : 14.3095 30.5920 33.6101 cm(-1)

Electronic energy : =-2142.649301
 Zero-point correction= 0.259098
 Thermal correction to Energy= 0.285478
 Thermal correction to Enthalpy= 0.286423
 Thermal correction to Gibbs Free Energy= 0.199756
 Sum of electronic and zero-point Energies= -2142.390203
 Sum of electronic and thermal Energies= -2142.363823
 Sum of electronic and thermal Enthalpies= -2142.362878
 Sum of electronic and thermal Free Energies= -2142.449544

 Cartesian Coordinates

6	-1.413813	-0.836323	-2.849773
6	-2.860463	-1.087716	-2.455417
44	-1.496563	0.643662	0.214372
1	-1.302886	-0.768319	-3.938503
1	-0.772387	-1.659729	-2.506219
1	-3.252602	-2.051126	-2.804534
1	-3.508509	-0.289984	-2.842241
6	-2.171664	2.719391	0.244168
6	-0.786633	2.740046	0.596854
6	-0.332864	1.929626	1.649725
6	-1.249968	1.145916	2.420711
6	-2.618282	1.169301	2.121020
6	-3.075957	1.931225	0.999499
1	-3.306271	0.532759	2.670219
1	-2.527544	3.278450	-0.616847
1	-0.059612	3.272340	-0.010036
1	0.736609	1.846919	1.818183
1	-0.876291	0.463849	3.177214
1	-4.123316	1.892786	0.709592
6	-0.089182	-1.834310	1.037934

8	-0.053145	-0.908239	0.148211
8	-0.773836	-1.926099	2.042811
6	0.846870	-2.989470	0.631773
1	-2.545141	-2.301929	-0.231730
6	2.809953	1.236599	-0.580993
8	2.157234	2.094442	-0.036478
8	2.466712	0.492443	-1.602266
6	4.230052	0.873283	-0.116322
1	1.516525	0.675727	-1.843856
15	-0.721517	0.725031	-2.068515
15	-2.895582	-0.985229	-0.614864
1	-4.270119	-0.999943	-0.275428
1	-1.624930	1.635111	-2.704910
9	0.332433	-3.587642	-0.458398
9	2.067011	-2.557905	0.320521
9	0.957808	-3.904778	1.584152
9	5.091053	0.968309	-1.127574
9	4.623844	1.685851	0.853207
9	4.252042	-0.376154	0.339659

 Bn-Ru-PP_2-CCl3COOH

Number of imaginary frequencies : 0
 The smallest frequencies are : 27.7992 40.8561 45.6900 cm(-1)

Electronic energy : =-4304.6832143
 Zero-point correction= 0.248084
 Thermal correction to Energy= 0.276734
 Thermal correction to Enthalpy= 0.277678
 Thermal correction to Gibbs Free Energy= 0.187487
 Sum of electronic and zero-point Energies= -4304.435131
 Sum of electronic and thermal Energies= -4304.406481
 Sum of electronic and thermal Enthalpies= -4304.405536
 Sum of electronic and thermal Free Energies= -4304.495727

 Cartesian Coordinates

6	-2.692975	-0.417220	-2.711198
6	-4.019681	-0.120908	-2.038153
44	-1.871843	0.939558	0.373881
1	-2.711156	-0.215931	-3.789237
1	-2.432243	-1.478996	-2.588289
1	-4.828792	-0.767362	-2.404826
1	-4.309729	0.925724	-2.208930
6	-2.605544	2.943964	0.246157
6	-1.182533	3.023210	0.142920
6	-0.359782	2.489532	1.157163
6	-0.961822	1.827419	2.258480
6	-2.366731	1.802033	2.430054
6	-3.184269	2.333514	1.399786
1	-2.811367	1.295684	3.280744
1	-3.241251	3.327457	-0.547636
1	-0.717536	3.438016	-0.748484
1	0.718759	2.502794	1.038322
1	-0.326022	1.305924	2.970982
1	-4.265905	2.246599	1.469545
6	-0.761720	-2.125730	0.494818
8	-0.629264	-0.930236	0.704411
8	-1.857474	-2.773867	0.259871
6	0.490621	-3.029341	0.404743
1	-2.648155	-2.131637	0.191687
6	2.212820	1.254913	-1.017988
8	1.675438	2.319564	-1.197893
8	1.759627	0.070219	-1.331347
6	3.566070	1.166954	-0.258042
1	0.827413	0.169183	-1.694757
15	-1.314005	0.588752	-1.935035
15	-3.726661	-0.414183	-0.217910
1	-4.906719	0.153764	0.342527
1	-1.664525	1.841392	-2.524602
17	0.169562	-4.643049	1.077109
17	0.826641	-3.152599	-1.353098
17	1.859785	-2.291950	1.236767
17	4.537418	-0.235493	-0.736092
17	3.107868	1.023641	1.482604
17	4.492548	2.655499	-0.500018

 Bn-Ru-PP_2-CH3COOH

Number of imaginary frequencies : 0
 The smallest frequencies are : 34.4025 41.2384 59.0800 cm(-1)

Electronic energy : =-1547.3705521
 Zero-point correction= 0.304418
 Thermal correction to Energy= 0.326783
 Thermal correction to Enthalpy= 0.327727
 Thermal correction to Gibbs Free Energy= 0.253027
 Sum of electronic and zero-point Energies= -1547.066134
 Sum of electronic and thermal Energies= -1547.043769
 Sum of electronic and thermal Enthalpies= -1547.042825
 Sum of electronic and thermal Free Energies= -1547.117526

 Cartesian Coordinates

6	-0.710518	2.499527	1.570595
6	-2.043730	2.620820	0.853892
44	-0.775668	-0.505045	-0.141326
1	-0.745204	2.996589	2.548498
1	0.074242	2.979690	0.979290
1	-2.195715	3.609776	0.405622
1	-2.871028	2.429639	1.549856
6	-1.504874	-2.156545	1.079880
6	-0.135785	-2.452470	0.787561
6	0.291928	-2.448560	-0.548475
6	-0.631772	-2.234519	-1.620376
6	-1.985889	-1.996278	-1.335510
6	-2.423753	-1.937012	0.025617
1	-2.686574	-1.786767	-2.139694
1	-1.839240	-2.077636	2.111068
1	0.604115	-2.542150	1.577130
1	1.358625	-2.514582	-0.745438
1	-0.270924	-2.183516	-2.642976
1	-3.456548	-1.684280	0.253100
6	0.935691	1.689439	-1.358729
8	0.913731	0.459315	-0.979136
8	-0.011186	2.482424	-1.299346
6	2.279971	2.139277	-1.883964
1	-2.343060	1.972236	-1.688046
6	3.321059	-0.583481	0.680823
8	2.757197	-1.613631	0.988048
8	3.035257	0.604906	1.209330
6	4.403295	-0.497947	-0.351355
1	2.201653	0.513596	1.729913
1	2.635092	1.455198	-2.661861
1	3.002679	2.108703	-1.059408
1	2.218026	3.154157	-2.281181
1	4.916494	-1.457598	-0.434803
1	5.110830	0.304902	-0.129641
1	3.924259	-0.271371	-1.311704
15	-0.163391	0.724213	1.851753
15	-2.175304	1.315688	-0.455588
1	-3.536971	0.917214	-0.286570
1	-1.224678	0.382034	2.751823

 Bn-Ru-PP-TS1_CCI3COOH

Number of imaginary frequencies : 1
 The smallest frequencies are : -426.1042 16.7834 21.9958 cm(-1)

Electronic energy : =-4345.1217598
 Zero-point correction= 0.292220
 Thermal correction to Energy= 0.323751
 Thermal correction to Enthalpy= 0.324695
 Thermal correction to Gibbs Free Energy= 0.225566
 Sum of electronic and zero-point Energies= -4344.829540
 Sum of electronic and thermal Energies= -4344.798009
 Sum of electronic and thermal Enthalpies= -4344.797064
 Sum of electronic and thermal Free Energies= -4344.896194

 Cartesian Coordinates

6	0.303410	3.475389	-1.785268
6	-0.828762	4.058703	-0.969382
44	-0.198288	0.886019	0.386341
1	0.940357	4.248537	-2.234720
1	-0.081326	2.857469	-2.609615
1	-1.529193	4.643656	-1.580458
1	-0.426661	4.721969	-0.193547
6	-0.007808	1.500942	2.566067
6	1.214709	0.861992	2.271200
6	1.206241	-0.417661	1.687877
6	-0.028020	-1.097284	1.480660
6	-1.243995	-0.528480	1.916538
6	-1.238257	0.792584	2.401596
1	-2.188987	-1.048149	1.781909
1	-0.017120	2.526292	2.926376
1	2.161806	1.384965	2.378828
1	2.144013	-0.872035	1.379133
1	-0.027006	-2.071607	0.996063
1	-2.184403	1.273691	2.635178
6	0.250900	-0.216867	-1.466217
1	0.209708	0.366851	-2.391707
1	-0.357956	-1.118853	-1.599322
1	-1.128752	0.511927	-0.833428
1	1.291462	-0.520392	-1.301502
6	-4.223497	-0.010479	-0.045940
8	-4.072132	0.363248	1.090588
8	-3.988809	0.664034	-1.141748
6	-4.663173	-1.463931	-0.370584
1	-3.485815	1.502849	-0.897526
6	4.192978	0.127621	-0.202784
8	3.985066	0.675091	0.852011
8	3.789368	0.505482	-1.387072

6	4.940811	-1.232067	-0.278212
1	3.128406	1.261876	-1.274690
15	1.343807	2.366425	-0.703864
15	-1.776779	2.649430	-0.165255
1	-1.984768	3.246339	1.114613
1	1.571369	3.336820	0.323288
17	-5.877134	-1.503045	-1.661952
17	-3.166051	-2.310915	-0.910645
17	-5.292406	-2.255746	1.080706
17	6.126751	-1.243141	-1.596403
17	3.664520	-2.467232	-0.591409
17	5.733908	-1.587007	1.260610

 Bn-Ru-PP-TS1_CH3COOH

Number of imaginary frequencies : 1
 The smallest frequencies are : -486.5685 20.3420 29.9801 cm(-1)

Electronic energy : =-1587.7891012
 Zero-point correction= 0.347947
 Thermal correction to Energy= 0.374098
 Thermal correction to Enthalpy= 0.375042
 Thermal correction to Gibbs Free Energy= 0.288435
 Sum of electronic and zero-point Energies= -1587.441155
 Sum of electronic and thermal Energies= -1587.415003
 Sum of electronic and thermal Enthalpies= -1587.414059
 Sum of electronic and thermal Free Energies= -1587.500666

 Cartesian Coordinates

6	0.163149	1.649275	-2.796447
6	-0.956541	2.460364	-2.178216
44	-0.142829	0.471094	0.449270
1	0.774322	2.229838	-3.499320
1	-0.246393	0.794932	-3.355462
1	-1.662022	2.847009	-2.927813
1	-0.545520	3.312651	-1.619278
6	0.810778	2.167723	1.681673
6	1.637626	1.007046	1.812302
6	1.093199	-0.194167	2.290374
6	-0.301403	-0.279192	2.539254
6	-1.125031	0.876590	2.419757
6	-0.547515	2.110888	2.035129
1	-2.195576	0.796933	2.588197
1	1.231116	3.091967	1.294274
1	2.679287	1.023940	1.502518
1	1.725843	-1.076475	2.334187
1	-0.754450	-1.232684	2.799212
1	-1.176933	2.988633	1.910967
6	0.023979	-1.507663	-0.467480
1	-0.294620	-1.532427	-1.516695
1	-0.499752	-2.305495	0.076246
1	-1.281953	-0.560413	0.114049
1	1.100860	-1.701602	-0.411092
6	-3.719260	-1.956089	-0.202132
8	-3.247169	-1.429764	0.787481
8	-3.641690	-1.447176	-1.427140
6	-4.454475	-3.263267	-0.193671
1	-3.165714	-0.575514	-1.399650
6	4.071720	-1.530528	-0.374740
8	3.526709	-1.059868	0.605751
8	3.741870	-1.232560	-1.624343
6	5.196433	-2.521580	-0.319777
1	2.997867	-0.571762	-1.621429
1	-3.924208	-3.987228	-0.820537
1	-5.450400	-3.133727	-0.627967
1	-4.533983	-3.641168	0.826196
1	6.067377	-2.124467	-0.850232
1	4.902773	-3.442263	-0.833654
1	5.454838	-2.738000	0.717401
15	1.284045	0.955877	-1.462731
15	-1.855817	1.282609	-1.031761
1	-2.514672	2.234583	-0.191772
1	1.779260	2.235861	-1.049006

 Bn-Ru-PP-TS1_TFA

Number of imaginary frequencies : 1
 The smallest frequencies are : -486.0042 14.7983 25.8319 cm(-1)

Electronic energy : =-2183.0590881
 Zero-point correction= 0.304250
 Thermal correction to Energy= 0.333425
 Thermal correction to Enthalpy= 0.334369
 Thermal correction to Gibbs Free Energy= 0.239763
 Sum of electronic and zero-point Energies= -2182.754838
 Sum of electronic and thermal Energies= -2182.725663
 Sum of electronic and thermal Enthalpies= -2182.724719
 Sum of electronic and thermal Free Energies= -2182.819325

 Cartesian Coordinates

6	0.094160	-1.900662	2.945217
6	-1.034157	-2.804488	2.494237
44	-0.311477	-1.141452	-0.408590
1	0.723913	-2.359342	3.717979
1	-0.303701	-0.965918	3.366761
1	-1.722067	-3.059679	3.312497
1	-0.631306	-3.738800	2.080329
6	0.676058	-2.906958	-1.539441
6	1.422969	-1.719560	-1.818906
6	0.781177	-0.604183	-2.380794
6	-0.624710	-0.619981	-2.560366
6	-1.371376	-1.796015	-2.267455
6	-0.699472	-2.957220	-1.808884
1	-2.451778	-1.793227	-2.383547
1	1.172764	-3.767081	-1.098701
1	2.480896	-1.655135	-1.579194
1	1.353042	0.303214	-2.556821
1	-1.146169	0.274900	-2.890671
1	-1.266869	-3.852685	-1.568222
6	-0.097716	0.915478	0.306665
1	-0.377176	1.052297	1.357940
1	-0.633784	1.660901	-0.296319
1	-1.430875	-0.089387	-0.107175
1	0.975646	1.096248	0.192132
6	-3.723521	1.254345	0.091890
8	-3.508330	0.592750	-0.895491
8	-3.625237	0.885106	1.346750
6	-4.111478	2.739346	0.008772
1	-3.266699	-0.051039	1.408255
6	3.872220	0.910194	0.179154
8	3.347660	0.423829	-0.795080
8	3.597179	0.682960	1.438135
6	5.009219	1.939625	0.062765
1	2.848406	0.013824	1.513650
15	1.173756	-1.439861	1.487755
15	-1.971368	-1.848343	1.185974
1	-2.589423	-2.932637	0.491487
1	1.624787	-2.775431	1.236980
9	-4.343738	3.092419	-1.245503
9	-5.195119	2.995073	0.734728
9	-3.103848	3.477265	0.478767
9	4.648007	3.085693	0.635908
9	6.102358	1.489285	0.675209
9	5.298909	2.172407	-1.207660

Role of Lewis Acids (Tables S4-S5)

AlMe3

Number of imaginary frequencies : 2
The smallest frequencies are : -16.4864 -4.8940 31.1108 cm(-1)

Electronic energy : =-362.0560365
Zero-point correction= 0.105570
Thermal correction to Energy= 0.112569
Thermal correction to Enthalpy= 0.113513
Thermal correction to Gibbs Free Energy= 0.074517
Sum of electronic and zero-point Energies= -361.950467
Sum of electronic and thermal Energies= -361.943468
Sum of electronic and thermal Enthalpies= -361.942523
Sum of electronic and thermal Free Energies= -361.981519

Cartesian Coordinates

13	0.000011	-0.000054	-0.000058
6	1.736290	-0.910361	0.000057
1	2.589989	-0.224007	0.001629
1	1.838167	-1.566024	0.874790
1	1.839406	-1.563258	-0.876616
6	-0.079697	1.958804	-0.000100
1	0.442537	2.375326	-0.871395
1	-1.100887	2.355044	-0.007424
1	0.428861	2.373994	0.879941
6	-1.656606	-1.048385	0.000070
1	-2.276126	-0.807476	0.873901
1	-2.272746	-0.812320	-0.877489
1	-1.489264	-2.130921	0.003254

BPh3

Number of imaginary frequencies : 0
The smallest frequencies are : 41.4446 44.2959 64.1652 cm(-1)

Electronic energy : =-719.2538928
Zero-point correction= 0.276365
Thermal correction to Energy= 0.291550
Thermal correction to Enthalpy= 0.292494
Thermal correction to Gibbs Free Energy= 0.232512
Sum of electronic and zero-point Energies= -718.977528
Sum of electronic and thermal Energies= -718.962343
Sum of electronic and thermal Enthalpies= -718.961399
Sum of electronic and thermal Free Energies= -719.021381

Cartesian Coordinates

5	-0.000495	-0.000382	0.000851
6	-0.134036	1.557067	-0.000043
6	0.816498	2.374364	0.637069
6	-1.209669	2.201237	-0.636736
6	0.694356	3.758501	0.652475
1	1.661280	1.907348	1.142120
6	-1.325103	3.585925	-0.650440
1	-1.962677	1.597906	-1.142529
6	-0.375000	4.367145	0.001378
1	1.435964	4.365437	1.167563
1	-2.159282	4.058263	-1.164945
1	-0.468045	5.451291	0.001910
6	1.415448	-0.662710	0.000763
6	2.509007	-0.054381	-0.640808
6	1.650757	-1.892039	0.641529
6	3.766123	-0.646212	-0.656889
1	2.360955	0.897947	-1.148726
6	2.910991	-2.477261	0.655190
1	0.825886	-2.389226	1.150682
6	3.970402	-1.857195	-0.001452
1	4.590333	-0.161172	-1.175557
1	3.068125	-3.420994	1.173218
1	4.956084	-2.318060	-0.002080
6	-1.282141	-0.895010	0.000172
6	-2.467005	-0.479409	0.633100
6	-1.300033	-2.150275	-0.633527
6	-3.604439	-1.277432	0.647276
1	-2.486678	0.486972	1.135657
6	-2.441238	-2.942829	-0.648561
1	-0.399595	-2.501531	-1.136093
6	-3.594738	-2.509430	-0.000883
1	-4.502321	-0.937813	1.159229
1	-2.431755	-3.902451	-1.161092
1	-4.486878	-3.132362	-0.001289

LiClO4

Number of imaginary frequencies : 0
The smallest frequencies are : 144.1000 387.0180 393.3788 cm(-1)

Electronic energy : =-768.1759106
Zero-point correction= 0.018419
Thermal correction to Energy= 0.023586
Thermal correction to Enthalpy= 0.024530
Thermal correction to Gibbs Free Energy= -0.010342
Sum of electronic and zero-point Energies= -768.157492
Sum of electronic and thermal Energies= -768.152325
Sum of electronic and thermal Enthalpies= -768.151380
Sum of electronic and thermal Free Energies= -768.186253

Cartesian Coordinates

3	-2.251518	0.000604	-0.000174
8	-0.767293	-0.000498	-1.178741
8	-0.766890	0.000200	1.179135
17	0.191626	-0.000039	-0.000003
8	0.985588	-1.211644	0.000178
8	0.985707	1.211799	-0.000501

SiMe3Cl

Number of imaginary frequencies : 0
The smallest frequencies are : 143.7972 152.8410 153.3734 cm(-1)

Electronic energy : =-869.3574273
Zero-point correction= 0.111919
Thermal correction to Energy= 0.120741
Thermal correction to Enthalpy= 0.121685
Thermal correction to Gibbs Free Energy= 0.078977
Sum of electronic and zero-point Energies= -869.245508
Sum of electronic and thermal Energies= -869.236687
Sum of electronic and thermal Enthalpies= -869.235742
Sum of electronic and thermal Free Energies= -869.278450

Cartesian Coordinates

14	-0.343442	0.000024	0.000018
6	-0.888716	1.732907	-0.432941
1	-1.983182	1.801857	-0.448810
1	-0.512843	2.455778	0.299034
1	-0.515054	2.025703	-1.419993
6	-0.889455	-1.241352	-1.283946
1	-0.515261	-0.968335	-2.276448
1	-0.514711	-2.242346	-1.044766
1	-1.983962	-1.290361	-1.334160
6	-0.888669	-0.491231	1.717264
1	-0.514697	-1.487465	1.976668
1	-0.513041	0.216076	2.464408
1	-1.983136	-0.509727	1.785570
17	1.755595	-0.000203	-0.000236

TiCl4

Number of imaginary frequencies : 0
The smallest frequencies are : 119.2499 119.4690 140.5926 cm(-1)

Electronic energy : =-1899.2327728
Zero-point correction= 0.005947
Thermal correction to Energy= 0.013100
Thermal correction to Enthalpy= 0.014044
Thermal correction to Gibbs Free Energy= -0.028102
Sum of electronic and zero-point Energies= -1899.226825
Sum of electronic and thermal Energies= -1899.219673
Sum of electronic and thermal Enthalpies= -1899.218729
Sum of electronic and thermal Free Energies= -1899.260875

Cartesian Coordinates

17	1.586766	-1.460045	-0.016566
17	-0.679093	0.346469	-2.016738
22	0.000062	-0.000077	0.000118
17	-1.639092	-0.733014	1.193954
17	0.731338	1.846690	0.839196

ZnCl2

Number of imaginary frequencies : 0
The smallest frequencies are : 107.4240 367.2329 526.5555 cm(-1)

Electronic energy : =-1147.6122886
Zero-point correction= 0.002281
Thermal correction to Energy= 0.006382
Thermal correction to Enthalpy= 0.007326
Thermal correction to Gibbs Free Energy= -0.020566

Sum of electronic and zero-point Energies= -1147.610008
Sum of electronic and thermal Energies= -1147.605907
Sum of electronic and thermal Enthalpies= -1147.604963
Sum of electronic and thermal Free Energies= -1147.632854

Cartesian Coordinates

30 -0.000000 0.000655 -0.000000
17 2.073579 0.080517 -0.000000
17 -2.073579 -0.081674 0.000000

Bn-Ru-PP-Presence-C-C_bond formation-TS3_LiCl

Number of imaginary frequencies : 1
The smallest frequencies are : -352.7875 39.0493 55.9635 cm(-1)

Electronic energy : =-1786.1239373
Zero-point correction= 0.240232
Thermal correction to Energy= 0.260167
Thermal correction to Enthalpy= 0.261111
Thermal correction to Gibbs Free Energy= 0.192564
Sum of electronic and zero-point Energies= -1785.883705
Sum of electronic and thermal Energies= -1785.863771
Sum of electronic and thermal Enthalpies= -1785.862827
Sum of electronic and thermal Free Energies= -1785.931373

Cartesian Coordinates

6 2.285573 -2.340860 0.084974
6 1.156331 -2.854628 -0.800314
44 0.433109 0.494999 0.066132
1 3.203507 -2.920973 -0.070406
1 1.995331 -2.455733 1.134404
1 0.617990 -3.686405 -0.336291
1 1.520429 -3.185735 -1.779237
6 0.554011 1.761376 -1.761224
6 1.368353 2.413389 -0.800038
6 0.836231 2.748384 0.457344
6 -0.527684 2.456217 0.741573
6 -1.382835 1.928671 -0.249218
6 -0.826382 1.537354 -1.482825
1 -2.413639 1.659519 -0.029509
1 0.987626 1.429104 -2.701435
1 2.424597 2.569366 -1.007669
1 1.476265 3.171061 1.226938
1 -0.916434 2.613641 1.743987
1 -1.466801 1.025502 -2.200074
6 0.894051 -0.087520 2.264420
1 1.456939 -1.017242 2.314415
1 0.289318 0.012443 3.169705
1 1.572457 0.771312 2.284125
8 -1.769800 0.101333 2.045490
6 -0.855357 -0.625025 1.609990
8 -0.883412 -1.860557 1.455013
1 -1.352343 -1.965980 -1.070460
15 2.627842 -0.529389 -0.313809
15 -0.036145 -1.467079 -1.085409
1 3.280504 -0.224604 0.920605
1 0.112698 -1.230220 -2.478037
3 -2.971341 -1.178558 1.175567
17 -3.623220 -0.730156 -0.880084

Bn-Ru-PP-Presence-C-C_bond formation-TS3_BPh3

Number of imaginary frequencies : 1
The smallest frequencies are : -352.2491 22.4014 35.9744 cm(-1)

Electronic energy : =-2037.5810912
Zero-point correction= 0.514868
Thermal correction to Energy= 0.547450
Thermal correction to Enthalpy= 0.548394
Thermal correction to Gibbs Free Energy= 0.452134
Sum of electronic and zero-point Energies= -2037.066224
Sum of electronic and thermal Energies= -2037.033642
Sum of electronic and thermal Enthalpies= -2037.032697
Sum of electronic and thermal Free Energies= -2037.128957

Cartesian Coordinates

6 -3.440362 -2.533473 -1.032241
6 -3.033265 -2.825309 0.403979
44 -2.151763 0.496932 -0.365323
1 -4.220520 -3.227265 -1.368931
1 -2.567008 -2.654924 -1.682279
1 -2.378459 -3.698578 0.484242
1 -3.907424 -2.990910 1.044460
6 -3.226204 1.807711 1.083756
6 -3.622705 2.254261 -0.196698
6 -2.647299 2.611805 -1.148512
6 -1.272483 2.582814 -0.786138
6 -0.870017 2.274291 0.528092

6	-1.840452	1.817319	1.438625
1	0.191938	2.246252	0.766124
1	-3.973465	1.455138	1.790462
1	-4.673224	2.222539	-0.475917
1	-2.942657	2.867560	-2.162449
1	-0.505746	2.792413	-1.529800
1	-1.528098	1.463761	2.420484
6	-1.317529	-0.148756	-2.446310
1	-1.736720	-1.098522	-2.772916
1	-0.320506	-0.022838	-2.882306
1	-1.904279	0.681552	-2.850971
8	0.697297	0.146896	-0.776044
6	-0.237830	-0.701192	-0.947951
8	-0.255338	-1.910178	-0.881685
1	-0.910580	-1.807410	1.583023
15	-4.098538	-0.774360	-1.102578
15	-2.134138	-1.343269	1.064617
1	-3.994199	-0.614004	-2.518948
1	-2.827668	-1.055372	2.268811
5	2.040675	-0.097782	0.066465
6	3.035047	-1.013692	-0.807555
6	4.194548	-1.545180	-0.225265
6	2.860427	-1.240598	-2.177183
6	5.122161	-2.274008	-0.961798
1	4.374503	-1.381598	0.839262
6	3.778873	-1.969639	-2.927649
1	1.979493	-0.832629	-2.676306
6	4.915654	-2.492928	-2.321042
1	6.010391	-2.673258	-0.474428
1	3.606132	-2.130203	-3.990925
1	5.636474	-3.064536	-2.902589
6	2.639096	1.405314	0.169852
6	3.416277	1.836003	1.253637
6	2.470623	2.322810	-0.879960
6	3.972630	3.112179	1.304143
1	3.590987	1.152171	2.085571
6	3.014503	3.603126	-0.840680
1	1.907641	2.011003	-1.762785
6	3.766113	4.007138	0.259842
1	4.569142	3.409499	2.165258
1	2.863708	4.285360	-1.676558
1	4.195230	5.006502	0.297003
6	1.582930	-0.743510	1.488478
6	1.077084	0.042387	2.536629
6	1.581977	-2.130294	1.703851
6	0.587892	-0.508556	3.720583
1	1.092261	1.129899	2.435715
6	1.103773	-2.698862	2.884006
1	1.963479	-2.779735	0.916689
6	0.598422	-1.889517	3.899095
1	0.219736	0.142065	4.513956
1	1.127961	-3.779875	3.012388
1	0.230853	-2.329322	4.824268

 Bn-Ru-PP-Presence-C-C_bond formation-TS3_LiClO4

Number of imaginary frequencies : 1
 The smallest frequencies are : -350.0685 32.2337 43.5439 cm(-1)

Electronic energy : =-2086.5384507
 Zero-point correction= 0.257832
 Thermal correction to Energy= 0.280979
 Thermal correction to Enthalpy= 0.281924
 Thermal correction to Gibbs Free Energy= 0.206002
 Sum of electronic and zero-point Energies= -2086.280619
 Sum of electronic and thermal Energies= -2086.257471
 Sum of electronic and thermal Enthalpies= -2086.256527
 Sum of electronic and thermal Free Energies= -2086.332449

 Cartesian Coordinates

6	-1.987542	2.963000	0.107094
6	-0.658962	3.057472	-0.632046
44	-1.320040	-0.358459	0.006341
1	-2.604848	3.850818	-0.076872
1	-1.793565	2.912361	1.183419
1	0.091963	3.610483	-0.060079
1	-0.765848	3.537863	-1.610812
6	-1.686298	-1.403598	-1.925186
6	-2.799432	-1.724194	-1.107716
6	-2.595977	-2.286943	0.164961
6	-1.271022	-2.559379	0.606454
6	-0.163214	-2.370469	-0.247703
6	-0.370229	-1.744110	-1.492330
1	0.847571	-2.547880	0.106425
1	-1.839565	-0.894816	-2.873762
1	-3.800753	-1.449380	-1.431537
1	-3.438682	-2.456283	0.829532
1	-1.098075	-2.894756	1.625517
1	0.491465	-1.496756	-2.109350
6	-1.785040	0.254070	2.198436
1	-1.980970	1.322167	2.259421

1	-1.364330	-0.083628	3.149318
1	-2.720166	-0.304557	2.093703
8	0.621893	-0.914684	2.208065
6	0.092253	0.118353	1.757016
8	0.586397	1.262813	1.721411
1	1.365200	1.365943	-0.735473
15	-2.924318	1.435254	-0.476131
15	-0.027069	1.341460	-0.918169
1	-3.778469	1.333518	0.664816
1	-0.072704	1.237088	-2.333557
3	2.313237	0.030549	1.809083
8	4.037492	0.628124	1.034658
8	2.588303	-0.832454	-0.141646
17	3.854172	-0.034514	-0.302480
8	4.977091	-0.906717	-0.599489
8	3.652135	0.981565	-1.336024

 Bn-Ru-PP-Presence-C-C_bond formation-TS3_TiCl4

Number of imaginary frequencies : 1
 The smallest frequencies are : -280.2871 36.5314 39.8380 cm(-1)

Electronic energy : =-3217.5766842
 Zero-point correction= 0.245206
 Thermal correction to Energy= 0.270102
 Thermal correction to Enthalpy= 0.271046
 Thermal correction to Gibbs Free Energy= 0.190556
 Sum of electronic and zero-point Energies= -3217.331479
 Sum of electronic and thermal Energies= -3217.306582
 Sum of electronic and thermal Enthalpies= -3217.305638
 Sum of electronic and thermal Free Energies= -3217.386128

 Cartesian Coordinates

6	-2.113938	3.049118	0.416428
6	-1.407036	3.020132	-0.934795
44	-1.787452	-0.318667	0.154895
1	-2.694420	3.971799	0.537156
1	-1.363479	3.032540	1.213191
1	-0.411420	3.470994	-0.884228
1	-1.979717	3.534194	-1.714133
6	-3.274203	-1.372408	-1.154637
6	-3.744070	-1.594839	0.162922
6	-2.882224	-2.144965	1.126402
6	-1.561918	-2.519381	0.754378
6	-1.134146	-2.441319	-0.590656
6	-1.976644	-1.829669	-1.534082
1	-0.109340	-2.688555	-0.858220
1	-3.910658	-0.867192	-1.877008
1	-4.734607	-1.247574	0.446789
1	-3.205006	-2.238617	2.159730
1	-0.858176	-2.858591	1.510118
1	-1.616058	-1.674032	-2.549120
6	-0.827895	0.379778	2.137473
1	-1.067007	1.434956	2.231768
1	0.148392	0.220817	2.611949
1	-1.525859	-0.253184	2.692474
8	0.973116	-1.001440	0.816816
6	0.254606	0.039351	0.667161
8	0.810261	1.109289	0.272231
1	0.032671	1.087189	-2.098194
15	-3.290709	1.583808	0.562638
15	-1.208159	1.258811	-1.455688
1	-3.336764	1.554970	1.989918
1	-2.108016	1.154053	-2.548894
17	3.071959	0.601893	2.186003
17	1.734133	-0.779536	-2.045835
22	2.671053	-0.043805	0.038991
17	3.668359	1.681701	-0.923884
17	4.104665	-1.719629	0.068617

 Bn-Ru-PP-Presence-C-C_bond formation-TS3_ZnCl2

Number of imaginary frequencies : 1
 The smallest frequencies are : -338.8805 30.0722 37.0670 cm(-1)

Electronic energy : =-2465.9609136
 Zero-point correction= 0.241113
 Thermal correction to Energy= 0.263350
 Thermal correction to Enthalpy= 0.264294
 Thermal correction to Gibbs Free Energy= 0.188690
 Sum of electronic and zero-point Energies= -2465.719801
 Sum of electronic and thermal Energies= -2465.697564
 Sum of electronic and thermal Enthalpies= -2465.696620
 Sum of electronic and thermal Free Energies= -2465.772223

 Cartesian Coordinates

6	1.904793	3.048619	-0.142752
6	1.124714	2.948251	1.162561
44	1.408616	-0.299589	-0.201966

1	2.523999	3.953711	-0.162099
1	1.197317	3.114776	-0.975527
1	0.178820	3.495712	1.118031
1	1.700667	3.322504	2.016037
6	2.726712	-1.538877	1.104896
6	3.260640	-1.692757	-0.199531
6	2.428321	-2.118744	-1.247928
6	1.064332	-2.426053	-0.983019
6	0.556644	-2.412196	0.333866
6	1.378606	-1.923914	1.367039
1	-0.495011	-2.608640	0.528661
1	3.347145	-1.132656	1.900032
1	4.286882	-1.393859	-0.399852
1	2.807484	-2.158347	-2.265409
1	0.391710	-2.657151	-1.804526
1	0.963563	-1.813689	2.367271
6	0.700124	0.599367	-2.217782
1	0.861808	1.674453	-2.225732
1	-0.162529	0.364669	-2.846372
1	1.541159	0.075657	-2.682126
8	-1.345829	-0.720721	-1.151385
6	-0.641300	0.293116	-0.884113
8	-1.072603	1.379627	-0.457243
1	-0.548157	1.041980	1.995708
15	3.023042	1.542659	-0.328855
15	0.755048	1.163614	1.479255
1	3.187838	1.644556	-1.744245
1	1.515596	0.900974	2.650352
30	-2.956875	-0.106244	-0.001281
17	-4.758938	0.530441	-0.956894
17	-2.353800	-0.882300	1.975030

Bn-Ru-PP-Presence-C-C_bond formation-TS3_AIMe3

Number of imaginary frequencies : 1
The smallest frequencies are : -349.3010 35.0315 54.1915 cm(-1)

Electronic energy = -1680.4012059
Zero-point correction= 0.344982
Thermal correction to Energy= 0.370930
Thermal correction to Enthalpy= 0.371874
Thermal correction to Gibbs Free Energy= 0.290936
Sum of electronic and zero-point Energies= -1680.056224
Sum of electronic and thermal Energies= -1680.030276
Sum of electronic and thermal Enthalpies= -1680.029332
Sum of electronic and thermal Free Energies= -1680.110269

Cartesian Coordinates

6	-2.524273	-2.489529	-0.481624
6	-1.876892	-2.799711	0.861083
44	-0.934156	0.464987	-0.095767
1	-3.402760	-3.124918	-0.648044
1	-1.803896	-2.696036	-1.279732
1	-1.218650	-3.672255	0.811487
1	-2.624404	-2.976115	1.642743
6	-1.867363	1.955454	1.264774
6	-2.177855	2.387745	-0.050661
6	-1.144465	2.586877	-0.982537
6	0.212973	2.393040	-0.592614
6	0.544457	2.080481	0.737174
6	-0.503741	1.803392	1.645132
1	1.582076	1.917844	1.018165
1	-2.665184	1.726617	1.966910
1	-3.217347	2.482173	-0.356394
1	-1.382408	2.834629	-2.013269
1	1.007421	2.460488	-1.332254
1	-0.262272	1.466189	2.651744
6	-0.441867	-0.361725	-2.213117
1	-0.948645	-1.306041	-2.402395
1	0.490223	-0.340320	-2.786935
1	-1.030557	0.467866	-2.617013
8	1.876673	-0.097182	-0.908783
6	0.910543	-0.889222	-0.859349
8	0.794387	-2.079910	-0.681247
1	0.359072	-1.806749	1.850852
13	3.554126	-0.220859	0.107092
15	-3.054909	-0.682236	-0.507411
15	-0.875683	-1.326062	1.373889
1	-3.148885	-0.568813	-1.928514
1	-1.473331	-0.966622	2.611279
6	4.168097	1.659234	-0.129354
1	5.216271	1.781582	0.175436
1	4.122045	1.949700	-1.189164
1	3.603982	2.419508	0.432343
6	4.590807	-1.632392	-0.804425
1	4.851553	-1.363499	-1.836351
1	5.533877	-1.857846	-0.288747
1	4.022498	-2.571222	-0.850374
6	2.880792	-0.683409	1.933523
1	3.674428	-0.617223	2.690143
1	2.066870	-0.027952	2.286542

1 2.510368 -1.719435 1.968129

Bn-Ru-PP-Presence-C-C_bond formation-TS3_SiMe3Cl-TS

Number of imaginary frequencies : 1
The smallest frequencies are : -341.9406 41.1296 43.5241 cm(-1)

Electronic energy : =-2187.6682081
Zero-point correction= 0.351397
Thermal correction to Energy= 0.377757
Thermal correction to Enthalpy= 0.378702
Thermal correction to Gibbs Free Energy= 0.297005
Sum of electronic and zero-point Energies= -2187.316811
Sum of electronic and thermal Energies= -2187.290451
Sum of electronic and thermal Enthalpies= -2187.289506
Sum of electronic and thermal Free Energies= -2187.371204

Cartesian Coordinates

6 2.189100 2.814513 0.311011
6 1.601205 2.521138 1.681783
44 1.132759 -0.302990 -0.339821
1 2.936486 3.616215 0.364681
1 1.388442 3.135017 -0.363523
1 0.889525 3.288226 2.003766
1 2.387355 2.450037 2.443408
6 2.354229 -1.910098 0.600729
6 2.736898 -1.920487 -0.767756
6 1.752044 -2.056927 -1.755365
6 0.384143 -2.226784 -1.384029
6 0.017664 -2.356643 -0.034695
6 1.001333 -2.164634 0.957508
1 -1.016099 -2.439593 0.298927
1 3.100101 -1.722638 1.369398
1 3.770910 -1.730024 -1.045310
1 2.024094 -1.976053 -2.805083
1 -0.383208 -2.243369 -2.154737
1 0.640953 -2.138842 1.990265
6 0.409686 0.964610 -2.181046
1 0.897627 1.935885 -2.143240
1 -0.520285 1.047860 -2.752565
1 1.009165 0.243499 -2.742430
8 -1.665915 0.028115 -0.956480
6 -0.692972 0.912780 -0.767486
8 -0.870152 2.038657 -0.328560
1 -0.596415 1.050592 2.037876
15 3.013883 1.243351 -0.304546
15 0.737266 0.875780 1.641397
1 3.063889 1.606962 -1.687979
1 1.265492 0.199145 2.760991
14 -3.323676 0.315380 -0.492428
6 -3.510591 1.234955 1.108717
1 -3.120467 2.254924 1.051311
1 -4.576461 1.278234 1.367796
1 -2.995689 0.674955 1.902822
6 -4.009461 1.272820 -1.950092
1 -3.905647 0.712833 -2.886585
1 -5.071134 1.508013 -1.813267
1 -3.470066 2.222533 -2.055056
6 -3.955996 -1.430240 -0.354643
1 -3.516229 -1.868894 0.552816
1 -5.046603 -1.462200 -0.254372
1 -3.675420 -2.038372 -1.223023
17 -1.554861 -1.349404 2.651117

Bn-Ru-NNTs.AA-CO2-insertion-TS2_AICl3

Number of imaginary frequencies : 1
The smallest frequencies are : -152.3554 8.8432 9.5774 cm(-1)

Electronic energy : =-3186.9253212
Zero-point correction= 0.378530
Thermal correction to Energy= 0.410197
Thermal correction to Enthalpy= 0.411141
Thermal correction to Gibbs Free Energy= 0.311374
Sum of electronic and zero-point Energies= -3186.546791
Sum of electronic and thermal Energies= -3186.515124
Sum of electronic and thermal Enthalpies= -3186.514180
Sum of electronic and thermal Free Energies= -3186.613947

Cartesian Coordinates

6 2.649101 -1.371942 1.833516
6 1.708580 -2.376978 2.441257
44 0.211119 -1.336953 0.052890
1 3.690346 -1.687252 1.968096
1 2.521920 -0.402212 2.358798
1 1.855241 -2.481247 3.524323
1 1.845363 -3.354687 1.964786
6 0.084591 -3.400726 -1.035251
6 0.819376 -2.503239 -1.818413

6	0.304506	-1.216549	-2.160890
6	-0.999385	-0.862536	-1.760258
6	-1.780685	-1.780779	-1.006455
6	-1.187335	-2.990722	-0.561984
1	-2.829267	-1.576189	-0.796416
1	0.518786	-4.344918	-0.721122
1	1.851531	-2.716235	-2.078364
1	0.939116	-0.526191	-2.704931
1	-1.409595	0.117149	-2.002418
1	-1.749950	-3.630074	0.116168
6	0.285437	0.680606	0.742878
1	-0.140895	0.826864	1.747719
1	-0.255210	1.340019	0.055035
1	1.329522	0.992925	0.789739
8	-2.526639	0.487919	0.698487
6	-2.163997	-0.555049	1.203262
8	-2.335099	-1.378125	2.030624
1	0.145789	-1.077701	2.697419
13	-4.122848	1.241088	-0.059888
17	-4.786904	2.626194	1.374385
17	-3.365415	2.026537	-1.876569
17	-5.275513	-0.533733	-0.280283
1	-0.369949	-2.588066	2.376519
16	3.508415	-0.659216	-0.520369
6	3.517780	1.112265	-0.321365
6	4.132320	1.668369	0.797325
6	2.837791	1.916799	-1.231466
6	4.035787	3.037199	1.015159
1	4.694049	1.031699	1.477320
6	2.754857	3.282821	-1.003050
1	2.383591	1.464661	-2.109736
6	3.343128	3.861848	0.125407
1	4.512877	3.479491	1.888701
1	2.223411	3.917662	-1.710844
6	3.261411	5.341136	0.350456
1	4.017390	5.871437	-0.242552
1	2.284157	5.737655	0.054585
1	3.430211	5.599290	1.400863
8	3.172217	-0.906811	-1.923816
8	4.784453	-1.138354	0.009437
7	2.311069	-1.289089	0.418382
7	0.343050	-1.903766	2.131176

 Bn-Ru-NNTs-C-C_bond formation-TS3_AIC3

Number of imaginary frequencies : 1
 The smallest frequencies are : -293.4604 15.8942 26.5902 cm(-1)

Electronic energy : =-3186.9295505
 Zero-point correction= 0.379988
 Thermal correction to Energy= 0.410986
 Thermal correction to Enthalpy= 0.411930
 Thermal correction to Gibbs Free Energy= 0.316104
 Sum of electronic and zero-point Energies= -3186.549562
 Sum of electronic and thermal Energies= -3186.518565
 Sum of electronic and thermal Enthalpies= -3186.517620
 Sum of electronic and thermal Free Energies= -3186.613447

 Cartesian Coordinates

6	1.682885	-0.841646	2.205349
6	0.474252	-1.507769	2.807586
44	-0.253085	-1.043906	-0.093136
1	2.600272	-1.218397	2.673327
1	1.621711	0.249812	2.380801
1	0.348766	-1.267714	3.871179
1	0.549315	-2.595321	2.691924
6	-0.715239	-3.266245	-0.270316
6	0.291603	-3.007750	-1.212281
6	0.149182	-1.935776	-2.126350
6	-1.070908	-1.213409	-2.175009
6	-2.153864	-1.579316	-1.341098
6	-1.944618	-2.535807	-0.339769
1	-3.091280	-1.030708	-1.394574
1	-0.561510	-4.013909	0.503090
1	1.255297	-3.504222	-1.144830
1	0.994774	-1.660552	-2.748158
1	-1.184990	-0.363675	-2.844321
1	-2.733425	-2.707418	0.390615
6	0.595804	0.965739	-0.736217
1	1.250249	1.316194	0.060856
1	0.066856	1.807692	-1.191180
1	1.171511	0.497118	-1.538344
8	-2.114154	1.183302	-0.608180
6	-1.156159	0.974508	0.231806
8	-0.982601	1.521617	1.301175
13	-3.832125	1.387356	-0.010965
17	-4.018187	-0.181709	1.492154
17	-4.936834	0.811847	-1.754484
17	-4.229055	3.325431	0.723156
7	-0.674662	-1.014755	2.026275
7	1.660196	-1.168174	0.783510

16	3.126969	-1.296199	0.057843
6	3.824013	0.336360	-0.133254
6	4.269345	1.026486	0.992514
6	3.891488	0.920455	-1.393510
6	4.744600	2.322822	0.851435
1	4.269511	0.542875	1.966622
6	4.378235	2.215535	-1.519324
1	3.577321	0.349904	-2.264090
6	4.796123	2.940930	-0.401558
1	5.094933	2.866298	1.727744
1	4.441631	2.673601	-2.505313
6	5.282368	4.351657	-0.535654
1	5.647421	4.557825	-1.546901
1	4.475758	5.065909	-0.327397
1	6.092066	4.565889	0.170113
8	2.909255	-1.812389	-1.296491
8	4.013678	-2.010756	0.973812
1	-1.546942	-1.493732	2.251439
1	-0.830918	-0.021096	2.241267

 Bn-Ru-NNTs-AA-C-C_bond formation-TS3_LiClO4

Number of imaginary frequencies : 1
 The smallest frequencies are : -303.9712 14.3526 21.3084 cm(-1)

Electronic energy : =-2560.9743698
 Zero-point correction= 0.457614
 Thermal correction to Energy= 0.494645
 Thermal correction to Enthalpy= 0.495589
 Thermal correction to Gibbs Free Energy= 0.385799
 Sum of electronic and zero-point Energies= -2560.516756
 Sum of electronic and thermal Energies= -2560.479725
 Sum of electronic and thermal Enthalpies= -2560.478781
 Sum of electronic and thermal Free Energies= -2560.588571

 Cartesian Coordinates

6	-1.141315	-0.062294	-2.014412
6	0.340821	-0.224194	-2.215155
44	-0.055109	-0.783743	0.714741
1	-1.689425	-0.414529	-2.897410
1	-1.375989	1.009951	-1.862718
1	0.732327	0.419193	-3.014117
1	0.582094	-1.266766	-2.453062
6	0.902315	-2.811965	0.393434
6	-0.378954	-3.051657	0.920934
6	-0.806388	-2.398270	2.102423
6	0.096053	-1.552496	2.794105
6	1.435967	-1.413641	2.347300
6	1.811664	-1.987490	1.125337
1	2.104778	-0.732929	2.861209
1	1.196681	-3.225603	-0.566841
1	-1.112619	-3.613930	0.349857
1	-1.840715	-2.496125	2.413949
1	-0.235479	-0.981133	3.657225
1	2.784940	-1.768370	0.695010
6	-1.564502	0.739164	1.462701
1	-1.912077	1.301997	0.596744
1	-1.503725	1.392658	2.336976
1	-2.264930	-0.059467	1.721240
8	0.887845	1.325507	2.661494
6	0.386306	1.313625	1.521837
8	0.496776	2.202336	0.657097
7	0.969554	0.123203	-0.932164
7	-1.483268	-0.860791	-0.841302
16	-3.007059	-1.449867	-0.808760
6	-4.156942	-0.087773	-0.653786
6	-4.405911	0.728120	-1.755292
6	-4.793534	0.153575	0.559408
6	-5.266242	1.809759	-1.623034
1	-3.954462	0.497891	-2.717291
6	-5.658650	1.234290	0.673938
1	-4.623846	-0.521450	1.394467
6	-5.897261	2.085488	-0.407256
1	-5.465378	2.447578	-2.483211
1	-6.167953	1.418530	1.618997
6	-6.802960	3.271248	-0.267871
1	-7.343657	3.475385	-1.198273
1	-7.539274	3.123975	0.529100
1	-6.232322	4.175647	-0.021076
8	-3.150343	-2.252855	0.410380
8	-3.293634	-2.055421	-2.109082
1	1.961281	-0.138432	-0.944132
1	0.913289	1.135427	-0.773411
6	4.595399	-1.408093	-1.384222
8	5.244769	-0.761236	-0.428923
8	3.381199	-1.385768	-1.508906
6	5.518043	-2.166203	-2.282542
1	4.622336	-0.170378	0.054692
1	4.949504	-2.833974	-2.930272
1	6.078637	-1.452739	-2.895577
1	6.249267	-2.725720	-1.692725

3	2.184448	2.570930	1.687427
8	3.456325	3.561727	0.519172
8	3.504998	1.187267	0.624761
17	4.000929	2.372485	-0.199236
8	5.452846	2.382891	-0.201456
8	3.440203	2.267649	-1.541527

 Bn-Ru-NNTs.AA-C-C_bond formation-TS3_LiCl

Number of imaginary frequencies : 1
 The smallest frequencies are : -271.9733 17.4748 24.0323 cm(-1)

Electronic energy : =-2260.5661529
 Zero-point correction= 0.440132
 Thermal correction to Energy= 0.473760
 Thermal correction to Enthalpy= 0.474704
 Thermal correction to Gibbs Free Energy= 0.372729
 Sum of electronic and zero-point Energies= -2260.126020
 Sum of electronic and thermal Energies= -2260.092393
 Sum of electronic and thermal Enthalpies= -2260.091449
 Sum of electronic and thermal Free Energies= -2260.193424

 Cartesian Coordinates

6	-0.725781	-1.640427	-1.360139
6	0.763008	-1.754218	-1.542572
44	0.444030	0.304428	0.634239
1	-1.211619	-2.609290	-1.529700
1	-1.128065	-0.916972	-2.097936
1	1.039535	-2.006198	-2.575260
1	1.168398	-2.522710	-0.874132
6	1.731689	-0.999115	1.980969
6	0.497895	-0.836884	2.634051
6	-0.056313	0.454172	2.828071
6	0.689647	1.591410	2.435662
6	1.996830	1.440222	1.899402
6	2.483990	0.157643	1.614238
1	2.557683	2.302624	1.553831
1	2.100517	-1.989566	1.729215
1	-0.126921	-1.698723	2.850530
1	-1.066334	0.541960	3.214800
1	0.259602	2.586673	2.505989
1	3.410958	0.055103	1.051741
6	-1.274121	1.569512	-0.101499
1	-1.642301	1.097721	-1.013600
1	-1.329484	2.655444	-0.202184
1	-1.900310	1.311091	0.755819
8	0.954430	3.232569	0.039430
6	0.637258	2.213993	-0.595864
8	0.795849	2.035469	-1.823167
7	1.330445	-0.454910	-1.156348
7	-0.932952	-1.189689	0.011512
16	-2.338856	-1.662628	0.700351
6	-3.697180	-0.775420	-0.053894
6	-4.097562	-1.101790	-1.347400
6	-4.327362	0.251680	0.641057
6	-5.109225	-0.368310	-1.953551
1	-3.635168	-1.938236	-1.866393
6	-5.343304	0.970821	0.025149
1	-4.022355	0.468707	1.661917
6	-5.744026	0.678720	-1.280620
1	-5.422536	-0.617319	-2.966644
1	-5.840887	1.773899	0.567520
6	-6.858097	1.442389	-1.930188
1	-7.827698	0.966430	-1.735292
1	-6.918368	2.467481	-1.549637
1	-6.733489	1.488979	-3.017250
8	-2.315769	-1.248304	2.106543
8	-2.559267	-3.069500	0.365225
1	2.346737	-0.532210	-1.034247
1	1.142347	0.269466	-1.860337
6	5.060172	-1.560454	-1.078723
8	5.694874	-0.493236	-1.512844
8	3.943857	-1.544869	-0.577429
6	5.864131	-2.810585	-1.264056
1	5.168138	0.330613	-1.330823
1	5.292966	-3.679785	-0.936732
1	6.146687	-2.916525	-2.315802
1	6.793859	-2.735783	-0.691387
3	2.397296	3.211738	-1.399434
17	4.248614	2.123186	-0.780976

 Bn-Ru-OO-C-C_bond formation-TS3_LiClO4

Number of imaginary frequencies : 1
 The smallest frequencies are : -298.5365 43.3648 59.4142 cm(-1)

Electronic energy : =-1553.0483859
 Zero-point correction= 0.248307
 Thermal correction to Energy= 0.269437
 Thermal correction to Enthalpy= 0.270381

Thermal correction to Gibbs Free Energy= 0.199141
 Sum of electronic and zero-point Energies= -1552.800079
 Sum of electronic and thermal Energies= -1552.778949
 Sum of electronic and thermal Enthalpies= -1552.778005
 Sum of electronic and thermal Free Energies= -1552.849245

 Cartesian Coordinates

8	-2.992502	0.958498	-0.439352
6	-2.673623	2.307962	-0.479761
6	-1.472814	2.491151	-1.374862
8	-0.473580	1.559616	-0.929497
44	-1.368454	-0.183083	0.013757
1	-3.536721	2.879268	-0.859264
1	-2.432457	2.715283	0.525116
1	-1.052877	3.504025	-1.365927
1	-1.711957	2.210211	-2.407447
6	-1.206248	-1.351629	-1.902103
6	-2.417011	-1.699507	-1.286675
6	-2.448523	-2.073873	0.088279
6	-1.218521	-2.237826	0.784230
6	0.017843	-2.017956	0.127228
6	0.020914	-1.472346	-1.167810
1	0.952708	-2.077017	0.674026
1	-1.203724	-0.921469	-2.899404
1	-3.353454	-1.491782	-1.797905
1	-3.397047	-2.215760	0.597502
1	-1.218413	-2.478885	1.843691
1	0.959768	-1.115679	-1.592698
6	-1.981711	0.539353	2.072770
1	-1.621811	1.435761	2.586502
1	-2.007591	-0.298839	2.770037
1	-2.968760	0.763262	1.659823
8	0.481306	-0.375418	2.464396
6	0.043875	0.463007	1.682814
8	0.566148	1.561049	1.363653
1	0.050721	1.914330	-0.165084
3	2.314616	0.633314	1.773147
8	3.643530	1.324298	0.398545
8	2.843358	-0.894229	0.550516
17	3.597883	0.037252	-0.366858
8	2.829504	0.210079	-1.603000
8	4.934815	-0.467684	-0.620483

 Bn-Ru-OO.2TFA-C-C_bond formation-TS3_LiCl

Number of imaginary frequencies : 1
 The smallest frequencies are : -324.1204 18.6661 20.2028 cm(-1)

Electronic energy : =-2305.8887555
 Zero-point correction= 0.313529
 Thermal correction to Energy= 0.346377
 Thermal correction to Enthalpy= 0.347322
 Thermal correction to Gibbs Free Energy= 0.246841
 Sum of electronic and zero-point Energies= -2305.575226
 Sum of electronic and thermal Energies= -2305.542378
 Sum of electronic and thermal Enthalpies= -2305.541434
 Sum of electronic and thermal Free Energies= -2305.641914

 Cartesian Coordinates

8	1.644628	-0.846518	-0.969368
6	0.911257	-2.013904	-1.237253
6	-0.273527	-1.625860	-2.084994
8	-0.912274	-0.503204	-1.453688
44	0.478117	0.646314	-0.186529
1	1.556581	-2.726642	-1.775021
1	0.559082	-2.500434	-0.313093
1	-1.005363	-2.433668	-2.201690
1	0.055510	-1.286033	-3.075096
6	0.610325	2.153669	-1.844612
6	1.857661	2.137250	-1.195985
6	1.925519	2.258611	0.215455
6	0.737819	2.508344	0.962703
6	-0.503259	2.651685	0.304333
6	-0.573102	2.397515	-1.077394
1	-1.437315	2.771345	0.846859
1	0.535189	1.920454	-2.902841
1	2.762710	1.854492	-1.728606
1	2.884223	2.111379	0.703365
1	0.776512	2.536437	2.049008
1	-1.563438	2.318395	-1.525485
6	1.198003	-0.418708	1.712403
1	1.261072	-1.491351	1.533450
1	0.889661	-0.209021	2.739151
1	2.181819	0.037636	1.572064
8	-1.350763	0.526954	2.208881
6	-0.820403	-0.290052	1.444010
8	-1.173780	-1.431275	1.111200
6	-4.144012	-1.208514	0.063732
8	-3.713032	-1.240837	1.319551
8	-3.479484	-1.436332	-0.918117

1	-1.754665	-0.799334	-1.046895
6	-5.663698	-1.004787	-0.009566
9	-6.118994	-0.271200	0.999115
9	-6.223242	-2.217618	0.076270
9	-6.012548	-0.457213	-1.153229
1	-2.728306	-1.499875	1.304393
6	4.735554	-0.431668	-0.045484
8	3.954567	-1.459603	-0.190038
8	4.457580	0.740050	-0.193522
6	6.148539	-0.874784	0.370059
9	6.945044	0.170688	0.528446
9	6.671763	-1.672664	-0.559253
9	6.096590	-1.547861	1.519440
1	3.007649	-1.159648	-0.490812
3	-3.259121	0.763777	1.909929
17	-3.751048	1.856640	0.076943

Bn-Ru-OO.2TFA-C-C_bond formation-TS3_LiClO4

Number of imaginary frequencies : 1
The smallest frequencies are : -331.2372 16.2862 20.3125 cm(-1)

Electronic energy : ==-2606.3057771
Zero-point correction= 0.330773
Thermal correction to Energy= 0.366841
Thermal correction to Enthalpy= 0.367785
Thermal correction to Gibbs Free Energy= 0.260720
Sum of electronic and zero-point Energies= -2605.975004
Sum of electronic and thermal Energies= -2605.938936
Sum of electronic and thermal Enthalpies= -2605.937992
Sum of electronic and thermal Free Energies= -2606.045057

Cartesian Coordinates

8	2.214042	-1.073261	-0.813201
6	1.611576	-2.321235	-1.033761
6	0.438866	-2.102495	-1.955000
8	-0.350642	-1.029849	-1.408634
44	0.878861	0.354202	-0.207180
1	2.347161	-2.998341	-1.495672
1	1.261937	-2.782846	-0.095611
1	-0.196886	-2.987896	-2.071053
1	0.781242	-1.767244	-2.941843
6	0.839564	1.739681	-1.982020
6	2.106609	1.857862	-1.395586
6	2.218862	2.076644	0.005183
6	1.048748	2.319249	0.779252
6	-0.223416	2.332934	0.165553
6	-0.332247	1.952772	-1.182327
1	-1.121556	2.482883	0.754329
1	0.737937	1.425937	-3.017073
1	3.010085	1.603126	-1.944393
1	3.204127	2.036423	0.460887
1	1.125146	2.447148	1.856550
1	-1.325301	1.791684	-1.596203
6	1.595957	-0.483356	1.804404
1	1.803481	-1.545368	1.682727
1	1.205791	-0.273382	2.803308
1	2.521157	0.090846	1.702708
8	-1.045741	0.261435	2.096697
6	-0.395926	-0.567654	1.445939
8	-0.618865	-1.766040	1.213915
6	-3.537168	-1.926355	0.090399
8	-3.166165	-1.825935	1.357891
8	-2.820606	-2.204989	-0.840232
1	-1.134083	-1.415525	-0.963333
6	-5.048828	-1.712785	-0.071293
9	-5.506292	-0.841895	0.826936
9	-5.658429	-2.881395	0.134256
9	-5.330918	-1.284351	-1.282211
1	-2.162938	-1.993461	1.402240
6	5.257147	-0.176492	-0.108892
8	4.552549	-1.246728	0.115072
8	4.896342	0.856833	-0.630886
6	6.692441	-0.353545	0.415130
9	7.428666	0.713342	0.148306
9	7.264285	-1.418243	-0.142004
9	6.667799	-0.533965	1.736760
1	3.593324	-1.140976	-0.255860
3	-2.959329	0.312197	1.813434
8	-3.962204	2.003652	1.559443
8	-3.177316	0.653461	-0.223922
17	-3.946709	1.926125	0.059666
8	-3.200944	3.057628	-0.488796
8	-5.291395	1.834873	-0.472438

Bn-Ru-OO-C-C_bond formation-TS3_AlCl3

Number of imaginary frequencies : 1
The smallest frequencies are : -303.0834 22.0045 36.3093 cm(-1)

Electronic energy : =-2407.9949399
 Zero-point correction= 0.235085
 Thermal correction to Energy= 0.256160
 Thermal correction to Enthalpy= 0.257104
 Thermal correction to Gibbs Free Energy= 0.184112
 Sum of electronic and zero-point Energies= -2407.759855
 Sum of electronic and thermal Energies= -2407.738780
 Sum of electronic and thermal Enthalpies= -2407.737836
 Sum of electronic and thermal Free Energies= -2407.810828

.....
 Cartesian Coordinates

.....
 8 3.242928 0.694040 -0.826622
 6 3.283321 2.045197 -0.508053
 6 3.013566 2.193584 0.968324
 8 1.801736 1.464402 1.244684
 44 1.541578 -0.181663 -0.153159
 1 4.272804 2.452285 -0.771077
 1 2.529392 2.634011 -1.070924
 1 2.892892 3.229686 1.305263
 1 3.801003 1.710689 1.558446
 6 2.515484 -1.641356 1.246605
 6 2.868600 -2.015130 -0.059951
 6 1.870976 -2.151742 -1.062527
 6 0.498745 -2.062358 -0.691333
 6 0.130739 -1.836726 0.656290
 6 1.128801 -1.521183 1.591904
 1 -0.915373 -1.733473 0.934685
 1 3.284434 -1.393837 1.972451
 1 3.915241 -2.002278 -0.352775
 1 2.152325 -2.309457 -2.099500
 1 -0.284329 -2.126641 -1.443375
 1 0.840183 -1.167582 2.578908
 6 0.817164 0.746096 -2.099966
 1 0.328789 1.711245 -2.258259
 1 0.284360 -0.024070 -2.657882
 1 1.862049 0.841029 -2.402193
 8 -1.358808 0.218229 -0.813299
 6 -0.371098 0.931689 -0.444918
 8 -0.379126 2.018337 0.110928
 1 1.004035 2.008948 1.010709
 13 -3.002329 0.115938 0.013314
 17 -2.500771 0.023829 2.107828
 17 -3.625460 -1.812685 -0.674992
 17 -4.212510 1.751616 -0.552975

.....
 Bn-Ru-OO-C-C_bond formation-TS3_2.AIC13

.....
 Number of imaginary frequencies : 1
 The smallest frequencies are : -223.4535 20.0701 36.4284 cm(-1)

Electronic energy : =-4031.1587958
 Zero-point correction= 0.241762
 Thermal correction to Energy= 0.269595
 Thermal correction to Enthalpy= 0.270539
 Thermal correction to Gibbs Free Energy= 0.181571
 Sum of electronic and zero-point Energies= -4030.917033
 Sum of electronic and thermal Energies= -4030.889201
 Sum of electronic and thermal Enthalpies= -4030.888256
 Sum of electronic and thermal Free Energies= -4030.977225

.....
 Cartesian Coordinates

.....
 8 3.182945 -0.500020 -1.556449
 6 3.148270 0.733617 -2.203744
 6 3.278666 1.813245 -1.163575
 8 2.278512 1.515900 -0.160349
 44 1.840264 -0.599601 -0.048586
 1 3.973785 0.774021 -2.930927
 1 2.204888 0.882464 -2.766649
 1 3.108712 2.831686 -1.530474
 1 4.248750 1.759967 -0.656641
 6 3.353125 -0.771266 1.674819
 6 3.520977 -1.916978 0.891974
 6 2.385974 -2.676071 0.494309
 6 1.117154 -2.389765 1.069830
 6 0.977284 -1.320799 1.991088
 6 2.056696 -0.451672 2.202318
 1 -0.005659 -1.064180 2.379135
 1 4.188316 -0.098999 1.849843
 1 4.482185 -2.111271 0.423895
 1 2.486762 -3.480471 -0.228739
 1 0.237246 -2.961531 0.770556
 1 1.901306 0.470939 2.757248
 6 0.597845 -1.225435 -1.825749
 1 -0.122595 -0.588286 -2.350405
 1 0.130166 -2.180791 -1.578876
 1 1.491763 -1.333962 -2.440961
 8 -1.082367 -0.696406 0.149279
 6 -0.144976 -0.016999 -0.332790
 8 -0.282758 1.195959 -0.694030
 1 1.467004 2.025882 -0.368934

13	-1.123359	2.545564	0.285648
17	0.207086	4.112137	-0.355210
17	-3.150423	2.713860	-0.201692
17	-0.658164	1.970293	2.306166
13	-2.674528	-1.543633	-0.271169
17	-3.932794	-1.189439	1.381229
17	-3.166926	-0.740654	-2.168065
17	-1.999277	-3.593189	-0.378721

SiCl4

Number of imaginary frequencies : 0
The smallest frequencies are : 145.4720 145.5443 217.6404 cm(-1)

Electronic energy : =-2130.3173326
Zero-point correction= 0.007366
Thermal correction to Energy= 0.013833
Thermal correction to Enthalpy= 0.014777
Thermal correction to Gibbs Free Energy= -0.025193
Sum of electronic and zero-point Energies= -2130.309967
Sum of electronic and thermal Energies= -2130.303500
Sum of electronic and thermal Enthalpies= -2130.302555
Sum of electronic and thermal Free Energies= -2130.342526

Cartesian Coordinates

14	-0.000117	-0.000069	0.000064
17	-1.506160	-1.359655	0.155478
17	0.324755	0.431172	-1.961899
17	1.697606	-0.771854	0.814734
17	-0.516104	1.700394	0.991634

Bn-Ru-PP-C-C_bond formation-TS3_SiCl4

Number of imaginary frequencies : 1
The smallest frequencies are : -311.7768 31.1264 39.8466 cm(-1)

Electronic energy : =-3448.6308003
Zero-point correction= 0.246811
Thermal correction to Energy= 0.270972
Thermal correction to Enthalpy= 0.271916
Thermal correction to Gibbs Free Energy= 0.192882
Sum of electronic and zero-point Energies= -3448.383989
Sum of electronic and thermal Energies= -3448.359829
Sum of electronic and thermal Enthalpies= -3448.358884
Sum of electronic and thermal Free Energies= -3448.437918

Cartesian Coordinates

6	-2.634717	2.787012	0.512269
6	-2.120732	2.928286	-0.914032
44	-1.614868	-0.393042	0.145220
1	-3.363745	3.572403	0.746140
1	-1.792402	2.889839	1.204325
1	-1.331279	3.681044	-0.996719
1	-2.923381	3.189512	-1.612791
6	-2.854541	-1.724956	-1.154513
6	-3.225938	-2.075224	0.165593
6	-2.234117	-2.437408	1.091682
6	-0.874173	-2.516506	0.676972
6	-0.514416	-2.324471	-0.671666
6	-1.496213	-1.872957	-1.570961
1	0.527858	-2.354609	-0.982431
1	-3.606802	-1.361991	-1.850618
1	-4.259591	-1.962940	0.483518
1	-2.497785	-2.616523	2.130653
1	-0.094761	-2.722748	1.407168
1	-1.204296	-1.617817	-2.588070
6	-0.745565	0.376243	2.164984
1	-1.190180	1.342935	2.387699
1	0.256973	0.333720	2.608264
1	-1.300151	-0.437230	2.640581
8	1.192609	-0.326949	0.594461
6	0.267585	0.608243	0.638349
8	0.465572	1.791587	0.415741
1	-0.166428	1.477284	-2.023872
15	-3.463833	1.108192	0.692178
15	-1.436891	1.292158	-1.447196
1	-3.418606	1.051809	2.119077
1	-2.207298	0.975726	-2.595153
14	2.815188	0.024974	0.026100
17	1.899850	-0.266611	-2.059320
17	3.911174	1.635962	-0.726719
17	3.771967	-1.822802	-0.021036
17	3.302645	0.529446	2.088178

Effect in Solvent Phase Optimization (Table S8)

Solvent (DCM) Optimization of Bn-Ru-NNTs

Bn-Ru-NNTs

Number of imaginary frequencies : 1
The smallest frequencies are : -31.2577 15.4300 35.4394 cm(-1)

Electronic energy : =-1563.8434045
Zero-point correction= 0.372862
Thermal correction to Energy= 0.397647
Thermal correction to Enthalpy= 0.398591
Thermal correction to Gibbs Free Energy= 0.316595
Sum of electronic and zero-point Energies= -1563.470542
Sum of electronic and thermal Energies= -1563.445758
Sum of electronic and thermal Enthalpies= -1563.444813
Sum of electronic and thermal Free Energies= -1563.526810

Cartesian Coordinates

6	0.619305	0.134505	2.194750
6	-0.797598	0.382377	2.644266
44	-1.095072	-0.686131	-0.099721
1	1.206680	-0.329510	2.996362
1	1.107984	1.084815	1.920251
1	-0.844423	1.200422	3.374280
1	-1.201116	-0.523025	3.113520
6	-2.575503	-2.114267	-0.845396
6	-1.310757	-2.443323	-1.424020
6	-0.577494	-1.461882	-2.113020
6	-1.086602	-0.132129	-2.188583
6	-2.371244	0.177798	-1.665276
6	-3.124959	-0.822149	-1.008917
1	-2.707268	1.212128	-1.628419
1	-3.090837	-2.844817	-0.228217
1	-0.870968	-3.419572	-1.243184
1	0.428381	-1.683918	-2.455189
1	-0.474396	0.660446	-2.610793
1	-4.029547	-0.538254	-0.476024
7	-1.605084	0.670582	1.452406
1	-1.466369	1.622403	1.092221
7	0.550487	-0.752655	1.011274
16	1.999078	-1.500975	0.649157
6	3.058502	-0.179659	0.110858
6	3.943087	0.404851	1.011289
6	2.952432	0.285679	-1.199528
6	4.731832	1.469224	0.588624
1	4.016861	0.023526	2.027091
6	3.746445	1.348612	-1.603657
1	2.266476	-0.193353	-1.896093
6	4.645913	1.955682	-0.717847
1	5.429062	1.931171	1.285650
1	3.677011	1.716762	-2.626345
6	5.511376	3.086501	-1.178532
1	4.947670	3.793868	-1.797303
1	5.943723	3.633456	-0.334594
1	6.342058	2.716035	-1.793165
8	1.768816	-2.393661	-0.484991
8	2.568441	-2.056631	1.879234
6	-4.150152	2.123723	0.414972
8	-4.304871	1.151042	1.210929
8	-3.069644	2.706745	0.148268
6	-5.392009	2.577148	-0.342982
1	-2.637742	0.680870	1.606504
1	-6.303660	2.411613	0.239884
1	-5.319433	3.628639	-0.638223
1	-5.477439	1.980082	-1.262267

Bn-Ru-NNTs-AA-Presence-TS1_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 31.0436 35.8522 45.6509 cm(-1)

Electronic energy : =-1604.3293529
Zero-point correction= 0.419704
Thermal correction to Energy= 0.448918
Thermal correction to Enthalpy= 0.449862
Thermal correction to Gibbs Free Energy= 0.359488
Sum of electronic and zero-point Energies= -1603.909649
Sum of electronic and thermal Energies= -1603.880435
Sum of electronic and thermal Enthalpies= -1603.879491
Sum of electronic and thermal Free Energies= -1603.969865

 Cartesian Coordinates

6	0.480842	-0.400699	2.327573
6	-0.964310	-0.263455	2.733030
44	-1.067102	-0.814587	-0.177930
1	1.044128	-0.973903	3.072948
1	0.949269	0.595303	2.237112
1	-1.072494	0.416936	3.587207
1	-1.363578	-1.244135	3.018542
6	-2.587615	-2.018136	-1.199398
6	-1.305594	-2.370762	-1.724964
6	-0.457568	-1.377010	-2.246573
6	-0.863147	-0.014858	-2.183441
6	-2.153904	0.333961	-1.696691
6	-3.027809	-0.676337	-1.231784
1	-2.416088	1.379719	-1.547971
1	-3.199397	-2.776027	-0.718607
1	-0.949449	-3.393110	-1.636230
1	0.548290	-1.639220	-2.558068
1	-0.165927	0.772588	-2.460310
1	-3.945147	-0.389135	-0.721592
6	0.546193	2.722260	-0.001495
1	1.092222	3.194884	0.820980
1	0.883641	3.151099	-0.950531
1	-0.528884	2.896708	0.120303
1	0.746492	1.644018	0.000704
6	-4.028621	2.020766	0.585495
8	-4.350340	0.939716	1.156373
8	-2.880883	2.537173	0.549527
6	-5.131614	2.728924	-0.190950
1	-1.593763	1.218796	1.376929
7	-1.714218	0.210715	1.562893
7	0.497445	-1.084321	1.014682
16	1.982114	-1.729591	0.595793
6	2.957890	-0.319442	0.127371
6	3.642147	0.397594	1.106376
6	2.976582	0.089217	-1.204550
6	4.335679	1.545285	0.741846
1	3.644358	0.052373	2.137818
6	3.678705	1.235026	-1.551525
1	2.458742	-0.494902	-1.962014
6	4.355680	1.986472	-0.584606
1	4.876498	2.109956	1.499719
1	3.706859	1.556166	-2.591830
6	5.062740	3.249997	-0.962409
1	5.471461	3.193852	-1.977097
1	4.368163	4.100613	-0.940378
1	5.879368	3.478755	-0.269755
8	1.784823	-2.563094	-0.588905
8	2.595159	-2.325296	1.785452
1	-2.748119	0.184557	1.657755
1	-6.110410	2.574836	0.274423
1	-5.179545	2.299662	-1.201966
1	-4.928309	3.799349	-0.294285

 Bn-Ru-NNTs-AA-Presence-TS1

Number of imaginary frequencies : 1
 The smallest frequencies are : -1667.7019 20.3750 25.7173 cm(-1)

Electronic energy : =-1604.2904756
 Zero-point correction= 0.415686
 Thermal correction to Energy= 0.443614
 Thermal correction to Enthalpy= 0.444558
 Thermal correction to Gibbs Free Energy= 0.355821
 Sum of electronic and zero-point Energies= -1603.874790
 Sum of electronic and thermal Energies= -1603.846862
 Sum of electronic and thermal Enthalpies= -1603.845918
 Sum of electronic and thermal Free Energies= -1603.934655

 Cartesian Coordinates

6	0.095883	-0.477372	2.420302
6	-1.366606	-0.748346	2.667639
44	-1.055291	-0.698252	-0.353631
1	0.704439	-0.875309	3.240911
1	0.259655	0.615840	2.375835
1	-1.726422	-0.243260	3.573171
1	-1.529662	-1.827537	2.773970
6	-2.350096	-2.383537	-0.855521
6	-1.015562	-2.744250	-1.134500
6	-0.218136	-1.929039	-1.998232
6	-0.755968	-0.753075	-2.547353
6	-2.105634	-0.377006	-2.260165
6	-2.897032	-1.190038	-1.424914
1	-2.489300	0.580338	-2.598918
1	-2.931077	-2.961482	-0.140843
1	-0.559270	-3.588524	-0.626827
1	0.831672	-2.170046	-2.128184
1	-0.116601	-0.078341	-3.112123

1	-3.889497	-0.854706	-1.133506
6	-0.267964	1.518459	-0.288958
1	-0.262545	2.175794	0.589781
1	-0.170746	2.117417	-1.204216
1	-1.585767	1.462924	-0.346463
1	0.645085	0.920498	-0.227409
6	-3.191822	2.697284	0.527863
8	-2.793271	2.058025	-0.513525
8	-2.791471	2.480956	1.685139
6	-4.222243	3.769079	0.266305
1	-2.268237	0.746026	1.566691
7	-2.108136	-0.275764	1.481071
7	0.411286	-1.135746	1.155324
16	1.951494	-1.569320	0.916567
6	2.822392	-0.144969	0.280403
6	3.164454	0.886321	1.156530
6	3.043262	-0.011020	-1.086681
6	3.712276	2.056419	0.650991
1	3.006888	0.766557	2.226739
6	3.596492	1.167044	-1.579260
1	2.789299	-0.829564	-1.756433
6	3.930608	2.218429	-0.723078
1	3.982414	2.864217	1.330401
1	3.777716	1.272008	-2.648247
6	4.530530	3.486676	-1.246687
1	4.553055	3.500334	-2.341138
1	3.966630	4.363299	-0.905738
1	5.559940	3.613050	-0.887963
8	2.000940	-2.584975	-0.143023
8	2.581436	-1.892131	2.205161
1	-3.032815	-0.704542	1.455610
1	-5.087584	3.335841	-0.247479
1	-3.802986	4.529266	-0.402261
1	-4.547535	4.241343	1.196450

 Bn-Ru-NNTs-AA-Presence-TS1_for

Number of imaginary frequencies : 0
 The smallest frequencies are : 25.1120 30.9130 36.1271 cm(-1)

Electronic energy : =-1604.3241984
 Zero-point correction= 0.421674
 Thermal correction to Energy= 0.449865
 Thermal correction to Enthalpy= 0.450809
 Thermal correction to Gibbs Free Energy= 0.361774
 Sum of electronic and zero-point Energies= -1603.902524
 Sum of electronic and thermal Energies= -1603.874334
 Sum of electronic and thermal Enthalpies= -1603.873390
 Sum of electronic and thermal Free Energies= -1603.962424

 Cartesian Coordinates

6	0.273656	-0.529186	2.418335
6	-1.166684	-0.865323	2.713190
44	-0.966646	-0.746906	-0.312498
1	0.920195	-0.922456	3.212362
1	0.395253	0.570132	2.398369
1	-1.505254	-0.411716	3.653302
1	-1.279888	-1.953505	2.786575
6	-2.173118	-2.608581	-0.928380
6	-0.831227	-2.828288	-1.245267
6	-0.103270	-1.856998	-2.009153
6	-0.741941	-0.699811	-2.495886
6	-2.107917	-0.453931	-2.163144
6	-2.789754	-1.381424	-1.335544
1	-2.602202	0.453356	-2.500178
1	-2.711954	-3.305372	-0.291392
1	-0.303373	-3.687902	-0.841991
1	0.958644	-2.008410	-2.171478
1	-0.172832	0.042689	-3.050889
1	-3.803697	-1.156813	-1.008055
6	-0.353479	1.291956	-0.182363
1	-0.856547	1.858944	0.616672
1	-0.515791	1.828796	-1.130655
1	-2.676968	1.361462	-0.444743
1	0.721129	1.324173	0.032395
6	-3.797971	2.559344	0.528348
8	-3.430334	1.970637	-0.613426
8	-3.293536	2.291271	1.602627
6	-4.878706	3.564214	0.317597
1	-2.205619	0.598621	1.700437
7	-1.989656	-0.395830	1.576208
7	0.577546	-1.142696	1.129071
16	2.131197	-1.462388	0.835172
6	2.916094	0.026682	0.231742
6	3.325953	0.997621	1.144390
6	3.018020	0.260139	-1.136957
6	3.823801	2.207965	0.678448
1	3.261086	0.800191	2.212601
6	3.518753	1.475446	-1.589827
1	2.710262	-0.510804	-1.839944
6	3.923938	2.467846	-0.692678

1	4.146068	2.968699	1.388723
1	3.602749	1.659614	-2.660436
6	4.488091	3.765511	-1.183878
1	4.147340	3.993568	-2.199507
1	4.206487	4.598548	-0.530128
1	5.585428	3.732820	-1.207744
8	2.222734	-2.436540	-0.260945
8	2.820901	-1.791987	2.093491
1	-2.889930	-0.874406	1.587283
1	-5.729336	3.098603	-0.190377
1	-4.511362	4.365154	-0.332931
1	-5.195373	3.981627	1.274143

Bn-Ru-NNTs.AA-AICl3-Presence-CO2-insertion-TS2_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 20.7418 33.6285 36.3192 cm(-1)

Electronic energy : =-3415.9724145
Zero-point correction= 0.442236
Thermal correction to Energy= 0.480319
Thermal correction to Enthalpy= 0.481263
Thermal correction to Gibbs Free Energy= 0.370388
Sum of electronic and zero-point Energies= -3415.530179
Sum of electronic and thermal Energies= -3415.492096
Sum of electronic and thermal Enthalpies= -3415.491152
Sum of electronic and thermal Free Energies= -3415.602026

Cartesian Coordinates

6	2.530254	0.723813	1.830415
6	2.302562	-0.472308	2.717626
44	1.706148	-1.538065	-0.016601
1	3.351781	1.337445	2.223905
1	1.614229	1.349060	1.852103
1	2.018415	-0.163172	3.733171
1	3.211977	-1.082577	2.777044
6	3.343311	-3.156669	-0.201840
6	3.335710	-2.282782	-1.313795
6	2.159545	-2.073273	-2.091910
6	0.950959	-2.706492	-1.695338
6	0.908320	-3.524276	-0.538436
6	2.103976	-3.695373	0.223937
1	-0.030826	-3.955608	-0.200296
1	4.242104	-3.294693	0.391766
1	4.224796	-1.707699	-1.558502
1	2.176758	-1.383723	-2.930465
1	0.030220	-2.493579	-2.235074
1	2.055499	-4.247784	1.161280
6	0.008441	-0.306208	-0.304968
1	-0.886426	-0.867973	0.010825
1	-0.127282	-0.064675	-1.367770
1	0.050070	0.636578	0.256104
8	-3.324967	-0.864993	1.200243
6	-2.507758	-1.525581	1.742400
8	-1.770099	-2.228524	2.272936
1	0.353285	-0.796711	2.207170
13	-4.121664	-0.684109	-0.626197
17	-6.173185	-0.762434	-0.171357
17	-3.354134	1.209516	-1.175206
17	-3.270277	-2.371342	-1.563942
1	1.153395	-2.179939	2.574684
16	3.328736	1.364982	-0.544868
6	1.938124	2.424436	-0.913557
6	1.546082	3.387126	0.019876
6	1.182568	2.210064	-2.060442
6	0.371803	4.097479	-0.184427
1	2.166999	3.584610	0.891622
6	0.014682	2.940301	-2.259871
1	1.507778	1.468344	-2.786816
6	-0.418979	3.875341	-1.318185
1	0.053188	4.840468	0.547014
1	-0.579690	2.772796	-3.157762
6	-1.696232	4.636306	-1.496915
1	-1.512972	5.717527	-1.539348
1	-2.217724	4.347443	-2.415519
1	-2.373530	4.465366	-0.649600
8	3.719112	0.724772	-1.806880
8	4.319456	2.231271	0.116476
7	2.826264	0.227482	0.488954
7	1.242726	-1.287536	2.091179
6	-1.218920	1.745617	2.548782
8	-1.842961	2.425643	1.591251
8	-1.231657	0.525949	2.610975
6	-0.507170	2.641362	3.501417
1	-2.213345	1.802629	0.938365
1	0.318923	3.134960	2.973976
1	-1.179566	3.428061	3.857316
1	-0.115272	2.067965	4.342741

Bn-Ru-NNTs.AA-AICl3-Presence-CO2-insertion-TS2

Number of imaginary frequencies : 1
The smallest frequencies are : -185.2472 14.4988 25.6075 cm(-1)

Electronic energy : =-3415.9540974
Zero-point correction= 0.442258
Thermal correction to Energy= 0.479640
Thermal correction to Enthalpy= 0.480584
Thermal correction to Gibbs Free Energy= 0.370531
Sum of electronic and zero-point Energies= -3415.511839
Sum of electronic and thermal Energies= -3415.474458
Sum of electronic and thermal Enthalpies= -3415.473514
Sum of electronic and thermal Free Energies= -3415.583566

Cartesian Coordinates

6	2.495927	-1.278148	1.637160
6	1.470766	-1.605054	2.688498
44	-0.199261	-1.540945	0.225803
1	3.432580	-1.812641	1.843386
1	2.713792	-0.193801	1.682745
1	1.777014	-1.227852	3.672796
1	1.315245	-2.688311	2.756884
6	-0.600611	-3.819423	0.294765
6	-0.018324	-3.453064	-0.935534
6	-0.582080	-2.447520	-1.768287
6	-1.757861	-1.796065	-1.341986
6	-2.372286	-2.154068	-0.111540
6	-1.738452	-3.106893	0.733088
1	-3.342597	-1.747196	0.163546
1	-0.124701	-4.556264	0.934525
1	0.934446	-3.884795	-1.226766
1	-0.076091	-2.152973	-2.680869
1	-2.183147	-0.994082	-1.942195
1	-2.154914	-3.298612	1.720393
6	0.124237	0.513631	-0.244099
1	-0.257728	1.211146	0.516616
1	-0.335132	0.776129	-1.206488
1	1.205095	0.659636	-0.313018
8	-2.770596	0.761637	0.065534
6	-2.393024	0.208996	1.073366
8	-2.387158	0.017709	2.224780
1	0.309719	0.033704	2.340114
13	-4.483289	1.437586	-0.486304
17	-4.204266	3.532661	-0.533007
17	-4.743516	0.504610	-2.369363
17	-5.736631	0.702547	1.062102
1	-0.554047	-1.255094	2.885989
16	3.020199	-1.635136	-0.870113
6	3.566922	0.048189	-1.132123
6	4.537842	0.599507	-0.296100
6	2.980082	0.818454	-2.133451
6	4.897107	1.932455	-0.453243
1	5.025163	-0.017163	0.456339
6	3.353074	2.148798	-2.281426
1	2.236476	0.370963	-2.789930
6	4.302952	2.729306	-1.436209
1	5.657597	2.366255	0.195974
1	2.899154	2.751448	-3.067084
6	4.652361	4.180145	-1.547169
1	5.718811	4.353958	-1.364422
1	4.399077	4.584961	-2.532616
1	4.097725	4.763962	-0.799539
8	2.358525	-2.056637	-2.110038
8	4.223529	-2.369091	-0.449478
7	1.936833	-1.667612	0.341454
7	0.202219	-0.983565	2.259395
6	2.126125	2.530861	2.155924
8	1.916759	3.050206	0.945962
8	1.341915	1.773205	2.698026
6	3.429386	2.955211	2.744532
1	1.098244	2.660812	0.583938
1	4.153577	2.145835	2.585643
1	3.815310	3.862243	2.273438
1	3.319393	3.096091	3.822363

Bn-Ru-NNTs-AA-AICl3-Presence-CO2-insertion-TS2_for

Number of imaginary frequencies : 0
The smallest frequencies are : 14.6259 26.4057 30.1830 cm(-1)

Electronic energy : =-3415.9734237
Zero-point correction= 0.444358
Thermal correction to Energy= 0.481888
Thermal correction to Enthalpy= 0.482833
Thermal correction to Gibbs Free Energy= 0.372490
Sum of electronic and zero-point Energies= -3415.529065
Sum of electronic and thermal Energies= -3415.491535
Sum of electronic and thermal Enthalpies= -3415.490591
Sum of electronic and thermal Free Energies= -3415.600933

Cartesian Coordinates

6	2.207382	-1.433491	1.678012
6	1.112157	-1.482829	2.707322
44	-0.509320	-1.451188	0.253180
1	2.982694	-2.178218	1.900127
1	2.676373	-0.434599	1.709007
1	1.440601	-1.055591	3.662864
1	0.761969	-2.506640	2.878805
6	-0.768495	-3.810632	0.653039
6	-0.212735	-3.641925	-0.628596
6	-0.822734	-2.823454	-1.606347
6	-2.034716	-2.191076	-1.296331
6	-2.626195	-2.389263	-0.018061
6	-1.977344	-3.164379	0.965448
1	-3.579464	-1.921500	0.212780
1	-0.243531	-4.395943	1.401561
1	0.754177	-4.086161	-0.847367
1	-0.336692	-2.665900	-2.561884
1	-2.513355	-1.532215	-2.013424
1	-2.408464	-3.243858	1.960062
6	0.039918	0.432669	-0.617435
1	-0.437949	1.316144	-0.178250
1	-0.224467	0.386778	-1.679261
1	1.119188	0.520387	-0.492195
8	-2.720899	0.427852	-0.464070
6	-2.104118	0.018421	0.598548
8	-2.361501	0.346684	1.738416
1	0.302982	0.277525	2.051251
13	-4.074190	1.623151	-0.421308
17	-3.360731	3.489482	0.365361
17	-4.623816	1.827137	-2.492779
17	-5.717963	0.804357	0.697744
1	-0.826530	-0.691039	2.745235
16	2.676560	-1.776534	-0.860034
6	3.544106	-0.221604	-1.000806
6	4.567906	0.081712	-0.105877
6	3.175664	0.688090	-1.992759
6	5.194286	1.321824	-0.183740
1	4.891286	-0.651478	0.629416
6	3.814711	1.916778	-2.059627
1	2.397477	0.425739	-2.705465
6	4.816049	2.261601	-1.144594
1	5.997252	1.562536	0.512316
1	3.530202	2.630697	-2.831620
6	5.440116	3.620581	-1.186854
1	6.312325	3.687733	-0.528114
1	5.753508	3.887935	-2.202914
1	4.718020	4.383977	-0.866756
8	1.942681	-1.980785	-2.110901
8	3.692304	-2.766513	-0.479280
7	1.590316	-1.690332	0.368767
7	-0.000684	-0.700722	2.145729
6	2.295373	2.613380	1.722886
8	2.109311	3.034120	0.471665
8	1.597824	1.764297	2.247221
6	3.445405	3.299820	2.376178
1	1.360571	2.541155	0.088875
1	4.370550	3.017090	1.859125
1	3.339003	4.385082	2.282683
1	3.508940	3.014476	3.426887

Bn-Ru-NNTs.AA-AICl3-Presence-C-C_bond formation-TS3_rev

Number of imaginary frequencies : 1
 The smallest frequencies are : -19.9606 17.8112 22.4536 cm(-1)

Electronic energy = -3415.977006
 Zero-point correction= 0.443707
 Thermal correction to Energy= 0.480620
 Thermal correction to Enthalpy= 0.481564
 Thermal correction to Gibbs Free Energy= 0.372163
 Sum of electronic and zero-point Energies= -3415.533299
 Sum of electronic and thermal Energies= -3415.496386
 Sum of electronic and thermal Enthalpies= -3415.495442
 Sum of electronic and thermal Free Energies= -3415.604843

Cartesian Coordinates

6	-1.627127	-1.302938	-1.838054
6	-0.239704	-1.795434	-2.131762
44	0.001484	-0.660341	0.643808
1	-2.369654	-1.966468	-2.295612
1	-1.759403	-0.290952	-2.262183
1	0.004057	-1.754411	-3.200381
1	-0.105283	-2.821791	-1.770652
6	1.321577	-2.621416	1.059484
6	0.109987	-2.863519	1.700014
6	-0.420972	-1.880887	2.574094
6	0.354890	-0.757051	2.938673
6	1.606619	-0.538191	2.337209
6	2.037874	-1.411257	1.322128
1	2.180433	0.350664	2.575314

1	1.700285	-3.309034	0.306707
1	-0.478948	-3.743091	1.454045
1	-1.420777	-2.003182	2.975902
1	-0.039818	-0.035981	3.649160
1	2.958945	-1.198033	0.783755
6	-1.391434	0.851170	1.359852
1	-1.934987	1.257102	0.505709
1	-0.891839	1.652182	1.913268
1	-2.062664	0.297600	2.019802
8	1.437974	1.831914	0.796840
6	0.526600	1.269170	0.034830
8	0.110758	1.765839	-0.995060
13	2.896306	2.587202	0.096699
17	3.481786	1.328967	-1.592156
17	4.383579	2.425144	1.639751
17	2.628604	4.609782	-0.540194
7	0.663874	-0.904642	-1.380547
7	-1.755707	-1.294610	-0.377950
16	-3.257637	-1.598215	0.177460
6	-4.321789	-0.207993	-0.189415
6	-4.724597	0.015770	-1.505886
6	-4.746641	0.637801	0.831387
6	-5.531983	1.107707	-1.795907
1	-4.431439	-0.669644	-2.297807
6	-5.561512	1.721322	0.526072
1	-4.452926	0.436883	1.858542
6	-5.956840	1.980397	-0.789098
1	-5.850293	1.283056	-2.822646
1	-5.904039	2.377862	1.324801
6	-6.805095	3.169740	-1.116651
1	-7.466832	2.969103	-1.966389
1	-7.419954	3.472682	-0.262402
1	-6.181215	4.030904	-1.389914
8	-3.207687	-1.723103	1.637865
8	-3.813673	-2.722774	-0.587107
1	1.632988	-1.245338	-1.425538
1	0.636476	0.018295	-1.822327
6	4.342343	-2.532362	-1.502159
8	5.128165	-1.472300	-1.351521
8	3.123238	-2.459260	-1.504203
6	5.116458	-3.793253	-1.668978
1	4.575582	-0.665736	-1.290272
1	4.442705	-4.650347	-1.696634
1	5.689312	-3.744229	-2.601309
1	5.837469	-3.901914	-0.852737

Bn-Ru-NNTs.AA-AICl3-Presence-C-C_bond formation-TS3

Number of imaginary frequencies : 1

The smallest frequencies are : -270.1953 15.1802 18.8931 cm(-1)

Electronic energy : =-3415.970909
Zero-point correction= 0.443122
Thermal correction to Energy= 0.480362
Thermal correction to Enthalpy= 0.481306
Thermal correction to Gibbs Free Energy= 0.369923
Sum of electronic and zero-point Energies= -3415.527787
Sum of electronic and thermal Energies= -3415.490547
Sum of electronic and thermal Enthalpies= -3415.489603
Sum of electronic and thermal Free Energies= -3415.600986

Cartesian Coordinates

6	-1.815296	-1.453625	-1.550205
6	-0.464542	-1.996633	-1.922102
44	0.045535	-0.610190	0.693405
1	-2.601028	-2.159517	-1.848010
1	-1.992680	-0.498738	-2.080280
1	-0.324004	-2.058538	-3.008104
1	-0.315805	-2.991826	-1.487261
6	0.785959	-2.636596	1.435179
6	-0.259886	-2.283621	2.305614
6	-0.267347	-1.017314	2.929135
6	0.835027	-0.145377	2.756963
6	1.966922	-0.563761	2.016426
6	1.916509	-1.773324	1.314938
1	2.816503	0.101451	1.899056
1	0.747509	-3.565219	0.872364
1	-1.133676	-2.923774	2.392673
1	-1.135777	-0.702487	3.497244
1	0.816307	0.848947	3.195266
1	2.728074	-2.044925	0.645398
6	-1.124926	1.330414	0.781105
1	-1.780382	1.339290	-0.089170
1	-0.782360	2.343557	1.008679
1	-1.644970	0.976171	1.675072
8	1.501388	1.932139	0.713353
6	0.629525	1.327807	-0.068997
8	0.501387	1.603852	-1.253821
13	3.004040	2.556637	-0.030987
17	3.807055	1.014857	-1.353302
17	4.336468	2.772755	1.649902

17	2.787555	4.412758	-1.075173
7	0.522074	-1.074290	-1.333759
7	-1.796110	-1.264276	-0.099395
16	-3.246724	-1.359356	0.634724
6	-4.340319	-0.129498	-0.065890
6	-5.001372	-0.396368	-1.262662
6	-4.523931	1.088158	0.587445
6	-5.833275	0.571645	-1.813418
1	-4.882493	-1.359723	-1.752968
6	-5.363442	2.041539	0.028160
1	-4.023452	1.278063	1.533946
6	-6.026500	1.801754	-1.180520
1	-6.350110	0.366032	-2.749666
1	-5.515138	2.991522	0.539166
6	-6.944710	2.832611	-1.759624
1	-7.900871	2.851441	-1.220614
1	-6.515605	3.838104	-1.682619
1	-7.164029	2.630827	-2.813145
8	-3.065793	-1.022634	2.051281
8	-3.859495	-2.653423	0.306256
1	1.466145	-1.468236	-1.416183
1	0.507397	-0.181030	-1.839256
6	4.034484	-3.003769	-1.667308
8	4.924463	-2.059265	-1.375903
8	2.829918	-2.820534	-1.598992
6	4.678998	-4.281528	-2.077768
1	4.454693	-1.227282	-1.166570
1	3.925619	-5.058121	-2.213963
1	5.223133	-4.126003	-3.015683
1	5.412252	-4.590680	-1.326379

Bn-Ru-NNTs.AA-AlCl3-Presence-C-C_bond formation-TS3_for

Number of imaginary frequencies : 1
The smallest frequencies are : -10.3131 18.5024 28.3408 cm(-1)

Electronic energy : =-3416.0557913
Zero-point correction= 0.444111
Thermal correction to Energy= 0.481603
Thermal correction to Enthalpy= 0.482547
Thermal correction to Gibbs Free Energy= 0.370490
Sum of electronic and zero-point Energies= -3415.611681
Sum of electronic and thermal Energies= -3415.574188
Sum of electronic and thermal Enthalpies= -3415.573244
Sum of electronic and thermal Free Energies= -3415.685301

Cartesian Coordinates

6	-1.323059	-1.061251	-2.162705
6	0.083964	-1.539895	-2.414378
44	-0.182025	-1.390223	0.554713
1	-2.019595	-1.530077	-2.866180
1	-1.380165	0.032200	-2.286661
1	0.476767	-1.139587	-3.357356
1	0.104084	-2.634889	-2.459415
6	0.898783	-2.821793	1.796824
6	-0.479195	-2.814721	2.173456
6	-1.105838	-1.611798	2.568117
6	-0.374166	-0.401520	2.499282
6	1.003664	-0.405251	2.144550
6	1.643449	-1.621008	1.824754
1	1.535909	0.535663	2.032864
1	1.355834	-3.734015	1.424563
1	-1.067528	-3.723034	2.080703
1	-2.170169	-1.602114	2.776899
1	-0.878966	0.548117	2.664679
1	2.658041	-1.610067	1.435936
6	-1.340967	2.381039	-0.214651
1	-1.848168	2.823383	-1.078220
1	-1.529546	2.979253	0.679644
1	-1.760643	1.374262	-0.075982
8	0.929838	2.696786	0.413982
6	0.120381	2.244779	-0.513077
8	0.522499	1.725096	-1.552734
13	2.701565	2.766635	0.142367
17	3.550498	0.779620	-0.107462
17	3.465638	3.552411	1.999551
17	3.220400	4.055085	-1.492789
7	0.911359	-1.114964	-1.268372
7	-1.654244	-1.426121	-0.765119
16	-3.266332	-1.792334	-0.486229
6	-4.061308	-0.213780	-0.325231
6	-4.498251	0.454263	-1.466825
6	-4.199543	0.353961	0.939647
6	-5.073585	1.711599	-1.331485
1	-4.406000	-0.011853	-2.445397
6	-4.780080	1.609528	1.055396
1	-3.873119	-0.193878	1.821302
6	-5.217311	2.309049	-0.075033
1	-5.426024	2.239541	-2.216141
1	-4.905246	2.057076	2.040276
6	-5.805151	3.678496	0.059053

1	-6.483003	3.908980	-0.769378
1	-6.354262	3.789015	1.000332
1	-5.014043	4.440144	0.054819
8	-3.347817	-2.473710	0.804019
8	-3.813616	-2.456061	-1.671311
1	1.810987	-1.606633	-1.233137
1	1.105177	-0.108651	-1.349243
6	4.518281	-2.699920	-0.991022
8	5.092952	-1.680300	-1.626104
8	3.333902	-2.715659	-0.701519
6	5.489134	-3.785557	-0.679915
1	4.429595	-0.976434	-1.750322
1	4.971141	-4.645047	-0.253096
1	6.027484	-4.079010	-1.586459
1	6.233344	-3.411357	0.031638

Solvent (DCM) Optimization of Bn-Ru-PP

CH4

Number of imaginary frequencies : 0
The smallest frequencies are : 1306.9134 1307.9284 1308.6481 cm(-1)

Electronic energy : =-40.4778172
Zero-point correction= 0.044450
Thermal correction to Energy= 0.047325
Thermal correction to Enthalpy= 0.048269
Thermal correction to Gibbs Free Energy= 0.024780
Sum of electronic and zero-point Energies= -40.433367
Sum of electronic and thermal Energies= -40.430493
Sum of electronic and thermal Enthalpies= -40.429548
Sum of electronic and thermal Free Energies= -40.453038

Cartesian Coordinates

6	0.000031	-0.000005	-0.000056
1	0.579175	0.919061	-0.121866
1	0.648458	-0.864128	-0.166517
1	-0.818751	-0.013656	-0.724133
1	-0.409066	-0.041248	1.012851

CO2

Number of imaginary frequencies : 0
The smallest frequencies are : 668.6616 668.6616 1404.2216 cm(-1)

Electronic energy : =-188.4972854
Zero-point correction= 0.011930
Thermal correction to Energy= 0.014549
Thermal correction to Enthalpy= 0.015493
Thermal correction to Gibbs Free Energy= -0.009425
Sum of electronic and zero-point Energies= -188.485356
Sum of electronic and thermal Energies= -188.482736
Sum of electronic and thermal Enthalpies= -188.481792
Sum of electronic and thermal Free Energies= -188.506710

Cartesian Coordinates

8	0.000000	0.000000	1.164686
6	0.000000	0.000000	-0.000007
8	0.000000	0.000000	-1.164681

AlCl3

Number of imaginary frequencies : 0
The smallest frequencies are : 137.9990 138.5440 184.5938 cm(-1)

Electronic energy : =-1623.1152937
Zero-point correction= 0.004713
Thermal correction to Energy= 0.010091
Thermal correction to Enthalpy= 0.011035
Thermal correction to Gibbs Free Energy= -0.024722
Sum of electronic and zero-point Energies= -1623.110580
Sum of electronic and thermal Energies= -1623.105203
Sum of electronic and thermal Enthalpies= -1623.104258
Sum of electronic and thermal Free Energies= -1623.140016

Cartesian Coordinates

13	0.000000	0.000000	0.000000
17	0.000000	2.081030	0.000000
17	1.802225	-1.040515	0.000000
17	-1.802225	-1.040515	0.000000

Bn-Ru-PP

Number of imaginary frequencies : 0
The smallest frequencies are : 56.5400 67.5750 113.9436 cm(-1)

Electronic energy : =-1089.3841471
Zero-point correction= 0.175759
Thermal correction to Energy= 0.187761
Thermal correction to Enthalpy= 0.188705
Thermal correction to Gibbs Free Energy= 0.137402
Sum of electronic and zero-point Energies= -1089.208388
Sum of electronic and thermal Energies= -1089.196386
Sum of electronic and thermal Enthalpies= -1089.195442
Sum of electronic and thermal Free Energies= -1089.246745

Cartesian Coordinates

```

6      3.034802 -0.650761  0.266008
6      2.970928  0.690929 -0.430646
44     -0.302488  0.001380 -0.209615
1      2.901511  0.546163 -1.517425
1      3.861390  1.304823 -0.229866
6     -1.527369  0.569167  1.426562
6     -1.579515 -0.854556  1.283251
6     -2.060347 -1.436222  0.079330
6     -2.340621 -0.587079 -1.004106
6     -2.331099  0.839653 -0.854749
6     -1.982771  1.418167  0.372272
1     -2.555555  1.468438 -1.711750
1     -1.145417  1.001390  2.347684
1     -1.230772 -1.487502  2.095265
1     -2.063158 -2.514938 -0.049215
1     -2.565499 -1.013858 -1.978227
1     -1.933426  2.498385  0.481895
15     1.441261  1.574093  0.227008
15     1.440309 -1.630782  0.038307
1      3.882754 -1.260934 -0.073468
1      3.158793 -0.515704  1.351872
1      1.486027 -1.603950 -1.407748
1      1.185250  2.431530 -0.893217

```

Bn-Ru-PP-TS1_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 51.6312 59.9962 99.3176 cm(-1)

```

Electronic energy :      =-1129.8444469
Zero-point correction=      0.221920
Thermal correction to Energy=      0.236094
Thermal correction to Enthalpy=      0.237038
Thermal correction to Gibbs Free Energy=      0.181469
Sum of electronic and zero-point Energies= -1129.622526
Sum of electronic and thermal Energies= -1129.608353
Sum of electronic and thermal Enthalpies= -1129.607408
Sum of electronic and thermal Free Energies= -1129.662977

```

Cartesian Coordinates

```

6     -2.901139 -0.420921 -0.880103
6     -3.049900  0.598263  0.227612
44     0.328328 -0.020310  0.250254
1     -3.193130  0.098797  1.194924
1     -3.899072  1.280326  0.069250
6      1.441453  1.045622 -1.543749
6      1.474179 -0.338945 -1.752311
6      1.982420 -1.201995 -0.739747
6      2.512846 -0.646642  0.449474
6      2.468732  0.743835  0.678666
6      1.868429  1.577330 -0.298079
1      2.835892  1.161406  1.611500
1      1.000218  1.701760 -2.289382
1      1.072519 -0.762206 -2.669476
1      1.976729 -2.278467 -0.886999
1      2.894898 -1.308410  1.223503
1      1.768145  2.643619 -0.109333
6      0.034436 -1.222925  2.001095
1     -0.978088 -1.184900  2.419408
1      0.734540 -0.883440  2.777151
1     -0.494995  0.752236  1.423273
1      0.262156 -2.270945  1.759581
15     -1.494737  1.635225  0.223780
15     -1.387856 -1.503316 -0.601687
1     -3.777855 -1.078047 -0.959248
1     -2.785851  0.080914 -1.852323
1     -1.917172 -2.093065  0.589193
1     -1.695211  2.253684  1.499275

```

Bn-Ru-PP-TS1

Number of imaginary frequencies : 1
The smallest frequencies are : -564.6540 41.4296 62.5597 cm(-1)

```

Electronic energy :      =-1129.8412467
Zero-point correction=      0.219960
Thermal correction to Energy=      0.234098
Thermal correction to Enthalpy=      0.235042
Thermal correction to Gibbs Free Energy=      0.179433
Sum of electronic and zero-point Energies= -1129.621287
Sum of electronic and thermal Energies= -1129.607149
Sum of electronic and thermal Enthalpies= -1129.606204
Sum of electronic and thermal Free Energies= -1129.661814

```

Cartesian Coordinates

```

6     -2.848956 -0.532035 -0.885883

```

6	-3.045929	0.636162	0.056328
44	0.330788	-0.011348	0.220051
1	-3.279907	0.272676	1.066052
1	-3.865898	1.297415	-0.260890
6	1.401709	0.782471	-1.665866
6	1.476139	-0.620060	-1.663852
6	2.035360	-1.305302	-0.546997
6	2.511252	-0.559107	0.552425
6	2.448949	0.857905	0.558514
6	1.856736	1.519531	-0.536625
1	2.797402	1.419289	1.420575
1	0.924542	1.300935	-2.493315
1	1.072133	-1.187396	-2.498248
1	2.063196	-2.390972	-0.529261
1	2.886858	-1.081325	1.429838
1	1.740891	2.600544	-0.521230
6	-0.054664	-0.688683	2.270990
1	-1.061876	-0.625895	2.704998
1	0.635985	-0.165483	2.943245
1	-0.674539	0.545736	1.353848
1	0.208364	-1.752479	2.231367
15	-1.462133	1.646549	0.054740
15	-1.384092	-1.598015	-0.371543
1	-3.741565	-1.171137	-0.936393
1	-2.651565	-0.176122	-1.908530
1	-1.947653	-1.930621	0.903871
1	-1.651248	2.270836	1.329681

Bn-Ru-PP-TS1_for

Number of imaginary frequencies : 0

The smallest frequencies are : 49.4850 72.9301 82.8561 cm(-1)

Electronic energy : =-1129.8690919
 Zero-point correction= 0.223493
 Thermal correction to Energy= 0.238889
 Thermal correction to Enthalpy= 0.239833
 Thermal correction to Gibbs Free Energy= 0.181139
 Sum of electronic and zero-point Energies= -1129.645599
 Sum of electronic and thermal Energies= -1129.630203
 Sum of electronic and thermal Enthalpies= -1129.629258
 Sum of electronic and thermal Free Energies= -1129.687953

Cartesian Coordinates

6	2.980957	-0.833730	-0.431960
6	2.969933	0.272110	0.601536
44	-0.333250	0.025270	-0.021266
1	2.961251	1.251728	0.102523
1	3.852690	0.236562	1.257552
6	-1.502564	-1.378144	1.063295
6	-1.546930	-1.708923	-0.327230
6	-2.069537	-0.779577	-1.271430
6	-2.406739	0.507075	-0.822935
6	-2.383449	0.837206	0.572423
6	-1.987750	-0.114409	1.522030
1	-2.630507	1.849209	0.883833
1	-1.093016	-2.093680	1.771667
1	-1.167409	-2.671420	-0.661202
1	-2.074648	-1.015183	-2.332065
1	-2.669340	1.278893	-1.542658
1	-1.936845	0.141383	2.577221
6	0.295911	3.156579	-0.794621
1	1.210873	3.583693	-1.215948
1	0.458625	2.922885	0.262871
1	0.039842	2.246227	-1.353700
1	-0.526230	3.873027	-0.884350
15	1.414024	0.028547	1.633198
15	1.410535	-0.812146	-1.474685
1	3.851331	-0.778094	-1.099952
1	3.021325	-1.818849	0.058076
1	1.654148	0.503447	-2.005788
1	1.243552	1.383151	2.073267

Bn-Ru-PP-TS2_rev

Number of imaginary frequencies : 0

The smallest frequencies are : 35.8604 49.6972 64.4587 cm(-1)

Electronic energy : =-1318.3850253
 Zero-point correction= 0.236219
 Thermal correction to Energy= 0.254273
 Thermal correction to Enthalpy= 0.255217
 Thermal correction to Gibbs Free Energy= 0.189614
 Sum of electronic and zero-point Energies= -1318.148807
 Sum of electronic and thermal Energies= -1318.130752
 Sum of electronic and thermal Enthalpies= -1318.129808
 Sum of electronic and thermal Free Energies= -1318.195411

Cartesian Coordinates

6	2.821866	1.759570	-0.449181
6	2.180137	2.218990	0.847269
44	0.193068	-0.433969	-0.066642
1	3.911163	1.891372	-0.424525
1	2.449482	2.359362	-1.291839
1	2.255116	3.301114	1.017938
1	2.632332	1.701745	1.704623
6	0.485564	-2.036637	1.544291
6	0.770730	-2.571221	0.262977
6	-0.187780	-2.519148	-0.781965
6	-1.447307	-1.898619	-0.539744
6	-1.752950	-1.363707	0.727906
6	-0.750448	-1.373580	1.740593
1	-2.717611	-0.901539	0.916735
1	1.233608	-2.059305	2.331386
1	1.750262	-3.003397	0.066393
1	0.055480	-2.904851	-1.767797
1	-2.167435	-1.809186	-1.350911
1	-0.950727	-0.886593	2.692831
6	-0.256263	0.579192	-1.909005
1	0.394944	1.431562	-2.153117
1	-1.291733	0.954436	-1.899736
1	-0.168875	-0.141659	-2.735114
8	-3.798466	0.750803	-0.905604
6	-3.316217	1.531078	-0.187321
8	-2.849842	2.316305	0.536331
15	0.414613	1.683176	0.766614
1	-0.101094	2.041886	2.037288
1	-0.154317	2.736763	0.003885
15	2.458368	-0.053809	-0.839653
1	3.182161	-0.549971	0.299036

Bn-Ru-PP-TS2

Number of imaginary frequencies : 1
The smallest frequencies are : -423.2554 33.7434 69.6296 cm(-1)

Electronic energy : =-1318.332822
Zero-point correction= 0.235776
Thermal correction to Energy= 0.252733
Thermal correction to Enthalpy= 0.253677
Thermal correction to Gibbs Free Energy= 0.191710
Sum of electronic and zero-point Energies= -1318.097046
Sum of electronic and thermal Energies= -1318.080089
Sum of electronic and thermal Enthalpies= -1318.079145
Sum of electronic and thermal Free Energies= -1318.141112

Cartesian Coordinates

6	3.187745	0.529948	-0.558848
6	2.998678	0.638119	0.944334
44	-0.158990	-0.309846	-0.066013
1	4.180601	0.139934	-0.815583
1	3.103941	1.522230	-1.024666
1	3.647122	1.386583	1.418211
1	3.168654	-0.331482	1.431979
6	-0.079172	-2.141841	1.153080
6	-0.289172	-2.524530	-0.195746
6	-1.394615	-2.022403	-0.927308
6	-2.276993	-1.113415	-0.295871
6	-2.118536	-0.750302	1.063375
6	-0.987762	-1.228754	1.765687
1	-2.797221	-0.039103	1.523034
1	0.790155	-2.502347	1.696805
1	0.430316	-3.175204	-0.687688
1	-1.520961	-2.276076	-1.975318
1	-3.060867	-0.637410	-0.876907
1	-0.800323	-0.891817	2.782924
6	-0.441144	1.503245	-1.606252
1	0.593578	1.864181	-1.598216
1	-1.001189	2.351006	-2.027883
1	-0.597943	0.731745	-2.371718
8	-2.824727	1.738334	-0.604676
6	-1.726488	2.092547	-0.248622
8	-1.167509	2.828602	0.530373
15	1.225695	1.078780	1.147469
1	1.018600	1.201400	2.540597
1	1.225874	2.435416	0.765791
15	1.902175	-0.599210	-1.357310
1	2.399802	-1.770544	-0.697702

Bn-Ru-PP-TS2_for

Number of imaginary frequencies : 0
The smallest frequencies are : 20.9308 38.0940 55.9192 cm(-1)

Electronic energy : =-1318.3782369
Zero-point correction= 0.239559
Thermal correction to Energy= 0.257506
Thermal correction to Enthalpy= 0.258450
Thermal correction to Gibbs Free Energy= 0.191447

Sum of electronic and zero-point Energies= -1318.138678
Sum of electronic and thermal Energies= -1318.120731
Sum of electronic and thermal Enthalpies= -1318.119787
Sum of electronic and thermal Free Energies= -1318.186790

.....
Cartesian Coordinates

.....
6 0.049026 3.086200 0.589734
6 -0.150639 3.135318 -0.910783
44 -0.766351 -0.210270 -0.120033
1 -0.253707 4.027014 1.067960
1 1.111481 2.929614 0.823136
1 0.614859 3.722563 -1.435321
1 -1.132659 3.562025 -1.166219
6 -2.639967 -1.350599 -0.133513
6 -2.158498 -1.331911 1.201310
6 -0.853169 -1.799378 1.500026
6 -0.025444 -2.258896 0.451495
6 -0.525848 -2.347834 -0.879546
6 -1.823165 -1.887102 -1.174134
1 0.126780 -2.689184 -1.678233
1 -3.624497 -0.953147 -0.361262
1 -2.765791 -0.885971 1.985216
1 -0.458851 -1.709081 2.508345
1 1.001645 -2.547849 0.659235
1 -2.184283 -1.889936 -2.198456
6 3.063192 0.327516 1.183713
1 2.916175 1.343091 0.795359
1 3.815924 0.346601 1.973750
1 2.101146 -0.002532 1.597577
8 4.557825 -1.183292 0.067247
6 3.507590 -0.584941 0.078262
8 2.656566 -0.710118 -0.953200
15 -0.145386 1.376803 -1.487344
1 -0.068516 1.479344 -2.902620
15 -0.886912 1.674806 1.419032
1 -2.190843 2.173654 1.086998
1 1.821420 -0.211400 -0.801085

.....
Bn-Ru-PP-ALCl3-Presence-CO2-insertion-TS2_rev

.....
Number of imaginary frequencies : 0
The smallest frequencies are : 21.3895 30.5439 46.4357 cm(-1)

Electronic energy : =-2941.5200567
Zero-point correction= 0.243047
Thermal correction to Energy= 0.267824
Thermal correction to Enthalpy= 0.268768
Thermal correction to Gibbs Free Energy= 0.185891
Sum of electronic and zero-point Energies= -2941.277010
Sum of electronic and thermal Energies= -2941.252233
Sum of electronic and thermal Enthalpies= -2941.251289
Sum of electronic and thermal Free Energies= -2941.334166

.....
Cartesian Coordinates

.....
6 3.744689 2.272573 -0.966485
6 3.436982 2.577948 0.487186
44 1.773971 -0.393121 -0.042253
1 4.726954 2.671839 -1.248627
1 2.997747 2.747964 -1.616785
1 3.349955 3.649484 0.703031
1 4.208714 2.157632 1.147827
6 2.521322 -1.912111 1.539580
6 2.856427 -2.356303 0.247267
6 1.854885 -2.521815 -0.756064
6 0.508634 -2.220899 -0.442333
6 0.150445 -1.754080 0.844751
6 1.176285 -1.535705 1.802873
1 -0.887780 -1.530880 1.080483
1 3.290446 -1.777675 2.294449
1 3.896982 -2.550252 -0.002917
1 2.127964 -2.854907 -1.753225
1 -0.254864 -2.305502 -1.213625
1 0.921702 -1.108812 2.771285
6 0.707444 0.579144 -1.621234
1 1.091776 1.566954 -1.912133
1 -0.348560 0.707686 -1.335446
1 0.731779 -0.058582 -2.517358
8 -2.282827 1.115419 0.428408
6 -1.681324 1.321943 1.420281
8 -1.094980 1.550948 2.382302
1 0.893116 2.634924 0.455111
13 -3.817265 0.030023 -0.332538
17 -5.116442 1.584760 -0.898968
17 -2.851834 -1.029202 -1.871095
17 -4.328641 -1.062804 1.399836
1 3.316394 0.429574 -2.576804
1 1.735542 1.881396 2.283265
15 3.745337 0.393256 -1.211554
15 1.867141 1.689027 0.884677

Bn-Ru-PP-AlCl3-Presence-CO2-insertion-TS2

Number of imaginary frequencies : 1
 The smallest frequencies are : -170.2759 10.3888 28.0404 cm(-1)

Electronic energy : =-2941.5156176
 Zero-point correction= 0.241938
 Thermal correction to Energy= 0.266179
 Thermal correction to Enthalpy= 0.267123
 Thermal correction to Gibbs Free Energy= 0.184874
 Sum of electronic and zero-point Energies= -2941.273679
 Sum of electronic and thermal Energies= -2941.249438
 Sum of electronic and thermal Enthalpies= -2941.248494
 Sum of electronic and thermal Free Energies= -2941.330743

Cartesian Coordinates

6	3.571863	2.374606	-0.730204
6	3.348278	2.496841	0.763587
44	1.544222	-0.352047	-0.068705
1	4.548993	2.781233	-1.019239
1	2.801863	2.934057	-1.278656
1	3.301149	3.531599	1.121833
1	4.133392	1.971891	1.325459
6	2.458980	-2.068213	1.240997
6	2.765348	-2.284816	-0.112990
6	1.740706	-2.336213	-1.099656
6	0.389644	-2.206230	-0.700169
6	0.058610	-2.012167	0.660104
6	1.108527	-1.849902	1.605626
1	-0.983964	-2.000027	0.974015
1	3.249719	-1.998770	1.981906
1	3.804294	-2.364129	-0.423429
1	1.994435	-2.472419	-2.147244
1	-0.398535	-2.234211	-1.449481
1	0.866228	-1.613726	2.639113
6	0.547889	0.721046	-1.618112
1	0.653978	1.814766	-1.569229
1	-0.522717	0.485024	-1.578816
1	0.919991	0.393890	-2.598020
8	-1.757213	0.753869	0.335217
6	-1.079803	0.519986	1.302591
8	-0.824519	0.460702	2.437795
1	0.825778	2.650953	0.794411
13	-3.513222	0.218266	-0.253814
17	-4.346282	2.043782	-0.913873
17	-3.132844	-1.212096	-1.768212
17	-4.303769	-0.591226	1.541905
1	3.095659	0.720905	-2.521447
1	1.652473	1.640191	2.508108
15	3.526181	0.542246	-1.171380
15	1.759567	1.622913	1.097489

Bn-Ru-PP-AlCl3-Presence-CO2-insertion-TS2_for

Number of imaginary frequencies : 0
 The smallest frequencies are : 23.0046 31.6360 35.2071 cm(-1)

Electronic energy : =-2941.5516781
 Zero-point correction= 0.244800
 Thermal correction to Energy= 0.268658
 Thermal correction to Enthalpy= 0.269602
 Thermal correction to Gibbs Free Energy= 0.189637
 Sum of electronic and zero-point Energies= -2941.306878
 Sum of electronic and thermal Energies= -2941.283020
 Sum of electronic and thermal Enthalpies= -2941.282076
 Sum of electronic and thermal Free Energies= -2941.362041

Cartesian Coordinates

6	-2.437272	2.947497	0.190092
6	-1.773502	2.763925	-1.176334
44	-1.444518	-0.358461	0.164493
1	-3.528412	2.929422	0.096138
1	-2.174438	3.916132	0.632024
1	-1.280181	3.669206	-1.547699
1	-2.490699	2.441812	-1.940031
6	-3.036524	-0.563800	-1.555751
6	-3.760570	-0.368881	-0.365198
6	-3.521139	-1.211538	0.742386
6	-2.652697	-2.323828	0.611250
6	-1.960710	-2.539434	-0.589106
6	-2.100396	-1.623114	-1.656263
1	-1.242282	-3.348641	-0.664137
1	-3.166846	0.123507	-2.388607
1	-4.446396	0.469541	-0.273005
1	-4.009973	-1.011975	1.692431
1	-2.481934	-2.977535	1.462106
1	-1.510827	-1.746352	-2.560600
6	-0.710597	-0.704503	2.186861
1	-0.001258	0.054772	2.522685

1	-0.215172	-1.682789	2.209763
1	-1.580029	-0.732002	2.853462
8	1.476461	-0.016322	0.523313
6	0.593541	-0.852940	0.028725
8	0.902002	-1.899095	-0.518399
1	0.594846	2.050107	-0.433356
13	3.200130	-0.015788	0.040544
17	3.315959	0.171408	-2.108994
17	3.951675	1.800991	0.941340
17	4.313762	-1.705218	0.767778
1	-0.650208	2.154453	1.715875
1	-0.078887	1.120922	-2.291717
15	-1.966193	1.651003	1.483393
15	-0.535969	1.428190	-0.989492

 Bn-Ru-PP-AlCl3-Presence-C-C_bond formation-TS3_rev

Number of imaginary frequencies : 1
 The smallest frequencies are : -16.8443 17.7175 35.0003 cm(-1)

Electronic energy : =-2941.5504722
 Zero-point correction= 0.245126
 Thermal correction to Energy= 0.267844
 Thermal correction to Enthalpy= 0.268788
 Thermal correction to Gibbs Free Energy= 0.192473
 Sum of electronic and zero-point Energies= -2941.305346
 Sum of electronic and thermal Energies= -2941.282629
 Sum of electronic and thermal Enthalpies= -2941.281684
 Sum of electronic and thermal Free Energies= -2941.357999

 Cartesian Coordinates

6	-2.623623	-2.690974	-0.569210
6	-2.026790	-2.933952	0.808117
44	-1.337232	0.405528	-0.157599
1	-3.423677	-3.409114	-0.787746
1	-1.849421	-2.794319	-1.336947
1	-1.244149	-3.698033	0.804204
1	-2.789174	-3.223526	1.539775
6	-2.463366	1.798569	1.331565
6	-2.885144	2.217021	0.054663
6	-1.921076	2.547584	-0.914312
6	-0.541526	2.548971	-0.585385
6	-0.132147	2.265041	0.732503
6	-1.085267	1.850836	1.677136
1	0.923873	2.270800	0.988851
1	-3.192512	1.448435	2.058123
1	-3.939370	2.193541	-0.207672
1	-2.230147	2.779361	-1.929715
1	0.199759	2.773128	-1.347267
1	-0.765386	1.551201	2.673057
6	-1.182064	-0.010549	-2.293696
1	-1.182493	-1.073646	-2.544794
1	-0.257955	0.447995	-2.664505
1	-2.035384	0.476887	-2.776286
8	1.428487	0.196284	-0.747012
6	0.418026	-0.632006	-0.573705
8	0.539985	-1.846476	-0.604407
1	-0.047313	-1.622765	1.980016
13	3.051897	-0.102154	-0.075245
17	2.773096	-0.687884	1.991675
17	4.003804	1.834967	-0.157273
17	4.221529	-1.545385	-1.154710
15	-3.335444	-0.961361	-0.586992
15	-1.296570	-1.342634	1.398126
1	-3.530111	-0.863353	-1.992641
1	-2.055993	-1.002452	2.539598

 Bn-Ru-PP-AlCl3-Presence-C-C_bond formation-TS3

Number of imaginary frequencies : 1
 The smallest frequencies are : -322.3504 22.5365 36.0822 cm(-1)

Electronic energy : =-2941.5358563
 Zero-point correction= 0.244337
 Thermal correction to Energy= 0.267365
 Thermal correction to Enthalpy= 0.268309
 Thermal correction to Gibbs Free Energy= 0.191096
 Sum of electronic and zero-point Energies= -2941.291519
 Sum of electronic and thermal Energies= -2941.268492
 Sum of electronic and thermal Enthalpies= -2941.267547
 Sum of electronic and thermal Free Energies= -2941.344760

 Cartesian Coordinates

6	-2.663429	-2.661366	-0.508778
6	-2.114189	-2.859872	0.894375
44	-1.354314	0.421652	-0.144309
1	-3.470804	-3.373902	-0.719665
1	-1.867294	-2.824620	-1.243527
1	-1.416749	-3.700619	0.961016

1	-2.916179	-3.024556	1.623015
6	-2.443065	1.773248	1.273126
6	-2.879958	2.200653	-0.003096
6	-1.934203	2.548483	-0.979353
6	-0.550486	2.540378	-0.655105
6	-0.118553	2.280336	0.660943
6	-1.058715	1.845498	1.610540
1	0.940273	2.300123	0.903230
1	-3.164156	1.420914	2.006414
1	-3.937145	2.164272	-0.253680
1	-2.253194	2.782288	-1.991231
1	0.184918	2.750127	-1.427850
1	-0.730358	1.550019	2.604853
6	-0.693536	-0.353760	-2.232475
1	-1.181404	-1.302496	-2.445246
1	0.252029	-0.304204	-2.779769
1	-1.273686	0.488446	-2.622629
8	1.436006	0.203502	-0.866063
6	0.425852	-0.651986	-0.811186
8	0.577585	-1.853234	-0.609180
1	0.034023	-1.658897	1.871617
13	2.987521	-0.101312	-0.049668
17	2.634145	-0.590731	2.029744
17	3.972610	1.823256	-0.151557
17	4.199265	-1.593188	-1.014269
15	-3.345281	-0.917045	-0.629662
15	-1.243297	-1.307533	1.401197
1	-3.370596	-0.830441	-2.053716
1	-1.878324	-0.943956	2.610838

Bn-Ru-PP-AlCl3-Presence-C-C_bond formation-TS3_for

Number of imaginary frequencies : 0
The smallest frequencies are : 15.6903 24.0191 29.2752 cm(-1)

Electronic energy : =-2941.6127573
Zero-point correction= 0.245585
Thermal correction to Energy= 0.269562
Thermal correction to Enthalpy= 0.270506
Thermal correction to Gibbs Free Energy= 0.188760
Sum of electronic and zero-point Energies= -2941.367173
Sum of electronic and thermal Energies= -2941.343195
Sum of electronic and thermal Enthalpies= -2941.342251
Sum of electronic and thermal Free Energies= -2941.423997

Cartesian Coordinates

6	3.033759	2.680336	-0.086335
6	2.643235	2.526350	1.373655
44	1.547816	-0.399701	-0.101812
1	3.919326	3.320030	-0.187026
1	2.216636	3.153002	-0.648814
1	2.374596	3.471433	1.859136
1	3.451512	2.058282	1.952567
6	2.869576	-1.930717	0.726061
6	2.759913	-2.214722	-0.666313
6	1.488497	-2.350970	-1.248396
6	0.312105	-2.295455	-0.431420
6	0.406546	-2.103547	0.951748
6	1.692823	-1.848721	1.517269
1	-0.490475	-2.029462	1.561667
1	3.842317	-1.744204	1.172315
1	3.650513	-2.226911	-1.289738
1	1.391575	-2.467626	-2.323797
1	-0.667694	-2.358882	-0.901664
1	1.777427	-1.595730	2.571578
6	-1.613163	1.468032	-2.579548
1	-0.956789	1.746913	-3.405009
1	-2.153957	2.348916	-2.216608
1	-2.363478	0.750011	-2.933861
8	-1.468266	0.495505	-0.398241
6	-0.840045	0.858428	-1.459612
8	0.395376	0.718052	-1.560238
1	0.143509	2.213880	1.030672
13	-3.084706	0.068602	0.213615
17	-2.807962	-0.158103	2.331955
17	-3.614115	-1.792477	-0.725138
17	-4.503885	1.614831	-0.228449
15	3.429070	0.971804	-0.794476
15	1.220274	1.360086	1.362983
1	3.006216	1.254693	-2.129306
1	0.920844	1.087555	2.715900

Solvent (toluene) Optimization of Bn-Ru-NNTs

Bn-Ru-NNTs-AA

Number of imaginary frequencies : 0
The smallest frequencies are : 17.4074 24.6509 35.7828 cm(-1)

Electronic energy : =-1563.8301864
Zero-point correction= 0.373631
Thermal correction to Energy= 0.399141
Thermal correction to Enthalpy= 0.400085
Thermal correction to Gibbs Free Energy= 0.315678
Sum of electronic and zero-point Energies= -1563.456555
Sum of electronic and thermal Energies= -1563.431045
Sum of electronic and thermal Enthalpies= -1563.430101
Sum of electronic and thermal Free Energies= -1563.514508

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Cartesian Coordinates

6	0.621862	0.240127	2.144260
6	-0.790070	0.478700	2.617266
44	-1.096901	-0.656552	-0.103238
1	1.235186	-0.195001	2.942893
1	1.091707	1.187022	1.828906
1	-0.840442	1.327351	3.311467
1	-1.157928	-0.413684	3.138142
6	-2.589312	-2.124711	-0.723804
6	-1.334255	-2.483808	-1.308026
6	-0.625862	-1.548074	-2.082756
6	-1.146250	-0.229980	-2.227292
6	-2.417567	0.111302	-1.691840
6	-3.150591	-0.848179	-0.956505
1	-2.753005	1.146411	-1.702191
1	-3.086331	-2.816405	-0.049520
1	-0.877705	-3.440255	-1.070939
1	0.371167	-1.791063	-2.435699
1	-0.549475	0.539250	-2.710642
1	-4.036250	-0.527915	-0.410618
7	-1.633242	0.692309	1.435856
1	-1.579598	1.643492	1.038096
7	0.540360	-0.679654	0.986896
16	1.978798	-1.484456	0.661717
6	3.068110	-0.189412	0.115384
6	4.001034	0.344250	0.996023
6	2.943661	0.300280	-1.184299
6	4.819267	1.383501	0.565169
1	4.089866	-0.061736	2.000872
6	3.765611	1.336698	-1.596574
1	2.220769	-0.144107	-1.865548
6	4.713059	1.894962	-0.728724
1	5.557157	1.804329	1.246133
1	3.683051	1.722579	-2.611932
6	5.590172	3.013765	-1.197492
1	4.993773	3.881298	-1.505800
1	6.282006	3.342107	-0.415652
1	6.184549	2.711759	-2.068582
8	1.733204	-2.381780	-0.463278
8	2.512730	-2.022362	1.911559
6	-4.127238	2.117409	0.377987
8	-4.299735	1.141910	1.166651
8	-3.028964	2.649276	0.072712
6	-5.373513	2.640792	-0.322510
1	-2.665347	0.658594	1.605794
1	-6.256165	2.552590	0.318292
1	-5.243359	3.676126	-0.650941
1	-5.557149	2.026168	-1.215569

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Bn-Ru-NNTs-AA-Presence-TS1_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 30.5010 34.0808 45.2737 cm(-1)

Electronic energy : =-1604.3164162
Zero-point correction= 0.420743
Thermal correction to Energy= 0.449662
Thermal correction to Enthalpy= 0.450606
Thermal correction to Gibbs Free Energy= 0.361074
Sum of electronic and zero-point Energies= -1603.895673
Sum of electronic and thermal Energies= -1603.866754
Sum of electronic and thermal Enthalpies= -1603.865810
Sum of electronic and thermal Free Energies= -1603.955342

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Cartesian Coordinates

6	0.476248	-0.352732	2.315995
6	-0.967775	-0.218571	2.729156

44	-1.074253	-0.809077	-0.172027
1	1.048974	-0.920918	3.058157
1	0.940795	0.644233	2.213270
1	-1.078696	0.480342	3.568210
1	-1.353492	-1.196682	3.041483
6	-2.604438	-2.020458	-1.171319
6	-1.320809	-2.383778	-1.687485
6	-0.473414	-1.400965	-2.232587
6	-0.876726	-0.037422	-2.187299
6	-2.165328	0.322668	-1.702684
6	-3.042323	-0.679076	-1.224034
1	-2.420839	1.370986	-1.558267
1	-3.218133	-2.769070	-0.678540
1	-0.961818	-3.403212	-1.579047
1	0.532219	-1.672465	-2.536951
1	-0.177222	0.745587	-2.471359
1	-3.953545	-0.377974	-0.709164
6	0.552156	2.707106	-0.058226
1	1.098087	3.189829	0.758317
1	0.889616	3.129915	-1.010088
1	-0.523290	2.880312	0.062161
1	0.760670	1.630457	-0.047240
6	-4.000244	2.025818	0.568256
8	-4.329120	0.931668	1.108889
8	-2.841231	2.517371	0.513984
6	-5.107472	2.783817	-0.150290
1	-1.641220	1.229851	1.341370
7	-1.729279	0.219581	1.554388
7	0.487889	-1.042017	1.007213
16	1.968038	-1.729222	0.601687
6	2.962820	-0.331875	0.132296
6	3.651595	0.380955	1.109983
6	2.991710	0.070672	-1.200452
6	4.355409	1.521441	0.743911
1	3.650305	0.033130	2.140440
6	3.704101	1.208766	-1.549585
1	2.474271	-0.518598	-1.954346
6	4.382622	1.958417	-0.583115
1	4.899503	2.083562	1.501335
1	3.740215	1.525651	-2.591022
6	5.099636	3.216000	-0.962948
1	5.519793	3.151711	-1.972531
1	4.410647	4.071232	-0.953490
1	5.912462	3.445897	-0.266213
8	1.756200	-2.554221	-0.584146
8	2.555155	-2.320962	1.802118
1	-2.765873	0.181571	1.646985
1	-6.073684	2.634539	0.341173
1	-5.196661	2.387493	-1.172042
1	-4.879480	3.851076	-0.225814

Bn-Ru-NNTs-AA-Presence-TS1

Number of imaginary frequencies : 1
The smallest frequencies are : -1660.2236 21.9564 28.3928 cm(-1)

Electronic energy = -1604.2791829
Zero-point correction= 0.416629
Thermal correction to Energy= 0.444343
Thermal correction to Enthalpy= 0.445287
Thermal correction to Gibbs Free Energy= 0.357673
Sum of electronic and zero-point Energies= -1603.862554
Sum of electronic and thermal Energies= -1603.834840
Sum of electronic and thermal Enthalpies= -1603.833895
Sum of electronic and thermal Free Energies= -1603.921510

Cartesian Coordinates

6	0.127913	-0.437326	2.406702
6	-1.332822	-0.685093	2.686054
44	-1.074321	-0.690025	-0.337710
1	0.748849	-0.842669	3.214307
1	0.305642	0.653938	2.355132
1	-1.670196	-0.165392	3.592188
1	-1.504941	-1.761867	2.804802
6	-2.332681	-2.421190	-0.777648
6	-0.998854	-2.739035	-1.104482
6	-0.261937	-1.906131	-2.004023
6	-0.857858	-0.750192	-2.536566
6	-2.208276	-0.415306	-2.207009
6	-2.936338	-1.246747	-1.332707
1	-2.634407	0.530267	-2.527214
1	-2.867683	-3.015609	-0.040812
1	-0.486419	-3.554201	-0.602867
1	0.788991	-2.118057	-2.167807
1	-0.259654	-0.057025	-3.123699
1	-3.926467	-0.936610	-1.006169
6	-0.264414	1.517981	-0.334692
1	-0.259025	2.204352	0.521361
1	-0.171395	2.089264	-1.267312
1	-1.575131	1.455157	-0.373840
1	0.650550	0.925742	-0.253035

6	-3.161921	2.718466	0.499765
8	-2.801119	2.046362	-0.534480
8	-2.746258	2.516214	1.653834
6	-4.160058	3.819945	0.235432
1	-2.224232	0.817487	1.576301
7	-2.086624	-0.212783	1.507159
7	0.407703	-1.105137	1.140770
16	1.936955	-1.586786	0.888316
6	2.830805	-0.170639	0.261657
6	3.194076	0.845847	1.145529
6	3.053465	-0.028244	-1.103624
6	3.756799	2.012207	0.649214
1	3.044172	0.713164	2.215054
6	3.622799	1.145489	-1.587187
1	2.792744	-0.842188	-1.776162
6	3.972110	2.184580	-0.723334
1	4.042340	2.808907	1.335478
1	3.806127	1.256296	-2.655303
6	4.584870	3.451326	-1.236467
1	4.630291	3.465117	-2.330259
1	4.014306	4.329803	-0.911354
1	5.606967	3.578832	-0.858086
8	1.945555	-2.582516	-0.188874
8	2.558272	-1.931442	2.170955
1	-3.022974	-0.614009	1.507858
1	-5.014832	3.427213	-0.325508
1	-3.695921	4.589545	-0.391608
1	-4.504048	4.273078	1.168052

 Bn-Ru-NNTs-AA-Presence-TS1_for

Number of imaginary frequencies : 0
 The smallest frequencies are : 19.5683 27.0235 34.4254 cm(-1)

Electronic energy : =-1604.3129582
 Zero-point correction= 0.422261
 Thermal correction to Energy= 0.450472
 Thermal correction to Enthalpy= 0.451416
 Thermal correction to Gibbs Free Energy= 0.361818
 Sum of electronic and zero-point Energies= -1603.890697
 Sum of electronic and thermal Energies= -1603.862486
 Sum of electronic and thermal Enthalpies= -1603.861542
 Sum of electronic and thermal Free Energies= -1603.951140

 Cartesian Coordinates

6	0.292126	-0.498759	2.407209
6	-1.142430	-0.839911	2.722973
44	-0.970500	-0.744551	-0.306704
1	0.952316	-0.889839	3.191019
1	0.409196	0.601751	2.384970
1	-1.475296	-0.383030	3.664031
1	-1.245281	-1.928727	2.800688
6	-2.152448	-2.629957	-0.908755
6	-0.808882	-2.830917	-1.227188
6	-0.097985	-1.852291	-1.997767
6	-0.754249	-0.706991	-2.488209
6	-2.122890	-0.479191	-2.154797
6	-2.787328	-1.412548	-1.319264
1	-2.633272	0.418087	-2.494649
1	-2.678667	-3.332897	-0.267905
1	-0.261879	-3.674273	-0.816110
1	0.966270	-1.990891	-2.154214
1	-0.195284	0.042944	-3.043409
1	-3.804877	-1.199724	-0.994113
6	-0.365134	1.295072	-0.196440
1	-0.853339	1.868959	0.607475
1	-0.537092	1.830450	-1.143791
1	-2.649516	1.424446	-0.470862
1	0.712434	1.328562	0.000479
6	-3.833887	2.545842	0.511190
8	-3.413922	2.019389	-0.642048
8	-3.367722	2.237869	1.590635
6	-4.925209	3.542505	0.305483
1	-2.198929	0.613547	1.701641
7	-1.979645	-0.381704	1.590716
7	0.579297	-1.113288	1.118009
16	2.131844	-1.464043	0.822835
6	2.924636	0.025564	0.227604
6	3.338317	0.989377	1.145145
6	3.033316	0.264697	-1.138675
6	3.841867	2.199416	0.686279
1	3.274543	0.781950	2.211354
6	3.541040	1.479139	-1.584857
1	2.728884	-0.506118	-1.842940
6	3.946626	2.465485	-0.682644
1	4.167084	2.954876	1.400978
1	3.631662	1.666729	-2.654406
6	4.518497	3.763440	-1.165171
1	4.201994	3.988191	-2.189401
1	4.216197	4.599376	-0.524233
1	5.616234	3.737379	-1.161741

8	2.202313	-2.425105	-0.283605
8	2.808486	-1.800164	2.082023
1	-2.879273	-0.859266	1.616273
1	-5.736102	3.099374	-0.280957
1	-4.539993	4.392126	-0.268276
1	-5.302227	3.890156	1.267912

 Bn-Ru-NNTs_AA-AICI3-Presence-CO2-insertion-TS2_rev

Number of imaginary frequencies : 0
 The smallest frequencies are : 22.1019 29.8913 35.6793 cm(-1)

Electronic energy : =-3415.9596312
 Zero-point correction= 0.442830
 Thermal correction to Energy= 0.480747
 Thermal correction to Enthalpy= 0.481691
 Thermal correction to Gibbs Free Energy= 0.371212
 Sum of electronic and zero-point Energies= -3415.516802
 Sum of electronic and thermal Energies= -3415.478884
 Sum of electronic and thermal Enthalpies= -3415.477940
 Sum of electronic and thermal Free Energies= -3415.588419

 Cartesian Coordinates

6	2.521436	0.690431	1.839351
6	2.301757	-0.514426	2.717841
44	1.668455	-1.538286	-0.024632
1	3.354901	1.293931	2.223221
1	1.609462	1.323398	1.886897
1	2.032476	-0.217495	3.741790
1	3.212001	-1.125204	2.753694
6	3.300187	-3.153665	-0.255836
6	3.293649	-2.251911	-1.343475
6	2.114881	-2.017853	-2.110737
6	0.905352	-2.659591	-1.732190
6	0.863621	-3.511841	-0.600994
6	2.059550	-3.701798	0.155196
1	-0.074773	-3.954059	-0.276261
1	4.198786	-3.306572	0.333931
1	4.178796	-1.664456	-1.571292
1	2.135520	-1.300616	-2.925177
1	-0.017701	-2.428016	-2.260701
1	2.012549	-4.283410	1.075352
6	-0.016074	-0.284126	-0.273931
1	-0.912073	-0.840197	0.047546
1	-0.163734	-0.026955	-1.330810
1	0.048510	0.653957	0.293211
8	-3.340684	-0.824386	1.220201
6	-2.529957	-1.518389	1.730337
8	-1.816843	-2.267546	2.232120
1	0.344285	-0.830373	2.223886
13	-4.071797	-0.651439	-0.665683
17	-6.128480	-0.812377	-0.285756
17	-3.333524	1.269608	-1.138797
17	-3.111595	-2.320286	-1.527084
1	1.144134	-2.218951	2.567479
16	3.319597	1.348919	-0.533830
6	1.935422	2.421063	-0.898811
6	1.551726	3.388131	0.032368
6	1.184641	2.220894	-2.050644
6	0.390063	4.117428	-0.179348
1	2.178194	3.579174	0.901751
6	0.028854	2.967064	-2.256122
1	1.510553	1.480030	-2.777062
6	-0.396474	3.908894	-1.318112
1	0.080930	4.869249	0.547408
1	-0.562101	2.809514	-3.158014
6	-1.655641	4.696372	-1.515036
1	-1.448426	5.772408	-1.575846
1	-2.178134	4.404769	-2.432283
1	-2.346757	4.554153	-0.674134
8	3.696180	0.707782	-1.796990
8	4.306606	2.195956	0.148974
7	2.789810	0.208458	0.492293
7	1.232009	-1.321022	2.095795
6	-1.222438	1.677200	2.628496
8	-1.851876	2.357516	1.679436
8	-1.226240	0.457166	2.692323
6	-0.510645	2.574931	3.581547
1	-2.201535	1.746320	1.004516
1	0.305999	3.078548	3.048883
1	-1.185152	3.355275	3.947293
1	-0.107038	2.001316	4.416971

 Bn-Ru-NNTs_AA-AICI3-Presence-CO2-insertion-TS2

Number of imaginary frequencies : 1
 The smallest frequencies are : -163.8327 16.5096 21.2346 cm(-1)

Electronic energy : =-3415.9419504
 Zero-point correction= 0.442334

Thermal correction to Energy= 0.480009
 Thermal correction to Enthalpy= 0.480953
 Thermal correction to Gibbs Free Energy= 0.369529
 Sum of electronic and zero-point Energies= -3415.499616
 Sum of electronic and thermal Energies= -3415.461942
 Sum of electronic and thermal Enthalpies= -3415.460998
 Sum of electronic and thermal Free Energies= -3415.572421

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 Cartesian Coordinates

6	2.458298	-1.374667	1.629875
6	1.427722	-1.587353	2.705150
44	-0.286232	-1.496649	0.281747
1	3.338550	-2.004343	1.817033
1	2.786227	-0.318230	1.668104
1	1.781804	-1.210811	3.673933
1	1.178674	-2.650726	2.805394
6	-0.760455	-3.762596	0.425471
6	-0.187046	-3.449195	-0.823495
6	-0.734596	-2.452509	-1.675699
6	-1.884707	-1.755482	-1.252196
6	-2.488558	-2.057429	-0.002872
6	-1.868035	-3.002652	0.860434
1	-3.444467	-1.615496	0.271995
1	-0.295494	-4.495467	1.077558
1	0.749346	-3.914687	-1.117011
1	-0.226556	-2.195693	-2.598098
1	-2.299981	-0.961190	-1.870372
1	-2.279196	-3.157468	1.856478
6	0.103742	0.513679	-0.291721
1	-0.228149	1.257304	0.447231
1	-0.373877	0.752987	-1.251213
1	1.188448	0.590856	-0.403843
8	-2.730717	0.904213	0.182870
6	-2.402249	0.287414	1.168258
8	-2.434162	0.055646	2.314461
1	0.436149	0.136511	2.277477
13	-4.419465	1.512542	-0.538831
17	-4.468665	3.558955	-0.037032
17	-4.185751	1.045015	-2.588077
17	-5.743092	0.247730	0.537649
1	-0.547183	-1.009075	2.932563
16	2.891838	-1.753963	-0.894370
6	3.575944	-0.114915	-1.115907
6	4.596074	0.323444	-0.274795
6	3.047111	0.736344	-2.084921
6	5.054318	1.632382	-0.379838
1	5.045812	-0.364597	0.437250
6	3.518786	2.037770	-2.181625
1	2.270582	0.369119	-2.752727
6	4.510529	2.512517	-1.316806
1	5.857384	1.975380	0.272463
1	3.106874	2.706443	-2.936653
6	4.939921	3.944761	-1.369015
1	5.904515	4.100141	-0.873608
1	5.022483	4.307998	-2.399716
1	4.200025	4.580246	-0.863076
8	2.155671	-2.074080	-2.120318
8	4.026764	-2.600684	-0.510255
7	1.836244	-1.706588	0.348508
7	0.214306	-0.866392	2.272083
6	2.260909	2.644646	1.932826
8	2.056530	2.971945	0.657770
8	1.633345	1.777001	2.511576
6	3.346067	3.466205	2.543924
1	1.397875	2.357474	0.281142
1	4.287129	3.260426	2.019910
1	3.131258	4.531662	2.413970
1	3.451270	3.229631	3.603263

.....
 Bn-Ru-NNTs_AA-AICl3-Presence-CO2-insertion-TS2_for

Number of imaginary frequencies : 0
 The smallest frequencies are : 9.7407 18.0157 27.5247 cm(-1)

Electronic energy : =-3415.955008
 Zero-point correction= 0.444778
 Thermal correction to Energy= 0.482448
 Thermal correction to Enthalpy= 0.483392
 Thermal correction to Gibbs Free Energy= 0.371424
 Sum of electronic and zero-point Energies= -3415.510230
 Sum of electronic and thermal Energies= -3415.472560
 Sum of electronic and thermal Enthalpies= -3415.471616
 Sum of electronic and thermal Free Energies= -3415.583584

.....
 Cartesian Coordinates

6	2.195180	-1.503984	1.734565
6	1.086465	-1.427735	2.750069
44	-0.502425	-1.301923	0.284534
1	2.875428	-2.336025	1.958424
1	2.773955	-0.565514	1.782056

1	1.446605	-1.024053	3.704962
1	0.631895	-2.408836	2.931211
6	-0.901699	-3.677141	0.585543
6	-0.339458	-3.457811	-0.688647
6	-0.911868	-2.561164	-1.616070
6	-2.087467	-1.883054	-1.256402
6	-2.678180	-2.117918	0.015016
6	-2.069271	-2.987670	0.944956
1	-3.605991	-1.611616	0.278375
1	-0.402777	-4.334948	1.290659
1	0.606338	-3.929023	-0.940373
1	-0.418025	-2.374629	-2.562673
1	-2.537974	-1.159398	-1.930159
1	-2.504240	-3.104445	1.934433
6	0.133561	0.525927	-0.603409
1	-0.229902	1.422459	-0.087777
1	-0.236300	0.546359	-1.633785
1	1.222916	0.512215	-0.589624
8	-2.605618	0.751615	-0.330812
6	-2.067394	0.237011	0.712146
8	-2.341469	0.445688	1.873412
1	0.484413	0.386312	2.032987
13	-4.225351	1.578796	-0.430200
17	-4.180033	3.443727	0.599476
17	-4.502870	1.781488	-2.544651
17	-5.626606	0.165429	0.392838
1	-0.763236	-0.423989	2.743615
16	2.659737	-1.843077	-0.808511
6	3.609690	-0.338083	-0.964984
6	4.629321	-0.067148	-0.056109
6	3.313502	0.562664	-1.988567
6	5.319965	1.137406	-0.147318
1	4.902652	-0.803060	0.696257
6	4.018395	1.753401	-2.070868
1	2.538730	0.318633	-2.711646
6	5.014870	2.069396	-1.140689
1	6.121769	1.351469	0.558919
1	3.789990	2.461193	-2.866642
6	5.710251	3.392570	-1.206759
1	6.564543	3.440280	-0.523007
1	6.072557	3.606749	-2.219058
1	5.018993	4.203186	-0.939263
8	1.915101	-2.011706	-2.057129
8	3.611785	-2.880031	-0.401169
7	1.571549	-1.675953	0.415409
7	0.067840	-0.545909	2.162038
6	2.512970	2.632492	1.562508
8	2.258937	3.009688	0.310755
8	1.915284	1.730959	2.120828
6	3.613111	3.431284	2.175006
1	1.575687	2.418748	-0.054832
1	4.561191	3.139289	1.706183
1	3.467533	4.498342	1.983271
1	3.665830	3.239524	3.247347

Bn-Ru-NNTs.AA-AlCl3-Presence-C-C_bond formation-TS3_rev

Number of imaginary frequencies : 0

The smallest frequencies are : 13.3249 19.7684 22.0614 cm(-1)

Electronic energy : =-3415.9617639

Zero-point correction= 0.444437

Thermal correction to Energy= 0.482255

Thermal correction to Enthalpy= 0.483199

Thermal correction to Gibbs Free Energy= 0.369964

Sum of electronic and zero-point Energies= -3415.517327

Sum of electronic and thermal Energies= -3415.479509

Sum of electronic and thermal Enthalpies= -3415.478565

Sum of electronic and thermal Free Energies= -3415.591800

.....
Cartesian Coordinates

6	-1.539963	-1.311744	-1.864297
6	-0.159560	-1.855415	-2.102694
44	-0.025065	-0.517385	0.613374
1	-2.291306	-1.958754	-2.330919
1	-1.623998	-0.300052	-2.300642
1	0.122142	-1.853854	-3.163026
1	-0.077915	-2.876285	-1.711313
6	1.089114	-2.496524	1.374427
6	-0.124456	-2.489716	2.055135
6	-0.540406	-1.303332	2.708944
6	0.352819	-0.211613	2.855295
6	1.636086	-0.271305	2.282578
6	1.951778	-1.355519	1.452566
1	2.319361	0.568303	2.370731
1	1.383627	-3.343591	0.759319
1	-0.816689	-3.322607	1.972647
1	-1.544752	-1.247713	3.113420
1	0.039248	0.677859	3.395707
1	2.887081	-1.356295	0.897819
6	-1.481999	1.050866	1.008516

1	-1.972767	1.322402	0.072778
1	-1.042978	1.936190	1.478381
1	-2.192737	0.583151	1.693161
8	1.358397	2.002920	0.610428
6	0.533909	1.352218	-0.172000
8	0.208867	1.710218	-1.284582
13	2.946558	2.580928	0.003281
17	3.576680	1.052620	-1.440087
17	4.223610	2.461912	1.727094
17	2.901583	4.504205	-0.893757
7	0.751420	-0.979356	-1.342246
7	-1.704827	-1.282674	-0.411723
16	-3.201088	-1.648712	0.141652
6	-4.318696	-0.293860	-0.194725
6	-4.657187	0.002892	-1.514430
6	-4.845491	0.452848	0.853385
6	-5.499582	1.073456	-1.777323
1	-4.284675	-0.611038	-2.331237
6	-5.694998	1.516789	0.574248
1	-4.599300	0.188749	1.878718
6	-6.024731	1.851570	-0.740389
1	-5.766191	1.308338	-2.806927
1	-6.115051	2.098276	1.393718
6	-6.910948	3.020185	-1.041442
1	-7.491954	3.323267	-0.164200
1	-6.320271	3.888972	-1.359792
1	-7.611085	2.794776	-1.853857
8	-3.130510	-1.781940	1.599750
8	-3.702655	-2.778573	-0.645298
1	1.692020	-1.388790	-1.287714
1	0.827757	-0.088591	-1.839660
6	4.328831	-2.788158	-1.272069
8	5.167093	-1.763077	-1.236717
8	3.118856	-2.669377	-1.152426
6	5.031062	-4.087090	-1.476770
1	4.664812	-0.925579	-1.152405
1	4.326910	-4.915596	-1.393510
1	5.491638	-4.095261	-2.470557
1	5.840198	-4.198960	-0.748624

Bn-Ru-NNTs.AA-AlCl3-Presence-C-C_bond formation-TS3_

Number of imaginary frequencies : 1
The smallest frequencies are : -292.3451 13.0903 19.8985 cm(-1)

Electronic energy : --3415.9556842
Zero-point correction= 0.443641
Thermal correction to Energy= 0.480848
Thermal correction to Enthalpy= 0.481792
Thermal correction to Gibbs Free Energy= 0.370093
Sum of electronic and zero-point Energies= -3415.512044
Sum of electronic and thermal Energies= -3415.474837
Sum of electronic and thermal Enthalpies= -3415.473892
Sum of electronic and thermal Free Energies= -3415.585591

Cartesian Coordinates

6	-1.553518	-1.526967	-1.793909
6	-0.150639	-2.004702	-2.047623
44	-0.006450	-0.619985	0.625445
1	-2.280435	-2.232703	-2.213067
1	-1.701833	-0.543187	-2.277613
1	0.099129	-2.025203	-3.115786
1	-0.008306	-3.008633	-1.630406
6	0.924619	-2.526224	1.463559
6	-0.249917	-2.327464	2.203126
6	-0.506915	-1.069237	2.797255
6	0.481745	-0.055367	2.751449
6	1.737377	-0.307589	2.149682
6	1.925355	-1.502942	1.448041
1	2.494171	0.471879	2.124419
1	1.082437	-3.448643	0.911222
1	-1.039370	-3.073431	2.195416
1	-1.474827	-0.884568	3.250798
1	0.279668	0.926094	3.173970
1	2.830660	-1.651804	0.864661
6	-1.354417	1.209575	0.609825
1	-1.970355	1.149814	-0.286311
1	-1.110311	2.253387	0.828222
1	-1.891485	0.842187	1.488627
8	1.215833	2.036722	0.629794
6	0.430010	1.364909	-0.175835
8	0.314007	1.588904	-1.367427
13	2.787877	2.652620	0.004443
17	3.603001	1.066905	-1.269142
17	3.993519	2.779214	1.780111
17	2.643079	4.496014	-1.043183
7	0.735257	-1.066149	-1.336338
7	-1.691694	-1.442271	-0.340770
16	-3.193537	-1.705391	0.251504
6	-4.245180	-0.320148	-0.160709
6	-4.627110	-0.117201	-1.486628

6	-4.654980	0.560983	0.834217
6	-5.390302	0.994911	-1.812142
1	-4.349543	-0.833670	-2.256273
6	-5.427123	1.665291	0.493384
1	-4.377789	0.370302	1.867962
6	-5.794347	1.907383	-0.831751
1	-5.690330	1.157786	-2.846517
1	-5.756346	2.352271	1.271668
6	-6.597958	3.114027	-1.205798
1	-7.051660	3.586114	-0.328302
1	-5.969598	3.867654	-1.697685
1	-7.399636	2.859462	-1.908609
8	-3.102851	-1.736565	1.714595
8	-3.760781	-2.859190	-0.450699
1	1.692634	-1.433600	-1.300364
1	0.755615	-0.173498	-1.840512
6	4.352326	-2.806170	-1.314935
8	5.174615	-1.775056	-1.180421
8	3.138517	-2.710856	-1.223498
6	5.080806	-4.077393	-1.589561
1	4.657185	-0.952632	-1.056451
1	4.389573	-4.920641	-1.572312
1	5.557534	-4.014176	-2.573690
1	5.879364	-4.222060	-0.855687

Bn-Ru-NNTs.AA-AlCl3-Presence-C-C_bond formation-TS3_for

Number of imaginary frequencies : 0

The smallest frequencies are : 15.8372 26.8113 27.5640 cm(-1)

Electronic energy : =-3416.0398336
 Zero-point correction= 0.444983
 Thermal correction to Energy= 0.483272
 Thermal correction to Enthalpy= 0.484216
 Thermal correction to Gibbs Free Energy= 0.369375
 Sum of electronic and zero-point Energies= -3415.594851
 Sum of electronic and thermal Energies= -3415.556562
 Sum of electronic and thermal Enthalpies= -3415.555617
 Sum of electronic and thermal Free Energies= -3415.670458

Cartesian Coordinates

6	-1.289746	-1.100243	-2.110879
6	0.129468	-1.543276	-2.362244
44	-0.130278	-1.364826	0.597379
1	-1.979583	-1.610091	-2.792198
1	-1.376744	-0.012152	-2.257509
1	0.507669	-1.144689	-3.312062
1	0.179014	-2.638222	-2.392002
6	0.975258	-2.787535	1.825340
6	-0.401502	-2.793718	2.209129
6	-1.033683	-1.597724	2.616989
6	-0.311533	-0.381478	2.547072
6	1.064035	-0.371589	2.185704
6	1.710213	-1.580772	1.855703
1	1.589364	0.573085	2.072058
1	1.439178	-3.692057	1.443020
1	-0.988551	-3.702644	2.112686
1	-2.097457	-1.600408	2.827879
1	-0.822179	0.563778	2.718717
1	2.720766	-1.558246	1.456547
6	-1.433436	2.455181	-0.191683
1	-1.927886	2.881469	-1.070496
1	-1.596885	3.095699	0.678035
1	-1.892880	1.472515	-0.013873
8	0.849852	2.712122	0.412087
6	0.022378	2.254567	-0.491988
8	0.387248	1.678497	-1.514946
13	2.623409	2.830093	0.145029
17	3.478449	0.825019	-0.083351
17	3.368680	3.600957	2.002742
17	3.099180	4.068302	-1.525481
7	0.946535	-1.079128	-1.225821
7	-1.598494	-1.437543	-0.701109
16	-3.206082	-1.859199	-0.409053
6	-4.044832	-0.296252	-0.331313
6	-4.490224	0.301543	-1.507485
6	-4.205617	0.332641	0.900825
6	-5.089516	1.552365	-1.441296
1	-4.385937	-0.216787	-2.457855
6	-4.811522	1.580535	0.948317
1	-3.876825	-0.165914	1.810263
6	-5.251315	2.212766	-0.219372
1	-5.446294	2.026588	-2.354145
1	-4.952174	2.076160	1.907725
6	-5.856961	3.580100	-0.164143
1	-6.562088	3.743560	-0.985804
1	-6.383549	3.751082	0.780706
1	-5.079312	4.351351	-0.245513
8	-3.262443	-2.470228	0.915524
8	-3.713871	-2.592784	-1.566132
1	1.859932	-1.542573	-1.182833

1	1.106143	-0.066077	-1.314388
6	4.555342	-2.649413	-1.088626
8	5.195564	-1.548992	-1.463871
8	3.387340	-2.657732	-0.735981
6	5.432524	-3.853991	-1.146981
1	4.607090	-0.778063	-1.343658
1	4.864193	-4.748925	-0.891547
1	5.862635	-3.953749	-2.148573
1	6.268544	-3.731720	-0.450229

Solvent (toluene) Optimization of Bn-Ru-PP

CH4

Number of imaginary frequencies : 0
The smallest frequencies are : 1316.3307 1316.7088 1316.8927 cm(-1)

Electronic energy : HF=-40.4775299
Zero-point correction= 0.044604 (Hartree/Particle)
Thermal correction to Energy= 0.047477
Thermal correction to Enthalpy= 0.048421
Thermal correction to Gibbs Free Energy= 0.024934
Sum of electronic and zero-point Energies= -40.432926
Sum of electronic and thermal Energies= -40.430053
Sum of electronic and thermal Enthalpies= -40.429109
Sum of electronic and thermal Free Energies= -40.452596

Cartesian Coordinates

6	0.000030	-0.000008	-0.000053
1	0.599016	0.899422	-0.163122
1	0.631396	-0.884342	-0.116795
1	-0.813014	-0.033697	-0.729521
1	-0.417579	0.018664	1.009758

CO2

Number of imaginary frequencies : 0
The smallest frequencies are : 670.9762 670.9762 1404.9454 cm(-1)

Electronic energy : HF=-188.4982379
Zero-point correction= 0.011973 (Hartree/Particle)
Thermal correction to Energy= 0.014590
Thermal correction to Enthalpy= 0.015535
Thermal correction to Gibbs Free Energy= -0.009380
Sum of electronic and zero-point Energies= -188.486265
Sum of electronic and thermal Energies= -188.483648
Sum of electronic and thermal Enthalpies= -188.482703
Sum of electronic and thermal Free Energies= -188.507618

Cartesian Coordinates

8	0.000000	0.000000	1.164497
6	0.000000	0.000000	-0.000001
8	0.000000	0.000000	-1.164496

AlCl3

Number of imaginary frequencies : 0
The smallest frequencies are : 142.4681 143.3310 198.0131 cm(-1)

Electronic energy : HF=-1623.1130127
Zero-point correction= 0.004822 (Hartree/Particle)
Thermal correction to Energy= 0.010147
Thermal correction to Enthalpy= 0.011091
Thermal correction to Gibbs Free Energy= -0.024518
Sum of electronic and zero-point Energies= -1623.108190
Sum of electronic and thermal Energies= -1623.102865
Sum of electronic and thermal Enthalpies= -1623.101921
Sum of electronic and thermal Free Energies= -1623.137530

Cartesian Coordinates

13	0.000000	0.000000	0.000000
17	0.000000	2.078176	0.000000
17	1.799753	-1.039088	0.000000
17	-1.799753	-1.039088	0.000000

Bn-Ru-PP

Number of imaginary frequencies : 0
The smallest frequencies are : 8.8360 72.5337 115.3776 cm(-1)

Electronic energy : HF=-1089.3748164
Zero-point correction= 0.175636 (Hartree/Particle)
Thermal correction to Energy= 0.187519
Thermal correction to Enthalpy= 0.188463
Thermal correction to Gibbs Free Energy= 0.135796
Sum of electronic and zero-point Energies= -1089.199180
Sum of electronic and thermal Energies= -1089.187298
Sum of electronic and thermal Enthalpies= -1089.186353
Sum of electronic and thermal Free Energies= -1089.239020

Cartesian Coordinates

```

6      3.039436 -0.684793  0.169933
6      2.956396  0.691828 -0.450080
44     -0.274520 -0.068476 -0.105682
1      2.854782  0.603720 -1.540242
1      3.859232  1.283464 -0.243795
6     -1.687173  0.699736  1.325685
6     -1.827581 -0.724127  1.267013
6     -2.164409 -1.355105  0.045640
6     -2.203412 -0.568740 -1.125152
6     -2.118485  0.860109 -1.071310
6     -1.900885  1.491464  0.162063
1     -2.165681  1.440443 -1.987564
1     -1.401730  1.176251  2.259090
1     -1.660050 -1.315417  2.162921
1     -2.234314 -2.437064 -0.015782
1     -2.311785 -1.053461 -2.092018
1     -1.761337  2.568583  0.210113
15     1.452063  1.554001  0.285609
15     1.419732 -1.634342  0.051393
1      3.850490 -1.293747 -0.251003
1      3.235383 -0.610027  1.252908
1      0.997647 -1.034558 -1.286625
1      1.176027  2.427629 -0.815774

```

Bn-Ru-PP-TS1_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 44.4903 59.2627 126.3393 cm(-1)

```

Electronic energy : HF=-1129.8587226
Zero-point correction= 0.224032 (Hartree/Particle)
Thermal correction to Energy= 0.238931
Thermal correction to Enthalpy= 0.239875
Thermal correction to Gibbs Free Energy= 0.182707
Sum of electronic and zero-point Energies= -1129.634691
Sum of electronic and thermal Energies= -1129.619792
Sum of electronic and thermal Enthalpies= -1129.618847
Sum of electronic and thermal Free Energies= -1129.676016

```

Cartesian Coordinates

```

6     -2.911127 -0.596424 -0.777520
6     -2.993826  0.662540  0.057713
44     0.351545 -0.000593  0.153193
1     -3.110389  0.400769  1.118958
1     -3.848371  1.294810 -0.226802
6     1.320290  0.677926 -1.632887
6     1.388887 -0.743348 -1.583114
6     2.047105 -1.397283 -0.500410
6     2.530697 -0.614705  0.559027
6     2.478609  0.815135  0.510437
6     1.908897  1.464350 -0.594017
1     2.839485  1.393646  1.356859
1     0.797896  1.165493 -2.451901
1     0.917894 -1.331318 -2.367121
1     2.073422 -2.481984 -0.448208
1     2.926431 -1.099188  1.448957
1     1.832439  2.548303 -0.622335
6     -0.253064 -0.254740  2.800836
1     -1.201304 -0.464579  3.305702
1     0.382193  0.383896  3.419086
1     -0.561143  0.333074  1.899613
1     0.246907 -1.200719  2.585644
15     -1.402920  1.623290 -0.237722
15     -1.398855 -1.618274 -0.317715
1     -3.803909 -1.228977 -0.676132
1     -2.820145 -0.345973 -1.845531
1     -1.830285 -1.818351  1.037753
1     -1.381284  2.321244  1.016155

```

Bn-Ru-PP-TS1

Number of imaginary frequencies : 1
The smallest frequencies are : -551.6649 34.9992 64.4611 cm(-1)

```

Electronic energy : HF=-1129.8357332
Zero-point correction= 0.220379 (Hartree/Particle)
Thermal correction to Energy= 0.234433
Thermal correction to Enthalpy= 0.235377
Thermal correction to Gibbs Free Energy= 0.179841
Sum of electronic and zero-point Energies= -1129.615355
Sum of electronic and thermal Energies= -1129.601300
Sum of electronic and thermal Enthalpies= -1129.600356
Sum of electronic and thermal Free Energies= -1129.655893

```

Cartesian Coordinates

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6     -2.831190 -0.553101 -0.880761
6     -3.041759  0.633840  0.034608

```

44	0.335039	-0.006211	0.222946
1	-3.288718	0.289906	1.048064
1	-3.859777	1.286013	-0.305824
6	1.378552	0.741615	-1.686187
6	1.450852	-0.661228	-1.648569
6	2.025113	-1.319296	-0.522450
6	2.511174	-0.545022	0.553045
6	2.452544	0.872676	0.523579
6	1.847791	1.506423	-0.581095
1	2.808156	1.455220	1.368378
1	0.883763	1.239802	-2.515628
1	1.028687	-1.250370	-2.458395
1	2.044468	-2.404055	-0.475613
1	2.891474	-1.045361	1.441259
1	1.726582	2.586901	-0.590177
6	-0.054899	-0.617711	2.292709
1	-1.060184	-0.546735	2.730116
1	0.634286	-0.070609	2.947219
1	-0.698131	0.561085	1.332676
1	0.208539	-1.681888	2.285997
15	-1.460587	1.650389	0.029924
15	-1.375489	-1.614953	-0.332566
1	-3.723590	-1.192531	-0.930788
1	-2.622107	-0.217441	-1.907884
1	-1.944387	-1.901692	0.951663
1	-1.658694	2.284308	1.299689

 Bn-Ru-PP-TS1_for

Number of imaginary frequencies : 0
 The smallest frequencies are : 41.0627 55.5713 102.6459 cm(-1)

Electronic energy : HF=-1129.8388036
 Zero-point correction= 0.221536 (Hartree/Particle)
 Thermal correction to Energy= 0.235940
 Thermal correction to Enthalpy= 0.236884
 Thermal correction to Gibbs Free Energy= 0.180552
 Sum of electronic and zero-point Energies= -1129.617268
 Sum of electronic and thermal Energies= -1129.602863
 Sum of electronic and thermal Enthalpies= -1129.601919
 Sum of electronic and thermal Free Energies= -1129.658252

 Cartesian Coordinates

6	-2.873910	-0.434748	-0.885588
6	-3.048238	0.596231	0.207885
44	0.336908	-0.022481	0.248881
1	-3.211284	0.106736	1.176916
1	-3.896969	1.272505	0.023617
6	1.396781	1.003350	-1.579713
6	1.449710	-0.388171	-1.738881
6	1.986447	-1.206644	-0.703972
6	2.516078	-0.598457	0.461677
6	2.460920	0.799839	0.639317
6	1.831712	1.585213	-0.358641
1	2.830340	1.256595	1.552518
1	0.924915	1.624126	-2.336591
1	1.034768	-0.852685	-2.629775
1	1.986977	-2.287913	-0.808937
1	2.908087	-1.226970	1.258384
1	1.708756	2.654938	-0.205449
6	0.054920	-1.183702	2.030220
1	-0.958609	-1.155219	2.446324
1	0.744916	-0.808986	2.799110
1	-0.577512	0.738930	1.385687
1	0.300768	-2.233562	1.817134
15	-1.500239	1.644029	0.227968
15	-1.375649	-1.530311	-0.572016
1	-3.753517	-1.086086	-0.979905
1	-2.734544	0.057362	-1.859701
1	-1.916014	-2.074470	0.635432
1	-1.723252	2.260642	1.501368

 Bn-Ru-PP-ALCl3-Presence-CO2-insertion-TS2_rev

Number of imaginary frequencies : 0
 The smallest frequencies are : 15.5431 33.1878 36.5478 cm(-1)

Electronic energy : HF=-2941.5117738
 Zero-point correction= 0.243043 (Hartree/Particle)
 Thermal correction to Energy= 0.267868
 Thermal correction to Enthalpy= 0.268812
 Thermal correction to Gibbs Free Energy= 0.185456
 Sum of electronic and zero-point Energies= -2941.268731
 Sum of electronic and thermal Energies= -2941.243906
 Sum of electronic and thermal Enthalpies= -2941.242962
 Sum of electronic and thermal Free Energies= -2941.326318

 Cartesian Coordinates

6	3.816339	2.186598	-0.937852
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6	3.517271	2.500454	0.515637
44	1.693694	-0.370991	-0.041977
1	4.821814	2.529823	-1.211360
1	3.102971	2.707388	-1.591196
1	3.492081	3.573344	0.741534
1	4.258986	2.029174	1.176300
6	2.383882	-1.948460	1.512465
6	2.705092	-2.375182	0.211547
6	1.700801	-2.479751	-0.796336
6	0.363727	-2.144754	-0.476189
6	0.019817	-1.699731	0.821492
6	1.053522	-1.530469	1.781959
1	-1.017320	-1.480828	1.069754
1	3.157295	-1.853702	2.268680
1	3.739695	-2.591854	-0.044028
1	1.965119	-2.790326	-1.802954
1	-0.401674	-2.185677	-1.248983
1	0.812158	-1.118109	2.759932
6	0.716707	0.633711	-1.654597
1	1.102756	1.633346	-1.898568
1	-0.356617	0.737567	-1.438112
1	0.809568	0.020539	-2.562173
8	-2.127092	1.168881	0.299946
6	-1.565481	1.193704	1.337751
8	-1.052486	1.263303	2.365741
1	0.989659	2.706894	0.447569
13	-3.752888	0.064044	-0.342882
17	-5.120585	1.612843	-0.693383
17	-2.932397	-0.950372	-1.983395
17	-3.965956	-1.033430	1.453523
1	3.294237	0.378686	-2.553171
1	1.753604	1.908562	2.284845
15	3.719879	0.310427	-1.189372
15	1.895399	1.697461	0.888104

 Bn-Ru-PP-AICl3-Presence-CO2-insertion-TS2

Number of imaginary frequencies : 1

The smallest frequencies are : -150.2675 21.7668 27.7744 cm(-1)

Electronic energy : HF=-2941.5079875
 Zero-point correction= 0.242404 (Hartree/Particle)
 Thermal correction to Energy= 0.266528
 Thermal correction to Enthalpy= 0.267472
 Thermal correction to Gibbs Free Energy= 0.186172
 Sum of electronic and zero-point Energies= -2941.265583
 Sum of electronic and thermal Energies= -2941.241459
 Sum of electronic and thermal Enthalpies= -2941.240515
 Sum of electronic and thermal Free Energies= -2941.321815

 Cartesian Coordinates

6	3.723321	2.219865	-0.790714
6	3.475304	2.416746	0.691152
44	1.504678	-0.342334	-0.052595
1	4.735036	2.539685	-1.069279
1	3.013319	2.815644	-1.379945
1	3.496941	3.465316	1.010297
1	4.208539	1.859098	1.290578
6	2.309176	-2.060188	1.333240
6	2.623932	-2.337640	-0.007073
6	1.613450	-2.366501	-1.009027
6	0.264279	-2.154474	-0.638535
6	-0.074973	-1.900084	0.709373
6	0.966877	-1.760672	1.666776
1	-1.119536	-1.824543	1.007559
1	3.091773	-2.005861	2.083775
1	3.662432	-2.474905	-0.298068
1	1.877310	-2.544307	-2.047814
1	-0.513526	-2.161417	-1.399505
1	0.718468	-1.476480	2.686409
6	0.609489	0.707082	-1.675237
1	0.834253	1.782102	-1.722892
1	-0.478200	0.592670	-1.615635
1	0.934694	0.259656	-2.623329
8	-1.743807	0.896212	0.241335
6	-1.056077	0.695762	1.211875
8	-0.814728	0.703800	2.353887
1	0.972983	2.740474	0.623399
13	-3.495108	0.219388	-0.263893
17	-4.632939	1.978161	-0.484920
17	-3.098052	-0.884098	-2.022312
17	-3.910284	-0.973570	1.445380
1	3.136548	0.547403	-2.524205
1	1.673086	1.778045	2.415847
15	3.553795	0.379840	-1.169454
15	1.821389	1.667507	1.012544

 Bn-Ru-PP-AICl3-Presence-CO2-insertion-TS2_for

Number of imaginary frequencies : 0

The smallest frequencies are : 30.5071 39.2618 45.6202 cm(-1)

Electronic energy : HF=-2941.5340971
Zero-point correction= 0.245617 (Hartree/Particle)
Thermal correction to Energy= 0.269209
Thermal correction to Enthalpy= 0.270153
Thermal correction to Gibbs Free Energy= 0.191736
Sum of electronic and zero-point Energies= -2941.288480
Sum of electronic and thermal Energies= -2941.264888
Sum of electronic and thermal Enthalpies= -2941.263944
Sum of electronic and thermal Free Energies= -2941.342361

Cartesian Coordinates

6	-4.052448	1.390453	-0.555696
6	-2.996591	1.981883	-1.495955
44	-1.208933	-0.325272	0.281167
1	-4.646453	0.623190	-1.066161
1	-4.763834	2.154918	-0.219921
1	-3.160328	3.043601	-1.713861
1	-2.960259	1.459423	-2.459474
6	-2.221679	-1.531638	-1.444929
6	-2.618715	-2.177476	-0.254358
6	-1.646402	-2.599053	0.667920
6	-0.272668	-2.454833	0.357671
6	0.118491	-1.947380	-0.900328
6	-0.846227	-1.444145	-1.782621
1	1.175716	-1.867706	-1.140682
1	-2.973532	-1.150052	-2.130569
1	-3.674189	-2.263920	-0.008707
1	-1.948036	-3.009407	1.627689
1	0.487794	-2.745829	1.076851
1	-0.539019	-0.982199	-2.717961
6	-1.101090	-0.123305	2.443257
1	-1.107455	0.918255	2.775947
1	-0.178215	-0.600439	2.793438
1	-1.954556	-0.653458	2.883579
8	1.578566	-0.192882	0.805859
6	0.589244	0.664675	0.831880
8	0.712608	1.842360	1.099201
1	-1.298910	2.846988	0.230742
13	3.136750	0.172923	-0.016882
17	4.490637	1.360264	1.121928
17	3.905705	-1.806032	-0.403467
17	2.568012	1.104238	-1.889244
1	-2.954297	1.815832	1.630207
1	-0.383021	2.096909	-1.607601
15	-3.364948	0.594631	1.017554
15	-1.377786	1.767565	-0.660464

Bn-Ru-PP-AICl3-Presence-C-C_bond formation-TS3_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 27.2517 36.3207 37.5383 cm(-1)

Electronic energy : HF=-2941.5335974
Zero-point correction= 0.245371 (Hartree/Particle)
Thermal correction to Energy= 0.268944
Thermal correction to Enthalpy= 0.269888
Thermal correction to Gibbs Free Energy= 0.191254
Sum of electronic and zero-point Energies= -2941.288227
Sum of electronic and thermal Energies= -2941.264653
Sum of electronic and thermal Enthalpies= -2941.263709
Sum of electronic and thermal Free Energies= -2941.342344

Cartesian Coordinates

6	-2.750867	-2.609824	-0.559420
6	-2.105704	-2.908089	0.785063
44	-1.301934	0.410187	-0.158240
1	-3.590107	-3.288052	-0.757441
1	-2.012826	-2.733495	-1.359117
1	-1.359591	-3.705647	0.727915
1	-2.846896	-3.179395	1.545181
6	-2.283486	1.862596	1.379437
6	-2.743534	2.301790	0.123254
6	-1.811408	2.576342	-0.892961
6	-0.418747	2.513813	-0.628170
6	0.037107	2.217376	0.670606
6	-0.889033	1.844184	1.657549
1	1.104446	2.181389	0.875607
1	-2.996170	1.553735	2.140268
1	-3.809213	2.330194	-0.087995
1	-2.156401	2.820164	-1.894079
1	0.299786	2.696664	-1.422648
1	-0.533699	1.530773	2.637289
6	-1.231678	-0.019813	-2.296349
1	-1.295369	-1.080609	-2.547608
1	-0.294806	0.383671	-2.697040
1	-2.070712	0.510219	-2.759650
8	1.423340	0.063225	-0.842114
6	0.397522	-0.722314	-0.641781

8	0.434553	-1.938699	-0.679245
1	-0.021474	-1.706361	1.902976
13	3.035303	-0.146638	-0.082217
17	2.619998	-0.694438	1.975107
17	3.842050	1.852254	-0.147752
17	4.288765	-1.563697	-1.064446
15	-3.380503	-0.848048	-0.516179
15	-1.273524	-1.362489	1.364076
1	-3.628233	-0.719077	-1.911733
1	-1.980196	-1.010649	2.539034

Bn-Ru-PP-AICl3-Presence-C-C_bond formation-TS3

Number of imaginary frequencies : 1
The smallest frequencies are : -333.1378 15.6620 38.1181 cm(-1)

Electronic energy : HF=-2941.5193757
Zero-point correction= 0.244642 (Hartree/Particle)
Thermal correction to Energy= 0.267691
Thermal correction to Enthalpy= 0.268635
Thermal correction to Gibbs Free Energy= 0.191237
Sum of electronic and zero-point Energies= -2941.274733
Sum of electronic and thermal Energies= -2941.251685
Sum of electronic and thermal Enthalpies= -2941.250741
Sum of electronic and thermal Free Energies= -2941.328139

Cartesian Coordinates

6	-2.802018	-2.571763	-0.504821
6	-2.214216	-2.823470	0.874359
44	-1.318047	0.430970	-0.142735
1	-3.653672	-3.236590	-0.696542
1	-2.040817	-2.771447	-1.266715
1	-1.556458	-3.697782	0.897143
1	-2.996989	-2.966025	1.628348
6	-2.317886	1.843079	1.277393
6	-2.723958	2.289594	-0.003321
6	-1.755282	2.582697	-0.975397
6	-0.374769	2.493564	-0.647652
6	0.037334	2.205884	0.667998
6	-0.932426	1.827386	1.613483
1	1.095827	2.163089	0.913076
1	-3.062495	1.537008	2.008028
1	-3.780881	2.313120	-0.257328
1	-2.057728	2.837202	-1.987541
1	0.377127	2.656740	-1.416039
1	-0.621259	1.511627	2.607434
6	-0.759110	-0.365338	-2.247050
1	-1.302857	-1.284935	-2.451467
1	0.176364	-0.376909	-2.814257
1	-1.295879	0.504806	-2.637085
8	1.439603	0.056030	-0.934940
6	0.410930	-0.752868	-0.861984
8	0.470850	-1.957436	-0.669609
1	0.018484	-1.745301	1.822033
13	2.986757	-0.148150	-0.050339
17	2.497456	-0.590287	2.012443
17	3.825505	1.837257	-0.160834
17	4.266739	-1.615697	-0.922924
15	-3.390660	-0.789875	-0.582036
15	-1.246423	-1.325854	1.373956
1	-3.454139	-0.689279	-2.004836
1	-1.842259	-0.949097	2.602383

Bn-Ru-PP-AICl3-Presence-C-C_bond formation-TS3_for

Number of imaginary frequencies : 0
The smallest frequencies are : 33.9476 36.3557 48.8225 cm(-1)

Electronic energy : HF=-2941.6021936
Zero-point correction= 0.246318 (Hartree/Particle)
Thermal correction to Energy= 0.270023
Thermal correction to Enthalpy= 0.270968
Thermal correction to Gibbs Free Energy= 0.191460
Sum of electronic and zero-point Energies= -2941.355876
Sum of electronic and thermal Energies= -2941.332170
Sum of electronic and thermal Enthalpies= -2941.331226
Sum of electronic and thermal Free Energies= -2941.410733

Cartesian Coordinates

6	2.983916	2.679770	-0.106193
6	2.574899	2.555496	1.351822
44	1.518999	-0.397196	-0.098771
1	3.861026	3.330471	-0.210019
1	2.169120	3.125973	-0.693118
1	2.292179	3.508387	1.813913
1	3.383094	2.110929	1.949446
6	2.820452	-1.925710	0.758901
6	2.742840	-2.204707	-0.636270
6	1.484414	-2.342967	-1.246362

6	0.289018	-2.299559	-0.455849
6	0.351145	-2.111180	0.928484
6	1.623651	-1.847274	1.520833
1	-0.561032	-2.038512	1.516794
1	3.782544	-1.734274	1.225587
1	3.647539	-2.208122	-1.239186
1	1.412490	-2.451225	-2.324523
1	-0.682099	-2.366266	-0.944096
1	1.682091	-1.597325	2.577854
6	-1.607526	1.440497	-2.620922
1	-0.954620	1.717432	-3.449674
1	-2.168028	2.314359	-2.271191
1	-2.346799	0.705659	-2.963770
8	-1.450528	0.516324	-0.423379
6	-0.828531	0.857025	-1.490232
8	0.408839	0.716827	-1.592237
1	0.074130	2.205690	1.020125
13	-3.054225	0.066261	0.230967
17	-2.681619	-0.134902	2.335197
17	-3.525143	-1.810698	-0.701463
17	-4.477732	1.595404	-0.217387
15	3.417270	0.960232	-0.765162
15	1.166103	1.369788	1.349359
1	3.018299	1.212495	-2.112778
1	0.872682	1.109011	2.706773

Solvent (benzene) Optimization of Bn-Ru-NNTs

CH4

Number of imaginary frequencies : 0
The smallest frequencies are : 1316.8047 1317.1844 1317.3798 cm(-1)

Electronic energy : =-40.4776221
Zero-point correction= 0.044611
Thermal correction to Energy= 0.047484
Thermal correction to Enthalpy= 0.048428
Thermal correction to Gibbs Free Energy= 0.024941
Sum of electronic and zero-point Energies= -40.433011
Sum of electronic and thermal Energies= -40.430139
Sum of electronic and thermal Enthalpies= -40.429194
Sum of electronic and thermal Free Energies= -40.452681

Cartesian Coordinates

6	0.000030	-0.000008	-0.000053
1	0.599741	0.898539	-0.165298
1	0.630633	-0.885138	-0.114864
1	-0.813167	-0.034698	-0.729301
1	-0.417388	0.021342	1.009783

CO2

Number of imaginary frequencies : 0
The smallest frequencies are : 671.2946 671.2946 1404.9382 cm(-1)

Electronic energy : =-188.4983181
Zero-point correction= 0.011975
Thermal correction to Energy= 0.014592
Thermal correction to Enthalpy= 0.015536
Thermal correction to Gibbs Free Energy= -0.009378
Sum of electronic and zero-point Energies= -188.486343
Sum of electronic and thermal Energies= -188.483726
Sum of electronic and thermal Enthalpies= -188.482782
Sum of electronic and thermal Free Energies= -188.507696

Cartesian Coordinates

8	0.000000	0.000000	1.164500
6	0.000000	0.000000	-0.000001
8	0.000000	0.000000	-1.164499

CH3COOH

Number of imaginary frequencies : 0
The smallest frequencies are : 101.4568 430.4567 551.7067 cm(-1)

Electronic energy : =-228.9692241
Zero-point correction= 0.062187
Thermal correction to Energy= 0.066669
Thermal correction to Enthalpy= 0.067613
Thermal correction to Gibbs Free Energy= 0.035282
Sum of electronic and zero-point Energies= -228.907037
Sum of electronic and thermal Energies= -228.902555
Sum of electronic and thermal Enthalpies= -228.901611
Sum of electronic and thermal Free Energies= -228.933942

Cartesian Coordinates

6	-0.091771	0.122440	-0.000006
8	-0.653595	1.191675	-0.000046
8	-0.760973	-1.045018	-0.000004
1	-1.704750	-0.818389	-0.000037
6	1.385583	-0.098346	0.000048
1	1.676695	-0.680011	0.880794
1	1.676754	-0.680057	-0.880646
1	1.904972	0.860628	0.000041

Bn-Ru-NNTs-AA

Number of imaginary frequencies : 0
The smallest frequencies are : 12.4507 22.9060 39.2007 cm(-1)

Electronic energy : =-1563.830033
Zero-point correction= 0.373475
Thermal correction to Energy= 0.399092
Thermal correction to Enthalpy= 0.400036
Thermal correction to Gibbs Free Energy= 0.314887
Sum of electronic and zero-point Energies= -1563.456558
Sum of electronic and thermal Energies= -1563.430941
Sum of electronic and thermal Enthalpies= -1563.429997

Sum of electronic and thermal Free Energies= -1563.515146

Cartesian Coordinates

```
6 0.644002 0.398038 2.055089
6 -0.755179 0.626398 2.569688
44 -1.125898 -0.649296 -0.084289
1 1.297682 0.021014 2.851447
1 1.075928 1.337523 1.672024
1 -0.802919 1.510153 3.218910
1 -1.079267 -0.245855 3.150213
6 -2.645101 -2.149066 -0.543216
6 -1.406765 -2.560968 -1.129554
6 -0.718994 -1.697527 -2.002353
6 -1.236836 -0.392507 -2.235093
6 -2.488136 0.002767 -1.689115
6 -3.205716 -0.890833 -0.861464
1 -2.817591 1.036336 -1.772643
1 -3.127217 -2.781465 0.196812
1 -0.947765 -3.498050 -0.828179
1 0.266140 -1.972739 -2.363803
1 -0.649641 0.330934 -2.794918
1 -4.072680 -0.520145 -0.316801
7 -1.643298 0.756408 1.409708
1 -1.625766 1.686142 0.954760
7 0.543142 -0.582046 0.949334
16 1.962123 -1.439231 0.673363
6 3.099786 -0.194543 0.111867
6 4.063122 0.301522 0.981320
6 2.984308 0.292559 -1.189549
6 4.924423 1.299004 0.536349
1 4.139621 -0.100991 1.988558
6 3.849064 1.287700 -1.615521
1 2.233035 -0.120217 -1.860227
6 4.830444 1.805696 -0.760317
1 5.686243 1.690635 1.208376
1 3.773308 1.672617 -2.631726
6 5.759357 2.874255 -1.246358
1 5.204057 3.740953 -1.624865
1 6.428357 3.221911 -0.452985
1 6.381216 2.509518 -2.073436
8 1.708868 -2.361500 -0.429646
8 2.457188 -1.957414 1.947364
6 -4.117717 2.167005 0.300815
8 -4.309696 1.231635 1.131282
8 -3.008301 2.660895 -0.030594
6 -5.353583 2.689618 -0.418711
1 -2.665885 0.717513 1.614729
1 -6.231155 2.667883 0.234753
1 -5.194182 3.699290 -0.808367
1 -5.568227 2.029596 -1.271506
```

AIC13

Number of imaginary frequencies : 0
The smallest frequencies are : 142.6277 143.5242 198.4249 cm(-1)

```
Electronic energy : =-1623.1131315
Zero-point correction= 0.004827
Thermal correction to Energy= 0.010150
Thermal correction to Enthalpy= 0.011094
Thermal correction to Gibbs Free Energy= -0.024510
Sum of electronic and zero-point Energies= -1623.108305
Sum of electronic and thermal Energies= -1623.102982
Sum of electronic and thermal Enthalpies= -1623.102038
Sum of electronic and thermal Free Energies= -1623.137641
```

Cartesian Coordinates

```
13 0.000000 0.000000 0.000000
17 0.000000 2.078063 0.000000
17 1.799656 -1.039032 0.000000
17 -1.799656 -1.039032 0.000000
```

Bn-Ru-NNTs

Number of imaginary frequencies : 0
The smallest frequencies are : 20.3936 39.2629 41.6663 cm(-1)

```
Electronic energy : =-1334.8398333
Zero-point correction= 0.308717
Thermal correction to Energy= 0.328568
Thermal correction to Enthalpy= 0.329512
Thermal correction to Gibbs Free Energy= 0.259014
Sum of electronic and zero-point Energies= -1334.531116
Sum of electronic and thermal Energies= -1334.511265
Sum of electronic and thermal Enthalpies= -1334.510321
Sum of electronic and thermal Free Energies= -1334.580820
```

Cartesian Coordinates

6	-0.069339	2.155210	-1.163032
6	-1.392341	2.299694	-1.869374
44	-1.718147	-0.157303	-0.305907
1	0.355473	3.134234	-0.908469
1	0.642802	1.626051	-1.825750
1	-1.243922	2.614259	-2.912722
1	-2.000704	3.076398	-1.371440
6	-2.564646	-0.844700	1.602016
6	-1.355931	-1.562414	1.450495
6	-1.073392	-2.222139	0.240165
6	-2.048950	-2.235292	-0.805352
6	-3.317637	-1.631860	-0.610814
6	-3.552983	-0.886718	0.571590
1	-4.039485	-1.609333	-1.422870
1	-2.713856	-0.218422	2.476153
1	-0.581036	-1.436448	2.199649
1	-0.091240	-2.653558	0.067593
1	-1.806842	-2.689882	-1.761920
1	-4.464398	-0.304178	0.674173
7	-2.058149	1.008930	-1.791802
1	-2.860011	0.928112	-2.412755
7	-0.340759	1.361604	0.042531
16	0.831103	1.400504	1.175353
6	2.180666	0.415840	0.531310
6	3.094268	0.992861	-0.348261
6	2.283260	-0.931549	0.863828
6	4.097815	0.209048	-0.904016
1	3.029079	2.054574	-0.575031
6	3.294266	-1.703377	0.304759
1	1.585545	-1.360642	1.579397
6	4.213143	-1.147736	-0.589420
1	4.814983	0.658581	-1.589994
1	3.382528	-2.755684	0.573930
6	5.321993	-1.973952	-1.165505
1	5.068202	-3.039451	-1.177673
1	5.561360	-1.668826	-2.190312
1	6.241523	-1.866068	-0.575263
8	0.340149	0.715116	2.373342
8	1.353852	2.763922	1.301925

 Bn-Ru-NNTs-TS1_rev

Number of imaginary frequencies : 0
 The smallest frequencies are : 32.9023 34.0233 57.2173 cm(-1)

Electronic energy : --1375.3245528
 Zero-point correction= 0.355521
 Thermal correction to Energy= 0.379117
 Thermal correction to Enthalpy= 0.380061
 Thermal correction to Gibbs Free Energy= 0.302286
 Sum of electronic and zero-point Energies= -1374.969032
 Sum of electronic and thermal Energies= -1374.945436
 Sum of electronic and thermal Enthalpies= -1374.944491
 Sum of electronic and thermal Free Energies= -1375.022267

 Cartesian Coordinates

6	0.157725	1.866963	1.617816
6	1.456216	1.729533	2.369438
44	1.724265	-0.211873	0.189841
1	-0.209510	2.900415	1.638414
1	-0.605538	1.215590	2.088204
1	1.280856	1.753990	3.454959
1	2.124739	2.573952	2.121161
6	2.656832	-0.368352	-1.790793
6	1.404391	-1.012343	-1.918469
6	1.008372	-1.978631	-0.975815
6	1.907826	-2.361944	0.067284
6	3.217799	-1.820087	0.122297
6	3.571963	-0.781699	-0.774317
1	3.883021	-2.086258	0.939306
1	2.897116	0.475100	-2.430793
1	0.688464	-0.617051	-2.631603
1	-0.005509	-2.371285	-0.985046
1	1.576669	-3.056697	0.834839
1	4.517784	-0.260266	-0.655789
7	2.054618	0.469720	1.955651
1	2.832622	0.179373	2.543498
7	0.441548	1.429654	0.244912
16	-0.679435	1.845711	-0.865454
6	-2.070066	0.752732	-0.590401
6	-2.981957	1.038939	0.423783
6	-2.192864	-0.417408	-1.333971
6	-3.990972	0.128192	0.712193
1	-2.908831	1.978103	0.967655
6	-3.207690	-1.318450	-1.036948
1	-1.505664	-0.603448	-2.156378
6	-4.109007	-1.069500	0.001660
1	-4.704931	0.348676	1.505158
1	-3.308954	-2.231638	-1.623176
6	-5.154376	-2.076223	0.370675
1	-5.427084	-2.710028	-0.480141

1	-4.788688	-2.739766	1.166685
1	-6.065222	-1.596440	0.745486
8	-0.151788	1.533268	-2.196056
8	-1.166625	3.201146	-0.594429
6	-1.224091	-1.840949	2.178126
1	-1.458135	-2.814382	1.734512
1	-0.932360	-1.135541	1.392582
1	-2.106214	-1.460586	2.701515
1	-0.397800	-1.946338	2.887787

Bn-Ru-NNTs-TS1

Number of imaginary frequencies : 1
The smallest frequencies are : -1558.6257 16.9021 20.2679 cm(-1)

Electronic energy : =-1375.2716168
Zero-point correction= 0.351504
Thermal correction to Energy= 0.373494
Thermal correction to Enthalpy= 0.374439
Thermal correction to Gibbs Free Energy= 0.299615
Sum of electronic and zero-point Energies= -1374.920113
Sum of electronic and thermal Energies= -1374.898122
Sum of electronic and thermal Enthalpies= -1374.897178
Sum of electronic and thermal Free Energies= -1374.972002

Cartesian Coordinates

6	0.128138	2.078847	1.333079
6	1.423682	1.950863	2.098081
44	1.555175	-0.365652	0.269742
1	-0.117830	3.129098	1.135930
1	-0.687862	1.646788	1.944583
1	1.316132	2.392038	3.101690
1	2.208300	2.516231	1.561492
6	2.362284	-0.061797	-1.741145
6	1.631407	-1.282848	-1.774800
6	1.906279	-2.266905	-0.801190
6	2.947934	-2.086067	0.155535
6	3.670384	-0.869684	0.160501
6	3.399280	0.148208	-0.801678
1	4.395010	-0.681229	0.949771
1	2.040211	0.751652	-2.384263
1	0.801275	-1.390601	-2.464451
1	1.274490	-3.150429	-0.735216
1	3.118051	-2.830662	0.927722
1	3.915629	1.102303	-0.755589
7	1.719731	0.531796	2.176324
1	2.614475	0.329561	2.611865
7	0.324313	1.345732	0.081578
16	-0.826976	1.551405	-1.043823
6	-2.227011	0.542073	-0.571324
6	-3.100501	0.995992	0.415286
6	-2.398518	-0.719089	-1.134685
6	-4.129166	0.169974	0.850373
1	-2.984051	1.998363	0.821555
6	-3.435676	-1.532725	-0.694505
1	-1.726545	-1.045311	-1.925225
6	-4.310984	-1.105351	0.307234
1	-4.814666	0.522712	1.620263
1	-3.576879	-2.517061	-1.140099
6	-5.446909	-1.972425	0.757080
1	-5.227086	-3.035384	0.609403
1	-5.678428	-1.816189	1.816536
1	-6.361222	-1.748845	0.191651
8	-0.349622	1.003496	-2.318388
8	-1.301238	2.938574	-1.005121
6	-0.124527	-1.373237	1.587509
1	0.204612	-2.303231	2.064070
1	-0.581871	-1.598574	0.618510
1	-0.926682	-0.917708	2.184619
1	0.720855	-0.461557	1.988369

Bn-Ru-NNTs-TS1_for

Number of imaginary frequencies : 0
The smallest frequencies are : 26.1176 28.0371 29.7117 cm(-1)

Electronic energy : =-1375.3269461
Zero-point correction= 0.358419
Thermal correction to Energy= 0.380498
Thermal correction to Enthalpy= 0.381442
Thermal correction to Gibbs Free Energy= 0.306797
Sum of electronic and zero-point Energies= -1374.968527
Sum of electronic and thermal Energies= -1374.946448
Sum of electronic and thermal Enthalpies= -1374.945504
Sum of electronic and thermal Free Energies= -1375.020149

Cartesian Coordinates

6	0.108404	2.138332	1.202575
6	1.427233	2.167478	1.933918

44	1.562834	-0.360667	0.307004
1	-0.204647	3.160151	0.952959
1	-0.663462	1.715211	1.877423
1	1.349554	2.710439	2.885488
1	2.186410	2.653310	1.309450
6	2.368142	-0.225715	-1.779410
6	1.546929	-1.387339	-1.626956
6	1.841773	-2.321650	-0.604801
6	2.920574	-2.095306	0.291044
6	3.675603	-0.897280	0.147424
6	3.474981	-0.003536	-0.944958
1	4.440208	-0.667542	0.888756
1	2.065840	0.524408	-2.504734
1	0.674535	-1.508130	-2.260619
1	1.184826	-3.174655	-0.448543
1	3.112643	-2.777726	1.113991
1	4.073553	0.897270	-1.041860
7	1.856811	0.767127	2.145926
1	2.819147	0.736365	2.476462
7	0.305094	1.337667	0.002304
16	-0.855202	1.476052	-1.121035
6	-2.255230	0.497333	-0.589485
6	-3.130401	1.012691	0.365185
6	-2.423721	-0.797424	-1.068965
6	-4.155551	0.214156	0.855413
1	-3.015502	2.039852	0.705011
6	-3.459847	-1.582438	-0.577860
1	-1.745705	-1.175781	-1.830427
6	-4.334015	-1.094411	0.396299
1	-4.841125	0.613354	1.602496
1	-3.596917	-2.594774	-0.957101
6	-5.464319	-1.934368	0.908087
1	-5.258823	-3.003785	0.789584
1	-5.661178	-1.741443	1.968777
1	-6.394210	-1.719906	0.364908
8	-0.382941	0.861001	-2.365763
8	-1.333668	2.864043	-1.158956
6	-0.028995	-1.215594	1.416380
1	0.385779	-1.823110	2.237623
1	-0.646342	-1.874631	0.792317
1	-0.700212	-0.460254	1.848398
1	1.284351	0.340436	2.874796

Bn-Ru-NNTs-TS2_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 10.9971 26.7586 30.7286 cm(-1)

Electronic energy : =-1563.8302902
Zero-point correction= 0.371788
Thermal correction to Energy= 0.398046
Thermal correction to Enthalpy= 0.398991
Thermal correction to Gibbs Free Energy= 0.312283
Sum of electronic and zero-point Energies= -1563.458502
Sum of electronic and thermal Energies= -1563.432244
Sum of electronic and thermal Enthalpies= -1563.431300
Sum of electronic and thermal Free Energies= -1563.518007

Cartesian Coordinates

6	0.694482	1.319583	1.010987
6	-0.229695	1.159298	2.197260
44	-1.563905	-0.291157	-0.110009
1	1.731328	1.434208	1.360867
1	0.445937	2.245496	0.470853
1	-0.185604	2.020738	2.878144
1	0.043838	0.252944	2.748849
6	-1.387363	-2.579944	-0.026332
6	-1.396387	-2.081183	-1.372853
6	-2.464761	-1.286631	-1.833074
6	-3.494204	-0.890372	-0.926974
6	-3.412256	-1.299748	0.427430
6	-2.395051	-2.210900	0.864887
1	-4.147223	-0.929640	1.140855
1	-0.535905	-3.162840	0.311598
1	-0.550499	-2.294548	-2.016896
1	-2.453647	-0.895765	-2.847185
1	-4.285075	-0.220888	-1.255424
1	-2.348203	-2.522846	1.905164
7	-1.596434	0.974915	1.661180
1	-2.211300	0.595045	2.378311
7	0.534700	0.198594	0.080489
16	1.613237	-0.988157	0.354804
6	3.193669	-0.206316	0.038223
6	4.197451	-0.247542	0.995671
6	3.414258	0.394242	-1.200780
6	5.437034	0.318656	0.709049
1	3.999503	-0.722739	1.953512
6	4.652470	0.954495	-1.471803
1	2.613039	0.422751	-1.936770
6	5.682868	0.923333	-0.523189
1	6.228821	0.289859	1.456604

1	4.833385	1.427160	-2.436962
6	7.017453	1.524217	-0.842984
1	7.509871	0.982542	-1.660616
1	6.918927	2.567149	-1.168448
1	7.689142	1.502910	0.021454
8	1.449891	-2.025792	-0.671127
8	1.654025	-1.444735	1.758305
6	-1.580652	1.529888	-1.198316
1	-2.341703	1.520391	-1.992019
1	-0.599125	1.658075	-1.672992
1	-1.765897	2.421311	-0.574304
1	-1.991121	1.877035	1.397817
6	-4.561631	2.440427	-0.153572
8	-4.975226	2.387413	-1.239378
8	-4.175241	2.504298	0.945661

Bn-Ru-NNTs-TS2

Number of imaginary frequencies : 2
The smallest frequencies are : -481.9957 -36.3230 21.0494 cm(-1)

Electronic energy : =-1563.7825219
Zero-point correction= 0.371731
Thermal correction to Energy= 0.395804
Thermal correction to Enthalpy= 0.396748
Thermal correction to Gibbs Free Energy= 0.317117
Sum of electronic and zero-point Energies= -1563.410791
Sum of electronic and thermal Energies= -1563.386718
Sum of electronic and thermal Enthalpies= -1563.385774
Sum of electronic and thermal Free Energies= -1563.465405

Cartesian Coordinates

6	0.664868	1.198848	1.107750
6	-0.172767	0.925378	2.333878
44	-1.697887	-0.203447	-0.061675
1	1.727264	1.290608	1.375397
1	0.368436	2.164846	0.670222
1	-0.095682	1.730685	3.076617
1	0.140641	-0.019022	2.791408
6	-1.664552	-2.399524	0.061524
6	-1.576838	-2.031365	-1.317563
6	-2.532035	-1.173063	-1.881791
6	-3.597297	-0.663723	-1.079880
6	-3.705234	-1.031083	0.276079
6	-2.722873	-1.897501	0.849860
1	-4.477203	-0.582702	0.896986
1	-0.876746	-2.996797	0.510747
1	-0.701548	-2.330552	-1.882219
1	-2.407320	-0.817115	-2.900484
1	-4.258804	0.096322	-1.483368
1	-2.745398	-2.114635	1.915606
7	-1.562513	0.788221	1.856510
1	-2.136882	0.319506	2.553863
7	0.430834	0.160578	0.097039
16	1.467895	-1.096901	0.245199
6	3.072591	-0.353906	-0.016070
6	4.050276	-0.446728	0.964729
6	3.333851	0.278936	-1.230841
6	5.306776	0.103073	0.725638
1	3.821414	-0.949524	1.901284
6	4.588809	0.822559	-1.453005
1	2.554875	0.342259	-1.987922
6	5.593539	0.742836	-0.479835
1	6.079540	0.033458	1.489953
1	4.803511	1.319964	-2.398380
6	6.943061	1.336250	-0.743896
1	7.415089	0.873700	-1.619644
1	6.870968	2.410747	-0.953465
1	7.617553	1.204937	0.108328
8	1.242842	-2.023843	-0.869500
8	1.488071	-1.680840	1.599221
6	-1.631915	1.838592	-1.273074
1	-2.088021	1.668902	-2.251787
1	-0.601328	1.449066	-1.294761
1	-1.443165	2.916921	-1.164325
1	-1.975686	1.716388	1.697549
6	-3.236408	2.425966	-0.237557
8	-4.156991	2.285331	-0.991867
8	-2.915442	2.929257	0.815698

Bn-Ru-NNTs-TS2_for

Number of imaginary frequencies : 1
The smallest frequencies are : -12.3805 31.8995 48.1074 cm(-1)

Electronic energy : =-1563.831404
Zero-point correction= 0.373085
Thermal correction to Energy= 0.397412
Thermal correction to Enthalpy= 0.398356
Thermal correction to Gibbs Free Energy= 0.319781

Sum of electronic and zero-point Energies= -1563.458319
 Sum of electronic and thermal Energies= -1563.433992
 Sum of electronic and thermal Enthalpies= -1563.433048
 Sum of electronic and thermal Free Energies= -1563.511623

 Cartesian Coordinates

6	-0.090272	-0.973749	2.215686
6	-1.186741	-0.185547	2.888296
44	-1.854915	0.121227	0.052184
1	0.118038	-1.906347	2.754088
1	0.839310	-0.376699	2.191757
1	-0.796647	0.318604	3.786426
1	-1.990459	-0.868518	3.214784
6	-2.909524	-0.900997	-1.588115
6	-1.822838	-0.224937	-2.182754
6	-1.597766	1.134947	-1.869948
6	-2.530499	1.861703	-1.069898
6	-3.668914	1.206842	-0.550236
6	-3.828998	-0.189628	-0.762217
1	-4.334440	1.728963	0.132004
1	-2.987585	-1.979476	-1.683329
1	-1.073942	-0.800421	-2.717069
1	-0.680022	1.631828	-2.172600
1	-2.301555	2.885880	-0.791267
1	-4.624943	-0.726713	-0.254017
7	-1.683566	0.776128	1.906814
1	-2.388674	1.396215	2.299556
7	-0.558564	-1.248654	0.845579
16	0.395239	-2.295560	0.016490
6	1.904855	-1.385170	-0.287848
6	3.017300	-1.599569	0.516927
6	1.936367	-0.425343	-1.298260
6	4.171672	-0.853209	0.298765
1	2.975191	-2.354949	1.298066
6	3.092364	0.311878	-1.504965
1	1.058551	-0.266327	-1.920504
6	4.229650	0.104684	-0.714427
1	5.047102	-1.021985	0.924380
1	3.119612	1.065979	-2.291555
6	5.480037	0.890178	-0.966292
1	6.038962	0.479761	-1.817525
1	5.257114	1.936395	-1.207881
1	6.148746	0.875189	-0.099105
8	-0.226865	-2.559069	-1.281975
8	0.760219	-3.427949	0.871119
6	2.579610	3.147140	0.611042
1	2.871442	3.626037	-0.325799
1	3.191866	2.253782	0.783592
1	2.757836	3.829695	1.448853
6	1.134037	2.756833	0.565450
8	0.397918	2.959686	-0.381637
8	0.751265	2.165854	1.692262
1	-0.180492	1.811281	1.615048

 Bn-Ru-NNTs-AA-Presence-TS1_rev

Number of imaginary frequencies : 0
 The smallest frequencies are : 30.3337 32.8634 45.2216 cm(-1)

Electronic energy : =-1604.3164772
 Zero-point correction= 0.420730
 Thermal correction to Energy= 0.449671
 Thermal correction to Enthalpy= 0.450616
 Thermal correction to Gibbs Free Energy= 0.360939
 Sum of electronic and zero-point Energies= -1603.895747
 Sum of electronic and thermal Energies= -1603.866806
 Sum of electronic and thermal Enthalpies= -1603.865862
 Sum of electronic and thermal Free Energies= -1603.955538

 Cartesian Coordinates

6	0.476903	-0.348484	2.315141
6	-0.966896	-0.212304	2.728735
44	-1.074959	-0.807974	-0.171357
1	1.049267	-0.917010	3.057342
1	0.942752	0.647779	2.211493
1	-1.076940	0.488556	3.566312
1	-1.353184	-1.189423	3.043480
6	-2.604456	-2.022783	-1.166840
6	-1.320680	-2.385579	-1.683062
6	-0.475087	-1.402721	-2.230920
6	-0.880204	-0.039569	-2.188004
6	-2.168970	0.319857	-1.703411
6	-3.044199	-0.682056	-1.221958
1	-2.425455	1.368158	-1.560343
1	-3.216933	-2.771076	-0.672043
1	-0.959976	-3.404191	-1.572516
1	0.530776	-1.673523	-2.535136
1	-0.181812	0.743741	-2.473981
1	-3.955238	-0.380912	-0.706709
6	0.552880	2.709302	-0.062583

1	1.101441	3.191756	0.752366
1	0.891462	3.128682	-1.015574
1	-0.521666	2.887744	0.058056
1	0.757235	1.631898	-0.049363
6	-4.001585	2.025513	0.566184
8	-4.328637	0.930975	1.107435
8	-2.842804	2.517079	0.508557
6	-5.111262	2.783153	-0.148819
1	-1.640064	1.233388	1.337637
7	-1.728641	0.223710	1.553481
7	0.487325	-1.038632	1.006828
16	1.966967	-1.728568	0.602021
6	2.963524	-0.332500	0.132606
6	3.654324	0.378725	1.109924
6	2.992434	0.070272	-1.200077
6	4.360216	1.517886	0.743626
1	3.653020	0.030567	2.140267
6	3.706977	1.206877	-1.549455
1	2.473414	-0.517870	-1.953768
6	4.387736	1.954933	-0.583314
1	4.905918	2.078709	1.500864
1	3.743118	1.523831	-2.590882
6	5.107688	3.210688	-0.963726
1	5.530639	3.143659	-1.971988
1	4.420113	4.067088	-0.958093
1	5.919047	3.440805	-0.265358
8	1.754181	-2.553247	-0.583816
8	2.552564	-2.320357	1.803067
1	-2.765530	0.186918	1.646051
1	-6.074900	2.637384	0.348738
1	-5.207358	2.383171	-1.168517
1	-4.881720	3.849702	-0.229334

Bn-Ru-NNTs-AA-Presence-TS1

Number of imaginary frequencies : 1
The smallest frequencies are : -1659.5211 22.3425 28.3713 cm(-1)

Electronic energy : =-1604.2793132
Zero-point correction= 0.416665
Thermal correction to Energy= 0.444370
Thermal correction to Enthalpy= 0.445314
Thermal correction to Gibbs Free Energy= 0.357727
Sum of electronic and zero-point Energies= -1603.862648
Sum of electronic and thermal Energies= -1603.834943
Sum of electronic and thermal Enthalpies= -1603.833999
Sum of electronic and thermal Free Energies= -1603.921586

Cartesian Coordinates

6	0.129341	-0.435553	2.406124
6	-1.331250	-0.682621	2.686824
44	-1.075227	-0.689518	-0.337077
1	0.750843	-0.841211	3.213146
1	0.307473	0.655659	2.354418
1	-1.667753	-0.162475	3.593050
1	-1.503581	-1.759339	2.805986
6	-2.333971	-2.421002	-0.774853
6	-1.000400	-2.739114	-1.102438
6	-0.264211	-1.906845	-2.003158
6	-0.860528	-0.751233	-2.535990
6	-2.210718	-0.416072	-2.205767
6	-2.938061	-1.246930	-1.330331
1	-2.637068	0.529423	-2.525947
1	-2.868432	-3.014980	-0.037242
1	-0.487346	-3.553724	-0.600536
1	0.786604	-2.118990	-2.167330
1	-0.262690	-0.058461	-3.123968
1	-3.927958	-0.936458	-1.003367
6	-0.264804	1.518367	-0.336248
1	-0.259772	2.206225	0.518617
1	-0.171493	2.088215	-1.269703
1	-1.575207	1.455202	-0.374797
1	0.650204	0.926406	-0.253036
6	-3.161969	2.718914	0.498579
8	-2.801982	2.046011	-0.535439
8	-2.745712	2.517218	1.652531
6	-4.159859	3.820610	0.234251
1	-2.222577	0.820286	1.576859
7	-2.085669	-0.210293	1.508338
7	0.407745	-1.103537	1.140067
16	1.936513	-1.587220	0.887166
6	2.831603	-0.171610	0.260861
6	3.196492	0.843935	1.145115
6	3.054135	-0.028811	-1.104374
6	3.760420	2.009871	0.649212
1	3.047121	0.710631	2.214633
6	3.624713	1.144474	-1.587526
1	2.792592	-0.842324	-1.777109
6	3.975414	2.182748	-0.723298
1	4.047243	2.805822	1.335830
1	3.807982	1.255512	-2.655638

6	4.589005	3.449306	-1.235981
1	4.638612	3.461626	-2.329619
1	4.016245	4.327741	-0.914550
1	5.609497	3.578540	-0.853882
8	1.943448	-2.582235	-0.190622
8	2.557380	-1.932767	2.169612
1	-3.022438	-0.610468	1.510093
1	-5.015265	3.427784	-0.325672
1	-3.695954	4.589494	-0.393837
1	-4.502812	4.274579	1.166843

Bn-Ru-NNTs-AA-Presence-TS1_for

Number of imaginary frequencies : 0
The smallest frequencies are : 18.5233 26.7911 33.8229 cm(-1)

Electronic energy : =-1604.3130992
Zero-point correction= 0.422260
Thermal correction to Energy= 0.450484
Thermal correction to Enthalpy= 0.451428
Thermal correction to Gibbs Free Energy= 0.361692
Sum of electronic and zero-point Energies= -1603.890840
Sum of electronic and thermal Energies= -1603.862615
Sum of electronic and thermal Enthalpies= -1603.861671
Sum of electronic and thermal Free Energies= -1603.951407

Cartesian Coordinates

6	0.293327	-0.497362	2.406620
6	-1.141056	-0.838001	2.723663
44	-0.971829	-0.743382	-0.306156
1	0.954122	-0.889052	3.189625
1	0.410808	0.603154	2.384759
1	-1.473007	-0.381336	3.665187
1	-1.244197	-1.926837	2.800923
6	-2.154386	-2.629205	-0.906035
6	-0.811115	-2.830460	-1.225375
6	-0.100802	-1.852408	-1.997213
6	-0.757323	-0.707372	-2.487843
6	-2.125665	-0.479212	-2.153547
6	-2.789490	-1.412007	-1.316887
1	-2.636340	0.417825	-2.493597
1	-2.680160	-3.331705	-0.264316
1	-0.263577	-3.673287	-0.813926
1	0.963307	-1.991355	-2.154276
1	-0.198647	0.042173	-3.043864
1	-3.806872	-1.198934	-0.991316
6	-0.365076	1.295853	-0.197776
1	-0.851521	1.870603	0.606601
1	-0.537858	1.831101	-1.145046
1	-2.648115	1.425155	-0.470814
1	0.712815	1.328518	-0.002528
6	-3.833594	2.546352	0.510308
8	-3.412874	2.019584	-0.642468
8	-3.368251	2.238968	1.590226
6	-4.924914	3.542913	0.303499
1	-2.196995	0.616581	1.702997
7	-1.978943	-0.378964	1.592212
7	0.578954	-1.111539	1.117045
16	2.131005	-1.465018	0.821275
6	2.925694	0.023939	0.226750
6	3.340798	0.986635	1.144812
6	3.034903	0.263635	-1.139346
6	3.845995	2.196210	0.686633
1	3.276982	0.778505	2.210879
6	3.544354	1.477602	-1.584855
1	2.729683	-0.506554	-1.843943
6	3.951161	2.462913	-0.682126
1	4.172313	2.950785	1.401783
1	3.635401	1.665553	-2.654313
6	4.524782	3.760440	-1.163814
1	4.210461	3.985267	-2.188709
1	4.221613	4.596773	-0.523769
1	5.622506	3.733880	-1.158153
8	2.199281	-2.425249	-0.285923
8	2.807148	-1.802634	2.080165
1	-2.879157	-0.855315	1.618760
1	-5.734948	3.099993	-0.284287
1	-4.539047	4.392863	-0.269352
1	-5.303247	3.890120	1.265579

Bn-Ru-NNTs-AA-AICl3-Presence-CO2-insertion-TS2_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 26.3350 36.1826 38.1980 cm(-1)

Electronic energy : =-3415.959923
Zero-point correction= 0.443196
Thermal correction to Energy= 0.480979
Thermal correction to Enthalpy= 0.481923
Thermal correction to Gibbs Free Energy= 0.372399

Sum of electronic and zero-point Energies= -3415.516727
 Sum of electronic and thermal Energies= -3415.478944
 Sum of electronic and thermal Enthalpies= -3415.478000
 Sum of electronic and thermal Free Energies= -3415.587524

 Cartesian Coordinates

6	2.466521	0.721190	1.851515
6	2.271849	-0.491374	2.725852
44	1.709103	-1.527385	-0.030334
1	3.274230	1.350255	2.249303
1	1.533766	1.325341	1.883032
1	1.976658	-0.205946	3.745994
1	3.201146	-1.071751	2.774947
6	3.373783	-3.112647	-0.227039
6	3.387968	-2.202618	-1.306030
6	2.228885	-1.977630	-2.106509
6	1.019218	-2.642051	-1.773207
6	0.954790	-3.506693	-0.651825
6	2.128119	-3.682478	0.140855
1	0.015174	-3.969617	-0.362029
1	4.255607	-3.257618	0.389519
1	4.271077	-1.600870	-1.502036
1	2.264418	-1.250259	-2.911380
1	0.110724	-2.419756	-2.329686
1	2.061197	-4.272437	1.054471
6	-0.005256	-0.316313	-0.297341
1	-0.892904	-0.899183	0.000584
1	-0.141068	-0.049820	-1.353582
1	0.026772	0.616360	0.281561
8	-3.331093	-0.870866	1.195223
6	-2.515827	-1.568000	1.692941
8	-1.797909	-2.320151	2.183528
1	0.334780	-0.868512	2.201466
13	-4.099352	-0.672300	-0.671691
17	-6.149519	-0.804557	-0.248056
17	-3.341701	1.240586	-1.146406
17	-3.179119	-2.345006	-1.566765
1	1.171419	-2.232786	2.553311
16	3.307982	1.396447	-0.503224
6	1.915230	2.449314	-0.888620
6	1.516690	3.420814	0.031030
6	1.171435	2.228156	-2.041249
6	0.347993	4.134573	-0.192894
1	2.136097	3.625261	0.902153
6	0.007659	2.958332	-2.258728
1	1.508661	1.483748	-2.758917
6	-0.431701	3.904925	-1.331906
1	0.026442	4.888887	0.525769
1	-0.578292	2.784206	-3.160839
6	-1.701110	4.673771	-1.536252
1	-1.509070	5.752592	-1.597929
1	-2.216323	4.373890	-2.454855
1	-2.391925	4.523175	-0.696285
8	3.716022	0.763187	-1.760510
8	4.270436	2.255024	0.199688
7	2.774111	0.246577	0.510399
7	1.238846	-1.330969	2.085495
6	-1.259427	1.622604	2.642021
8	-1.854010	2.310903	1.676522
8	-1.236171	0.401598	2.677645
6	-0.630678	2.511621	3.659536
1	-2.165024	1.706355	0.976620
1	0.168588	3.094434	3.186797
1	-1.366127	3.227807	4.039693
1	-0.222690	1.920725	4.480494

 Bn-Ru-NNTs.AA-AICl3-Presence-CO2-insertion-TS2

Number of imaginary frequencies : 1
 The smallest frequencies are : -169.8478 14.2614 21.7775 cm(-1)

Electronic energy : -3415.942174
 Zero-point correction= 0.442261
 Thermal correction to Energy= 0.479788
 Thermal correction to Enthalpy= 0.480732
 Thermal correction to Gibbs Free Energy= 0.370245
 Sum of electronic and zero-point Energies= -3415.499913
 Sum of electronic and thermal Energies= -3415.462386
 Sum of electronic and thermal Enthalpies= -3415.461442
 Sum of electronic and thermal Free Energies= -3415.571929

 Cartesian Coordinates

6	2.476878	-1.456826	1.556953
6	1.481734	-1.707073	2.657199
44	-0.309266	-1.520089	0.297691
1	3.360637	-2.094944	1.691447
1	2.809995	-0.403399	1.622338
1	1.869407	-1.368708	3.627190
1	1.232473	-2.772980	2.725306
6	-0.773616	-3.792701	0.355176

6	-0.249866	-3.420490	-0.899851
6	-0.832243	-2.389122	-1.684410
6	-1.967300	-1.717718	-1.185008
6	-2.520586	-2.078679	0.072260
6	-1.864379	-3.058901	0.867394
1	-3.467805	-1.654996	0.400170
1	-0.281187	-4.552509	0.954144
1	0.675786	-3.867422	-1.250430
1	-0.361005	-2.088658	-2.613379
1	-2.405696	-0.898214	-1.753271
1	-2.235059	-3.259959	1.871196
6	0.076389	0.509201	-0.205744
1	-0.252886	1.221967	0.564047
1	-0.411685	0.781976	-1.150598
1	1.159320	0.595963	-0.323955
8	-2.740890	0.871130	0.356045
6	-2.391455	0.210015	1.302913
8	-2.398376	-0.055801	2.443882
1	0.479484	0.034030	2.331238
13	-4.296358	1.568498	-0.538687
17	-4.660719	3.394836	0.451153
17	-3.614257	1.693184	-2.535919
17	-5.684654	0.006528	-0.158428
1	-0.484436	-1.136659	2.970976
16	2.825812	-1.734866	-0.993764
6	3.492868	-0.084304	-1.175760
6	4.539817	0.327490	-0.354794
6	2.920603	0.802472	-2.086676
6	4.981517	1.644939	-0.419253
1	5.022245	-0.386214	0.309037
6	3.375021	2.112142	-2.142524
1	2.122811	0.456434	-2.740539
6	4.393776	2.559683	-1.294442
1	5.806906	1.967104	0.215593
1	2.928630	2.808538	-2.851499
6	4.809967	3.996912	-1.302933
1	5.775155	4.145264	-0.806464
1	4.886431	4.392158	-2.322388
1	4.066751	4.610919	-0.776063
8	2.049005	-2.014390	-2.204421
8	3.976569	-2.588051	-0.678175
7	1.812214	-1.741091	0.285616
7	0.256361	-0.967954	2.293140
6	2.281668	2.566629	2.024841
8	1.988348	2.980314	0.792713
8	1.689612	1.664615	2.588076
6	3.413832	3.342810	2.609608
1	1.299532	2.394474	0.425266
1	4.312821	3.173447	2.004656
1	3.195795	4.414822	2.569566
1	3.594765	3.033449	3.639518

 Bn-Ru-NNTs-AA-AlCl3-Presence-CO2-insertion-TS2_for

Number of imaginary frequencies : 0
 The smallest frequencies are : 8.9661 18.1524 27.3310 cm(-1)

Electronic energy : =-3415.9549283
 Zero-point correction= 0.444829
 Thermal correction to Energy= 0.482483
 Thermal correction to Enthalpy= 0.483427
 Thermal correction to Gibbs Free Energy= 0.371479
 Sum of electronic and zero-point Energies= -3415.510100
 Sum of electronic and thermal Energies= -3415.472445
 Sum of electronic and thermal Enthalpies= -3415.471501
 Sum of electronic and thermal Free Energies= -3415.583450

 Cartesian Coordinates

6	2.195953	-1.501091	1.734783
6	1.087642	-1.424507	2.750763
44	-0.502130	-1.301261	0.285295
1	2.876918	-2.332433	1.959172
1	2.774157	-0.562137	1.781176
1	1.448015	-1.019661	3.705113
1	0.633845	-2.405753	2.933203
6	-0.902285	-3.675194	0.586796
6	-0.339944	-3.456137	-0.687440
6	-0.912109	-2.559533	-1.615095
6	-2.087559	-1.881017	-1.255500
6	-2.678671	-2.115832	0.015724
6	-2.069768	-2.985341	0.945939
1	-3.606643	-1.609503	0.278643
1	-0.403543	-4.333106	1.291955
1	0.605972	-3.927213	-0.939012
1	-0.417793	-2.373115	-2.561487
1	-2.537736	-1.156878	-1.929024
1	-2.504966	-3.101803	1.935375
6	0.133475	0.526877	-0.602019
1	-0.229717	1.423057	-0.085582
1	-0.236984	0.548273	-1.632167
1	1.222878	0.512778	-0.588962

8	-2.605904	0.753458	-0.328360
6	-2.069234	0.238171	0.714249
8	-2.342721	0.444053	1.875998
1	0.484486	0.388513	2.032845
13	-4.227580	1.578810	-0.431994
17	-4.185071	3.442735	0.598543
17	-4.498810	1.778640	-2.547094
17	-5.626099	0.161794	0.389202
1	-0.762922	-0.421803	2.743690
16	2.659843	-1.844081	-0.807859
6	3.610502	-0.339636	-0.965675
6	4.631762	-0.069565	-0.058443
6	3.313229	0.561524	-1.988581
6	5.322840	1.134717	-0.150298
1	4.905962	-0.806108	0.692992
6	4.018409	1.752027	-2.071449
1	2.537458	0.317850	-2.710712
6	5.016431	2.067304	-1.142658
1	6.125929	1.348082	0.554702
1	3.789051	2.460238	-2.866589
6	5.712173	3.390291	-1.209408
1	6.566062	3.438487	-0.525170
1	6.075418	3.603483	-2.221597
1	5.020947	4.201350	-0.943184
8	1.914658	-2.013172	-2.056050
8	3.611238	-2.881090	-0.399479
7	1.571939	-1.674811	0.416200
7	0.068280	-0.543843	2.162309
6	2.512061	2.634289	1.563691
8	2.260758	3.008709	0.310613
8	1.912528	1.734891	2.123421
6	3.612168	3.433356	2.176059
1	1.577533	2.417764	-0.054972
1	4.560577	3.139923	1.708808
1	3.467593	4.500194	1.982288
1	3.663505	3.243454	3.248799

 Bn-Ru-NNTs.AA-AlCl3-Presence-C-C_bond formation-TS3_rev

Number of imaginary frequencies : 0

The smallest frequencies are : 13.6686 16.8659 21.7514 cm(-1)

Electronic energy : =-3415.9618411

Zero-point correction= 0.444473

Thermal correction to Energy= 0.482286

Thermal correction to Enthalpy= 0.483230

Thermal correction to Gibbs Free Energy= 0.369895

Sum of electronic and zero-point Energies= -3415.517369

Sum of electronic and thermal Energies= -3415.479555

Sum of electronic and thermal Enthalpies= -3415.478611

Sum of electronic and thermal Free Energies= -3415.591946

 Cartesian Coordinates

6	-1.540209	-1.307664	-1.865610
6	-0.159969	-1.851833	-2.104173
44	-0.025507	-0.515517	0.612849
1	-2.291760	-1.954205	-2.332566
1	-1.623761	-0.295708	-2.301462
1	0.121969	-1.849855	-3.164482
1	-0.079014	-2.873015	-1.713429
6	1.088804	-2.494735	1.373802
6	-0.125174	-2.488540	2.053688
6	-0.541849	-1.302434	2.707664
6	0.351113	-0.210693	2.855254
6	1.634712	-0.269721	2.283289
6	1.950953	-1.353337	1.452669
1	2.317783	0.570023	2.372030
1	1.384027	-3.341352	0.758394
1	-0.817472	-3.321288	1.970144
1	-1.546621	-1.247324	3.111160
1	0.037057	0.678425	3.395984
1	2.886450	-1.353501	0.898208
6	-1.482147	1.053087	1.007428
1	-1.972224	1.324996	0.071457
1	-1.043035	1.938241	1.477599
1	-2.193544	0.585526	1.691533
8	1.360545	2.003219	0.610258
6	0.534940	1.354500	-0.172140
8	0.209242	1.712851	-1.284278
13	2.950364	2.578600	0.003120
17	3.574169	1.050977	-1.444182
17	4.227928	2.449218	1.725648
17	2.908211	4.503654	-0.888967
7	0.751184	-0.976693	-1.343024
7	-1.705189	-1.279250	-0.413132
16	-3.200840	-1.648263	0.140289
6	-4.320113	-0.294368	-0.194523
6	-4.660129	0.002650	-1.513753
6	-4.846731	0.451303	0.854382
6	-5.503712	1.072548	-1.775384
1	-4.287954	-0.610737	-2.331120

6	-5.697435	1.514615	0.576503
1	-4.599573	0.186680	1.879344
6	-6.028628	1.849727	-0.737644
1	-5.771475	1.307639	-2.804651
1	-6.117304	2.095295	1.396648
6	-6.916209	3.017646	-1.037507
1	-7.495096	3.321411	-0.159095
1	-6.326875	3.886415	-1.358401
1	-7.618528	2.791100	-1.847740
8	-3.129536	-1.782384	1.598262
8	-3.700806	-2.777933	-0.647727
1	1.691782	-1.386127	-1.288428
1	0.827840	-0.085438	-1.839559
6	4.328303	-2.786773	-1.270481
8	5.166873	-1.762062	-1.237476
8	3.118245	-2.667651	-1.151834
6	5.030458	-4.086558	-1.470724
1	4.665227	-0.923836	-1.155536
1	4.325049	-4.914398	-1.391495
1	5.497760	-4.095501	-2.461318
1	5.834730	-4.198987	-0.737224

 Bn-Ru-NNTs.AA-AICI3-Presence-C-C_bond formation-TS3

Number of imaginary frequencies : 1
 The smallest frequencies are : -292.8946 13.2641 18.9545 cm(-1)

Electronic energy : =-3415.955757
 Zero-point correction= 0.443698
 Thermal correction to Energy= 0.480889
 Thermal correction to Enthalpy= 0.481833
 Thermal correction to Gibbs Free Energy= 0.370189
 Sum of electronic and zero-point Energies= -3415.512059
 Sum of electronic and thermal Energies= -3415.474868
 Sum of electronic and thermal Enthalpies= -3415.473924
 Sum of electronic and thermal Free Energies= -3415.585568

 Cartesian Coordinates

6	-1.556129	-1.524211	-1.790240
6	-0.153622	-2.002549	-2.045167
44	-0.005964	-0.617515	0.627452
1	-2.283505	-2.230569	-2.207653
1	-1.705014	-0.541035	-2.275066
1	0.095016	-2.023796	-3.113616
1	-0.011351	-3.006382	-1.627686
6	0.923298	-2.524352	1.465124
6	-0.250179	-2.323486	2.205897
6	-0.504480	-1.064724	2.800019
6	0.485653	-0.052320	2.752385
6	1.740262	-0.306574	2.149389
6	1.925509	-1.502514	1.447982
1	2.498149	0.471863	2.122920
1	1.079188	-3.447165	0.912902
1	-1.040979	-3.068062	2.199214
1	-1.471717	-0.878490	3.254351
1	0.285636	0.929746	3.174526
1	2.829668	-1.652903	0.863162
6	-1.352635	1.213232	0.612830
1	-1.969257	1.154210	-0.282878
1	-1.107629	2.256786	0.831558
1	-1.889540	0.845419	1.491564
8	1.219094	2.037984	0.628043
6	0.430834	1.368010	-0.176075
8	0.311932	1.591119	-1.367341
13	2.794190	2.649096	0.003771
17	3.599473	1.063388	-1.276573
17	4.001373	2.761548	1.779213
17	2.656412	4.496431	-1.036558
7	0.733488	-1.064138	-1.335253
7	-1.692686	-1.437703	-0.337184
16	-3.193890	-1.700691	0.256965
6	-4.247533	-0.318441	-0.160736
6	-4.633636	-0.123869	-1.486105
6	-4.657245	0.567351	0.830828
6	-5.401095	0.984755	-1.815864
1	-4.357462	-0.844466	-2.252369
6	-5.433165	1.667078	0.486148
1	-4.378057	0.381947	1.864993
6	-5.804332	1.901358	-0.839952
1	-5.704979	1.140157	-2.850138
1	-5.763421	2.356914	1.261588
6	-6.606472	3.108873	-1.214146
1	-7.307403	2.890183	-2.027333
1	-7.178921	3.493168	-0.363370
1	-5.954332	3.920727	-1.561757
8	-3.102073	-1.725179	1.720114
8	-3.759745	-2.858116	-0.440131
1	1.690814	-1.431828	-1.300219
1	0.753582	-0.171559	-1.839574
6	4.349390	-2.806657	-1.320577
8	5.173111	-1.776194	-1.191825

8	3.136035	-2.710653	-1.223448
6	5.075558	-4.078974	-1.596878
1	4.657326	-0.952818	-1.066618
1	4.384174	-4.921935	-1.572415
1	5.545004	-4.018656	-2.584709
1	5.879461	-4.221931	-0.868537

 Bn-Ru-NNTs.AA-AICl3-Presence-C-C_bond formation-TS3_for

Number of imaginary frequencies : 0
 The smallest frequencies are : 16.2599 22.8384 29.9905 cm(-1)

Electronic energy : =-3416.0398711
 Zero-point correction= 0.444997
 Thermal correction to Energy= 0.483255
 Thermal correction to Enthalpy= 0.484199
 Thermal correction to Gibbs Free Energy= 0.369587
 Sum of electronic and zero-point Energies= -3415.594875
 Sum of electronic and thermal Energies= -3415.556616
 Sum of electronic and thermal Enthalpies= -3415.555672
 Sum of electronic and thermal Free Energies= -3415.670284

 Cartesian Coordinates

6	-1.289716	-1.101824	-2.105278
6	0.130686	-1.538802	-2.360291
44	-0.122310	-1.365609	0.599469
1	-1.979133	-1.615046	-2.784522
1	-1.381696	-0.014133	-2.251851
1	0.505013	-1.138040	-3.310749
1	0.184817	-2.633543	-2.390779
6	0.991664	-2.786614	1.822058
6	-0.383918	-2.797601	2.210102
6	-1.018517	-1.604238	2.621737
6	-0.300397	-0.385657	2.550922
6	1.073995	-0.370882	2.185613
6	1.722889	-1.577591	1.851907
1	1.596356	0.575410	2.071761
1	1.457254	-3.689245	1.437281
1	-0.968468	-3.708233	2.114403
1	-2.081572	-1.610642	2.835915
1	-0.813616	0.557630	2.725295
1	2.732100	-1.550934	1.449494
6	-1.445672	2.465511	-0.196261
1	-1.940361	2.881277	-1.079921
1	-1.609545	3.115436	0.666358
1	-1.904668	1.484758	-0.007033
8	0.837107	2.721265	0.409695
6	0.010324	2.262302	-0.494222
8	0.375230	1.682401	-1.514976
13	2.610892	2.842634	0.144046
17	3.466949	0.837129	-0.086122
17	3.354541	3.610365	2.003039
17	3.084730	4.080136	-1.526763
7	0.948259	-1.071805	-1.225579
7	-1.593487	-1.439994	-0.694566
16	-3.199569	-1.867088	-0.399435
6	-4.044204	-0.306902	-0.328457
6	-4.492314	0.283703	-1.507238
6	-4.207338	0.327001	0.900752
6	-5.096057	1.532614	-1.446754
1	-4.386703	-0.238911	-2.455100
6	-4.817815	1.572901	0.942568
1	-3.876753	-0.166224	1.812431
6	-5.259948	2.198180	-0.227918
1	-5.454772	2.001207	-2.361760
1	-4.960020	2.072428	1.899720
6	-5.870244	3.563733	-0.179393
1	-6.579912	3.718845	-0.998794
1	-6.393042	3.739683	0.766637
1	-5.095824	4.337209	-0.270152
8	-3.252449	-2.472180	0.927943
8	-3.704788	-2.607595	-1.553084
1	1.863928	-1.530623	-1.185829
1	1.103082	-0.057856	-1.313587
6	4.565034	-2.648383	-1.091534
8	5.233544	-1.545590	-1.404341
8	3.392869	-2.648455	-0.752907
6	5.414855	-3.868863	-1.204586
1	4.655711	-0.769255	-1.267347
1	4.835082	-4.757898	-0.954321
1	5.807778	-3.952646	-2.223056
1	6.277034	-3.782126	-0.535391

Solvent (benzene) Optimization of Bn-Ru-PP

Bn-Ru-PP

Number of imaginary frequencies : 0
The smallest frequencies are : 13.3517 73.4879 115.4803 cm(-1)

Electronic energy : =-1089.3748392
Zero-point correction= 0.175678
Thermal correction to Energy= 0.187538
Thermal correction to Enthalpy= 0.188482
Thermal correction to Gibbs Free Energy= 0.136239
Sum of electronic and zero-point Energies= -1089.199161
Sum of electronic and thermal Energies= -1089.187301
Sum of electronic and thermal Enthalpies= -1089.186357
Sum of electronic and thermal Free Energies= -1089.238600

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Cartesian Coordinates

6	3.039140	-0.684920	0.169369
6	2.956050	0.691855	-0.450269
44	-0.274345	-0.068711	-0.105799
1	2.854332	0.604058	-1.540449
1	3.858954	1.283397	-0.243965
6	-1.686742	0.700465	1.325463
6	-1.827249	-0.723414	1.267350
6	-2.164575	-1.354844	0.046337
6	-2.203495	-0.568964	-1.124791
6	-2.118351	0.859903	-1.071588
6	-1.900473	1.491682	0.161513
1	-2.165561	1.439887	-1.988062
1	-1.400806	1.177346	2.258534
1	-1.659554	-1.314398	2.163440
1	-2.234564	-2.436831	-0.014622
1	-2.312130	-1.054102	-2.091428
1	-1.760650	2.568795	0.209087
15	1.451909	1.554017	0.285951
15	1.419314	-1.634370	0.051640
1	3.849996	-1.293966	-0.251852
1	3.235470	-0.610368	1.252318
1	0.995899	-1.032820	-1.286082
1	1.175622	2.426997	-0.815952

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Bn-Ru-PP-TS1_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 41.5437 60.4429 126.4895 cm(-1)

Electronic energy : =-1129.8587716
Zero-point correction= 0.223956
Thermal correction to Energy= 0.238897
Thermal correction to Enthalpy= 0.239841
Thermal correction to Gibbs Free Energy= 0.182530
Sum of electronic and zero-point Energies= -1129.634815
Sum of electronic and thermal Energies= -1129.619875
Sum of electronic and thermal Enthalpies= -1129.618931
Sum of electronic and thermal Free Energies= -1129.676241

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Cartesian Coordinates

6	-2.910096	-0.608191	-0.768221
6	-2.993393	0.663016	0.048230
44	0.351348	0.001141	0.153861
1	-3.110776	0.416886	1.113220
1	-3.847585	1.290737	-0.246856
6	1.319097	0.653457	-1.642921
6	1.389089	-0.766851	-1.572077
6	2.048012	-1.403913	-0.479729
6	2.531264	-0.604830	0.567890
6	2.476873	0.823916	0.498316
6	1.906407	1.456003	-0.615802
1	2.837224	1.415480	1.335871
1	0.795249	1.128451	-2.468299
1	0.917970	-1.367203	-2.346601
1	2.075094	-2.487708	-0.411107
1	2.927913	-1.075593	1.464848
1	1.828011	2.539292	-0.660056
6	-0.252339	-0.211752	2.798922
1	-1.201002	-0.413108	3.306453
1	0.383809	0.434216	3.408296
1	-0.559910	0.365027	1.890372
1	0.245513	-1.161984	2.596932
15	-1.402567	1.619549	-0.260772
15	-1.397959	-1.623459	-0.293277
1	-3.803041	-1.238852	-0.657577

1	-2.819629	-0.373136	-1.839978
1	-1.828969	-1.804799	1.065142
1	-1.380766	2.335610	0.982568

Bn-Ru-PP-TS1

Number of imaginary frequencies : 1
The smallest frequencies are : -550.3222 34.7131 64.4689 cm(-1)

Electronic energy : =-1129.8358861
Zero-point correction= 0.220393
Thermal correction to Energy= 0.234445
Thermal correction to Enthalpy= 0.235389
Thermal correction to Gibbs Free Energy= 0.179853
Sum of electronic and zero-point Energies= -1129.615493
Sum of electronic and thermal Energies= -1129.601442
Sum of electronic and thermal Enthalpies= -1129.600497
Sum of electronic and thermal Free Energies= -1129.656033

Cartesian Coordinates

6	-2.830499	-0.554180	-0.880436
6	-3.041674	0.633746	0.033531
44	0.335240	-0.005982	0.223087
1	-3.289323	0.290885	1.047186
1	-3.859569	1.285482	-0.308085
6	1.377702	0.740130	-1.686851
6	1.449642	-0.662720	-1.648079
6	2.024556	-1.319979	-0.521790
6	2.511152	-0.544892	0.552841
6	2.452839	0.872845	0.522243
6	1.847770	1.505769	-0.582695
1	2.808852	1.456010	1.366451
1	0.882242	1.237762	-2.516235
1	1.026615	-1.252482	-2.457011
1	2.043425	-2.404704	-0.473987
1	2.891659	-1.044592	1.441341
1	1.726618	2.586255	-0.592573
6	-0.054961	-0.614039	2.293814
1	-1.060133	-0.542432	2.731401
1	0.634238	-0.065832	2.947397
1	-0.699097	0.562123	1.331639
1	0.208345	-1.678257	2.288892
15	-1.460590	1.650539	0.028534
15	-1.375171	-1.615779	-0.330634
1	-3.722897	-1.193642	-0.930326
1	-2.620951	-0.219583	-1.907821
1	-1.944289	-1.900435	0.953969
1	-1.659033	2.285179	1.297942

Bn-Ru-PP-TS1_for

Number of imaginary frequencies : 0
The smallest frequencies are : 40.1392 53.0974 103.3728 cm(-1)

Electronic energy : =-1129.8389514
Zero-point correction= 0.221507
Thermal correction to Energy= 0.235927
Thermal correction to Enthalpy= 0.236871
Thermal correction to Gibbs Free Energy= 0.180461
Sum of electronic and zero-point Energies= -1129.617444
Sum of electronic and thermal Energies= -1129.603025
Sum of electronic and thermal Enthalpies= -1129.602081
Sum of electronic and thermal Free Energies= -1129.658490

Cartesian Coordinates

6	-2.870577	-0.434154	-0.887617
6	-3.049031	0.596642	0.205553
44	0.337793	-0.024000	0.248543
1	-3.216472	0.106811	1.173662
1	-3.896863	1.273074	0.017828
6	1.389840	1.000914	-1.582876
6	1.447266	-0.391119	-1.737802
6	1.988671	-1.204410	-0.701349
6	2.517429	-0.590370	0.461962
6	2.459461	0.808499	0.634805
6	1.825617	1.588108	-0.364570
1	2.829628	1.269605	1.545488
1	0.914140	1.617674	-2.340632
1	1.032159	-0.859932	-2.626377
1	1.992349	-2.286023	-0.802668
1	2.912066	-1.215159	1.260327
1	1.699003	2.657888	-0.214642
6	0.060991	-1.185550	2.030980
1	-0.952176	-1.161607	2.448268
1	0.749993	-0.807392	2.799043
1	-0.594469	0.726593	1.381484
1	0.310926	-2.234460	1.818028
15	-1.501053	1.644479	0.233294
15	-1.374893	-1.532573	-0.569972

1	-3.750707	-1.084247	-0.985755
1	-2.726928	0.058286	-1.860959
1	-1.917584	-2.072191	0.638518
1	-1.726762	2.257128	1.508148

Bn-Ru-PP-TS2_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 46.4497 64.6115 77.2276 cm(-1)

Electronic energy : =-1318.3801661
Zero-point correction= 0.236906
Thermal correction to Energy= 0.254687
Thermal correction to Enthalpy= 0.255631
Thermal correction to Gibbs Free Energy= 0.191399
Sum of electronic and zero-point Energies= -1318.143260
Sum of electronic and thermal Energies= -1318.125479
Sum of electronic and thermal Enthalpies= -1318.124535
Sum of electronic and thermal Free Energies= -1318.188767

Cartesian Coordinates

6	2.858126	1.692464	-0.470094
6	2.250592	2.167916	0.836819
44	0.176307	-0.426172	-0.056165
1	3.950729	1.795681	-0.463182
1	2.490850	2.302511	-1.307476
1	2.356156	3.247653	1.009374
1	2.706046	1.637643	1.684510
6	0.427325	-2.040986	1.548435
6	0.727748	-2.566569	0.268328
6	-0.213985	-2.497888	-0.792240
6	-1.470806	-1.868974	-0.564328
6	-1.792758	-1.341970	0.702783
6	-0.804854	-1.364828	1.728572
1	-2.757689	-0.875496	0.877999
1	1.164169	-2.073423	2.345401
1	1.707200	-3.003604	0.082489
1	0.045734	-2.870058	-1.778756
1	-2.176113	-1.761966	-1.386101
1	-1.014906	-0.882069	2.681000
6	-0.254191	0.609260	-1.887988
1	0.393242	1.467543	-2.119003
1	-1.292223	0.976954	-1.890153
1	-0.148715	-0.101887	-2.719222
8	-3.797892	0.806348	-0.904721
6	-3.279524	1.568684	-0.192321
8	-2.788337	2.340281	0.529601
15	0.470955	1.672396	0.786585
1	-0.006302	2.043977	2.070465
1	-0.085182	2.748679	0.045694
15	2.446675	-0.112909	-0.855092
1	3.148857	-0.608543	0.298970

Bn-Ru-PP-TS2

Number of imaginary frequencies : 1
The smallest frequencies are : -358.9464 37.8134 57.0129 cm(-1)

Electronic energy : =-1318.3246571
Zero-point correction= 0.236132
Thermal correction to Energy= 0.253063
Thermal correction to Enthalpy= 0.254007
Thermal correction to Gibbs Free Energy= 0.191938
Sum of electronic and zero-point Energies= -1318.088526
Sum of electronic and thermal Energies= -1318.071594
Sum of electronic and thermal Enthalpies= -1318.070650
Sum of electronic and thermal Free Energies= -1318.132719

Cartesian Coordinates

6	3.191002	0.495408	-0.553933
6	2.998935	0.620879	0.947926
44	-0.161036	-0.319854	-0.060558
1	4.180141	0.092387	-0.804538
1	3.123331	1.484144	-1.029724
1	3.656253	1.365342	1.416701
1	3.158931	-0.346529	1.443620
6	-0.106139	-2.155249	1.138557
6	-0.331046	-2.526157	-0.212321
6	-1.427471	-1.993506	-0.933594
6	-2.290465	-1.071950	-0.289779
6	-2.123817	-0.728190	1.072012
6	-0.997206	-1.231493	1.763410
1	-2.779947	0.003332	1.531932
1	0.759736	-2.535668	1.674233
1	0.375674	-3.183471	-0.714029
1	-1.557598	-2.227718	-1.985527
1	-3.054924	-0.557024	-0.863617
1	-0.798877	-0.905324	2.782262
6	-0.464643	1.530292	-1.596302

1	0.567359	1.896861	-1.587108
1	-1.024542	2.332393	-2.097125
1	-0.598252	0.705940	-2.310688
8	-2.789074	1.762677	-0.570925
6	-1.668373	2.113477	-0.268302
8	-1.099827	2.850537	0.510853
15	1.227792	1.081937	1.134278
1	1.017865	1.238056	2.524549
1	1.235169	2.428244	0.722049
15	1.896802	-0.625323	-1.353470
1	2.382898	-1.793377	-0.676006

 Bn-Ru-PP-TS2_for

Number of imaginary frequencies : 0
 The smallest frequencies are : 12.1289 31.2313 42.7416 cm(-1)

Electronic energy : =-1318.3695558
 Zero-point correction= 0.239938
 Thermal correction to Energy= 0.258054
 Thermal correction to Enthalpy= 0.258998
 Thermal correction to Gibbs Free Energy= 0.190250
 Sum of electronic and zero-point Energies= -1318.129618
 Sum of electronic and thermal Energies= -1318.111502
 Sum of electronic and thermal Enthalpies= -1318.110557
 Sum of electronic and thermal Free Energies= -1318.179306

 Cartesian Coordinates

6	-0.535432	3.070304	0.613864
6	-0.745284	3.091863	-0.885700
44	-0.704072	-0.311406	-0.119805
1	-1.011965	3.931293	1.100665
1	0.537427	3.121864	0.845230
1	-0.115578	3.825228	-1.407463
1	-1.794201	3.315920	-1.133834
6	-2.332996	-1.773491	-0.107147
6	-1.832126	-1.683220	1.217747
6	-0.456960	-1.903243	1.480773
6	0.414821	-2.188936	0.405112
6	-0.090774	-2.359290	-0.914900
6	-1.457040	-2.141235	-1.173309
1	0.596374	-2.563714	-1.730803
1	-3.377566	-1.556410	-0.308619
1	-2.490860	-1.360863	2.020432
1	-0.061206	-1.747710	2.480247
1	1.482875	-2.283933	0.583793
1	-1.836375	-2.196582	-2.189465
6	2.989758	0.837889	1.121008
1	2.863171	1.842403	0.699272
1	3.687527	0.881964	1.958888
1	2.002681	0.513676	1.479519
8	4.546973	-0.719942	0.169492
6	3.514352	-0.104881	0.073789
8	2.749675	-0.234374	-1.025827
15	-0.396632	1.371153	-1.472087
1	-0.351534	1.494747	-2.887740
15	-1.181698	1.500086	1.436132
1	-2.553859	1.740038	1.089975
1	1.894123	0.235328	-0.926096

 Bn-Ru-PP-AICl3-Presence-CO2-insertion-TS2_rev

Number of imaginary frequencies : 0
 The smallest frequencies are : 15.9105 32.7820 36.0861 cm(-1)

Electronic energy : =-2941.5120308
 Zero-point correction= 0.243049
 Thermal correction to Energy= 0.267876
 Thermal correction to Enthalpy= 0.268820
 Thermal correction to Gibbs Free Energy= 0.185450
 Sum of electronic and zero-point Energies= -2941.268982
 Sum of electronic and thermal Energies= -2941.244155
 Sum of electronic and thermal Enthalpies= -2941.243211
 Sum of electronic and thermal Free Energies= -2941.326580

 Cartesian Coordinates

6	3.817182	2.185732	-0.938329
6	3.517715	2.500381	0.514918
44	1.693493	-0.370782	-0.041724
1	4.822929	2.528384	-1.211602
1	3.104362	2.706588	-1.592224
1	3.492941	3.573379	0.740448
1	4.259066	2.029018	1.175960
6	2.383950	-1.948103	1.512766
6	2.704831	-2.374957	0.211831
6	1.700312	-2.479422	-0.795823
6	0.363245	-2.144512	-0.475351
6	0.019634	-1.699554	0.822372
6	1.053667	-1.530002	1.782465

1	-1.017422	-1.480563	1.070890
1	3.157565	-1.853184	2.268759
1	3.739411	-2.591401	-0.044060
1	1.964416	-2.789857	-1.802546
1	-0.402365	-2.185388	-1.247950
1	0.812522	-1.117503	2.760444
6	0.717390	0.633079	-1.655379
1	1.103043	1.632816	-1.899514
1	-0.356150	0.736494	-1.439837
1	0.811349	0.019687	-2.562662
8	-2.126235	1.169669	0.297653
6	-1.565213	1.194108	1.335751
8	-1.053076	1.263781	2.364222
1	0.990333	2.707771	0.445804
13	-3.753722	0.063532	-0.343061
17	-5.120866	1.612517	-0.693709
17	-2.933784	-0.952735	-1.982532
17	-3.964426	-1.031142	1.455300
1	3.294777	0.377174	-2.552700
1	1.753151	1.910364	2.283653
15	3.720424	0.309389	-1.188902
15	1.895392	1.697926	0.887066

Bn-Ru-PP-AlCl3-Presence-CO2-insertion-TS2

Number of imaginary frequencies : 1
The smallest frequencies are : -149.5422 24.5199 27.6644 cm(-1)

Electronic energy : =-2941.5082062
Zero-point correction= 0.242481
Thermal correction to Energy= 0.266579
Thermal correction to Enthalpy= 0.267523
Thermal correction to Gibbs Free Energy= 0.186409
Sum of electronic and zero-point Energies= -2941.265725
Sum of electronic and thermal Energies= -2941.241627
Sum of electronic and thermal Enthalpies= -2941.240683
Sum of electronic and thermal Free Energies= -2941.321797

Cartesian Coordinates

6	3.725432	2.217515	-0.791443
6	3.476299	2.416253	0.689969
44	1.503306	-0.341954	-0.052291
1	4.737717	2.535977	-1.069523
1	3.016597	2.813394	-1.381993
1	3.498724	3.465148	1.008078
1	4.208515	1.858563	1.290618
6	2.302388	-2.058800	1.339380
6	2.623782	-2.336886	0.000931
6	1.618011	-2.367024	-1.005899
6	0.266995	-2.155587	-0.642123
6	-0.078784	-1.900174	0.703992
6	0.958322	-1.759824	1.666247
1	-1.124830	-1.824157	0.996972
1	3.081323	-2.003506	2.093655
1	3.663761	-2.473514	-0.285057
1	1.887010	-2.545447	-2.043278
1	-0.507290	-2.163300	-1.406676
1	0.704633	-1.474785	2.684355
6	0.610390	0.705434	-1.677394
1	0.831511	1.781275	-1.723526
1	-0.477050	0.587159	-1.620952
1	0.939838	0.259967	-2.624895
8	-1.742451	0.899171	0.236157
6	-1.053867	0.698653	1.206315
8	-0.814000	0.707668	2.348812
1	0.974652	2.742421	0.618743
13	-3.494667	0.219564	-0.263510
17	-4.634795	1.976324	-0.486490
17	-3.099056	-0.888547	-2.019391
17	-3.903738	-0.969935	1.449811
1	3.138662	0.543840	-2.523419
1	1.671510	1.781886	2.413362
15	3.554493	0.377173	-1.168150
15	1.821290	1.668915	1.010388

Bn-Ru-PP-AlCl3-Presence-CO2-insertion-TS2_for

Number of imaginary frequencies : 0
The smallest frequencies are : 27.4501 32.4102 41.7217 cm(-1)

Electronic energy : =-2941.5337642
Zero-point correction= 0.245446
Thermal correction to Energy= 0.269137
Thermal correction to Enthalpy= 0.270082
Thermal correction to Gibbs Free Energy= 0.191071
Sum of electronic and zero-point Energies= -2941.288319
Sum of electronic and thermal Energies= -2941.264627
Sum of electronic and thermal Enthalpies= -2941.263683
Sum of electronic and thermal Free Energies= -2941.342693

Cartesian Coordinates

6	-4.197741	1.207722	-0.450122
6	-3.226023	1.911090	-1.403440
44	-1.211213	-0.301124	0.259437
1	-4.724890	0.391751	-0.958738
1	-4.974158	1.893749	-0.089091
1	-3.472874	2.967147	-1.563044
1	-3.199707	1.437723	-2.392252
6	-2.184750	-1.565581	-1.451644
6	-2.567219	-2.202338	-0.253141
6	-1.589675	-2.569180	0.689458
6	-0.218822	-2.399842	0.379439
6	0.161891	-1.905839	-0.886710
6	-0.809945	-1.435735	-1.780499
1	1.216918	-1.801187	-1.125618
1	-2.944330	-1.218778	-2.147144
1	-3.621196	-2.319469	-0.013161
1	-1.886899	-2.965135	1.656719
1	0.547352	-2.656411	1.105506
1	-0.509107	-0.980073	-2.720481
6	-0.994621	0.018400	2.398150
1	-1.011440	1.076929	2.675819
1	-0.043147	-0.417355	2.721796
1	-1.807100	-0.504504	2.918363
8	1.582448	-0.094989	0.767676
6	0.593277	0.751407	0.662299
8	0.711540	1.958428	0.740987
1	-1.502837	2.857206	0.248627
13	3.185491	0.187766	-0.007491
17	4.470283	1.499386	-1.073072
17	3.967613	-1.820300	-0.116502
17	2.718166	0.886319	-2.002633
1	-3.052082	1.716424	1.688778
1	-0.643845	2.187378	-1.649231
15	-3.397837	0.467916	1.092918
15	-1.554955	1.782954	-0.651831

Bn-Ru-PP-AICl3-Presence-C-C_bond formation-TS3_rev

Number of imaginary frequencies : 0
 The smallest frequencies are : 14.5854 33.3946 34.3915 cm(-1)

Electronic energy : =-2941.533339
 Zero-point correction= 0.245313
 Thermal correction to Energy= 0.268927
 Thermal correction to Enthalpy= 0.269871
 Thermal correction to Gibbs Free Energy= 0.190516
 Sum of electronic and zero-point Energies= -2941.288026
 Sum of electronic and thermal Energies= -2941.264412
 Sum of electronic and thermal Enthalpies= -2941.263468
 Sum of electronic and thermal Free Energies= -2941.342823

Cartesian Coordinates

6	-2.755272	-2.607041	-0.557103
6	-2.107076	-2.906921	0.785595
44	-1.300299	0.410388	-0.158606
1	-3.596089	-3.283863	-0.753292
1	-2.019325	-2.731769	-1.358553
1	-1.362156	-3.705425	0.725928
1	-2.846637	-3.177757	1.547488
6	-2.273488	1.865178	1.382193
6	-2.736806	2.305666	0.127723
6	-1.807475	2.577831	-0.891666
6	-0.414043	2.512826	-0.631347
6	0.045533	2.215851	0.665890
6	-0.878070	1.843667	1.655568
1	1.113692	2.178055	0.866887
1	-2.984363	1.558053	2.145440
1	-3.803128	2.336352	-0.079980
1	-2.155329	2.822414	-1.891627
1	0.302487	2.694287	-1.427985
1	-0.519976	1.529513	2.634070
6	-1.235163	-0.019922	-2.296832
1	-1.301809	-1.080508	-2.548136
1	-0.298039	0.381084	-2.699442
1	-2.073757	0.512065	-2.758747
8	1.422681	0.057691	-0.846345
6	0.396258	-0.726253	-0.645921
8	0.429821	-1.942531	-0.684627
1	-0.018217	-1.708379	1.899463
13	3.033817	-0.148570	-0.082362
17	2.613238	-0.700148	1.972899
17	3.830874	1.854264	-0.141316
17	4.291683	-1.560480	-1.064959
15	-3.381834	-0.844094	-0.511916
15	-1.270934	-1.362791	1.362970
1	-3.632506	-0.714729	-1.906963
1	-1.974748	-1.010162	2.539579

Bn-Ru-PP-AICl3-Presence-C-C_bond formation-TS3

Number of imaginary frequencies : 1
The smallest frequencies are : -333.2744 8.4683 36.7526 cm(-1)

Electronic energy : =-2941.5191424
Zero-point correction= 0.244619
Thermal correction to Energy= 0.267689
Thermal correction to Enthalpy= 0.268633
Thermal correction to Gibbs Free Energy= 0.190623
Sum of electronic and zero-point Energies= -2941.274523
Sum of electronic and thermal Energies= -2941.251453
Sum of electronic and thermal Enthalpies= -2941.250509
Sum of electronic and thermal Free Energies= -2941.328519

Cartesian Coordinates

6	-2.803791	-2.570381	-0.504344
6	-2.214576	-2.823199	0.874058
44	-1.317382	0.431256	-0.142558
1	-3.656100	-3.234569	-0.695437
1	-2.043499	-2.770439	-1.267036
1	-1.557141	-3.697800	0.895436
1	-2.996587	-2.966023	1.628806
6	-2.313747	1.844705	1.278683
6	-2.721298	2.290631	-0.001716
6	-1.753795	2.582303	-0.975461
6	-0.372842	2.492540	-0.649563
6	0.041005	2.205376	0.665649
6	-0.927714	1.827766	1.612569
1	1.099898	2.161917	0.909059
1	-3.057626	1.539738	2.010543
1	-3.778593	2.314641	-0.254209
1	-2.057603	2.836448	-1.987306
1	0.378243	2.654605	-1.419017
1	-0.615223	1.512137	2.606162
6	-0.760773	-0.365202	-2.247490
1	-1.305435	-1.284288	-2.451774
1	0.174542	-0.377944	-2.814985
1	-1.296840	0.505246	-2.637798
8	1.439544	0.052611	-0.935982
6	0.411034	-0.755376	-0.863186
8	0.468178	-1.959934	-0.671324
1	0.019486	-1.746750	1.820777
13	2.987367	-0.148975	-0.050075
17	2.494368	-0.590203	2.012064
17	3.820713	1.838374	-0.160653
17	4.267554	-1.615846	-0.921687
15	-3.391281	-0.787967	-0.580166
15	-1.245362	-1.326337	1.373411
1	-3.456084	-0.686993	-2.002926
1	-1.840325	-0.949876	2.602482

Bn-Ru-PP-AICl3-Presence-C-C_bond formation-TS3_for

Number of imaginary frequencies : 0
The smallest frequencies are : 33.8845 35.9092 48.4704 cm(-1)

Electronic energy : =-2941.6022642
Zero-point correction= 0.246323
Thermal correction to Energy= 0.270033
Thermal correction to Enthalpy= 0.270977
Thermal correction to Gibbs Free Energy= 0.191424
Sum of electronic and zero-point Energies= -2941.355941
Sum of electronic and thermal Energies= -2941.332231
Sum of electronic and thermal Enthalpies= -2941.331287
Sum of electronic and thermal Free Energies= -2941.410840

Cartesian Coordinates

6	2.983820	2.679559	-0.106533
6	2.574488	2.555729	1.351454
44	1.518209	-0.397054	-0.098687
1	3.861165	3.329976	-0.210290
1	2.169336	3.126041	-0.693686
1	2.292057	3.508838	1.813333
1	3.382544	2.111133	1.949269
6	2.819835	-1.925586	0.758549
6	2.741621	-2.204537	-0.636600
6	1.482886	-2.342772	-1.246079
6	0.287772	-2.299782	-0.455062
6	0.350532	-2.111396	0.929177
6	1.623287	-1.847145	1.520887
1	-0.561450	-2.038679	1.517836
1	3.782140	-1.733964	1.224739
1	3.646072	-2.207768	-1.239906
1	1.410515	-2.450733	-2.324251
1	-0.683683	-2.366704	-0.942654
1	1.682117	-1.597303	2.577929
6	-1.608072	1.439456	-2.621175
1	-0.955147	1.717293	-3.449623
1	-2.170447	2.312252	-2.271806

1	-2.345947	0.703352	-2.964354
8	-1.450255	0.517778	-0.422665
6	-0.828778	0.857165	-1.490005
8	0.408673	0.716829	-1.592496
1	0.073742	2.206653	1.019312
13	-3.054253	0.066289	0.231763
17	-2.679756	-0.136199	2.335409
17	-3.521713	-1.810377	-0.702887
17	-4.477024	1.595589	-0.216694
15	3.416996	0.959772	-0.765168
15	1.165314	1.370343	1.348795
1	3.017730	1.212002	-2.112700
1	0.871418	1.110268	2.706305

NNTs_Diphenyl Ligand

Bn-Ru-NNTs_Diphenyl-AA

Number of imaginary frequencies : 2

The smallest frequencies are : -39.0215 -14.2796 9.8862 cm(-1)

Electronic energy : =-2025.5463532
Zero-point correction= 0.533958
Thermal correction to Energy= 0.567237
Thermal correction to Enthalpy= 0.568181
Thermal correction to Gibbs Free Energy= 0.466234
Sum of electronic and zero-point Energies= -2025.012395
Sum of electronic and thermal Energies= -2024.979116
Sum of electronic and thermal Enthalpies= -2024.978172
Sum of electronic and thermal Free Energies= -2025.080119

.....
Cartesian Coordinates

6 -0.604039 0.421690 -0.269528
6 0.464323 1.362285 -0.856973
44 1.920990 -1.166195 -0.477132
1 -0.769171 0.721748 0.781988
1 0.465080 1.195764 -1.945941
6 3.753593 -1.661338 -1.616671
6 2.821397 -2.741467 -1.681403
6 2.335954 -3.354102 -0.499861
6 2.681383 -2.787737 0.749356
6 3.579751 -1.678325 0.818962
6 4.151873 -1.148652 -0.364799
1 3.742137 -1.162961 1.762432
1 4.072839 -1.169036 -2.530298
1 2.441583 -3.064272 -2.647169
1 1.576854 -4.128370 -0.549835
1 2.170865 -3.133374 1.643101
1 4.705723 -0.211626 -0.297589
7 1.756560 0.909886 -0.339629
1 1.909570 1.073790 0.695713
7 -0.016923 -0.941492 -0.288999
16 -0.989455 -2.298923 0.040545
6 -2.440546 -1.699264 0.868435
6 -3.676655 -1.796975 0.241733
6 -2.315011 -1.175673 2.152922
6 -4.804428 -1.344663 0.912818
1 -3.736672 -2.206259 -0.763636
6 -3.451597 -0.715056 2.801593
1 -1.338678 -1.132048 2.632538
6 -4.709103 -0.794618 2.193418
1 -5.778589 -1.407233 0.430214
1 -3.368522 -0.292586 3.801795
6 -5.934166 -0.324944 2.917030
1 -5.710665 0.514726 3.583623
1 -6.717369 -0.010129 2.219606
1 -6.354359 -1.127027 3.537147
8 -0.256261 -3.119023 1.004371
8 -1.381527 -2.906227 -1.228710
6 3.944800 1.839136 1.549307
8 4.266777 1.802940 0.333675
8 2.862949 1.399110 2.048061
6 4.930086 2.490386 2.506736
1 2.579917 1.419895 -0.691410
1 4.895342 3.576600 2.363866
1 4.687900 2.266255 3.548746
1 5.951189 2.173051 2.273340
6 -1.894914 0.591071 -1.030925
6 -2.900454 1.400723 -0.504159
6 -2.057651 0.036544 -2.301640
6 -4.058028 1.650356 -1.230991
1 -2.767806 1.838299 0.485462
6 -3.219830 0.279185 -3.025924
1 -1.282004 -0.611143 -2.707565
6 -4.221434 1.086546 -2.493153
1 -4.835518 2.283653 -0.809692
1 -3.343978 -0.165352 -4.010786
1 -5.128651 1.276285 -3.062473
6 0.166123 2.817119 -0.584623
6 -0.566556 3.554690 -1.516996
6 0.574268 3.430643 0.602603
6 -0.895080 4.882116 -1.268958
1 -0.893825 3.076540 -2.440846
6 0.247247 4.761347 0.845504
1 1.169939 2.883014 1.335404
6 -0.488186 5.488580 -0.084650
1 -1.465773 5.444428 -2.004561
1 0.577075 5.232745 1.768511
1 -0.738403 6.529186 0.109665

Number of imaginary frequencies : 0
The smallest frequencies are : 9.5409 19.9212 31.4977 cm(-1)

Electronic energy : =-2066.0333221
Zero-point correction= 0.581086
Thermal correction to Energy= 0.619747
Thermal correction to Enthalpy= 0.620691
Thermal correction to Gibbs Free Energy= 0.506548
Sum of electronic and zero-point Energies= -2065.452236
Sum of electronic and thermal Energies= -2065.413575
Sum of electronic and thermal Enthalpies= -2065.412631
Sum of electronic and thermal Free Energies= -2065.526774

Cartesian Coordinates

6	-1.647808	-0.393825	0.380470
6	-1.971604	0.758972	-0.585862
44	0.566374	-0.262479	-1.623514
1	-1.427152	0.031300	1.375562
6	1.042296	-0.408186	-3.768107
6	1.370842	-1.639620	-3.117423
6	2.252022	-1.652909	-2.016434
6	2.718524	-0.414931	-1.495405
6	2.403274	0.815242	-2.142592
6	1.592762	0.804683	-3.300312
1	2.637719	1.775713	-1.684462
1	0.310689	-0.402657	-4.570708
1	0.879225	-2.560163	-3.420692
1	2.419452	-2.578707	-1.474307
1	3.260571	-0.397671	-0.550892
1	1.259242	1.754468	-3.710136
6	4.607475	2.234990	0.229354
1	5.068100	2.715168	1.097527
1	4.560101	2.955369	-0.591495
1	3.592667	1.917427	0.495001
1	5.207594	1.369657	-0.069382
6	1.385321	3.351427	0.171210
8	1.366916	3.405976	-1.076732
8	0.855805	2.429090	0.878160
6	2.059401	4.471907	0.946605
1	-0.116733	1.737612	-0.234564
7	-0.686572	1.316970	-1.032908
7	-0.439896	-1.062975	-0.151615
16	0.164361	-2.347006	0.775850
6	1.689343	-1.684028	1.423295
6	1.732192	-0.384047	1.923627
6	2.802222	-2.514659	1.484175
6	2.917515	0.088447	2.465301
1	0.882719	0.290798	1.845729
6	3.981544	-2.025124	2.039302
1	2.741284	-3.528002	1.093069
6	4.056937	-0.722256	2.535473
1	2.957425	1.117326	2.823223
1	4.859939	-2.667040	2.088411
6	5.324593	-0.188269	3.129083
1	6.142409	-0.912338	3.059418
1	5.640640	0.731668	2.621401
1	5.188288	0.063555	4.187697
8	0.511572	-3.438134	-0.133902
8	-0.735588	-2.583937	1.896679
1	-0.791895	2.081280	-1.698704
1	1.289995	5.154401	1.326457
1	2.740326	5.040324	0.307292
1	2.593296	4.074043	1.816435
6	-2.856233	-1.295192	0.487174
6	-3.744107	-1.138283	1.548577
6	-3.150813	-2.212455	-0.521628
6	-4.917468	-1.881615	1.599079
1	-3.512743	-0.421508	2.336006
6	-4.320623	-2.962028	-0.467321
1	-2.445632	-2.353293	-1.341308
6	-5.208763	-2.795315	0.590889
1	-5.603840	-1.750793	2.432489
1	-4.536771	-3.683360	-1.252359
1	-6.123415	-3.382264	0.633482
6	-2.910156	1.770422	0.022708
6	-2.450225	2.719082	0.940790
6	-4.267484	1.727649	-0.297227
6	-3.344598	3.614317	1.517898
1	-1.390142	2.762887	1.199882
6	-5.159235	2.620838	0.285879
1	-4.627901	0.972814	-0.996787
6	-4.697504	3.568123	1.193785
1	-2.979964	4.353538	2.227588
1	-6.215296	2.576645	0.029767
1	-5.391761	4.270965	1.648948
1	-2.460893	0.309986	-1.464742

Number of imaginary frequencies : 1
The smallest frequencies are : -1640.5703 15.3474 20.5161 cm(-1)

Electronic energy : =-2065.9901693
Zero-point correction= 0.577496
Thermal correction to Energy= 0.614502
Thermal correction to Enthalpy= 0.615446
Thermal correction to Gibbs Free Energy= 0.506379
Sum of electronic and zero-point Energies= -2065.412673
Sum of electronic and thermal Energies= -2065.375667
Sum of electronic and thermal Enthalpies= -2065.374723
Sum of electronic and thermal Free Energies= -2065.483790

Cartesian Coordinates

6	-1.157236	-0.539658	-0.165873
6	-1.660276	0.871428	-0.521317
44	1.312237	1.032597	-1.017701
1	-0.918274	-0.532893	0.918820
6	1.208025	1.871942	-3.035195
6	1.817236	0.601726	-3.104402
6	2.969408	0.306010	-2.312097
6	3.471295	1.274613	-1.425675
6	2.874405	2.568171	-1.343546
6	1.740640	2.850035	-2.133485
1	3.185838	3.275323	-0.581855
1	0.296350	2.073381	-3.592001
1	1.358786	-0.204513	-3.668927
1	3.352322	-0.707695	-2.314717
1	4.264849	1.007437	-0.731225
1	1.221004	3.794910	-1.985542
6	1.780283	0.704272	1.259448
1	1.053391	0.786760	2.077643
1	2.802044	0.769989	1.651686
1	1.671033	1.965949	0.955775
1	1.676082	-0.310583	0.871373
6	0.828531	3.662649	2.064712
8	1.754922	3.311887	1.245854
8	-0.232122	3.037835	2.233496
6	1.100757	4.922883	2.851363
1	-0.457925	2.083115	0.700542
7	-0.545757	1.819107	-0.303911
7	0.053810	-0.733292	-0.975516
16	0.676319	-2.250276	-1.119369
6	1.536191	-2.628836	0.401293
6	0.786488	-2.943733	1.533946
6	2.921970	-2.542262	0.471111
6	1.434842	-3.131939	2.745876
1	-0.294075	-3.053513	1.452050
6	3.558456	-2.743944	1.690838
1	3.487759	-2.324876	-0.432145
6	2.826748	-3.029030	2.844751
1	0.856013	-3.373412	3.636781
1	4.644457	-2.682440	1.750972
6	3.510136	-3.257245	4.159139
1	4.551973	-2.922016	4.136185
1	3.000752	-2.726508	4.971473
1	3.511745	-4.322166	4.423905
8	1.698516	-2.207572	-2.169639
8	-0.386308	-3.243702	-1.224249
1	-0.768570	2.699223	-0.768224
1	1.391510	5.732400	2.174349
1	1.947468	4.753739	3.525274
1	0.224608	5.215549	3.433335
6	-2.323813	-1.480882	-0.383668
6	-3.032817	-1.956004	0.715494
6	-2.812534	-1.737673	-1.665999
6	-4.216765	-2.669031	0.544322
1	-2.669219	-1.738865	1.720535
6	-3.989314	-2.450463	-1.840567
1	-2.245290	-1.393732	-2.529735
6	-4.699957	-2.913937	-0.734345
1	-4.762290	-3.028013	1.414199
1	-4.354981	-2.651900	-2.845224
1	-5.624750	-3.469527	-0.873022
6	-2.923293	1.255999	0.206263
6	-2.917568	1.519863	1.578311
6	-4.138162	1.261939	-0.480856
6	-4.110672	1.775072	2.245266
1	-1.980570	1.544149	2.132567
6	-5.330633	1.510415	0.188064
1	-4.150163	1.035898	-1.546671
6	-5.318887	1.764995	1.555498
1	-4.093237	1.983198	3.312550
1	-6.270217	1.501386	-0.359534
1	-6.250226	1.959234	2.082747
1	-1.855070	0.858593	-1.604931

Bn-Ru-NNTs_Diphenyl-AA-Presence-TS1_for

Number of imaginary frequencies : 1
The smallest frequencies are : -27.2106 15.9379 22.6656 cm(-1)

Electronic energy : =-2066.0246715
Zero-point correction= 0.583279
Thermal correction to Energy= 0.619953
Thermal correction to Enthalpy= 0.620897
Thermal correction to Gibbs Free Energy= 0.512175
Sum of electronic and zero-point Energies= -2065.441393
Sum of electronic and thermal Energies= -2065.404719
Sum of electronic and thermal Enthalpies= -2065.403775
Sum of electronic and thermal Free Energies= -2065.512497

.....
Cartesian Coordinates

.....
6 -1.182195 -0.556986 -0.181487
6 -1.641976 0.852503 -0.598481
44 1.358769 0.885899 -1.014105
1 -0.959389 -0.521527 0.905336
6 1.521716 1.684195 -3.167266
6 2.014849 0.377587 -3.133631
6 3.023505 0.004340 -2.186475
6 3.543711 0.951692 -1.287668
6 3.038159 2.283961 -1.283704
6 1.986916 2.612046 -2.180052
1 3.415815 3.022553 -0.582683
1 0.720339 1.958393 -3.847935
1 1.577817 -0.400590 -3.752476
1 3.323244 -1.035529 -2.138660
1 4.271507 0.643703 -0.540082
1 1.538137 3.603548 -2.118970
6 1.615103 0.634157 1.088391
1 0.909508 1.217586 1.702427
1 2.635791 0.891371 1.412452
1 1.780524 2.878452 0.849381
1 1.453166 -0.416244 1.343279
6 0.893718 4.223285 1.861682
8 1.981026 3.758706 1.239742
8 -0.178506 3.654080 1.841973
6 1.165227 5.509576 2.573657
1 -0.463948 2.152260 0.508418
7 -0.506204 1.795109 -0.451796
7 0.028209 -0.824273 -0.964845
16 0.584937 -2.368667 -1.021423
6 1.407165 -2.725876 0.526919
6 0.631687 -3.041547 1.640368
6 2.790466 -2.635735 0.632569
6 1.250261 -3.229799 2.869420
1 -0.446394 -3.150214 1.530260
6 3.396773 -2.833189 1.867154
1 3.379302 -2.419086 -0.255564
6 2.637783 -3.123742 3.002885
1 0.649555 -3.473459 3.745259
1 4.480866 -2.766563 1.954824
6 3.296251 -3.360534 4.328835
1 4.272412 -2.867544 4.387541
1 2.678592 -2.991737 5.155171
1 3.461162 -4.431659 4.503119
8 1.618745 -2.432301 -2.058473
8 -0.520748 -3.320602 -1.090160
1 -0.702388 2.619825 -1.018442
1 1.619587 6.231361 1.888557
1 1.885507 5.334456 3.379223
1 0.238439 5.908017 2.986712
6 -2.385363 -1.458415 -0.380004
6 -3.118259 -1.879651 0.725342
6 -2.876302 -1.729699 -1.658746
6 -4.326986 -2.552561 0.564164
1 -2.749488 -1.655384 1.727022
6 -4.077982 -2.401937 -1.823566
1 -2.288554 -1.432344 -2.526151
6 -4.812237 -2.810995 -0.711080
1 -4.889718 -2.870833 1.439105
1 -4.444363 -2.615972 -2.825454
1 -5.756148 -3.335594 -0.842074
6 -2.872222 1.316522 0.138496
6 -2.816228 1.620407 1.500997
6 -4.102359 1.378369 -0.516103
6 -3.968496 1.974919 2.192484
1 -1.867220 1.577593 2.035786
6 -5.256944 1.726715 0.175348
1 -4.157051 1.118765 -1.572709
6 -5.192283 2.025347 1.532385
1 -3.909759 2.209035 3.252920
1 -6.210153 1.760558 -0.347123
1 -6.094538 2.297081 2.075543
1 -1.855898 0.794204 -1.675773

.....
Bn-Ru-NNTs_Diphenyl_AA-AlCl3-Presence-CO2-insertion-TS2_rev

Number of imaginary frequencies : 0
The smallest frequencies are : 21.0607 28.3916 29.4923 cm(-1)

Electronic energy : =-3877.6758942
 Zero-point correction= 0.603540
 Thermal correction to Energy= 0.650948
 Thermal correction to Enthalpy= 0.651892
 Thermal correction to Gibbs Free Energy= 0.519951
 Sum of electronic and zero-point Energies= -3877.072354
 Sum of electronic and thermal Energies= -3877.024946
 Sum of electronic and thermal Enthalpies= -3877.024002
 Sum of electronic and thermal Free Energies= -3877.155944

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 Cartesian Coordinates

6	2.188887	-0.066603	0.052216
6	1.955322	-0.892437	1.335532
44	0.007561	-2.191008	-0.459892
1	1.723283	0.929437	0.241752
1	2.469438	-1.854959	1.190980
6	1.180718	-4.160051	-0.649215
6	0.795939	-3.635087	-1.909565
6	-0.564596	-3.356964	-2.218476
6	-1.547973	-3.527920	-1.206860
6	-1.182653	-3.962123	0.090252
6	0.196325	-4.233789	0.362848
1	-1.929288	-4.027690	0.877815
1	2.225474	-4.354269	-0.423880
1	1.555966	-3.381725	-2.645577
1	-0.815162	-2.903338	-3.171395
1	-2.576471	-3.227301	-1.398450
1	0.492695	-4.494620	1.378734
6	-1.419826	-0.653811	-0.650665
1	-2.240569	-0.833012	0.062393
1	-1.857696	-0.676661	-1.657432
1	-1.004669	0.346904	-0.477008
8	-3.813067	0.410065	1.873129
6	-2.927700	-0.221769	2.330694
8	-2.135233	-0.877004	2.847851
1	-0.018604	-0.317762	1.436082
13	-5.169751	0.250458	0.350422
17	-6.886551	0.908943	1.348341
17	-4.283859	1.610385	-1.005491
17	-4.985061	-1.814168	-0.020156
1	0.288190	-1.722071	2.223244
16	1.615266	-0.135535	-2.531565
6	1.066290	1.569537	-2.423575
6	1.994682	2.574401	-2.172002
6	-0.283526	1.878642	-2.582514
6	1.558411	3.891252	-2.040449
1	3.050077	2.319373	-2.095491
6	-0.703424	3.193333	-2.448144
1	-0.989551	1.087009	-2.820082
6	0.206478	4.216822	-2.161095
1	2.281815	4.681666	-1.841315
1	-1.759913	3.438196	-2.561563
6	-0.279467	5.622136	-1.976917
1	0.536358	6.302482	-1.711295
1	-0.751588	6.006035	-2.889441
1	-1.036537	5.669496	-1.183428
8	0.652885	-0.842601	-3.378209
8	3.006714	-0.055090	-2.979091
7	1.514398	-0.777002	-1.030452
7	0.510183	-1.192807	1.381602
6	-0.940284	2.613369	1.242368
8	-1.838596	3.237112	0.493291
8	-1.154849	1.533939	1.776102
6	0.344338	3.363637	1.324379
1	-2.606636	2.652829	0.342976
1	0.864975	3.244829	0.362457
1	0.158682	4.433606	1.454602
1	0.972845	2.972257	2.127371
6	3.680671	0.140451	-0.105531
6	4.496513	-0.908463	-0.532012
6	4.269310	1.335892	0.297506
6	5.877031	-0.766189	-0.538798
1	4.027296	-1.826791	-0.884570
6	5.653975	1.483993	0.289424
1	3.633136	2.152002	0.645498
6	6.460358	0.430293	-0.123678
1	6.504284	-1.587089	-0.879484
1	6.101269	2.422277	0.610189
1	7.542414	0.541238	-0.132544
6	2.482742	-0.245400	2.594657
6	3.798135	-0.494011	2.996490
6	1.700307	0.619916	3.363171
6	4.325578	0.120548	4.125066
1	4.422287	-1.158487	2.399325
6	2.228184	1.233712	4.496737
1	0.666855	0.826088	3.084042
6	3.542046	0.989222	4.879197
1	5.353595	-0.081241	4.416644
1	1.603772	1.903658	5.084536
1	3.953146	1.468887	5.764399

.....

Number of imaginary frequencies : 1

The smallest frequencies are : -157.8063 16.1884 22.4957 cm(-1)

Electronic energy : =-3877.655245
 Zero-point correction= 0.604508
 Thermal correction to Energy= 0.651042
 Thermal correction to Enthalpy= 0.651986
 Thermal correction to Gibbs Free Energy= 0.522212
 Sum of electronic and zero-point Energies= -3877.050737
 Sum of electronic and thermal Energies= -3877.004203
 Sum of electronic and thermal Enthalpies= -3877.003259
 Sum of electronic and thermal Free Energies= -3877.133033

Cartesian Coordinates

6	2.184957	-0.580105	-0.133465
6	1.520477	-1.665240	0.724680
44	-0.807636	-0.883764	-0.863038
1	2.362026	0.284275	0.541031
1	1.398197	-2.552511	0.086231
6	-0.536454	-2.847054	-2.073523
6	-0.549412	-1.722225	-2.929232
6	-1.626626	-0.800117	-2.944055
6	-2.704029	-1.006890	-2.058502
6	-2.715809	-2.127374	-1.187994
6	-1.591792	-2.999270	-1.152537
1	-3.598001	-2.346125	-0.588975
1	0.317798	-3.517621	-2.058176
1	0.322709	-1.502527	-3.540601
1	-1.566018	0.085680	-3.565100
1	-3.521262	-0.287062	-2.015241
1	-1.567273	-3.802190	-0.417716
6	-1.208125	1.106960	-0.242874
1	-1.387333	1.187614	0.837427
1	-2.085147	1.495281	-0.773829
1	-0.328097	1.698605	-0.503772
8	-3.623086	-0.055572	0.763892
6	-2.819062	-0.901143	1.089052
8	-2.439400	-1.697948	1.866932
1	0.220965	-0.271193	1.507809
13	-5.539284	0.131503	0.614209
17	-6.092363	1.155871	2.364952
17	-5.687477	1.193515	-1.209937
17	-6.074827	-1.922703	0.500349
1	-0.337851	-1.821399	1.628104
16	1.669576	0.892197	-2.285583
6	1.967857	2.447304	-1.448354
6	3.112733	2.609653	-0.673597
6	1.067919	3.499455	-1.612710
6	3.319608	3.817094	-0.011636
1	3.852725	1.812596	-0.620206
6	1.298513	4.701387	-0.961281
1	0.204190	3.361453	-2.259011
6	2.412173	4.870598	-0.132722
1	4.215144	3.951254	0.595601
1	0.597679	5.526348	-1.084261
6	2.597237	6.152179	0.620375
1	3.563182	6.187286	1.135498
1	2.535748	7.022446	-0.043165
1	1.807204	6.269681	1.374529
8	0.530932	1.114686	-3.178934
8	2.956614	0.519035	-2.867451
7	1.211991	-0.238041	-1.181258
7	0.157478	-1.172422	1.017231
6	0.842308	2.680636	2.417063
8	0.075952	3.472009	1.674316
8	0.804602	1.465192	2.357217
6	1.761871	3.456330	3.302345
1	-0.429803	2.912436	1.053221
1	2.589465	3.825898	2.683646
1	1.253299	4.324560	3.729091
1	2.160766	2.813311	4.087583
6	3.525217	-1.120607	-0.585679
6	3.608129	-2.086832	-1.588629
6	4.678580	-0.771028	0.111701
6	4.819861	-2.695338	-1.882619
1	2.713281	-2.331768	-2.159917
6	5.896775	-1.379383	-0.179749
1	4.614624	-0.035867	0.915255
6	5.968853	-2.345635	-1.175141
1	4.874023	-3.440436	-2.673376
1	6.788512	-1.098739	0.376123
1	6.918423	-2.822548	-1.406815
6	2.315631	-2.073155	1.939137
6	3.023227	-3.276677	1.908066
6	2.407174	-1.261439	3.072287
6	3.812704	-3.664733	2.983426
1	2.975943	-3.900569	1.015522
6	3.190681	-1.656158	4.152249
1	1.881173	-0.308721	3.107505

6	3.895335	-2.854775	4.111453
1	4.363596	-4.601224	2.939990
1	3.253627	-1.018479	5.031365
1	4.509018	-3.156894	4.956935

 Bn-Ru-NNTs_Diphenyl_AA-AlCl3-Presence-CO2-insertion-TS2_for

Number of imaginary frequencies : 0
 The smallest frequencies are : 18.2604 19.6133 24.3893 cm(-1)

Electronic energy : =-3877.6602545
 Zero-point correction= 0.605410
 Thermal correction to Energy= 0.652461
 Thermal correction to Enthalpy= 0.653405
 Thermal correction to Gibbs Free Energy= 0.521932
 Sum of electronic and zero-point Energies= -3877.054844
 Sum of electronic and thermal Energies= -3877.007793
 Sum of electronic and thermal Enthalpies= -3877.006849
 Sum of electronic and thermal Free Energies= -3877.138322

 Cartesian Coordinates

6	2.117523	-0.676479	-0.135800
6	1.390149	-1.642040	0.806434
44	-0.911582	-0.784994	-0.769655
1	2.401822	0.204988	0.472823
1	1.187416	-2.562301	0.239286
6	-0.629864	-2.831874	-1.988429
6	-0.602019	-1.737606	-2.880027
6	-1.652662	-0.796250	-2.945322
6	-2.759864	-0.964333	-2.095063
6	-2.813342	-2.078001	-1.214533
6	-1.730959	-2.982808	-1.130870
1	-3.693135	-2.228720	-0.588020
1	0.216176	-3.510958	-1.932298
1	0.289867	-1.556823	-3.475316
1	-1.558095	0.068176	-3.592163
1	-3.571043	-0.237044	-2.080935
1	-1.761516	-3.784007	-0.396357
6	-1.143991	1.287363	-0.359194
1	-1.419533	1.489328	0.681629
1	-1.935469	1.666323	-1.013163
1	-0.192860	1.764837	-0.586130
8	-3.521594	0.182795	0.429646
6	-2.588591	-0.584704	0.795967
8	-2.439453	-1.251296	1.790102
1	0.217995	-0.086095	1.490270
13	-5.345258	0.178879	0.678831
17	-5.811514	1.358295	2.370800
17	-5.964541	0.978318	-1.208796
17	-5.837207	-1.901825	0.844519
1	-0.504439	-1.557729	1.712620
16	1.648913	0.794105	-2.300145
6	2.074229	2.340938	-1.507389
6	3.231144	2.437915	-0.739993
6	1.260492	3.455491	-1.710924
6	3.532861	3.646970	-0.118487
1	3.909148	1.589856	-0.661013
6	1.587262	4.656617	-1.101799
1	0.387003	3.365406	-2.352362
6	2.711782	4.764618	-0.277194
1	4.436916	3.730018	0.484707
1	0.955043	5.530144	-1.255722
6	3.001760	6.054376	0.426720
1	3.966412	6.029507	0.944552
1	3.014285	6.899101	-0.271532
1	2.222447	6.267867	1.170778
8	0.512696	1.071691	-3.179294
8	2.890378	0.297650	-2.885868
7	1.131359	-0.293960	-1.162683
7	0.082459	-1.016392	1.072071
6	1.005579	2.844593	2.296505
8	0.251886	3.678509	1.586772
8	0.941223	1.634441	2.186730
6	1.945439	3.565906	3.205411
1	-0.276985	3.147099	0.963525
1	2.790635	3.921532	2.602512
1	1.464071	4.438996	3.652874
1	2.317501	2.889107	3.975439
6	3.383596	-1.357944	-0.608368
6	3.352814	-2.362573	-1.575499
6	4.582934	-1.089407	0.046737
6	4.496936	-3.088015	-1.876161
1	2.426899	-2.546384	-2.118980
6	5.733101	-1.815085	-0.251022
1	4.607459	-0.324842	0.824502
6	5.691351	-2.818750	-1.210490
1	4.462406	-3.862399	-2.639261
1	6.661093	-1.596469	0.272085
1	6.587513	-3.387554	-1.446715
6	2.172246	-2.021377	2.037840
6	2.783036	-3.276032	2.086498

6	2.347231	-1.137994	3.105346
6	3.559318	-3.645432	3.177936
1	2.669531	-3.959200	1.244658
6	3.116639	-1.513617	4.201884
1	1.895155	-0.147945	3.076640
6	3.724728	-2.764146	4.241399
1	4.033810	-4.623512	3.198163
1	3.243299	-0.821252	5.031232
1	4.326979	-3.051617	5.099994

Bn-Ru-NNTs_Diphenyl_AA-AlCl3-Presence-C-C_bond formation-TS3_rev

Number of imaginary frequencies : 0
 The smallest frequencies are : 16.7750 22.4135 28.1307 cm(-1)

Electronic energy : =-3877.6763012
 Zero-point correction= 0.606416
 Thermal correction to Energy= 0.652940
 Thermal correction to Enthalpy= 0.653884
 Thermal correction to Gibbs Free Energy= 0.524648
 Sum of electronic and zero-point Energies= -3877.069885
 Sum of electronic and thermal Energies= -3877.023361
 Sum of electronic and thermal Enthalpies= -3877.022417
 Sum of electronic and thermal Free Energies= -3877.151654

Cartesian Coordinates

6	-1.274183	0.598860	0.461900
6	-0.299179	1.434803	-0.360508
44	0.611152	-1.460139	-0.691534
1	-0.777438	0.392810	1.422134
1	-0.653576	1.482045	-1.400972
6	1.232999	-0.895073	-2.923552
6	0.213439	-1.827844	-3.092702
6	0.275975	-3.039266	-2.363986
6	1.448701	-3.391162	-1.647918
6	2.537135	-2.506054	-1.584153
6	2.378466	-1.221623	-2.124356
1	3.428836	-2.749086	-1.012366
1	1.162776	0.101012	-3.356571
1	-0.684381	-1.584956	-3.652625
1	-0.580263	-3.703851	-2.374544
1	1.496980	-4.344192	-1.128315
1	3.156477	-0.474369	-1.975509
6	-0.226341	-2.991850	0.624024
1	-0.692628	-2.486390	1.468256
1	0.532756	-3.704908	0.960058
1	-0.989129	-3.464441	-0.000313
8	2.652484	-2.009753	1.214356
6	1.498322	-1.402039	1.216772
8	1.038642	-0.755852	2.131766
13	4.194725	-1.198241	1.686945
17	3.862536	0.922337	1.192277
17	5.603455	-1.992442	0.277523
17	4.706829	-1.438808	3.718960
7	0.941436	0.617284	-0.352254
7	-1.346506	-0.744220	-0.176805
16	-2.519411	-0.974692	-1.311227
6	-4.047542	-1.080267	-0.400805
6	-5.129230	-0.296311	-0.774685
6	-4.160101	-2.030132	0.610642
6	-6.332941	-0.444161	-0.095600
1	-5.015448	0.426191	-1.578545
6	-5.368545	-2.166589	1.275684
1	-3.299731	-2.639538	0.880330
6	-6.468096	-1.369173	0.940081
1	-7.184878	0.176253	-0.371180
1	-5.466409	-2.901393	2.073729
6	-7.752487	-1.479064	1.703909
1	-8.616641	-1.231042	1.078509
1	-7.899207	-2.487227	2.105724
1	-7.759530	-0.785916	2.555708
8	-2.327066	-2.316583	-1.876867
8	-2.622583	0.140117	-2.266483
1	1.603094	1.008997	-1.034480
1	1.389394	0.735996	0.559766
6	2.935943	3.091163	-2.070600
8	3.618234	3.347822	-0.968512
8	2.462908	1.994962	-2.337288
6	2.807092	4.294943	-2.944224
1	3.708764	2.537224	-0.425895
1	2.249349	4.046377	-3.847457
1	2.289026	5.080536	-2.383300
1	3.798551	4.679161	-3.201571
6	-2.580524	1.271133	0.808879
6	-3.159022	2.272903	0.029093
6	-3.216557	0.888121	1.991900
6	-4.348546	2.876313	0.425580
1	-2.693691	2.571434	-0.907180
6	-4.414850	1.472244	2.379199
1	-2.765113	0.103661	2.600515
6	-4.981828	2.474535	1.596484

1	-4.785052	3.660225	-0.189392
1	-4.903896	1.149931	3.296115
1	-5.915067	2.943286	1.901042
6	0.043767	2.814859	0.134353
6	-0.065517	3.910721	-0.722771
6	0.552206	3.007448	1.422532
6	0.317187	5.180419	-0.301197
1	-0.452538	3.761691	-1.731869
6	0.947234	4.273491	1.838586
1	0.656725	2.162859	2.105672
6	0.830631	5.362213	0.978875
1	0.214073	6.029155	-0.974898
1	1.350812	4.408560	2.838813
1	1.140409	6.351198	1.307525

 Bn-Ru-NNTs_Diphenyl_AA-AlCl3-Presence-C-C_bond formation-TS3

Number of imaginary frequencies : 1
 The smallest frequencies are : -230.0324 15.7737 21.3254 cm(-1)

Electronic energy : =-3877.6687531
 Zero-point correction= 0.605149
 Thermal correction to Energy= 0.651241
 Thermal correction to Enthalpy= 0.652185
 Thermal correction to Gibbs Free Energy= 0.522373
 Sum of electronic and zero-point Energies= -3877.063604
 Sum of electronic and thermal Energies= -3877.017512
 Sum of electronic and thermal Enthalpies= -3877.016568
 Sum of electronic and thermal Free Energies= -3877.146380

 Cartesian Coordinates

6	-1.777464	0.410843	0.042910
6	-0.804440	1.480186	-0.461601
44	0.825690	-1.022961	-0.773078
1	-1.697509	0.402846	1.150925
1	-0.920100	1.548117	-1.553547
6	0.714687	-0.674505	-3.014474
6	0.272524	-2.000708	-2.806336
6	1.053023	-2.915722	-2.069252
6	2.320049	-2.508959	-1.591542
6	2.828640	-1.222703	-1.911244
6	2.013572	-0.294166	-2.579224
1	3.804777	-0.911878	-1.549641
1	0.060593	0.044739	-3.500293
1	-0.739369	-2.276161	-3.099608
1	0.639231	-3.885479	-1.814029
1	2.916114	-3.166372	-0.964647
1	2.359233	0.731964	-2.701328
6	0.548819	-2.092300	1.193451
1	-0.090163	-1.452544	1.805023
1	1.325563	-2.550683	1.809002
1	-0.019330	-2.891965	0.711644
8	3.223103	-1.543644	0.903288
6	2.160187	-0.816207	1.000200
8	2.003948	0.121752	1.761021
13	4.890580	-0.865543	1.165968
17	4.851726	0.994826	0.004173
17	6.086755	-2.278336	0.102363
17	5.370255	-0.566913	3.200124
7	0.546521	0.969425	-0.198584
7	-1.283387	-0.867036	-0.486232
16	-2.291353	-2.100125	-0.869311
6	-3.583153	-2.085767	0.354360
6	-4.906592	-1.958747	-0.049576
6	-3.250098	-2.242804	1.696614
6	-5.907501	-1.972634	0.912762
1	-5.131964	-1.830038	-1.105090
6	-4.262331	-2.248627	2.645462
1	-2.208106	-2.356946	1.991490
6	-5.602740	-2.114200	2.268431
1	-6.947573	-1.863493	0.608847
1	-4.013923	-2.364396	3.699547
6	-6.689948	-2.151089	3.298973
1	-7.573278	-1.592324	2.972667
1	-7.011224	-3.182428	3.492660
1	-6.353888	-1.733659	4.254118
8	-1.538568	-3.352774	-0.720009
8	-2.924309	-1.902657	-2.180938
1	1.237520	1.564297	-0.674702
1	0.778591	0.989763	0.803396
6	2.292958	3.783805	-0.733427
8	2.942361	3.548205	0.395808
8	2.074079	2.925364	-1.577595
6	1.822673	5.197041	-0.830299
1	3.326144	2.644005	0.390303
1	1.398396	5.382831	-1.817485
1	1.052646	5.362205	-0.065605
1	2.644501	5.887656	-0.622754
6	-3.182670	0.849077	-0.303843
6	-3.607838	0.950213	-1.630408
6	-4.026021	1.292888	0.713999

6	-4.863983	1.465952	-1.926600
1	-2.964991	0.589254	-2.431107
6	-5.279897	1.815393	0.419007
1	-3.692081	1.225664	1.749398
6	-5.703121	1.899581	-0.903321
1	-5.189979	1.528805	-2.962317
1	-5.927612	2.154428	1.224159
1	-6.685144	2.303922	-1.138096
6	-1.015935	2.844882	0.143250
6	-1.631963	3.847181	-0.608011
6	-0.633559	3.122037	1.458721
6	-1.862273	5.103292	-0.059540
1	-1.944117	3.631552	-1.629185
6	-0.854110	4.382328	2.005526
1	-0.153468	2.358119	2.072125
6	-1.469424	5.375145	1.248311
1	-2.346153	5.873057	-0.655952
1	-0.543818	4.586949	3.027168
1	-1.643559	6.358776	1.677923

 Bn-Ru-NNTs_Diphenyl_AA-AlCl3-Presence-C-C_bond formation-TS3_for

Number of imaginary frequencies : 0
 The smallest frequencies are : 12.8259 20.7130 28.2352 cm(-1)

Electronic energy : =-3877.756271
 Zero-point correction= 0.606669
 Thermal correction to Energy= 0.653930
 Thermal correction to Enthalpy= 0.654874
 Thermal correction to Gibbs Free Energy= 0.520741
 Sum of electronic and zero-point Energies= -3877.149602
 Sum of electronic and thermal Energies= -3877.102341
 Sum of electronic and thermal Enthalpies= -3877.101397
 Sum of electronic and thermal Free Energies= -3877.235530

 Cartesian Coordinates

6	-1.441890	0.507679	-0.332161
6	-0.289136	1.231960	-1.039594
44	0.246470	-1.580552	-1.626203
1	-1.253133	0.559932	0.753084
1	-0.562690	1.335725	-2.101476
6	0.053633	-2.919652	-3.331725
6	-0.196481	-3.684768	-2.167419
6	0.735647	-3.629137	-1.101728
6	1.952847	-2.897411	-1.238486
6	2.233742	-2.218916	-2.448638
6	1.278909	-2.202699	-3.485860
1	3.108416	-1.574851	-2.500085
1	-0.720142	-2.828238	-4.089361
1	-1.155778	-4.171676	-2.022336
1	0.472441	-4.074859	-0.146451
1	2.626672	-2.783182	-0.390925
1	1.433172	-1.571997	-4.356021
6	0.618289	-2.783294	2.697418
1	-0.245576	-2.986411	2.053445
1	0.238815	-2.537082	3.696175
1	1.257545	-3.664412	2.788914
8	2.677033	-1.709433	2.256100
6	1.382062	-1.601335	2.169579
8	0.796672	-0.624848	1.700698
13	3.941386	-0.472200	1.948050
17	4.054893	-0.279844	-0.239466
17	5.759895	-1.270746	2.689334
17	3.441503	1.450045	2.739018
7	0.875917	0.330965	-0.991422
7	-1.359644	-0.910459	-0.756477
16	-2.570648	-2.012526	-0.279058
6	-3.486273	-1.222485	1.015854
6	-4.825876	-0.916181	0.811550
6	-2.849577	-0.958862	2.227305
6	-5.540257	-0.327557	1.846280
1	-5.285003	-1.127582	-0.150976
6	-3.578356	-0.356869	3.242363
1	-1.792565	-1.192923	2.356721
6	-4.930308	-0.038954	3.069444
1	-6.589892	-0.077201	1.701121
1	-3.094248	-0.129201	4.190782
6	-5.713152	0.578181	4.187710
1	-6.561445	1.159760	3.812458
1	-6.117192	-0.194179	4.854459
1	-5.088562	1.237379	4.799798
8	-1.878910	-3.159284	0.314357
8	-3.446508	-2.257367	-1.421815
1	1.662872	0.742082	-1.510308
1	1.163744	0.177250	-0.014052
6	3.053047	2.974890	-1.972601
8	3.770664	2.895896	-0.862045
8	2.553476	2.011231	-2.531868
6	2.911410	4.386100	-2.442183
1	3.847257	1.959899	-0.581246
1	2.409954	4.409972	-3.410190

1	2.315786	4.936215	-1.703725
1	3.890743	4.869340	-2.499973
6	-2.746222	1.195979	-0.649693
6	-3.392247	0.991224	-1.869765
6	-3.270168	2.117836	0.256388
6	-4.561233	1.684272	-2.166246
1	-2.992624	0.262287	-2.573507
6	-4.432548	2.817126	-0.044082
1	-2.759261	2.282468	1.205078
6	-5.084148	2.596788	-1.254336
1	-5.066769	1.508964	-3.113151
1	-4.834086	3.531249	0.671253
1	-5.998703	3.137207	-1.487900
6	-0.013330	2.601161	-0.471288
6	-0.507762	3.733011	-1.121616
6	0.718394	2.755194	0.708245
6	-0.277461	5.002057	-0.601185
1	-1.088782	3.612691	-2.036299
6	0.967718	4.026099	1.216049
1	1.109017	1.889469	1.245500
6	0.467684	5.151010	0.566323
1	-0.673581	5.876382	-1.112969
1	1.560078	4.126958	2.122473
1	0.659212	6.143382	0.968295