Reactions of Carbene-Stabilized Borenium Cations

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Supporting Information

Table of Contents

General Considerations	1
NMR Spectra of 4	2
NMR Spectra of 5	4
In-situ NMR Spectra of Oxidation of 4	6
In-situ NMR Spectra of Oxidation of 5	7
NMR Spectra of 6	8
NMR Spectra of 7	10
NMR Spectra of 8a/8b	12
NMR Spectra of 9	14
NMR Spectra of 10	17
NMR Spectra of 11	
NMR Spectra of 12	21
NMR Spectra of 13	23
Computational Details	
Tables of Optimized Coordinates	27
References	

General Considerations

All manipulations were carried out under dry, O₂-free N₂ using an MBraun or an Innovative Technology glovebox and a Schlenk vacuum-line. Pentane and dichloromethane were collected from a Grubbs-type column system manufactured by Innovative Technology and into thick-walled glass Schlenk bombs with Young-type Teflon valve stopcocks. Spectrograde chloroform was obtained from ACP Chemicals, dried over CaH₂, and vacuum-transferred into Young bombs. Tetrahydrofuran was obtained from Sigma-Aldrich, dried over Na/benzophenone, and vacuumtransferred into Young bombs. Dichloromethane-d₂ and chloroform-d were obtained from Cambridge Isotope Laboratories, dried over CaH₂, and vacuum-transferred into Young bombs. All solvents were degassed after purification and stored over 4 Å molecular sieves. Commercial reagents were purchased from Sigma-Aldrich, TCI Chemicals, Strem Chemicals or Alfa Aesar, and used without further purification unless indicated otherwise. 1,3-dibenzylimidazolium bromide¹ 1,3-dibenzylimidazolyl-2-ylidene-borane², di-t-butyl(ethynyl)phosphane,³ di-tertbutyl(phenylethynyl)phosphane³ and dimesityl(1-phenylvinyl)phosphane⁴ were prepared using literature methods.

NMR spectra were recorded on a Bruker Avance 400 MHz spectrometer at 25 °C. Chemical shifts are given relative to SiMe₄ and referenced to the residual solvent signal (¹H, ¹³C) or relative to an external standard (¹¹B: 15% (Et₂O)BF₃, ³¹P: 85% H₃PO₄, ¹⁹F: CFCI₃). Chemical shifts are reported in ppm and coupling constants as scalar values in Hz. Mass spectrometry was carried out using an AB/Sciex QStar mass spectrometer with an ESI source. GC-MS spectra were obtained on an Agilent Technologies 5975C VL MSD with Triple Axis Detector and 7890A GC System. Column Agilent 19091S-433 (30m x 250 µm x 0.25 µm). Helium was used as the carrier gas. Elemental analyses (C, H, N) were performed in-house with a Perkin Elmer 2400 Series II CHNS Analyzer.



Figure S2. ¹³C{H} NMR spectrum of **4**. (* residual pentane)



Figure S4. ¹⁹F NMR spectrum of **4**.



Figure S6. ¹³C{H} NMR spectrum of **5** (in CDCl₃)



Figure S8. ¹⁹F NMR spectrum of **5**.





Figure S10. In-situ ¹³C{H} NMR spectrum of cyclohexanol in the reaction mixture. (in CDCl₃).



Figure S12. ¹³C{H} NMR spectrum 3,3-dimethylbutan-1-ol in the reaction mixture.





5.55

Figure S13. ¹H NMR spectrum of **6** with minor unknown impurities. (* residual pentane)



Figure S14. ¹³C{H} NMR spectrum of **6**. (* residual pentane) (in CDCl₃)



-30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220

Figure S16. ¹⁹F NMR spectrum of **6**.



Figure S18. ¹³C{H} NMR spectrum of **7**. (in CDCl₃)



Figure S20. ¹⁹F NMR spectrum of **7**.



Figure S21. ¹H NMR spectrum of **8a/8b** with minor unknown impurities. (* residual pentane)

 $\begin{bmatrix} 140.28\\ 133.62\\ 133.62\\ 133.62\\ 137.62\\ 137.62\\ 137.62\\ 137.62\\ 137.62\\ 137.62\\ 137.62\\ 137.62\\ 137.62\\ 137.62\\ 137.62\\ 137.62\\ 128.64\\ 1229.22\\ 128.65\\ 1229.22\\ 1229.22\\ 1229.22\\ 1226.25\\ 1226.25\\ 1226.25\\ 1226.39\\$



Figure S22. ¹³C{H} NMR spectrum of 8a/8b. (* residual pentane) (in CDCl₃)



Figure S24. ¹⁹F NMR spectrum of **8a/8b**.







Figure S26. ¹H{¹¹B} NMR spectrum of **9**.





Figure S28. ³¹P{H} NMR spectrum of **9**.



Figure S30. ¹⁹F NMR spectrum of **9**.

NMR Spectra of 10 5.88 5.89 5.90 5.95



Figure S32. ¹H{¹¹B} NMR spectrum of **10** with minor impurities.



Figure S34. ¹¹B NMR spectrum of **10**.



-30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220

Figure S35. ¹⁹F NMR spectrum of **10**.



Figure S36. ³¹P NMR spectrum of **11**.



Figure S38. ¹⁹F spectrum of **11**.



Figure S39. ¹H NMR spectrum of **12**. (* residual pentane, ⁺ residual toluene)



Figure S40. ¹³C{H} NMR spectrum of **12**. (in CDCl₃)



Figure S42. ¹⁹F NMR spectrum of **12**.



Figure S43. ³¹P{H} NMR spectrum of **12**.



Figure S44. 1H NMR spectrum of 13. (* residual pentane)



Figure S45. ¹³C{H} NMR spectrum of **13**. (* residual pentane)





Figure S46. ¹¹B NMR spectrum of **13**.



Figure S47. ¹⁹F NMR spectrum of **13**.



Figure S48. ³¹P{H} NMR spectrum of **13**.

Computational Details

Table S1. Isotropic shift of the boron centre.

	δ (absolute) _{comp}	δ (referenced) _{comp}	δ (CDCl ₃) _{expt}
2	-59.4461	48.1	48.1
11 ^a	-1091.43	-1.5966	-1.8

^a Isotropic shift calculated for both isomers were identical.

Table S2. Isotropic shift of the phosphorus centre.

	δ (absolute) _{comp}	δ (referenced) _{comp}	δ (CDCI ₃) _{expt}
H ₂ CC(Ph)PMes ₂	-227.545	40.3	40.3
11 ^a	-243.33	26.6	33

^a Isotropic shift calculated for both isomers were identical.

Tables of Optimized Coordinates

The following tables contain the optimized coordinates of the compounds. All calculations were carried out in the gas phase.

Center Number	Atomic Number	Atomic Type	Coorc x	linates (Ang: Y	stroms)
1	6	0	0.954465	0.576459	-3.640107
2	6	0	1.782385	1.265427	-4.494492
3	6	0	1.381343	2.581345	-2.728578
4	7	0	0.720379	1.397288	-2.565778
5	1	0	0.524485	-0.415656	-3.726373
6	1	0	2.191165	0.984862	-5.458843
7	7	0	2.033358	2.486661	-3.922927
8	6	0	-0.128064	1.069845	-1.411620
9	1	0	-1.138642	0.858194	-1.798208
10	1	0	0.254214	0.129742	-0.982127
11	6	0	-0.203987	2.133372	-0.337982
12	6	0	0.461533	3.385597	-0.450857
13	6	0	-0.974739	1.845979	0.792275
14	6	0	0.318109	4.319511	0.607495
15	6	0	-1.094649	2.787453	1.817953
16	1	0	-1.487666	0.884950	0.882532
17	6	0	-0.448218	4.028663	1.728999
18	1	0	0.826477	5.282524	0.527063
19	1	0	-1.698514	2.549527	2.695564
20	1	0	-0.548791	4.756283	2.535448
21	6	0	2.931689	3.529039	-4.501991
22	1	0	2.683893	4.463395	-3.983213
23	1	0	3.962834	3.254499	-4.235395
24	6	0	2.779906	3.654595	-5.997922
25	6	0	1.655180	4.289519	-6.549393
26	6	0	3.770641	3.146602	-6.850854
27	6	0	1.521406	4.405002	-7.933803
28	1	0	0.885708	4.706663	-5.894258
29	6	0	3.637327	3.265422	-8.237826
30	1	0	4.660112	2.670368	-6.429499
31	6	0	2.511718	3.891465	-8.779294
32	1	0	0.648765	4.906612	-8.355204
33	1	0	4.417346	2.875579	-8.893685
34	1	0	2.408968	3.989106	-9.861241
35	5	0	1.306565	3.707388	-1.677018
36	1	0	1.878387	4.745500	-1.836967

Table S3. Optimized Cartesian coordinates of 2.

Center	Atomic	Atomic	Coord	dinates (Ang	stroms)
Number	Number	Туре	Х	Y	Ζ
1	6	0	0.371462	-2.479575	-1.243612
2	1	0	-0.691990	-2.392382	-1.473783
3	1	0	0.921298	-3.305252	-1.703390
4	6	0	0.989170	-1.636616	-0.398575
5	6	0	2.446072	-1.773606	-0.112860
6	6	0	2.982622	-1.477379	1.148325
7	6	0	3.324923	-2.186754	-1.127296
8	6	0	4.350941	-1.599743	1.388157
9	1	0	2.318922	-1.155555	1.952532
10	6	0	4.689450	-2.310939	-0.887173
11	1	0	2.931916	-2.379443	-2.127417
12	6	0	5.210067	-2.016953	0.374061
13	1	0	4.745941	-1.366872	2.378246
14	1	0	5.353733	-2.625663	-1.693658
15	1	0	6.281046	-2.106536	0.561564
16	15	0	0.031548	-0.488124	0.678325
1/	6	0	0.3/048/	1.293695	0.301622
18	6	0	1.283/68	1.835664	-0.631//6
19	6	0	-0.3/8992	2.181290	1.11/463
20	6	0	_0 232026	3.223723	-0.743961
21	6	0	-0.232920	J.J01303	0.937104
22	0	0	2 099207	4.110009 3.629088	-1 179992
23	1	0	-0 830417	4 226879	1 585934
25	6	0	-1 708411	-0 753826	0 110597
26	6	0	-2.279467	-0.171637	-1.040555
23	6	0	-2.503727	-1.583839	0.936612
28	6	0	-3.636208	-0.391498	-1.311126
29	6	0	-3.848926	-1.780070	0.622246
30	6	0	-4.440957	-1.179143	-0.491030
31	1	0	-4.071301	0.062872	-2.205300
32	1	0	-4.453051	-2.425047	1.265977
33	6	0	-1.493550	0.662924	-2.019723
34	1	0	-1.373818	1.698336	-1.666301
35	1	0	-0.486056	0.254492	-2.172147
36	1	0	-2.008058	0.689947	-2.989329
37	6	0	-1.933312	-2.282576	2.147302
38	1	0	-1.073364	-2.912556	1.875788
39	1	0	-1.572506	-1.560276	2.893826
40	1	0	-2.693555	-2.920726	2.615931
41	6	0	-5.903846	-1.378948	-0.786207
42	1	0	-6.148034	-1.083600	-1.814919
43	1	0	-6.196521	-2.429197	-0.648045
44	1	0	-6.523609	-0.773772	-0.106806
45	6	0	2.1645//	1.01328/	-1.53/926
46	1	0	3.030800	0.612639	-0.991060
4 /	1	0	1.038047	1 620225	-1.9/8323
40 10	1	0	2.34/429 _1 350007	1 700562 1 700562	-2.30016U
49 50	ю 1	0	-1.338UZ/ -2.258520	1 262382	2.102328 1 707165
51	⊥ 1	0	_0 910337	1.202302 0 924328	2 801533
52	± 1	0	-1 671921	2 536261	2 800803
53	- 6	0	0.820145	5.600313	-0.101395
54	1	0	1.124470	5.877807	-1.119597
55	1	0	-0.111788	6.129750	0.138608
56	1	õ	1.596531	5.967339	0.587933

Table S4. Optimized Cartesian coordinates of dimesityl(1-phenylvinyl)phosphane.

Number Type X Y Z 1 6 0 2.989407 1.363575 -2.853952 2 6 0 3.608842 0.161232 -2.705709 3 6 0 2.043625 1.440921 -1.856440 4 7 0 2.043625 1.440921 -1.856440 5 1 0 3.149630 2.162333 -3.571206 6 1 0 4.428790 -0.291471 -3.255149 9 1 0 1.62236 3.472751 -2.03052 10 1 0 0.198995 2.437156 -1.778205 11 6 0 1.484669 4.106682 0.54462 14 6 0 1.631900 4.293860 1.904698 2.235379 15 6 0 1.654573 3.186688 2.761918 18 1 0 1.50564 3.207063 3.834066 21 <	Center	Atomic	Atomic	Coord	dinates (Ang	stroms)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Number	Number	Туре	X	Y	Z
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1	6		2,989407	1.363575	-2.853952
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	2	6	0	3.608842	0.161232	-2.705709
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3	6	0	2.054939	0.319730	-1.113278
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	4	7	0	2.043625	1.440921	-1.856440
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	5	1	0	3.149630	2.162533	-3.571206
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	6	1	0	4.428790	-0.291471	-3.255149
8 6 0 1.241715 2.608370 -1.473424 9 1 0 1.622326 3.472551 -2.03052 10 1 0 0.198995 2.437156 -1.778205 11 6 0 1.333138 2.822960 0.022252 12 6 0 1.446609 4.110632 0.541462 14 6 0 1.446609 4.10638 2.23379 15 6 0 1.654573 3.186688 2.761918 18 1 0 1.506227 1.048166 2.321941 20 1 0 1.756576 5.298642 2.321941 21 0 3.662432 -2.439722 -1.83593 23 1 0 3.662432 -2.439722 -1.815697 24 6 0 4.822308 -1.694453 0.710787 24 6 0 5.954185 -2.217223 -0.357468 27 6 </td <td>7</td> <td>7</td> <td>0</td> <td>3.018282</td> <td>-0.462792</td> <td>-1.626306</td>	7	7	0	3.018282	-0.462792	-1.626306
9 1 0 1.62226 3.472751 -2.03052 10 1 0 0.198995 2.437156 -1.778205 11 6 0 1.292021 1.697195 0.063568 13 6 0 1.484669 4.101632 0.541462 14 6 0 1.486038 1.904698 2.235379 15 6 0 1.651970 3.186688 2.761918 16 1 0 1.506277 1.048166 2.915167 19 1 0 1.756676 5.298642 2.321941 20 1 0 3.662432 -2.439722 -1.815697 24 6 0 4.322308 -1.694453 -0.771122 25 6 0 4.824679 -0.461345 0.710787 26 0 0 5.954185 -2.217283 -0.57668 27 6 0 6.69185 0.148918 0.935326 29 </td <td>8</td> <td>6</td> <td>0</td> <td>1.241715</td> <td>2.608370</td> <td>-1.473424</td>	8	6	0	1.241715	2.608370	-1.473424
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	9	1	0	1.622326	3.472751	-2.030052
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	10	1	0	0.198995	2.437156	-1.778205
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	11	6	0	1.333138	2.825960	0.022252
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	12	6	0	1.292021	1.697195	0.863568
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	13	6	0	1.484669	4.110632	0.541462
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	14	6	0	1.486038	1.904698	2.235379
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	15	6	0	1.631900	4.293860	1.916662
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	16	1	0	1.506801	4.973460	-0.127932
18101.509271.0481662.91516719101.7566765.2986422.32194120101.8055643.3207063.83408621603.528389 -1.694453 -1.020343 22102.75267 -2.059635 -0.336934 23103.662432 -2.439722 -1.815697 2460 4.822308 -1.451416 -0.277122 2560 4.884679 -0.643345 0.710787 2660 5.954185 -2.217283 -0.557868 2760 6.069185 -0.244528 1.408516 2810 4.003555 0.148918 0.935326 2960 7.140342 -2.002112 0.145492 3010 5.9511584 -2.991454 -1.3275433 3160 7.198765 -1.016232 1.127285 3210 8.1225964 -0.845910 1.675608 3550 1.117672 0.237121 0.181880 3660 0.948303 -1.013867 1.206718 3710 0.924922 -1.996789 0.710390 3810 1.666217 -1.086731 2.039854 3960 -1.314395 -1.758440 2.337832 4260 -2.78461 -2.490903 4.180288	17	6	0	1.654573	3.186688	2.761918
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	18	1	0	1.509227	1.048166	2.915167
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	19	1	0	1.756676	5.298642	2.321941
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	20	l	0	1.805564	3.320/06	3.834086
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	21	6	0	3.528389	-1.694453	-1.020343
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	22	1	0	2.752657	-2.059635	-0.336934
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	23		0	3.662432	-2.439/22	-1.815697
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	24	6	0	4.822308	-1.451416	-0.277122
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	20	6	0	4.0040/9	-0.401343	0.710767
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	20	6	0	5.954105 6 069185	-2.21/203	-0.557888
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	27	1	0	0.009105	-0.244J28	0 035326
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	20	6	0	7 140342	-2 002112	0.935320
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	30	1	0	5 911584	-2 991454	-1 327543
3210 6.112250 0.528444 2.176700 33 10 8.020627 -2.605730 -0.078433 34 10 8.125964 -0.845910 1.675608 35 50 1.117672 0.237121 0.181880 36 60 0.948303 -1.013865 1.206718 37 10 0.924922 -1.996789 0.710390 38 10 1.666217 -1.086731 2.039854 39 60 -0.426490 0.175893 2.375420 41 60 -1.314395 -1.758440 2.33383 42 60 -1.933919 -1.515902 3.567291 43 60 -2.718461 -2.490903 4.180288 45 10 -1.778795 -0.553112 4.063389 46 60 -2.262733 -3.993614 2.351543 47 10 -0.949741 -3.245128 0.788505 48 60 -2.892216 -3.731009 3.568174 49 10 -3.189071 -2.282936 5.142063 51 10 -3.506414 -4.966803 1.873375 51 10 -3.506414 -4.966803 1.873375 51 10 -3.506414 -4.966803 1.873375 51 10 -3.506414 -4.966803 1.873375 51 1	31	- 6	0	7 198705	-1 016232	1 127285
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	32	1	0	6.112250	0.528444	2.176700
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	33	1	0	8.020627	-2.605730	-0.078433
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	34	1	0	8.125964	-0.845910	1.675608
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	35	5	0	1.117672	0.237121	0.181880
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	36	6	0	0.948303	-1.013865	1.206718
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	37	1	0	0.924922	-1.996789	0.710390
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	38	1	0	1.666217	-1.086731	2.039854
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	39	6	0	-0.486508	-0.678528	1.696406
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	40	1	0	-0.426490	0.175893	2.375420
4260 -1.933919 -1.515902 3.567291 43 60 -1.476394 -3.018668 1.741620 44 60 -2.718461 -2.490903 4.180288 45 10 -1.788795 -0.553112 4.063389 46 60 -2.262733 -3.993614 2.351543 47 10 -0.994741 -3.245128 0.788505 48 60 -2.892216 -3.731009 3.568174 49 10 -3.189071 -2.282936 5.142063 50 10 -2.381926 -4.966803 1.873375 51 10 -3.506414 -4.496299 4.044342 52 150 -0.932834 0.045644 -0.000924 53 60 -2.284661 1.920411 -1.527218 54 60 -2.284661 1.920411 -1.527218 55 60 -3.041603 3.074650 -1.751281 57 60 -3.041603 3.074650 -1.751281 57 60 -3.501787 3.875773 -0.708976 59 10 -3.278595 3.351547 -2.781389 60 10 -3.278592 -1.989200 -0.902604	41	6	0	-1.314395	-1.758440	2.333383
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	42	6	0	-1.933919	-1.515902	3.567291
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	43	6	0	-1.476394	-3.018668	1.741620
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	44	6	0	-2.718461	-2.490903	4.180288
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	45	1	0	-1.788795	-0.553112	4.063389
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	46	6	0	-2.262733	-3.993614	2.351543
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	47	1	0	-0.994741	-3.245128	0.788505
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	48	6	0	-2.892216	-3.731009	3.568174
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	49	1	0	-3.189071	-2.282936	5.142063
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	50	1	0	-2.381926	-4.966803	1.873375
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	51	1	0	-3.506414	-4.496299	4.044342
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	52	15	0	-0.932834	0.045644	-0.000924
54 6 0 -2.284661 1.920411 -1.527218 55 6 0 -2.416020 2.356359 0.876107 56 6 0 -3.041603 3.074650 -1.751281 57 6 0 -3.171606 3.495113 0.592772 58 6 0 -3.278595 3.351547 -2.781389 60 1 0 -3.518120 4.108572 1.427876 61 6 0 -1.928242 -1.288820 -0.2020604	53	6	0	-1.967684	1.551999	-0.197631
55 6 0 -2.416020 2.356359 0.876107 56 6 0 -3.041603 3.074650 -1.751281 57 6 0 -3.171606 3.495113 0.592772 58 6 0 -3.501787 3.875773 -0.708976 59 1 0 -3.278595 3.351547 -2.781389 60 1 0 -3.518120 4.108572 1.427876 61 6 0 -1.828242 -1.288820 -0.802604	54	6	Û	-2.284661	1.920411	-1.527218
56 6 0 -3.041603 3.074650 -1.751281 57 6 0 -3.171606 3.495113 0.592772 58 6 0 -3.501787 3.875773 -0.708976 59 1 0 -3.278595 3.351547 -2.781389 60 1 0 -3.518120 4.108572 1.427876 61 6 0 -1.928242 -1.288820 -0.920604	55	6	Û	-2.416020	2.356359	0.876107
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	56	6	U	-3.041603	3.0/4650	-1./51281
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	5/	6	U	-3.1/16U6	3.495113	0.392//2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	20	b 1	U	-3.3U1/8/	3.0/3//3 2 2515/7	-0./089/6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	59	1	0	-3.2/0395 -3.510120	3.33134/ / 108572	-2.101309 1 /07976
	61	± 6	0	-1.828242	-1.288820	-0.890604

Table S5. Optimized Cartesian coordinates of **11(R)**.

62	6	0	-3.180194	-1.513288	-0.539550
63	6	0	-1.217621	-2.096229	-1.876712
64	6	0	-3.882709	-2.535922	-1.185410
65	6	0	-1.965073	-3.102244	-2.489014
66	6	0	-3.302278	-3.340741	-2.162684
67	1	0	-4.922911	-2.710381	-0.900693
68	1	0	-1.484853	-3.723859	-3.248459
69	6	0	0.216264	-1.933292	-2.307482
70	1	0	0.418642	-0.926125	-2.701736
71	1	0	0.904054	-2.106877	-1.470343
72	1	0	0.460384	-2.654209	-3.097074
73	6	0	-3.931653	-0.709512	0.491649
74	1	0	-4.328399	0.220436	0.055520
75	1	0	-4.776196	-1.295028	0.876216
76	1	0	-3.307484	-0.434874	1.350133
77	6	0	-4.088477	-4.415420	-2.861032
78	1	0	-4.469277	-4.045612	-3.825356
79	1	0	-3.463590	-5.294031	-3.068941
80	1	0	-4.951049	-4.732888	-2.261813
81	6	0	-1.860758	1.134259	-2.747251
82	1	0	-0.851435	0.707477	-2.652507
83	1	0	-2.544137	0.293349	-2.939031
84	1	0	-1.867703	1.784172	-3.631860
85	6	0	-2.143499	2.051340	2.326085
86	1	0	-2.447074	1.029544	2.592472
87	1	0	-1.077122	2.172516	2.565665
88	1	0	-2.706476	2.740937	2.966077
89	6	0	-4.337909	5.099112	-0.964473
90	1	0	-4.339100	5.370392	-2.027444
91	1	0	-5.380147	4.922838	-0.659029
92	1	0	-3.968608	5.956852	-0.385671

Center	Atomic	Atomic	Coord	dinates (Ang	stroms)
Number	Number	Туре	Х	Y	Z
	 6			1 363575	
2	6	0	-3.608842	0.161232	-2.705709
- 3	6	0	-2.054939	0.319730	-1.113278
4	7	0	-2.043625	1.440921	-1.856440
5	1	0	-3.149630	2.162533	-3.571206
6	1	0	-4.428790	-0.291471	-3.255149
7	7	0	-3.018282	-0.462792	-1.626306
8	6	0	-1.241715	2.608370	-1.473424
9	1	0	-1.622326	3.472751	-2.030052
10	1	0	-0.198995	2.437156	-1.778205
11	6	0	-1.333138	2.825960	0.022252
12	6	0	-1.292021	1.697195	0.863568
13	6	0	-1.484669	4.110632	0.541462
14	6	0	-1.486038	1.904698	2.235379
15	6	0	-1.631900	4.293860	1.916662
16	1	0	-1.506801	4.973460	-0.127932
17	6	0	-1.654573	3.186688	2.761918
18	1	0	-1.509227	1.048166	2.915167
19	1	0	-1.756676	5.298642	2.321941
20	1	0	-1.805564	3.320706	3.834086
21	6	0	-3.528389	-1.694453	-1.020343
22	1	0	-2.752657	-2.059635	-0.336934
23	1	0	-3.662432	-2.439722	-1.815697
24	6	0	-4.822308	-1.451416	-0.277122
25	6	0	-4.884679	-0.461345	0.710787
26	6	0	-5.954185	-2.21/283	-0.55/868
27	6	0	-6.069185	-0.244528	1.408516
28	1 G	0	-4.003565	0.148918	0.935326
29	0	0	-7.140342	-2.002112	-1 2075432
30	1 6	0	-7 198705	-2.991434	-1.327343
32	1	0	-6 112250	0 528444	2 176700
32	1	0	-8 020627	-2 605730	-0 078433
34	1	0	-8 125964	-0.845910	1 675608
35	5	0	-1.117672	0.237121	0.181880
36	6	0	-0.948303	-1.013865	1.206718
37	1	0	-0.924922	-1.996789	0.710390
38	1	0	-1.666217	-1.086731	2.039854
39	6	0	0.486508	-0.678528	1.696406
40	1	0	0.426490	0.175893	2.375420
41	6	0	1.314395	-1.758440	2.333383
42	6	0	1.933919	-1.515902	3.567291
43	6	0	1.476394	-3.018668	1.741620
44	6	0	2.718461	-2.490903	4.180288
45	1	0	1.788795	-0.553112	4.063389
46	6	0	2.262733	-3.993614	2.351543
47	1	0	0.994741	-3.245128	0.788505
48	6	0	2.892216	-3.731009	3.568174
49	1	0	3.189071	-2.282936	5.142063
50	1	0	2.381926	-4.966803	1.873375
51	1	0	3.506414	-4.496299	4.044342
52	15	0	0.932834	0.045644	-0.000924
53	6	0	1.967684	1.551999	-0.197631
54	6	U	2.284661	1.920411	-1.527218
55	6	U	2.416020	2.356359	0.876107
56	6	U	3.041603	3.0/4650	-1./51281
57	6	U	3.1/16U6 3.501707	3.495113	0.392//2
28 20	6 1	U	3.JUL/8/	3.0/3//3 2 2515/7	-0./089/6
59 60	1	0	J.∠/8395 3 519100	3.33134/ / 108572	-2./01305 1 /07974
00	1	U	J.JI0120	7.100012	1.12/0/0

Table S6. Optimized Cartesian coordinates of **11(S)**.

62	6	0	3.180194	-1.513288	-0.539550
63	6	0	1.217621	-2.096229	-1.876712
64	6	0	3.882709	-2.535922	-1.185410
65	6	0	1.965073	-3.102244	-2.489014
66	6	0	3.302278	-3.340741	-2.162684
67	1	0	4.922911	-2.710381	-0.900693
68	1	0	1.484853	-3.723859	-3.248459
69	6	0	-0.216264	-1.933292	-2.307482
70	1	0	-0.418642	-0.926125	-2.701736
71	1	0	-0.904054	-2.106877	-1.470343
72	1	0	-0.460384	-2.654209	-3.097074
73	6	0	3.931653	-0.709512	0.491649
74	1	0	4.328399	0.220436	0.055520
75	1	0	4.776196	-1.295028	0.876216
76	1	0	3.307484	-0.434874	1.350133
77	6	0	4.088477	-4.415420	-2.861032
78	1	0	4.469277	-4.045612	-3.825356
79	1	0	3.463590	-5.294031	-3.068941
80	1	0	4.951049	-4.732888	-2.261813
81	6	0	1.860758	1.134259	-2.747251
82	1	0	0.851435	0.707477	-2.652507
83	1	0	2.544137	0.293349	-2.939031
84	1	0	1.867703	1.784172	-3.631860
85	6	0	2.143499	2.051340	2.326085
86	1	0	2.447074	1.029544	2.592472
87	1	0	1.077122	2.172516	2.565665
88	1	0	2.706476	2.740937	2.966077
89	6	0	4.337909	5.099112	-0.964473
90	1	0	4.339100	5.370392	-2.027444
91	1	0	5.380147	4.922838	-0.659029
92	1	0	3.968608	5.956852	-0.385671

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