CARBONACEOUS NANOPARTICLE MOLECULAR INCEPTION FROM RADICAL ADDITION AND VAN DER WAALS COAGULATION OF POLYCYCLIC AROMATIC HYDROCARBON-BASED SYSTEMS. A THEORETICAL STUDY.

Anna Giordana, Andrea Maranzana, and Glauco Tonachini*

Dipartimento di Chimica Generale e Chimica Organica, Università di Torino, Corso Massimo D'Azeglio 48, I-10125 Torino, Italy

SUPPORTING INFORMATION

Table 1. Deformation energies in kcal mol^{-1}

	Deformation Energy		
	R	P	Total
SYSTEM 1			
adduct R–P·	2.1	40.7	42.8
SYSTEM 2			
syn adduct R–P·	28.4	31.1	59.5
gauche adduct R–P·	28.0	32.3	60.3
anti adduct R–P·	25.6	29.4	55.0
SYSTEM 4			
trans adduct R–P·	3.3	32.4	35.7
extended-cis adduct R–P·	3.7	36.6	40.3
packed-cis adduct R–P·	9.6	42.2	51.8
SYSTEM 3			
syn adduct R–P·	25.2	33.7	58.9
gauche adduct R–P·	24.3	30.6	54.8
anti adduct R–P·	24.1	29.0	53.1
SYSTEM 5			
syn adduct R–P·	17.7	43.1	60.8
gauche adduct R–P·	11.3	50.2	61.5

Table 2. Relative energies corrected by zero point vibrational energy ($\Delta \boldsymbol{E}_{ZPE}$), and entropy differences ($\Delta \boldsymbol{S}$).[a]

	$\Delta \boldsymbol{E}_{ZPE}$	$\Delta \boldsymbol{S}$					
T /K :		300	900	1300	1700	2100	2500
SYSTEM 1							
complex R•:P	-15.6	-49.8	-45.5	-44.0	-42.9	-42.1	-41.4
addition TS	0.6	-39.5	-37.3	-36.5	-35.9	-35.5	-35.1
adduct R–P•	-40.4	-42.6	-39.7	-38.3	-37.2	-36.4	-35.7
SYSTEM 2							
complex R•:P	-14.3	-56.2	-52.4	-51.1	-50.0	-49.2	-48.6
syn addition TS	7.1	-58.3	-56.5	-55.7	-55.2	-54.8	-54.5
syn adduct R–P•	5.7	-58.1	-55.3	-53.9	-52.9	-52.1	-51.5
gauche addition TS	17.5	-53.7	-51.8	-51.0	-50.5	-50.1	-49.8
gauche adduct R–P•	13.8	-53.8	-50.8	-49.5	-48.5	-47.7	-47.1
anti addition TS	18.4	-45.8	-44.2	-34.6	-43.1	-42.7	-42.4
anti adduct R–P•	12.3	-46.5	-43.9	-42.7	-41.7	-40.9	-40.3
SYSTEM 3							
complex R•:P	-26.3	-62.2	-58.1	-57.7	-55.6	-54.8	-54.1
syn addition TS	-5.2	-69.0	-66.8	-66.0	-65.5	-65.1	-64.8
syn adduct R–P•	-9.0	-67.8	-64.1	-62.7	-61.7	-60.9	-60.2
gauche addition TS	9.5	-52.5	-50.6	-44.9	-49.4	-49.0	-48.6
gauche adduct R–P•	4.6	-53.6	-50.6	-49.2	-48.2	-47.4	-46.6
anti addition TS	8.7	-48.6	-46.2	-45.3	-44.8	-44.3	-44.0
anti adduct R–P•	1.8	-49.7	-46.6	-45.2	-44.2	-43.3	-42.7
SYSTEM 4[b]							
complex R•:P	-12.4	-55.0	-50.9	-49.5	-48.5	-47.6	-47.0
trans addition TS	1.9	-42.4	-40.7	-40.1	-39.6	-39.2	-38.9
trans adduct R–P•	-38.1	-45.0	-43.3	-42.1	-41.2	-40.4	-39.8
extended-cis addition TS	2.4	-39.7	-37.8	-37.1	-36.6	-36.2	-35.9
extended-cis adduct R–P•	-37.9	-41.8	-39.9	-38.7	-37.7	-36.9	-36.3
packed-cis addition TS	-4.3	-60.7	-58.7	-58.0	-57.5	-57.1	-56.7
packed-cis adduct R–P•	-44.5	-62.1	-60.0	-58.6	-57.6	-56.8	-56.1
SYSTEM 5							
complex R•:P	-10.5	-55.7	-51.8	-50.4	-49.4	-48.5	-47.9
syn addition TS	4,0	-60.6	-59.5	-58.9	-58.4	-58.0	-57.7
syn adduct R–P•	-28.9	-64.1	-63.3	-62.2	-61.3	-60.5	-59.8
gauche addition TS	3.5	-56.9	-56.0	-55.4	-54.9	-54.5	-54.2
gauche adduct R–P•	-32.7	-61.5	-60.8	-59.7	-58.8	-58.0	-57.4

[a] With respect to reactants. Units: $\Delta \boldsymbol{E}_{ZPE}$ in kcal mol^{-1}, $\Delta \boldsymbol{S}$ in cal mol^{-1} K^{-1}. Thermochemistry (ZPE contribution, $\Delta \boldsymbol{H}$, $\Delta \boldsymbol{S}$) computed in correspondence of the 3-21G(d) energies and optimized structures. [b] R• from addition of the π radical PAH system R'• onto ethyne to give R'–CH=CH•, where the unpaired electron is localized in an approximately sp^2 orbital of the vinyl group terminal carbon.

Table 3. Relative energies corrected by zero point vibrational energy ($\Delta \boldsymbol{E}_{ZPE}$), and enthalpy differences ($\Delta \boldsymbol{H}$).[a]

	$\Delta \boldsymbol{E}_{ZPE}$	$\Delta \boldsymbol{H}$					
T /K :		300	900	1300	1700	2100	2500
SYSTEM 1							
complex R•:P	-15.6	-15.4	-13.1	-11.4	-9.8	-8.1	-6.5
addition TS	0.6	0.9	2.2	3.0	3.8	4.7	5.5
adduct R–P•	-40.4	-40.3	-38.6	-37.0	-35.4	-33.9	-32.3
SYSTEM 2							
complex R•:P	-14.3	-14.6	-12.5	-11.0	-9.5	-8.0	-6.4
syn addition TS	7.1	6.6	7.6	8.4	9.2	10.0	10.8
syn adduct R–P•	5.7	5.1	6.8	8.2	9.7	11.2	12.8
gauche addition TS	17.5	17.2	18.3	19.1	19.9	20.7	21.5
gauche adduct R–P•	13.8	13.4	15.1	16.5	18.0	19.5	21.0
anti addition TS	18.4	18.4	19.3	20.0	20.7	21.4	22.2
anti adduct R–P•	12.3	12.2	13.8	15.1	16.6	18.0	19.5
SYSTEM 3							
complex R•:P	-26.3	-26.6	-24.4	-22.8	-21.3	-19.7	-18.2
syn addition TS	-5.2	-6.1	-4.8	-4.0	-3.2	-2.5	-1.7
syn adduct R–P•	-9.0	-9.7	-7.6	-6.0	-4.5	-3.0	-1.4
gauche addition TS	9.5	9.4	10.5	11.3	12.0	12.8	13.6
gauche adduct R–P•	4.6	4.5	6.2	7.7	9.2	10.7	12.2
anti addition TS	8.7	8.8	10.2	11.1	12.0	12.8	13.6
anti adduct R–P•	1.8	1.8	3.7	5.2	6.7	8.3	9.9
SYSTEM 4[b]							
complex R•:P	-12.4	-12.5	-10.3	-8.7	-7.2	-5.6	-4.0
trans addition TS	1.9	2.0	3.0	3.6	4.3	5.0	5.7
trans adduct R–P•	-38.1	-38.1	-37.0	-35.7	-34.3	-32.9	-31.4
extended-cis addition TS	2.4	2.6	3.7	4.4	5.2	5.9	6.7
extended-cis adduct R–P•	-37.9	-37.8	-36.6	-35.3	-33.9	-32.4	-30.9
packed-cis addition TS	-4.3	-4.9	-3.8	-3.0	-2.2	-1.4	-0.6
packed-cis adduct R–P•	-44.5	-45.1	-43.8	-42.4	-40.8	-39.3	-38.7
SYSTEM 5							
complex R•:P	-10.5	-10.6	-8.4	-6.9	-5.3	-3.8	-2.2
syn addition TS	4.0	3.2	3.8	4.5	5.2	5.9	6.7
syn adduct R–P•	-28.9	-29.9	-29.2	-28.0	-26.6	-25.2	-23.7
gauche addition TS	3.5	2.8	3.4	4.1	4.8	5.5	6.2
gauche adduct R–P•	-32.7	-33.6	-33.0	-31.8	-30.4	-29.0	-27.5

[a] With respect to reactants. Units: $\Delta \boldsymbol{E}_{ZPE}$ and $\Delta \boldsymbol{H}$ in kcal mol^{-1}. Thermochemistry (ZPE contribution, $\Delta \boldsymbol{H}$) computed in correspondence of the 3-21G(d) energies and optimized structures. [b] R• from addition of the π radical PAH system R'• onto ethyne to give R'–CH=CH•, where the unpaired electron is localized in an approximately sp^2 orbital of the vinyl group terminal carbon.

Table 4. Equilibrium time (see text for more details).[a]

	t_{eq} /s				
T /K :	900	1300	1700	2100	2500
SYSTEM 1					
adduct R–P·	1.5×10^{-4}	9.3×10^{-8}	1.9×10^{-9}	1.7×10^{-10}	3.4×10^{-11}
SYSTEM 2					
syn adduct R–P·	[b]	[b]	[b]	[b]	[b]
gauche adduct R–P·	[b]	[b]	[b]	[b]	[b]
anti adduct R–P·	[b]	[b]	[b]	[b]	[b]
SYSTEM 3					
syn adduct R–P·	[b]	[b]	[b]	[b]	[b]
gauche adduct R–P·	[b]	[b]	[b]	[b]	[b]
anti adduct R–P·	[b]	[b]	[b]	2.3×10^{-15}	1.3×10^{-14}
SYSTEM 4[b]					
trans adduct R–P·	4.4×10^{-5}	3.0×10^{-8}	6.3×10^{-10}	5.9×10^{-11}	1.2×10^{-11}
extended-cis adduct R–P·	6.5×10^{-5}	4.5×10^{-8}	9.3×10^{-10}	8.3×10^{-11}	1.6×10^{-11}
packed-cis adduct R–P·	8.6×10^{-5}	6.1×10^{-8}	1.2×10^{-9}	1.1×10^{-10}	9.7×10^{-12}
SYSTEM 5					
syn adduct R–P·	4.3×10^{-7}	6.1×10^{-10}	[b]	[b]	[b]
gauche adduct R–P·	1.9×10^{-6}	2.6×10^{-9}	4.5×10^{-11}	1.0×10^{-11}	1.2×10^{-12}

[a] Assuming $[R_0] = 10^{-6}$ atm. [b] $t_{eq} < 10^{-16}$ s.

System 1:

C16H9 1-pyrenyl (grid=ultrafine)

Atom	X	Y	X (Angstrom)
6	-0.02276	0.00000	-0.00979
6	-0.01229	0.00000	1.41770
6	1.22214	0.00000	2.12603
6	2.44859	0.00000	1.36722
6	2.44047	0.00000	0.01470
6	1.20442	0.00000	-0.72771
6	1.21533	0.00000	3.52618
1	3.38927	0.00000	1.91498
1	3.37422	0.00000	-0.54466
6	1.17130	0.00000	-2.12614
6	-0.04076	0.00000	-2.80633
6	-1.24419	0.00000	-2.11054
6	-1.25939	0.00000	-0.71194
1	2.10915	0.00000	-2.67857
1	-0.04792	0.00000	-3.89366
1	-2.18889	0.00000	-2.65106
6	-2.48850	0.00000	0.04303
6	-2.48759	0.00000	1.39555
6	-1.24839	0.00000	2.13183
1	-3.42693	0.00000	-0.50854
1	-3.41763	0.00000	1.95846
6	0.01215	0.00000	4.23474
1	2.16264	0.00000	4.06305
1	0.00880	0.00000	5.32242
6	-1.15507	0.00000	3.51104

Energy -611.617299 (Hartree)

Frequencies cm-1:

99.799	154.873	208.012	255.294	259.266	361.418	406.385	413.298	462.345	489.243
500.169	509.492	514.168	529.638	550.229	590.371	608.436	694.200	706.022	722.780
746.930	772.155	798.144	807.072	826.657	836.029	848.578	862.379	927.697	961.576
983.360	997.433	1001.183	1008.235	1013.886	1115.465	1126.709	1144.616	1178.671	1185.862
1215.032	1222.750	1254.541	1275.185	1280.892	1328.049	1346.779	1395.380	1416.651	1447.001
1463.378	1474.562	1495.334	1523.347	1558.995	1627.703	1645.944	1669.054	1692.050	1717.879
3189.297	3191.150	3192.494	3196.523	3202.050	3204.177	3210.192	3213.617	3223.108	

C42H16 Tetrabenzoovalene (grid=ultrafine)

Atom	X	Y	X (Angstrom)
6	-4.97100	-2.43263	0.00000
6	-3.54291	-2.46801	0.00000
6	-2.83553	-1.23667	0.00000
6	-3.54954	0.00000	0.00000
6	-4.95990	0.00000	0.00000
6	-5.64857	-1.24911	0.00000
6	-1.41652	-1.23753	0.00000
6	-0.70143	0.00000	-0.00000
6	-1.41652	1.23753	0.00000
6	-2.83553	1.23667	0.00000
6	0.70143	0.00000	0.00000
6	1.41652	1.23753	0.00000
6	0.71113	2.46122	0.00000
6	-0.71113	2.46122	0.00000
6	1.41652	-1.23753	0.00000
6	2.83553	-1.23667	0.00000
6	3.54954	0.00000	0.00000
6	2.83553	1.23667	0.00000
6	3.54291	-2.46801	0.00000
6	2.81811	-3.67889	0.00000
6	1.43397	-3.69837	0.00000
6	0.71113	-2.46122	-0.00000
6	-0.71113	-2.46122	-0.00000
6	4.97100	-2.43263	0.00000
6	5.64857	-1.24911	0.00000
6	4.95990	0.00000	0.00000
6	5.64857	1.24911	0.00000
6	4.97100	2.43263	0.00000
6	3.54291	2.46801	0.00000
6	2.81811	3.67889	0.00000
6	1.43397	3.69837	0.00000
6	-1.43397	3.69837	0.00000
6	-0.67492	4.93113	-0.00000
6	0.67493	4.93113	-0.00000
6	-3.54291	2.46801	0.00000
6	-2.81811	3.67889	0.00000
6	-2.81811	-3.67889	0.00000
6	-1.43397	-3.69837	0.00000
6	0.67492	-4.93113	0.00000
6	-0.67492	-4.93113	0.00000
6	-5.64857	1.24911	0.00000
6	-4.97100	2.43263	0.00000
1	6.73715	-1.24043	0.00000
1	6.73715	1.24043	0.00000

```
  1   5.51258   3.37668   0.00000
  1   5.51258  -3.37668   0.00000
  1   3.36666   4.62030   0.00000
  1   1.22740   5.86894  -0.00000
  1  -1.22740   5.86894  -0.00000
  1   1.22740  -5.86894  -0.00000
  1   3.36666  -4.62030   0.00000
  1  -3.36666   4.62030   0.00000
  1  -3.36666  -4.62030   0.00000
  1  -1.22740  -5.86894   0.00000
  1  -5.51258   3.37668   0.00000
  1  -6.73715   1.24043   0.00000
  1  -6.73715  -1.24043   0.00000
  1  -5.51258  -3.37668   0.00000
Energy      -1601.339746          (Hartree)
Frequencies cm-1:
    44.431    54.230    70.203    98.647   114.395   166.817   173.611   180.064   190.338   248.026
   254.805   263.380   278.009   282.994   296.056   318.541   322.630   338.177   361.193   364.062
   368.275   372.835   380.461   382.332   384.567   432.918   446.683   464.155   476.320   489.004
   491.851   525.984   531.721   532.643   533.129   554.842   555.782   556.115   556.716   570.326
   572.579   582.603   604.656   607.000   628.508   633.774   637.497   639.111   640.898   643.429
   647.507   693.533   703.412   706.951   726.687   733.096   739.034   741.163   758.704   765.581
   798.174   798.223   804.903   807.101   808.358   813.278   823.373   823.824   827.360   842.846
   852.106   855.585   858.831   864.682   869.987   904.574   908.573   913.627   916.602   938.677
   939.131   949.384   989.663   989.818   999.727  1000.830  1000.861  1001.867  1006.211  1050.207
  1084.095  1087.147  1123.057  1125.562  1135.872  1141.891  1189.139  1193.918  1194.825  1198.346
  1211.109  1211.712  1220.402  1231.404  1250.750  1252.531  1264.003  1276.419  1292.716  1294.357
  1319.194  1335.081  1344.445  1346.220  1347.838  1373.520  1373.947  1408.758  1414.697  1415.843
  1420.392  1422.242  1444.687  1446.137  1451.399  1452.718  1456.662  1457.888  1461.029  1470.351
  1484.269  1493.732  1522.765  1524.794  1530.341  1539.738  1542.867  1550.220  1551.521  1566.425
  1577.268  1619.142  1638.475  1655.313  1662.561  1673.191  1675.645  1680.446  1693.505  1700.407
  1710.519  1713.302  3181.509  3181.528  3183.872  3183.947  3187.157  3187.167  3187.418  3187.527
  3193.770  3193.803  3207.010  3207.018  3207.329  3207.398  3211.131  3211.208

 Complex R:P (grid=ultrafine)
 Atom    X         Y         X   (Angstrom)
  6   4.61271  -2.69239  -0.98410
  6   3.19256  -2.57306  -1.06813
  6   2.61750  -1.27542  -1.04051
  6   3.45476  -0.12411  -0.94275
  6   4.85430  -0.27648  -0.84823
  6   5.40888  -1.59027  -0.87101
  6   1.20634  -1.12775  -1.05477
  6   0.62362   0.17449  -0.98271
  6   1.46341   1.32790  -0.90517
  6   2.87431   1.17905  -0.89509
  6  -0.77184   0.31729  -0.94401
  6  -1.35343   1.61570  -0.81366
  6  -0.52409   2.75338  -0.71498
  6   0.88944   2.61125  -0.77947
  6  -1.60969  -0.83836  -0.99666
  6  -3.01951  -0.69692  -0.91672
  6  -3.59884   0.59830  -0.76297
  6  -2.76199   1.75374  -0.71103
  6  -3.84838  -1.84889  -0.95030
  6  -3.25455  -3.12312  -1.07173
  6  -1.88172  -3.27981  -1.12990
  6  -1.03579  -2.12489  -1.08398
  6   0.37798  -2.26985  -1.10570
  6  -5.26081  -1.67626  -0.82569
  6  -5.80981  -0.43807  -0.66439
  6  -4.99685   0.73291  -0.62352
  6  -5.54913   2.03389  -0.43159
  6  -4.75220   3.13842  -0.36829
  6  -3.33311   3.03486  -0.49769
  6  -2.48510   4.15911  -0.39506
  6  -1.11007   4.04283  -0.49867
  6   1.73632   3.75938  -0.65414
  6   1.11308   5.05142  -0.46219
  6  -0.22734   5.18438  -0.38083
  6   3.70465   2.32320  -0.76993
  6   3.11022   3.59814  -0.66670
  6   2.34694  -3.69987  -1.12984
  6   0.96842  -3.57425  -1.14732
  6  -1.25549  -4.58180  -1.19083
  6   0.08777  -4.72093  -1.19415
  6   5.66837   0.88830  -0.72233
  6   5.11820   2.13601  -0.69153
  1  -6.88759  -0.32450  -0.56134
  1  -6.62862   2.12871  -0.32780
  1  -5.18790   4.12345  -0.21132
  1  -5.89578  -2.56007  -0.85432
  1  -2.92889   5.13969  -0.22467
  1  -0.67804   6.16239  -0.22192
  1   1.76113   5.92122  -0.36997
```

1	-1.90196	-5.45730	-1.22630
1	-3.89668	-4.00358	-1.09602
1	3.75302	4.47217	-0.56161
1	2.79458	-4.69355	-1.15289
1	0.54109	-5.71020	-1.23357
1	5.75310	3.01495	-0.59437
1	6.74735	0.76167	-0.65148
1	6.48974	-1.69840	-0.79857
1	5.05169	-3.68843	-1.00206
6	-0.24367	-1.13339	2.10746
6	-1.65576	-0.96546	2.12692
6	-2.47415	-2.09752	2.05464
6	-1.91590	-3.36729	1.97335
6	-0.53704	-3.54060	1.95856
6	0.31913	-2.43656	2.02318
1	-3.55545	-1.96878	2.03896
1	-2.56672	-4.23603	1.89770
1	-0.11078	-4.53847	1.87430
6	-2.19899	0.36933	2.17979
1	-3.28204	0.48356	2.15328
6	-1.39487	1.45638	2.22102
6	0.03909	1.31461	2.22402
1	-1.80925	2.46338	2.21952
6	0.61166	0.00847	2.15703
6	2.02477	-0.15100	2.10153
6	2.56130	-1.48504	1.98960
6	2.84857	0.98114	2.13054
1	3.64212	-1.59658	1.90036
6	1.75297	-2.56950	1.96589
1	2.17084	-3.56986	1.86925
6	2.30029	2.26155	2.22501
1	3.92893	0.85622	2.04902
1	2.94167	3.13968	2.23530
6	0.93164	2.36989	2.25815

Energy -2213.009996 (Hartree)

Frequencies cm-1:

25.881	35.516	43.737	46.334	67.026	74.098	94.819	102.603	125.469	145.359
147.399	162.245	181.398	190.289	195.738	199.174	206.363	239.672	258.620	264.582
269.692	277.715	280.075	281.518	287.854	296.198	328.651	331.540	338.483	362.696
369.278	370.268	378.740	381.458	382.151	383.132	384.580	413.940	415.885	432.389
446.333	463.176	463.777	477.278	488.764	490.639	495.421	500.200	510.246	521.293
525.146	531.686	532.938	533.971	535.803	549.450	554.255	555.746	557.219	559.935
570.125	574.111	582.510	591.329	604.141	607.592	609.720	627.707	633.103	635.012
638.807	639.754	644.222	647.166	691.287	692.587	702.607	705.265	707.554	711.428
718.704	720.206	730.347	741.695	745.873	758.887	759.876	770.823	779.548	794.363
795.086	798.684	805.046	805.881	806.674	808.179	810.214	816.302	824.032	824.655
832.823	835.886	842.649	851.937	854.527	856.376	858.075	864.413	869.879	900.975
904.873	911.349	914.178	919.752	939.899	940.146	949.693	955.431	982.792	987.599
989.004	989.943	992.593	998.290	999.101	1000.076	1000.489	1001.532	1006.297	1013.615
1049.556	1083.900	1087.083	1114.833	1125.540	1125.886	1126.196	1134.712	1145.010	1146.131
1176.858	1186.307	1187.849	1192.099	1195.039	1198.187	1211.686	1212.541	1213.402	1220.212
1220.919	1232.024	1252.038	1252.598	1253.035	1264.047	1274.577	1275.909	1279.615	1292.699
1294.939	1319.870	1329.534	1337.285	1343.996	1345.777	1347.085	1348.777	1374.949	1375.691
1395.861	1409.042	1415.770	1417.056	1419.792	1423.472	1424.734	1445.850	1446.157	1447.390
1451.574	1455.232	1455.930	1460.824	1461.167	1462.255	1471.822	1474.612	1486.517	1493.351
1493.878	1522.277	1523.751	1524.495	1533.308	1539.179	1544.021	1551.965	1552.206	1556.904
1567.540	1579.974	1619.173	1625.987	1640.178	1643.397	1655.834	1663.774	1665.737	1675.386
1675.802	1681.620	1689.314	1693.116	1698.675	1710.938	1713.737	1714.883	3162.247	3165.613
3166.774	3167.877	3168.226	3173.537	3173.572	3173.894	3177.950	3178.528	3179.685	3180.749
3182.787	3186.180	3186.614	3191.942	3192.015	3195.490	3197.433	3198.346	3198.418	3204.100
3205.183	3206.357	3213.233							

Addition TS (grid=ultrafine)

Atom	X	Y	X (Angstrom)
6	7.16809	-1.54703	1.52606
6	6.21491	-0.51410	1.26865
6	4.98823	-0.86542	0.64532
6	4.72698	-2.22429	0.29334
6	5.68962	-3.22022	0.56121
6	6.91516	-2.84294	1.18538
6	4.02144	0.13747	0.37395
6	2.78680	-0.21224	-0.25423
6	2.52699	-1.57175	-0.60810
6	3.49336	-2.57434	-0.33341
6	1.82855	0.77947	-0.52306
6	0.59677	0.43147	-1.15189
6	0.34274	-0.91243	-1.51602
6	1.31018	-1.91839	-1.23676
6	2.09164	2.14046	-0.17028
6	1.12515	3.14266	-0.44260
6	-0.11053	2.79348	-1.06723
6	-0.37351	1.43595	-1.42188
6	1.39107	4.49368	-0.09458
6	2.61825	4.81817	0.51870
6	3.57233	3.85266	0.79378

```
  6   3.31313   2.48718   0.44790
  6   4.28221   1.48170   0.72138
  6   0.39532   5.47963  -0.37778
  6  -0.78489   5.14122  -0.96939
  6  -1.07259   3.79080  -1.33308
  6  -2.29695   3.41574  -1.95456
  6  -2.54816   2.11835  -2.30015
  6  -1.59527   1.09085  -2.05008
  6  -1.84578  -0.26983  -2.38198
  6  -0.88436  -1.25676  -2.15976
  6   1.05436  -3.28364  -1.58785
  6  -0.20380  -3.59800  -2.22594
  6  -1.11795  -2.63917  -2.49612
  6   3.22988  -3.92538  -0.68421
  6   2.00658  -4.24994  -1.30566
  6   6.45368   0.83398   1.60806
  6   5.52261   1.82590   1.34844
  6   4.83596   4.16863   1.42446
  6   5.75415   3.21422   1.68660
  6   5.40348  -4.56974   0.19917
  6   4.22463  -4.90981  -0.39664
  6  -3.17441  -0.75187  -0.42918
  6  -4.54812  -0.59178  -0.36885
  6  -5.16070  -0.79224   0.90610
  6  -4.36300  -1.13480   2.03292
  6  -2.97758  -1.27393   1.88053
  6  -2.37316  -1.08225   0.63826
  6  -6.57516  -0.65154   1.04431
  6  -7.37118  -0.31181  -0.08405
  6  -6.72288  -0.11781  -1.35724
  6  -5.38386  -0.25155  -1.49354
  6  -8.75457  -0.18210   0.07413
  6  -9.34763  -0.38109   1.31572
  6  -8.57596  -0.71183   2.42363
  6  -7.18855  -0.85253   2.31171
  6  -5.01589  -1.33024   3.30345
  1  -1.53505   5.90364  -1.17362
  1  -3.04014   4.18780  -2.14706
  1  -3.49488   1.85062  -2.76651
  1   0.60002   6.51484  -0.10914
  1  -2.73213  -0.51771  -2.96557
  1  -2.37157  -1.53724   2.74664
  1  -1.29601  -1.19234   0.51395
  1  -7.34361   0.13797  -2.21455
  1  -4.39825  -1.59180   4.16123
  1  -9.04705  -0.86496   3.39339
  1 -10.42563  -0.27774   1.42075
  1  -9.36504   0.07766  -0.78923
  1  -2.06602  -2.89632  -2.96594
  1  -0.40198  -4.63793  -2.48035
  1   5.02964   5.20825   1.68420
  1   2.81721   5.85732   0.78122
  1   1.80918  -5.28875  -1.57038
  1   7.39707   1.09743   2.08625
  1   6.69873   3.47166   2.16306
  1   4.02191  -5.94544  -0.66508
  1   6.15275  -5.33225   0.40668
  1   7.65445  -3.61714   1.38520
  1   8.10881  -1.27651   2.00287
  6  -6.35541  -1.19628   3.43681
  1  -6.83409  -1.34673   4.40318
  1  -4.91284  -0.11197  -2.46444
Energy      -2212.965970          (Hartree)
Frequencies cm-1:
  -298.215     9.084    13.466    23.847    36.856    52.963    56.890    65.816    76.821    96.076
   107.655   110.846   144.714   171.205   175.181   182.598   189.678   214.431   241.645   250.678
   259.339   263.848   266.263   277.640   286.383   296.882   319.350   327.728   338.134   352.574
   364.382   369.091   370.723   375.212   381.738   382.554   384.702   407.671   412.801   425.854
   446.885   458.120   464.113   473.280   483.197   489.081   492.976   503.487   506.809   515.784
   525.512   530.951   531.374   533.034   533.616   541.915   555.822   556.916   558.717   562.734
   570.627   575.459   582.353   590.543   604.786   607.482   609.074   626.602   633.874   638.816
   640.122   643.985   646.306   650.800   693.428   695.332   702.935   705.593   708.169   724.247
   725.706   734.028   738.299   740.864   741.929   758.694   764.067   773.378   790.945   799.162
   802.744   805.024   805.323   808.649   812.151   815.700   823.349   824.560   826.283   827.711
   835.418   842.191   852.000   853.701   856.471   857.589   862.844   863.937   870.034   881.840
   910.166   914.225   919.628   927.466   939.595   940.532   950.684   970.795   983.013   983.831
   990.919   995.588   999.624  1000.127  1000.553  1001.771  1004.538  1006.504  1007.087  1010.801
  1050.397  1083.771  1088.744  1114.708  1125.203  1127.476  1127.986  1134.850  1144.441  1147.064
  1177.508  1185.269  1188.299  1193.138  1196.668  1199.842  1209.320  1213.700  1214.847  1222.488
  1222.912  1231.963  1251.215  1253.889  1254.188  1261.863  1274.436  1275.544  1280.461  1286.953
  1293.886  1316.152  1328.409  1332.229  1342.713  1344.861  1346.365  1349.258  1367.119  1370.062
  1397.272  1406.172  1414.169  1415.118  1418.345  1420.920  1423.724  1441.588  1445.933  1447.098
  1449.174  1451.748  1456.832  1460.377  1462.495  1462.848  1471.824  1474.412  1482.959  1490.319
  1496.142  1517.696  1521.026  1524.828  1527.761  1538.652  1540.153  1547.450  1553.516  1558.522
  1565.379  1576.799  1616.265  1625.938  1639.225  1643.490  1645.885  1659.938  1665.336  1666.765
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 1670.909  1677.994  1685.882  1691.555  1694.101  1699.397  1711.399  1716.507  3172.001  3172.690
 3172.939  3176.669  3179.079  3179.848  3180.145  3181.540  3181.817  3183.183  3185.861  3186.772
 3191.691  3192.421  3194.330  3194.384  3197.396  3198.174  3201.206  3201.404  3201.981  3202.604
 3206.115  3210.243  3211.795

Adduct R-P (grid=ultrafine)
Atom    X         Y         X   (Angstrom)
 6  -7.54444  -0.99095   2.68403
 6  -7.99889  -0.72334   1.34420
 6  -7.03323  -0.50937   0.32128
 6  -5.63670  -0.56085   0.62678
 6  -5.22619  -0.82176   1.96110
 6  -6.22493  -1.03620   2.97589
 6  -3.85793  -0.85955   2.25299
 6  -2.92034  -0.65170   1.25815
 6  -3.29936  -0.39920  -0.06240
 6  -4.66378  -0.34706  -0.39865
 6  -7.46623  -0.23847  -1.00478
 6  -6.46801  -0.02227  -2.01861
 6  -5.14678  -0.07498  -1.73467
 6  -9.35930  -0.66549   1.02072
 6  -9.77082  -0.40143  -0.27944
 6  -8.83501  -0.18853  -1.28485
 6  -2.18059  -0.14452  -1.07254
 6  -1.65750   1.26889  -0.87075
 6  -0.30312   1.52287  -0.60891
 6   0.65536   0.44637  -0.51139
 6   0.22533  -0.91296  -0.68809
 6  -1.12047  -1.22027  -0.95282
 6   1.17878  -1.96768  -0.58818
 6   2.54166  -1.67522  -0.31718
 6   2.95648  -0.32832  -0.14462
 6   2.00444   0.72698  -0.24354
 6   3.48829  -2.73211  -0.21970
 6   4.85401  -2.44225   0.05167
 6   5.27146  -1.08990   0.22548
 6   4.32628  -0.03690   0.12769
 6   5.79886  -3.49285   0.14942
 6   7.16000  -3.17317   0.42248
 6   7.56543  -1.88254   0.58995
 6   6.63839  -0.79639   0.49780
 6   4.74972   1.30417   0.30148
 6   6.11914   1.58730   0.57320
 6   7.03264   0.53953   0.66613
 6   3.06845  -4.08511  -0.39362
 6   4.04985  -5.12242  -0.28835
 6   5.35641  -4.83559  -0.02831
 6   3.80166   2.36766   0.20375
 6   2.44253   2.08638  -0.06551
 6   0.76926  -3.32638  -0.76024
 6   1.72339  -4.35549  -0.65921
 6   1.51100   3.14543  -0.16061
 6   0.13515   2.86634  -0.43224
 6  -1.50777  -2.55872  -1.11172
 6  -0.59874  -3.58860  -1.02489
 6   4.22689   3.71758   0.37779
 6   3.29357   4.74745   0.27934
 6   1.94611   4.49089   0.01390
 6   0.97708   5.54999  -0.08868
 6  -0.32450   5.28523  -0.34602
 6  -0.79161   3.93551  -0.52726
 6  -2.13637   3.64396  -0.79129
 6  -2.55553   2.33551  -0.95494
 6   6.51572   2.96389   0.74427
 6   5.61955   3.97199   0.65162
 1  -1.05063   6.09265  -0.42117
 1  -2.85343   4.45978  -0.86054
 1  -3.60875   2.12554  -1.13655
 1   1.31969   6.57417   0.04692
 1  -2.58223  -0.20917  -2.09396
 1  -3.53680  -1.05445   3.27451
 1  -1.85809  -0.68491   1.49588
 1  -6.80344   0.18556  -3.03327
 1  -5.88654  -1.23601   3.99102
 1 -10.09574  -0.82987   1.80519
 1 -10.83213  -0.35990  -0.51199
 1  -9.16057   0.01946  -2.30245
 1  -2.55916  -2.77609  -1.29665
 1  -0.92115  -4.61985  -1.15350
 1   5.93396   5.00573   0.78320
 1   3.62158   5.77796   0.41263
 1   1.40231  -5.38793  -0.79158
 1   8.07890   0.76111   0.87434
 1   7.56377   3.17213   0.95173
 1   3.72697  -6.15315  -0.42187
```

1	6.08946	-5.63680	0.04820
1	7.87832	-3.98791	0.49560
1	8.60912	-1.65468	0.79815
1	-8.29200	-1.15370	3.45822
1	-4.43175	0.09770	-2.53449

Energy -2213.038296 (Hartree)

Frequencies cm-1:

9.920	13.319	25.101	45.527	55.035	73.976	83.528	99.834	102.730	117.806
123.632	148.952	168.065	178.721	187.752	199.869	216.057	229.253	245.966	260.487
263.361	274.901	283.599	293.570	305.164	313.363	321.256	332.310	348.112	365.971
368.535	374.268	379.151	382.571	384.308	388.608	405.518	419.997	428.731	448.896
459.199	468.080	475.693	477.772	491.415	502.962	505.803	517.574	520.701	523.191
526.684	532.763	535.316	544.760	551.184	553.076	555.855	560.742	567.979	574.249
576.039	584.182	598.099	604.302	613.148	623.885	629.489	633.212	637.459	639.794
647.088	659.855	666.522	696.683	701.212	703.649	709.418	714.580	722.223	729.363
735.882	739.309	747.738	749.676	762.839	772.503	779.746	781.550	799.612	801.021
804.791	808.106	814.213	815.315	820.037	825.829	828.195	831.758	835.243	841.607
848.458	850.731	859.010	859.447	862.483	868.301	870.899	875.606	891.795	897.127
905.229	917.246	928.645	935.046	941.511	953.958	985.240	985.846	987.163	987.679
995.069	997.956	998.368	1001.008	1001.909	1002.099	1003.335	1008.572	1044.306	1073.533
1075.157	1093.383	1110.633	1124.582	1129.306	1130.905	1131.974	1156.377	1173.440	1176.408
1187.205	1191.306	1196.343	1198.853	1207.869	1208.768	1213.962	1216.091	1221.428	1227.155
1235.861	1240.148	1246.980	1254.889	1261.178	1262.490	1275.576	1278.460	1281.680	1285.664
1299.605	1301.613	1313.251	1319.972	1332.930	1337.603	1341.973	1346.788	1357.145	1362.098
1365.782	1369.375	1387.748	1402.087	1403.032	1409.047	1415.296	1432.092	1433.025	1438.456
1448.051	1451.149	1452.811	1456.377	1458.031	1461.373	1464.251	1472.900	1483.248	1485.455
1499.436	1505.111	1515.009	1521.947	1530.713	1533.096	1538.697	1556.992	1560.080	1570.473
1579.213	1583.247	1594.860	1612.660	1625.667	1628.006	1632.265	1642.094	1654.123	1659.946
1661.772	1669.766	1675.336	1680.634	1692.633	1700.172	1711.505	1720.155	3062.360	3174.430
3177.088	3177.228	3179.028	3180.414	3180.824	3182.465	3182.915	3183.090	3183.630	3186.602
3189.877	3191.840	3197.042	3197.907	3198.177	3198.478	3200.361	3200.761	3202.226	3203.851
3205.926	3213.201	3222.705							

System 2:

C16H11 1-H-pyrenyl

Atom	X	Y	X (Angstrom)
6	0.02289	-0.00957	-0.02871
6	0.04225	-0.00846	1.38181
6	1.27402	-0.00343	2.04982
6	2.46911	0.00041	1.36358
6	2.49165	-0.00063	-0.05446
6	1.25116	-0.00568	-0.75347
6	-1.24285	-0.01259	2.17749
1	1.27781	-0.00256	3.13949
1	3.41452	0.00435	1.90308
6	1.24090	-0.00681	-2.18201
6	-0.01250	-0.01180	-2.85608
6	2.46675	-0.00290	-2.87142
1	-0.01905	-0.01277	-3.94422
6	-1.19627	-0.01541	-2.15003
6	-1.21430	-0.01441	-0.74882
1	-2.14613	-0.01915	-2.68295
6	-2.45717	-0.01821	-0.00130
6	3.67426	0.00201	-2.17858
1	2.46029	-0.00375	-3.95973
1	4.61010	0.00498	-2.73258
6	3.69686	0.00318	-0.79406
1	4.64418	0.00705	-0.25813
6	-2.48607	-0.01745	1.33737
1	-1.25872	0.86722	2.84597
1	-3.43804	-0.02045	1.86532
1	-3.38678	-0.02182	-0.57021
1	-1.25248	-0.89191	2.84676

Energy -612.856459 (Hartree)

Frequencies cm-1:

93.294	101.058	189.168	202.777	253.499	326.490	348.935	404.711	434.074	453.306
491.328	491.969	501.200	510.833	538.839	539.185	602.626	664.070	669.404	688.704
734.402	741.470	759.131	802.982	804.927	826.476	834.628	854.707	895.048	938.331
954.586	964.372	978.969	985.931	993.474	997.768	1007.141	1118.123	1138.119	1151.773
1180.872	1205.864	1218.243	1223.295	1236.643	1242.496	1248.705	1268.972	1324.189	1344.382
1377.036	1392.542	1412.088	1448.332	1465.869	1471.695	1483.466	1527.464	1556.203	1576.803
1618.201	1631.359	1639.919	1724.444	3024.306	3041.478	3120.754	3147.838	3150.530	3152.073
3157.276	3163.457	3173.793	3183.686	3188.734					

C42H16 Tetrabenzoovalene

Atom	X	Y	X (Angstrom)
6	4.97101	-2.43228	0.00011
6	3.54294	-2.46741	0.00002
6	2.83555	-1.23639	-0.00002
6	3.54941	0.00000	0.00002
6	4.95971	0.00000	0.00008
6	5.64851	-1.24856	0.00013
6	1.41647	-1.23726	-0.00007

6	0.71118	-2.46069	-0.00007
6	1.43412	-3.69758	-0.00006
6	2.81822	-3.67809	-0.00003
6	2.83555	1.23639	-0.00002
6	1.41647	1.23726	-0.00007
6	0.70139	0.00000	-0.00008
6	-0.70139	0.00000	-0.00008
6	-1.41647	-1.23726	-0.00006
6	-0.71118	-2.46069	-0.00007
6	-1.43412	-3.69758	-0.00006
6	-0.67501	-4.93042	-0.00006
6	0.67501	-4.93042	-0.00006
6	0.71118	2.46069	-0.00007
6	-0.71118	2.46069	-0.00007
6	-1.41647	1.23726	-0.00006
6	-2.83555	1.23639	-0.00001
6	-3.54941	0.00000	0.00002
6	-2.83555	-1.23639	-0.00001
6	-3.54294	-2.46741	0.00002
6	-2.81822	-3.67809	-0.00003
6	-3.54294	2.46741	0.00002
6	-2.81822	3.67809	-0.00003
6	-1.43412	3.69758	-0.00006
6	-0.67501	4.93042	-0.00006
6	0.67501	4.93042	-0.00006
6	1.43412	3.69758	-0.00006
6	2.81822	3.67809	-0.00003
6	3.54294	2.46741	0.00002
6	4.97101	2.43228	0.00011
6	5.64851	1.24856	0.00013
6	-4.97101	2.43228	0.00011
6	-5.64851	1.24856	0.00012
6	-4.95971	0.00000	0.00008
6	-5.64851	-1.24856	0.00012
6	-4.97101	-2.43228	0.00011
1	-1.22847	5.86780	-0.00011
1	-3.36780	4.61911	0.00000
1	-3.36780	-4.61911	0.00000
1	3.36780	4.61911	0.00001
1	1.22847	5.86780	-0.00011
1	1.22847	-5.86780	-0.00011
1	-1.22847	-5.86780	-0.00011
1	3.36780	-4.61911	0.00001
1	-5.51364	3.37595	0.00015
1	-6.73705	1.23964	0.00017
1	-6.73705	-1.23964	0.00017
1	-5.51364	-3.37595	0.00015
1	5.51364	3.37595	0.00015
1	6.73705	1.23964	0.00018
1	6.73705	-1.23964	0.00018
1	5.51364	-3.37595	0.00015

Energy -1601.339590 (Hartree)

Frequencies cm-1:

44.107	54.401	69.410	98.414	113.415	167.342	172.059	178.006	191.241	247.009
254.965	262.531	277.072	283.808	295.181	318.549	322.109	335.936	361.945	365.549
368.671	372.165	380.152	381.428	383.544	433.910	444.674	461.853	477.553	486.677
493.041	522.418	530.979	531.196	531.898	554.110	554.598	555.490	556.424	568.446
571.907	582.192	601.278	606.754	628.190	630.716	636.828	637.573	640.678	642.045
647.591	691.720	701.027	705.378	726.960	732.416	738.691	740.788	757.730	764.920
796.230	798.289	802.810	805.644	806.116	813.006	822.771	822.829	827.413	841.353
848.676	852.328	856.176	862.816	867.602	902.604	906.519	911.807	914.664	936.906
939.563	946.960	987.505	987.610	999.068	999.437	1001.866	1002.187	1003.778	1046.182
1081.182	1082.144	1121.069	1121.940	1133.786	1139.220	1184.648	1190.757	1190.825	1194.370
1207.012	1207.017	1216.339	1227.203	1247.437	1249.463	1260.189	1274.048	1289.910	1291.594
1314.108	1337.372	1340.973	1342.154	1347.901	1372.689	1374.589	1405.186	1412.878	1415.236
1418.516	1422.746	1440.977	1442.449	1447.024	1447.076	1451.712	1456.360	1458.989	1467.424
1483.923	1491.597	1517.339	1521.921	1527.336	1535.177	1539.113	1546.577	1547.550	1562.503
1575.828	1618.271	1637.333	1653.305	1659.795	1675.442	1678.040	1681.134	1689.222	1696.676
1705.649	1707.863	3140.973	3140.996	3142.887	3142.964	3154.887	3154.887	3154.984	3155.068
3164.430	3164.456	3164.716	3164.821	3168.473	3168.503	3185.968	3186.027		

Complex R:P

Atom	X	Y	X (Angstrom)
6	2.30271	-0.13946	2.35381
6	0.80073	-0.02566	2.26153
6	0.00094	-1.17224	2.06803
6	0.59152	-2.46991	1.93520
6	2.03557	-2.58745	1.95999
6	2.83271	-1.52394	2.12638
6	-1.41605	-1.03920	1.99073
6	-2.01802	0.24807	2.08749
6	-1.17756	1.37797	2.25751
6	0.18995	1.23261	2.35218
6	-3.42333	0.35892	1.97997
6	-4.20790	-0.76865	1.80256

6	-3.62757	-2.02928	1.70035
6	-2.23323	-2.19209	1.78522
6	-1.60292	-3.46084	1.65685
6	-0.23285	-3.58441	1.73320
6	-3.26363	0.72085	-1.02743
6	-2.63833	-0.55247	-1.17792
6	-1.22652	-0.66372	-1.09944
6	-0.42848	0.50268	-0.89393
6	-1.05478	1.77694	-0.73979
6	-2.46846	1.88191	-0.78855
6	-0.26957	2.92549	-0.49592
6	1.14645	2.81662	-0.43201
6	1.76645	1.55947	-0.60739
6	0.96829	0.39387	-0.82454
6	1.94948	3.97344	-0.16606
6	3.32691	3.84680	-0.09730
6	3.96648	2.60258	-0.27487
6	3.17949	1.44905	-0.53458
6	3.80485	0.17085	-0.67268
6	5.20575	0.05562	-0.55729
6	5.97696	1.23246	-0.31480
6	5.38497	2.45263	-0.17961
6	1.59389	-0.88394	-0.95068
6	3.00757	-0.99339	-0.88414
6	3.62426	-2.26724	-0.99885
6	5.04451	-2.34809	-0.89235
6	5.80278	-1.23347	-0.67620
6	-0.90624	4.18895	-0.27749
6	-0.06830	5.34013	-0.01528
6	1.27711	5.23919	0.03497
6	2.81535	-3.40941	-1.17959
6	1.43615	-3.32106	-1.24677
6	0.80419	-2.03923	-1.13576
6	-0.61062	-1.92912	-1.21338
6	-3.09145	3.13867	-0.56676
6	-2.28876	4.27061	-0.30972
6	0.59266	-4.48265	-1.43517
6	-0.75057	-4.37554	-1.51657
6	-1.41728	-3.09519	-1.41386
6	-2.79251	-2.96774	-1.49761
6	-3.42794	-1.71349	-1.38447
6	-4.84685	-1.56976	-1.45054
6	-5.44087	-0.35093	-1.30291
6	-4.66945	0.82618	-1.07552
6	-5.27226	2.09960	-0.85852
6	-4.51812	3.20866	-0.60674
1	-1.63007	2.36971	2.28792
1	-1.36806	-5.26082	-1.66487
1	-3.40515	-3.85694	-1.65135
1	-2.77251	5.23252	-0.13954
1	3.29422	-4.38521	-1.26762
1	1.07592	-5.45526	-1.51989
1	0.82128	2.11477	2.46611
1	1.89070	6.11604	0.23630
1	-0.55625	6.30055	0.14331
1	3.93580	4.72684	0.11042
1	-5.45114	-2.46051	-1.61778
1	-6.52545	-0.25967	-1.34835
1	-6.35847	2.17152	-0.89161
1	-4.99497	4.17303	-0.43833
1	5.51660	-3.32543	-0.98235
1	6.88576	-1.31328	-0.59156
1	7.05881	1.13555	-0.23320
1	5.98740	3.33866	0.01469
1	0.23141	-4.56252	1.61307
1	-2.22631	-4.33620	1.47823
1	-4.25051	-2.90689	1.53013
1	-5.28730	-0.66572	1.71196
1	-3.87746	1.34949	2.01406
1	2.46347	-3.57628	1.79636
1	3.91644	-1.63692	2.08927
1	2.76291	0.55125	1.62865
1	2.63343	0.21416	3.34805

Energy -2214.251399 (Hartree)

Frequencies cm-1:

45.601	47.678	50.083	57.852	71.356	85.585	101.110	113.862	140.975	158.215
159.427	175.073	183.890	193.988	205.445	213.007	220.068	229.931	252.370	264.831
267.823	276.899	279.578	284.600	291.922	297.023	331.365	335.423	340.546	343.270
352.812	372.807	377.219	380.724	382.671	383.625	385.187	388.912	407.926	433.958
447.123	451.275	456.109	465.119	479.195	489.851	492.409	492.861	500.259	508.947
522.388	527.266	531.492	532.688	537.893	541.210	550.000	554.995	556.199	561.987
563.821	570.685	577.823	581.990	603.601	605.096	609.374	631.232	633.840	636.544
638.745	642.411	644.889	650.221	670.572	673.849	690.806	693.462	702.739	706.327
720.043	726.167	734.734	735.749	740.408	741.717	746.629	757.950	765.065	784.529
788.844	793.295	801.790	803.696	804.371	807.637	809.595	811.507	819.232	821.271

826.047	833.928	842.199	843.049	849.968	857.366	858.430	863.969	869.159	874.711
884.021	908.167	912.970	920.195	932.249	936.671	937.714	947.105	953.167	957.558
961.822	971.853	981.862	985.116	988.818	993.597	1000.057	1001.331	1005.025	1006.271
1007.480	1008.826	1048.841	1082.073	1085.063	1114.338	1121.536	1124.064	1133.056	1136.615
1141.728	1154.736	1179.886	1186.374	1190.702	1192.903	1197.255	1204.522	1208.773	1212.569
1216.823	1219.409	1225.890	1231.459	1237.049	1247.601	1248.502	1249.092	1250.553	1260.262
1270.422	1275.115	1291.587	1293.384	1316.355	1319.487	1336.039	1341.791	1344.264	1344.885
1348.391	1372.724	1375.793	1378.791	1389.546	1407.190	1411.333	1414.109	1414.238	1421.057
1421.661	1444.211	1444.859	1448.434	1449.198	1451.454	1455.026	1456.992	1459.444	1462.454
1468.522	1472.785	1482.324	1488.054	1492.213	1519.220	1522.608	1525.997	1529.255	1536.758
1539.911	1547.280	1550.245	1552.708	1564.519	1572.831	1576.972	1615.538	1617.900	1629.745
1632.816	1635.414	1655.332	1660.771	1671.375	1675.130	1678.275	1691.379	1696.147	1709.174
1712.234	1717.195	2994.620	3094.494	3112.411	3118.620	3119.939	3132.794	3134.240	3136.395
3137.824	3146.063	3170.470	3177.315	3177.801	3179.738	3180.144	3188.379	3191.937	3191.993
3196.390	3199.522	3202.443	3203.439	3212.137	3216.048	3217.665	3220.199	3237.878	

Syn addition TS

Atom	X	Y	X	(Angstrom)
6	-1.15739	2.76965	2.16065	
6	-2.11563	1.62196	1.94682	
6	-1.64296	0.28284	1.95418	
6	-0.25901	-0.01307	2.16716	
6	0.67987	1.09156	2.33455	
6	0.28058	2.36531	2.30393	
6	-2.54626	-0.77902	1.69300	
6	-3.93032	-0.50624	1.49907	
6	-4.36054	0.81603	1.50817	
6	-3.45947	1.86412	1.71799	
6	-4.83188	-1.61879	1.29481	
6	-4.36507	-2.87851	1.12818	
6	-2.94663	-3.11997	1.02224	
6	-2.05748	-2.11267	1.57181	
6	-0.71451	-2.36810	1.83175	
6	0.16740	-1.33176	2.15119	
6	-2.61212	0.74306	-1.32787	
6	-2.15270	-0.59782	-1.23998	
6	-0.76363	-0.86304	-1.03045	
6	0.14219	0.20619	-0.87715	
6	-0.32578	1.55945	-0.92475	
6	-1.69713	1.82351	-1.15150	
6	0.58022	2.63232	-0.74587	
6	1.96143	2.36920	-0.50728	
6	2.42744	1.03147	-0.46392	
6	1.52121	-0.05020	-0.65758	
6	2.86979	3.44435	-0.28555	
6	4.21316	3.17084	-0.03633	
6	4.70024	1.85411	0.00593	
6	3.79898	0.77146	-0.20750	
6	4.27270	-0.57312	-0.15567	
6	5.63973	-0.83194	0.10193	
6	6.52177	0.26707	0.30698	
6	6.07505	1.55507	0.26282	
6	1.99368	-1.39168	-0.61136	
6	3.36606	-1.65363	-0.35827	
6	3.83392	-3.00004	-0.29446	
6	5.22522	-3.22438	-0.03892	
6	6.08640	-2.18519	0.14966	
6	0.10379	3.97536	-0.78360	
6	1.04557	5.04230	-0.55679	
6	2.35431	4.79154	-0.31862	
6	2.92472	-4.05101	-0.46550	
6	1.56291	-3.81461	-0.69472	
6	1.08866	-2.47091	-0.78503	
6	-0.29921	-2.21310	-0.97505	
6	-2.16462	3.16965	-1.18704	
6	-1.25474	4.21549	-1.00067	
6	0.61065	-4.87504	-0.81174	
6	-0.72197	-4.61337	-0.96897	
6	-1.21751	-3.28536	-1.04675	
6	-2.62810	-3.00134	-0.98214	
6	-3.07689	-1.66451	-1.31387	
6	-4.42959	-1.37599	-1.57442	
6	-4.87180	-0.07527	-1.70818	
6	-3.98809	1.00609	-1.54632	
6	-4.43192	2.37252	-1.58320	
6	-3.56740	3.40176	-1.40516	
1	-5.41434	1.03315	1.33745	
1	-1.43400	-5.43648	-1.03109	
1	-3.30007	-3.81776	-1.25560	
1	-1.61525	5.24435	-1.02306	
1	3.28270	-5.07850	-0.40548	
1	0.96834	-5.90188	-0.75836	
1	-3.81601	2.89298	1.68605	
1	3.05179	5.60984	-0.14730	
1	0.67571	6.06620	-0.57964	

1	4.90440	3.99618	0.13237
1	-5.13370	-2.20107	-1.66432
1	-5.92338	0.12766	-1.90592
1	-5.49039	2.56452	-1.75313
1	-3.91980	4.43195	-1.43069
1	5.58281	-4.25176	0.00314
1	7.14072	-2.37537	0.34427
1	7.57221	0.05805	0.50392
1	6.76361	2.38252	0.42420
1	1.22179	-1.55206	2.31276
1	-0.33713	-3.38667	1.73614
1	-2.60549	-4.15318	1.11084
1	-5.05318	-3.70537	0.96056
1	-5.90209	-1.41466	1.28604
1	1.73694	0.84240	2.42839
1	1.01141	3.17136	2.37304
1	-1.25021	3.46938	1.31365
1	-1.46118	3.33659	3.05801

Energy -2214.224550 (Hartree)

Frequencies cm-1:

-498.576	33.746	37.634	56.367	69.211	88.998	96.531	115.252	126.656	142.095
148.171	164.131	176.519	184.907	193.404	197.073	212.358	232.856	242.408	260.543
267.480	268.107	277.149	290.496	294.955	305.105	328.199	332.450	336.589	340.514
355.292	371.853	377.440	379.749	380.439	381.668	384.478	391.600	411.415	428.793
445.120	456.303	462.367	463.397	475.144	479.796	483.335	485.427	496.049	504.142
516.952	519.821	527.618	529.379	530.687	542.513	553.092	555.225	556.229	558.422
567.633	570.996	577.250	581.582	602.625	606.643	608.853	620.732	632.721	636.809
637.942	641.255	644.248	653.490	663.353	676.775	678.230	691.135	698.455	702.799
707.407	716.087	726.198	729.877	739.843	746.750	754.960	757.174	782.746	790.524
793.026	796.983	800.443	801.531	803.229	805.630	807.844	811.319	822.188	826.833
831.158	839.813	846.863	850.444	852.859	857.266	858.052	860.618	866.149	890.500
895.692	896.919	914.756	933.031	937.951	946.957	950.948	963.439	966.717	968.243
973.960	983.385	984.756	987.555	989.653	996.359	997.773	999.920	1001.808	1004.828
1009.780	1045.039	1066.066	1071.776	1079.523	1090.139	1120.945	1127.417	1132.442	1151.724
1153.307	1158.137	1172.832	1176.024	1183.391	1191.214	1194.986	1200.340	1202.860	1203.387
1216.632	1221.622	1223.742	1234.345	1243.819	1248.443	1250.687	1256.413	1261.064	1263.548
1268.061	1277.713	1280.554	1288.291	1303.262	1315.552	1324.688	1329.038	1337.384	1342.482
1345.351	1362.381	1365.915	1380.269	1392.021	1394.695	1399.517	1408.640	1409.907	1412.829
1420.824	1426.506	1437.423	1440.549	1440.923	1445.012	1447.302	1451.531	1457.698	1462.360
1464.695	1471.386	1472.347	1475.553	1480.321	1498.198	1511.475	1515.308	1520.688	1526.341
1528.506	1534.304	1553.303	1563.189	1569.569	1574.229	1595.948	1606.445	1622.647	1631.047
1632.453	1635.762	1643.283	1648.083	1651.648	1656.450	1669.222	1672.437	1680.443	1689.404
1701.825	1752.245	3038.365	3058.968	3115.168	3131.928	3134.036	3145.425	3149.641	3151.756
3152.635	3153.603	3158.639	3160.274	3166.778	3170.517	3170.856	3172.034	3172.943	3173.187
3173.979	3176.925	3178.929	3183.149	3188.869	3194.432	3202.782	3207.383	3212.215	

Syn Adduct R-P

Atom	X	Y	X (Angstrom)
6	-1.19541	2.76509	2.16618
6	-2.15299	1.61589	1.94125
6	-1.67827	0.27441	1.96399
6	-0.30001	-0.02327	2.21260
6	0.63871	1.08615	2.38317
6	0.24116	2.35824	2.33399
6	-2.57223	-0.78584	1.67916
6	-3.95938	-0.51771	1.48768
6	-4.39232	0.79187	1.49369
6	-3.48828	1.85151	1.68917
6	-4.86410	-1.65822	1.32948
6	-4.40038	-2.88538	1.07182
6	-2.93939	-3.10875	0.80294
6	-2.07561	-2.11229	1.53418
6	-0.76550	-2.37587	1.85962
6	0.11708	-1.33725	2.21774
6	-2.59498	0.75442	-1.34921
6	-2.15248	-0.58606	-1.21428
6	-0.75730	-0.85512	-0.98954
6	0.14754	0.20622	-0.85083
6	-0.31457	1.56520	-0.90930
6	-1.67735	1.83321	-1.16668
6	0.59317	2.63408	-0.72666
6	1.97298	2.36703	-0.47315
6	2.43740	1.02839	-0.43291
6	1.52972	-0.05269	-0.63026
6	2.88104	3.43912	-0.24880
6	4.22581	3.16224	0.00176
6	4.71126	1.84709	0.03469
6	3.80845	0.76608	-0.18461
6	4.28357	-0.57859	-0.15353
6	5.65451	-0.83954	0.09043
6	6.53679	0.25795	0.30712
6	6.08854	1.54538	0.28248
6	2.00214	-1.39012	-0.60323
6	3.37843	-1.65507	-0.36679
6	3.85016	-3.00296	-0.33348

```
  6   5.24376  -3.22896  -0.09231
  6   6.10433  -2.19129   0.11107
  6   0.12463   3.97802  -0.77943
  6   1.06671   5.04256  -0.54369
  6   2.37143   4.78800  -0.28813
  6   2.94440  -4.05137  -0.51771
  6   1.57132  -3.81435  -0.72534
  6   1.09464  -2.46854  -0.78588
  6  -0.29280  -2.21133  -0.94815
  6  -2.13780   3.18104  -1.22287
  6  -1.22919   4.22337  -1.02570
  6   0.62739  -4.86618  -0.84405
  6  -0.72217  -4.59532  -0.94907
  6  -1.20720  -3.28204  -0.98160
  6  -2.66850  -2.99803  -0.77008
  6  -3.08368  -1.63737  -1.25921
  6  -4.40851  -1.35687  -1.59245
  6  -4.84328  -0.05249  -1.77708
  6  -3.96337   1.02283  -1.60832
  6  -4.40090   2.39407  -1.66367
  6  -3.53704   3.41870  -1.47159
  1  -5.44782   1.00769   1.33100
  1  -1.43519  -5.41930  -0.98401
  1  -3.28512  -3.77786  -1.24192
  1  -1.58454   5.25368  -1.06067
  1   3.30400  -5.07932  -0.48224
  1   0.98147  -5.89518  -0.81942
  1  -3.84979   2.87820   1.64236
  1   3.07005   5.60412  -0.11122
  1   0.70071   6.06762  -0.57500
  1   4.91754   3.98669   0.17306
  1  -5.12095  -2.17659  -1.66263
  1  -5.88797   0.14768  -2.01113
  1  -5.45465   2.58899  -1.85767
  1  -3.88334   4.45063  -1.50858
  1   5.60355  -4.25614  -0.07196
  1   7.16009  -2.38274   0.29575
  1   7.58836   0.04731   0.49550
  1   6.77703   2.37155   0.45080
  1   1.16442  -1.56634   2.41143
  1  -0.37464  -3.38807   1.74841
  1  -2.64329  -4.13239   1.07298
  1  -5.08042  -3.72844   0.95606
  1  -5.93301  -1.47407   1.43979
  1   1.69354   0.83710   2.49988
  1   0.97158   3.16449   2.40688
  1  -1.27373   3.46134   1.31632
  1  -1.51005   3.33335   3.05854
Energy      -2214.230889          (Hartree)
Frequencies cm-1:
    32.977    37.503    56.698    66.457    87.569    92.696   116.114   128.595   137.372   146.421
   165.956   177.355   186.074   197.236   201.115   213.579   232.542   240.187   259.336   268.166
   270.268   278.071   289.775   295.682   306.661   324.318   333.260   337.594   343.339   357.884
   371.837   376.670   379.237   380.180   384.767   385.926   397.548   410.587   427.431   446.172
   458.762   464.157   466.479   470.418   472.842   478.323   483.660   491.647   505.394   516.841
   519.103   525.771   529.297   530.487   545.461   552.079   555.538   556.404   561.785   569.001
   574.272   577.000   584.864   602.454   606.390   608.607   618.563   631.663   635.057   637.476
   638.982   642.010   657.448   663.305   667.596   681.932   693.988   699.436   701.516   711.186
   718.558   721.289   727.970   734.942   744.214   754.515   762.279   771.902   784.508   794.671
   797.096   798.421   802.216   806.145   806.801   809.716   818.738   825.285   826.515   828.423
   839.521   845.060   847.444   850.542   859.664   863.620   868.131   873.117   882.495   890.992
   898.861   914.984   931.868   935.467   937.528   949.430   950.112   958.153   970.869   974.578
   977.002   982.081   985.342   988.445   993.341   997.612   998.536  1000.393  1001.275  1007.766
  1030.286  1043.117  1073.218  1089.722  1105.967  1120.609  1128.073  1139.602  1146.899  1153.599
  1155.615  1171.801  1182.829  1183.307  1191.283  1195.735  1200.299  1201.305  1206.056  1211.681
  1219.473  1224.838  1234.483  1236.867  1239.272  1251.178  1253.675  1258.903  1262.924  1265.532
  1276.522  1278.310  1280.925  1291.092  1299.140  1312.670  1317.027  1322.210  1332.349  1342.731
  1344.447  1356.982  1357.446  1366.680  1383.221  1388.525  1396.182  1402.009  1407.634  1410.437
  1415.680  1418.561  1430.889  1433.503  1435.996  1444.449  1446.762  1451.446  1454.015  1455.084
  1460.028  1460.859  1470.216  1480.401  1481.609  1497.995  1510.492  1516.386  1520.882  1525.605
  1529.920  1534.529  1552.846  1571.675  1576.930  1580.812  1589.470  1612.048  1622.577  1630.779
  1639.025  1647.089  1658.621  1660.241  1664.020  1665.885  1672.426  1675.077  1687.535  1704.913
  1734.508  1761.659  3047.177  3062.323  3074.436  3090.908  3128.230  3132.090  3141.018  3146.709
  3154.941  3157.399  3160.058  3163.849  3164.086  3169.670  3170.991  3175.831  3177.668  3178.513
  3178.885  3179.066  3184.384  3191.863  3202.635  3203.681  3207.157  3207.538  3216.139

 Gauche Addition TS
 Atom    X         Y         X   (Angstrom)
  6  -5.94068  -1.93181   0.13684
  6  -5.10678  -0.76273   0.11350
  6  -3.73314  -0.91687  -0.21985
  6  -3.20468  -2.21561  -0.50493
  6  -4.04530  -3.35191  -0.43184
  6  -5.43348  -3.16492  -0.12019
  6  -2.88114   0.21460  -0.24021
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  6  -1.49742   0.06323  -0.58858
  6  -0.97850  -1.21650  -0.87820
  6  -1.82571  -2.37097  -0.81047
  6  -3.48178  -4.62901  -0.64519
  6  -2.13329  -4.77737  -0.88802
  6  -1.27882  -3.66114  -0.96925
  6   0.16643  -3.79737  -1.01356
  6   0.94238  -2.65717  -1.41620
  6   0.39487  -1.36336  -1.21828
  6   1.23073  -0.21890  -1.30690
  6   0.71389   1.05767  -0.98536
  6  -0.65352   1.19776  -0.61892
  6  -1.16780   2.48013  -0.25920
  6  -2.53155   2.62699   0.08930
  6  -3.39352   1.49009   0.08590
  6  -4.77397   1.63427   0.42415
  6  -5.59846   0.51460   0.42444
  6  -5.25967   2.95130   0.76671
  6  -4.44017   4.02576   0.78116
  6  -3.03833   3.91329   0.44657
  6  -2.18049   5.00631   0.46527
  6  -0.81873   4.88205   0.13423
  6  -0.30793   3.60836  -0.23997
  6   1.06955   3.46257  -0.58856
  6   1.57505   2.18620  -0.97054
  6   1.93068   4.58261  -0.54457
  6   1.39639   5.84777  -0.16068
  6   0.07958   5.99483   0.16153
  6   2.95048   2.03151  -1.30448
  6   3.79359   3.18679  -1.25200
  6   3.30361   4.40657  -0.88496
  6   2.61602  -0.36537  -1.63643
  6   3.44344   0.75872  -1.63304
  6   2.29957  -2.77453  -1.79933
  6   3.10849  -1.67629  -1.91214
  6   0.63853  -3.95033   0.98454
  6  -0.46043  -3.26970   1.64279
  6  -0.36599  -1.97068   1.99345
  6   0.86660  -1.23086   1.81447
  6   2.03380  -1.94257   1.40552
  6   1.95591  -3.33826   1.10608
  6   0.94484   0.13619   2.01812
  6   2.15696   0.82051   1.84171
  6   3.31492   0.15158   1.50049
  6   3.26420  -1.25467   1.27712
  6   4.43126  -1.97963   0.87906
  6   5.66234  -1.23490   0.62347
  6   5.75079   0.08317   0.82410
  6   4.62614   0.89804   1.39518
  6   3.12466  -4.01809   0.79162
  6   4.35230  -3.34829   0.69726
  1   0.04964   0.68935   2.30028
  1   2.70591  -3.76876  -1.97445
  1   0.55483  -4.77326  -1.31387
  1  -6.65140   0.62734   0.68272
  1   4.50304   0.63920  -1.85934
  1   4.15935  -1.78866  -2.17342
  1   2.18524   1.90148   1.97951
  1  -4.82327   5.00962   1.04741
  1  -6.31330   3.05604   1.02072
  1  -2.56851   5.98566   0.74512
  1  -1.70937  -5.77344  -1.01239
  1  -4.12849  -5.50369  -0.59637
  1  -6.07649  -4.04317  -0.08769
  1  -6.99530  -1.80752   0.37702
  1   4.84491   3.07086  -1.51390
  1   3.96065   5.27437  -0.85140
  1   2.06624   6.70568  -0.13162
  1  -0.31144   6.96899   0.45050
  1   5.24745  -3.90277   0.41834
  1   3.07905  -5.08670   0.58025
  1   0.61308  -5.04164   1.00330
  1  -1.40600  -3.79805   1.74937
  1  -1.22915  -1.44057   2.39613
  1   6.51752  -1.79621   0.24617
  1   6.68379   0.60613   0.61586
  1   4.47492   1.81311   0.80120
  1   4.92673   1.23477   2.40408
Energy      -2214.203237          (Hartree)
Frequencies cm-1:
  -640.012    24.265    34.006    42.961    51.881    73.064    80.332    94.370   106.807   124.745
   131.905   161.394   169.954   178.037   185.275   201.611   212.572   227.169   230.525   252.385
   261.532   268.835   277.337   289.874   296.806   302.315   323.500   337.430   339.844   344.430
   354.202   367.865   369.914   378.820   380.613   382.340   384.986   392.195   413.838   431.668
   446.026   454.757   458.880   466.610   474.467   476.615   482.445   487.588   493.850   505.008
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516.422	524.016	530.966	532.203	534.926	540.664	551.283	551.877	557.362	558.671
567.982	571.944	578.532	584.507	601.728	605.625	607.603	621.761	631.567	634.238
640.226	640.887	642.775	651.222	664.350	668.718	678.469	693.293	701.513	706.134
716.015	723.612	727.848	732.302	741.051	745.973	753.898	759.243	776.251	784.346
788.187	795.301	797.345	800.794	803.735	808.559	811.683	814.885	815.909	819.843
827.513	836.955	838.477	848.577	856.245	861.120	865.977	868.993	869.643	878.191
883.834	889.934	902.826	938.765	939.317	943.650	951.300	957.935	960.128	961.577
976.285	977.795	980.938	988.239	989.545	990.782	994.667	999.253	1002.351	1003.562
1008.328	1033.139	1050.783	1074.574	1080.032	1092.331	1120.326	1130.779	1132.992	1149.876
1152.350	1154.307	1169.415	1178.210	1185.450	1192.792	1195.257	1202.745	1204.463	1210.275
1216.754	1218.970	1224.947	1233.047	1244.373	1247.592	1249.665	1254.022	1258.651	1264.785
1267.538	1275.756	1280.142	1287.904	1308.811	1316.513	1323.629	1333.674	1337.491	1346.191
1346.873	1364.278	1364.694	1387.386	1396.282	1400.944	1404.025	1410.882	1412.005	1414.704
1423.332	1426.046	1439.319	1440.889	1441.400	1447.376	1448.202	1453.598	1460.444	1462.408
1465.355	1472.256	1475.173	1477.577	1484.374	1498.451	1513.278	1515.616	1521.792	1529.805
1533.341	1537.242	1553.115	1566.787	1567.526	1577.110	1601.607	1609.668	1624.409	1632.245
1639.321	1645.269	1650.173	1656.847	1658.763	1661.241	1672.768	1683.027	1688.276	1692.382
1706.760	1745.299	2994.823	3069.832	3115.534	3127.250	3128.042	3130.027	3132.150	3132.283
3132.518	3136.398	3143.936	3145.409	3147.352	3150.872	3151.981	3152.495	3154.161	3161.687
3175.972	3188.482	3198.606	3203.968	3207.869	3212.868	3214.901	3229.588	3233.417	

Gauche Adduct R-P

Atom	X	Y	X	(Angstrom)
6	-5.84670	-2.29809	0.02311	
6	-5.08151	-1.07712	0.05071	
6	-3.68838	-1.14414	-0.23139	
6	-3.06927	-2.40604	-0.50418	
6	-3.84453	-3.59474	-0.48155	
6	-5.26004	-3.49201	-0.22967	
6	-2.90912	0.03534	-0.21009	
6	-1.50720	-0.02788	-0.51913	
6	-0.89964	-1.26221	-0.78072	
6	-1.67374	-2.47763	-0.73818	
6	-3.20016	-4.82390	-0.67828	
6	-1.82201	-4.88597	-0.84229	
6	-1.04384	-3.72917	-0.85972	
6	0.45900	-3.78073	-0.76380	
6	1.12058	-2.55341	-1.32518	
6	0.48367	-1.31283	-1.13947	
6	1.22551	-0.11077	-1.27080	
6	0.62421	1.12712	-0.93507	
6	-0.74105	1.16958	-0.55332	
6	-1.34605	2.41269	-0.20397	
6	-2.72249	2.46719	0.12818	
6	-3.51066	1.27492	0.10284	
6	-4.90353	1.33030	0.39991	
6	-5.65911	0.15809	0.36055	
6	-5.47994	2.60879	0.73910	
6	-4.73010	3.73388	0.78035	
6	-3.31922	3.71341	0.47382	
6	-2.53488	4.86599	0.50153	
6	-1.16834	4.83525	0.18037	
6	-0.56791	3.59783	-0.18898	
6	0.81353	3.54956	-0.54710	
6	1.40261	2.31541	-0.93879	
6	1.59395	4.73080	-0.51479	
6	0.97350	5.95491	-0.12712	
6	-0.34821	6.00930	0.20197	
6	2.77996	2.26030	-1.30589	
6	3.53864	3.47378	-1.26166	
6	2.96943	4.65381	-0.87751	
6	2.60301	-0.15796	-1.64745	
6	3.35155	1.03204	-1.66159	
6	2.43739	-2.58028	-1.79620	
6	3.16890	-1.42054	-1.95542	
6	0.85059	-3.89613	0.83276	
6	-0.23247	-3.26914	1.67097	
6	-0.15147	-2.00575	2.08915	
6	1.03629	-1.19062	1.83581	
6	2.21992	-1.84786	1.38259	
6	2.19256	-3.23767	1.05368	
6	1.05610	0.17056	2.03988	
6	2.23124	0.91565	1.82001	
6	3.40605	0.30343	1.44841	
6	3.41314	-1.10576	1.22592	
6	4.60014	-1.77865	0.79551	
6	5.78814	-0.97517	0.49922	
6	5.82106	0.34479	0.69581	
6	4.67946	1.10896	1.30473	
6	3.37235	-3.87026	0.74039	
6	4.57666	-3.14571	0.62123	
1	0.14813	0.68084	2.36055	
1	2.91340	-3.54312	-1.97172	
1	0.85830	-4.68322	-1.24612	
1	-6.72473	0.20343	0.58526	

```
  1   4.40934   0.98952  -1.92303
  1   4.21184  -1.46532  -2.26481
  1   2.21047   1.99680   1.95719
  1  -5.18245   4.68923   1.04222
  1  -6.54385   2.64466   0.96805
  1  -2.99385   5.81637   0.77405
  1  -1.33426  -5.85568  -0.93986
  1  -3.79123  -5.73817  -0.67136
  1  -5.85064  -4.40665  -0.23583
  1  -6.91543  -2.23866   0.22184
  1   4.59020   3.43657  -1.54536
  1   3.56443   5.56547  -0.85129
  1   1.58147   6.85817  -0.10575
  1  -0.80658   6.95439   0.48909
  1   5.48723  -3.66360   0.32203
  1   3.36552  -4.93485   0.50338
  1   0.90965  -4.97333   1.04045
  1  -1.13180  -3.85561   1.85091
  1  -0.98104  -1.53835   2.61953
  1   6.65456  -1.49620   0.09125
  1   6.72065   0.91036   0.45446
  1   4.46757   2.01504   0.71649
  1   4.99735   1.45888   2.30309
Energy      -2214.213649          (Hartree)
Frequencies cm-1:
    22.093    37.508    41.987    52.545    75.998    80.365    93.398   108.760   123.086   135.909
   159.512   167.431   178.352   184.970   201.383   214.918   228.115   235.253   252.365   258.808
   271.210   276.953   292.230   295.469   306.151   321.558   334.596   344.286   346.220   359.023
   369.838   371.562   377.713   378.852   380.982   385.091   394.536   418.287   430.422   444.821
   457.470   459.758   467.944   471.839   472.856   479.186   483.537   489.531   502.777   516.756
   519.565   528.516   531.120   534.858   541.586   549.887   551.912   555.796   561.622   569.790
   573.977   584.102   588.671   596.785   604.955   610.047   618.220   628.881   631.358   633.506
   639.817   642.514   650.189   669.692   672.608   681.121   690.714   698.490   702.293   716.233
   720.922   721.401   732.381   738.934   743.468   757.479   760.462   765.981   774.890   792.661
   797.042   797.977   802.172   807.204   808.617   814.406   815.517   816.792   823.436   823.815
   829.905   844.191   849.785   854.784   861.130   865.027   866.652   869.801   876.457   879.757
   892.432   908.114   924.163   934.342   938.517   944.814   952.074   956.224   969.494   972.701
   974.157   981.282   986.949   990.156   994.421   996.959  1006.420  1006.982  1007.141  1007.672
  1018.865  1042.096  1074.495  1088.286  1108.667  1120.934  1129.613  1140.436  1149.441  1153.588
  1155.236  1169.844  1178.568  1185.208  1192.945  1195.067  1200.528  1202.802  1207.878  1209.051
  1213.832  1224.756  1235.415  1238.767  1241.930  1249.963  1252.932  1255.707  1260.399  1260.606
  1269.552  1278.545  1283.010  1291.754  1297.229  1312.171  1317.005  1321.786  1332.526  1340.430
  1345.987  1348.702  1360.370  1365.417  1381.145  1389.813  1397.385  1405.258  1407.133  1409.014
  1413.251  1421.015  1431.230  1435.981  1437.770  1445.513  1447.904  1453.036  1455.931  1456.561
  1460.651  1461.771  1470.969  1481.780  1487.427  1497.539  1513.700  1515.771  1522.173  1526.627
  1530.470  1535.445  1555.253  1574.743  1579.155  1582.359  1592.333  1615.141  1623.210  1631.136
  1639.175  1650.081  1659.250  1669.676  1673.153  1675.595  1676.877  1677.401  1689.676  1706.366
  1749.259  1756.779  3003.950  3050.139  3064.126  3086.979  3123.079  3133.762  3137.833  3148.260
  3150.440  3151.151  3153.336  3153.702  3162.640  3166.614  3190.122  3193.093  3194.378  3197.115
  3200.434  3202.850  3212.151  3213.363  3219.315  3223.858  3225.538  3231.152  3242.110

 Anti Addition TS
 Atom    X         Y         X   (Angstrom)
  6  -4.94516  -4.58935   0.06961
  6  -3.77495  -3.79227   0.27415
  6  -3.88116  -2.38187   0.10860
  6  -5.13164  -1.79456  -0.24317
  6  -6.26765  -2.61164  -0.43749
  6  -6.13674  -4.02201  -0.27299
  6  -2.73892  -1.56006   0.29645
  6  -1.49688  -2.14547   0.64284
  6  -1.40231  -3.56304   0.81739
  6  -2.53748  -4.35233   0.63123
  6  -0.34423  -1.32735   0.80369
  6  -0.45590   0.08454   0.65188
  6  -1.70673   0.66862   0.33753
  6  -2.84272  -0.14724   0.14146
  6   0.90763  -1.91313   1.12237
  6   2.08788  -1.09855   1.09171
  6   1.93536   0.33372   1.19601
  6   0.68268   0.91570   0.89183
  6   0.54976   2.33100   0.83494
  6   1.66530   3.15772   1.12074
  6   2.89200   2.55255   1.45682
  6   3.02972   1.17957   1.46851
  6  -0.70615   2.91856   0.49036
  6  -1.82842   2.09280   0.23519
  6  -0.13008  -4.11379   1.18128
  6   0.97143  -3.31997   1.32533
  6   1.50354   4.58206   1.04505
  6   0.31506   5.14191   0.70092
  6  -0.83538   4.33297   0.41061
  6  -2.07469   4.89054   0.06221
  6  -3.18770   4.09654  -0.19108
  6  -3.07319   2.67558  -0.09508
```

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  6  -4.21090   1.84765  -0.32100
  6  -4.09818   0.44289  -0.19345
  6  -5.47073   2.43105  -0.65806
  6  -5.54905   3.87015  -0.76623
  6  -4.47209   4.65611  -0.54293
  6  -6.57249   1.61039  -0.86162
  6  -6.48559   0.21130  -0.73372
  6  -5.23735  -0.37884  -0.39253
  6  -7.50556  -1.99787  -0.78715
  6  -7.61294  -0.64598  -0.92941
  6   2.65854  -1.31509  -0.88712
  6   3.84380  -0.49278  -0.97781
  6   5.12067  -1.08885  -0.72954
  6   5.23166  -2.50222  -0.58338
  6   4.04820  -3.31207  -0.77631
  6   2.83678  -2.74520  -0.97951
  6   3.77244   0.88024  -1.19045
  6   4.92697   1.67695  -1.15910
  6   6.16654   1.13517  -0.88560
  6   6.28483  -0.27782  -0.66502
  6   7.54426  -0.87331  -0.40299
  6   8.79835  -0.02823  -0.31907
  6   8.57606   1.43565  -0.57283
  6   7.37369   1.95512  -0.82890
  6   7.61740  -2.24650  -0.23179
  6   6.48383  -3.05512  -0.33179
  1   6.57727  -4.13536  -0.22649
  1   1.93377  -3.75786   1.58677
  1   3.00737  -1.53003   1.49285
  1  -2.16647   5.97491  -0.00426
  1  -2.46397  -5.43175   0.76344
  1  -0.06006  -5.18848   1.34088
  1   8.58613  -2.70611  -0.03618
  1  -6.50967   4.31080  -1.02885
  1  -4.55212   5.73942  -0.62221
  1  -7.53202   2.05842  -1.12004
  1   3.99953   0.73184   1.68387
  1   3.75123   3.18531   1.67424
  1   2.36411   5.21008   1.27086
  1   0.21116   6.22446   0.64409
  1  -4.86471  -5.66828   0.19327
  1  -7.01672  -4.64532  -0.42645
  1  -8.37482  -2.63642  -0.93855
  1  -8.56723  -0.19350  -1.19423
  1   4.83887   2.74904  -1.33022
  1   2.80302   1.34135  -1.37636
  1   1.95804  -3.36718  -1.13379
  1   4.16450  -4.39492  -0.78450
  1   7.26035   3.02365  -1.00951
  1   9.45518   2.07760  -0.54157
  1   9.25437  -0.15522   0.67777
  1   9.54033  -0.41053  -1.03988
  1   1.73406  -0.89309  -1.28463
Energy      -2214.189040          (Hartree)
Frequencies cm-1:
  -652.237    12.481    20.597    31.811    41.178    53.835    64.949    73.904    86.965   110.083
   117.344   127.399   155.279   169.206   176.421   186.007   199.525   202.547   224.309   247.318
   255.173   265.030   276.593   285.250   296.224   300.579   322.806   328.193   337.075   342.155
   356.724   364.108   367.891   369.847   377.790   381.261   383.791   386.588   410.938   430.284
   445.817   455.163   461.553   467.764   473.606   479.732   482.804   488.478   494.291   506.128
   513.528   524.020   529.629   532.598   535.150   539.088   552.929   555.461   556.146   562.198
   568.271   571.243   575.783   583.624   603.584   605.745   607.918   623.656   633.979   637.135
   639.032   642.078   644.745   652.465   670.075   678.791   683.482   694.618   702.223   707.351
   721.606   732.026   734.642   738.734   741.528   758.134   758.489   763.103   786.986   788.636
   797.190   801.510   803.171   804.905   807.273   813.851   819.339   821.223   823.183   824.487
   832.161   840.641   842.567   857.756   859.958   862.125   863.564   868.201   881.450   888.718
   893.531   919.230   937.109   938.766   946.606   951.235   954.669   971.946   975.193   976.177
   977.598   982.660   983.621   985.081   986.911   996.387   998.095  1001.985  1002.265  1005.737
  1020.345  1047.352  1068.142  1072.812  1079.254  1089.563  1119.952  1126.537  1130.758  1147.268
  1153.802  1157.696  1175.044  1175.912  1183.056  1191.997  1195.675  1202.685  1209.428  1211.303
  1217.743  1227.881  1228.324  1234.065  1244.374  1248.655  1254.278  1256.790  1264.208  1266.635
  1269.494  1274.332  1280.995  1284.775  1304.592  1315.492  1323.649  1330.147  1337.748  1343.751
  1347.246  1362.882  1371.015  1385.723  1387.406  1396.467  1403.781  1410.877  1412.916  1413.845
  1423.781  1434.337  1438.970  1440.799  1444.528  1446.245  1448.250  1452.779  1458.150  1465.112
  1467.040  1471.390  1475.608  1476.184  1495.208  1497.353  1514.571  1518.396  1519.214  1528.381
  1530.400  1535.725  1552.032  1559.534  1562.740  1572.264  1602.320  1605.076  1617.065  1629.656
  1637.111  1639.849  1642.269  1654.783  1657.235  1660.399  1673.179  1679.492  1682.499  1691.873
  1707.939  1757.851  3065.103  3083.829  3126.220  3127.849  3129.502  3135.267  3137.260  3144.134
  3147.776  3163.080  3168.001  3169.369  3171.214  3171.516  3179.776  3181.252  3185.287  3186.240
  3189.575  3192.884  3194.230  3196.951  3206.733  3208.189  3210.822  3214.803  3229.131
```

Anti Adduct R-P

Atom	X	Y	X	(Angstrom)
6	4.92360	1.65738	-1.21267	
6	6.16087	1.12896	-0.92434	
6	6.28119	-0.27510	-0.66870	
6	5.11697	-1.08473	-0.69544	
6	3.83898	-0.49242	-0.92126	
6	3.76580	0.85075	-1.20274	
6	2.60153	-1.31356	-0.67531	
6	2.83515	-2.77654	-0.93413	
6	4.04767	-3.32018	-0.79542	
6	5.23633	-2.50033	-0.55276	
6	7.54942	-0.86825	-0.41228	
6	7.62374	-2.23210	-0.22822	
6	6.48136	-3.04689	-0.32027	
6	7.37016	1.95431	-0.89309	
6	8.57365	1.44262	-0.63498	
6	8.80216	-0.01631	-0.35426	
6	2.15341	-1.15225	0.87280	
6	1.95158	0.31018	1.15353	
6	0.70603	0.89324	0.86230	
6	-0.44292	0.06633	0.58889	
6	-0.34402	-1.35599	0.74341	
6	0.89539	-1.96012	1.03910	
6	0.56677	2.30605	0.86279	
6	-0.68310	2.90488	0.51206	
6	-1.80026	2.08885	0.22109	
6	-1.68180	0.65850	0.29868	
6	1.67672	3.12525	1.19905	
6	1.51617	4.55722	1.15733	
6	0.34039	5.12530	0.79956	
6	-0.80855	4.32276	0.46407	
6	-3.03974	2.68200	-0.10995	
6	-3.14849	4.10129	-0.18426	
6	-2.03392	4.88965	0.10426	
6	3.01838	1.13093	1.51729	
6	2.88468	2.51260	1.55256	
6	-4.18412	1.86258	-0.35376	
6	-4.08495	0.45471	-0.22666	
6	-2.83682	-0.14908	0.10683	
6	-2.75328	-1.55527	0.27980	
6	-1.51415	-2.15403	0.62855	
6	-1.44267	-3.56549	0.84509	
6	-0.19337	-4.12220	1.21867	
6	0.93748	-3.33456	1.30745	
6	-2.60287	-4.34555	0.68151	
6	-3.82474	-3.77592	0.30863	
6	-3.90912	-2.36476	0.11147	
6	-5.14772	-1.76753	-0.25204	
6	-5.23340	-0.35346	-0.42035	
6	-6.47526	0.24994	-0.76967	
6	-6.54580	1.64525	-0.90379	
6	-5.43290	2.45751	-0.69300	
6	-5.50183	3.89565	-0.79159	
6	-4.42214	4.67311	-0.54596	
6	-6.29784	-2.57272	-0.43584	
6	-7.52535	-1.94718	-0.80005	
6	-7.61392	-0.59622	-0.96076	
6	-6.18923	-3.98043	-0.24363	
6	-5.00816	-4.55887	0.11678	
1	6.58348	-4.12790	-0.22977	
1	1.89529	-3.78782	1.55826	
1	2.97881	-1.56415	1.47004	
1	-2.12338	5.97505	0.05680	
1	-2.54465	-5.42152	0.84298	
1	-0.13542	-5.19024	1.42021	
1	8.59309	-2.69358	-0.04049	
1	-6.45648	4.34495	-1.06104	
1	-4.49498	5.75760	-0.61384	
1	-7.49870	2.10469	-1.16643	
1	3.98696	0.67816	1.72855	
1	3.73850	3.13266	1.82064	
1	2.37299	5.17624	1.41877	
1	0.23659	6.20861	0.76610	
1	-4.94488	-5.63571	0.26391	
1	-7.07833	-4.59294	-0.38765	
1	-8.40284	-2.57583	-0.94553	
1	-8.56092	-0.13415	-1.23490	
1	4.82989	2.72189	-1.42263	
1	2.79347	1.31309	-1.37248	
1	1.97138	-3.39686	-1.16144	
1	4.19542	-4.39341	-0.91638	
1	7.25235	3.01870	-1.09384	
1	9.45189	2.08651	-0.62122	
1	9.26320	-0.12133	0.64237	

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  1   9.54062  -0.40871  -1.07229
  1   1.75758  -0.93230  -1.26702
Energy      -2214.203743          (Hartree)
Frequencies cm-1:
    15.452    23.152    31.974    42.718    52.210    65.599    75.212    89.188   108.167   115.942
   133.848   157.116   172.508   177.584   183.120   200.204   203.518   217.613   245.729   254.485
   264.178   275.838   289.115   295.501   304.285   320.096   327.778   340.009   342.223   361.284
   363.891   368.266   369.712   379.399   381.619   385.116   388.018   416.226   429.050   444.598
   458.755   462.546   470.372   471.451   475.654   479.002   486.538   491.302   506.144   514.754
   519.186   525.645   532.619   536.778   539.515   549.737   553.949   556.521   562.870   570.519
   576.386   576.544   588.074   600.361   607.188   609.159   621.777   633.181   634.815   638.798
   640.429   644.328   655.851   663.609   672.774   681.883   696.229   702.106   709.608   717.814
   730.744   733.455   739.115   745.252   749.153   757.656   762.511   778.472   784.777   797.731
   800.318   801.576   803.575   808.322   812.851   819.255   820.927   822.788   824.955   831.549
   838.569   843.942   855.556   861.894   865.888   868.625   869.712   879.614   883.872   889.527
   906.071   916.087   933.830   937.337   947.008   951.848   957.882   968.151   969.538   976.743
   979.812   984.299   986.034   991.488   996.576   997.954  1000.293  1011.790  1015.143  1026.748
  1030.785  1046.310  1075.453  1091.193  1113.962  1121.028  1127.224  1148.992  1150.666  1154.640
  1157.931  1169.818  1182.207  1189.684  1194.284  1198.310  1203.075  1207.002  1210.151  1214.424
  1218.588  1225.540  1237.305  1239.142  1243.134  1254.762  1255.088  1262.123  1266.773  1268.392
  1275.950  1281.060  1282.779  1290.141  1293.186  1309.888  1315.186  1320.728  1331.389  1341.925
  1346.356  1353.694  1355.719  1364.282  1377.244  1385.408  1398.520  1401.360  1406.971  1413.238
  1414.041  1428.021  1429.889  1434.074  1438.554  1445.136  1446.397  1451.361  1451.775  1458.348
  1460.028  1465.633  1470.042  1480.358  1496.804  1497.661  1510.680  1518.961  1519.814  1523.956
  1529.167  1535.861  1552.862  1577.618  1578.189  1578.691  1585.975  1611.612  1617.750  1627.606
  1637.051  1647.937  1658.871  1666.402  1672.793  1673.815  1677.287  1679.215  1689.305  1709.124
  1748.399  1768.264  3069.200  3073.258  3087.761  3091.360  3120.345  3123.726  3132.619  3139.220
  3143.901  3151.230  3153.399  3157.100  3163.481  3163.630  3165.422  3172.472  3174.643  3184.528
  3185.408  3188.585  3200.567  3203.864  3226.684  3233.068  3238.691  3240.605  3245.753
```

System3:

```
 C32H14  7-H-ovalenyl
 Atom    X         Y         X   (Angstrom)
  6   0.01840  -0.02934  -0.03511
  6  -0.05304  -0.00238   1.47319
  6   1.27987  -0.03883   2.18082
  6   1.31060  -0.01820   3.57946
  6   2.50214  -0.04920   4.27589
  6  -1.16845   0.00028  -0.77527
  6  -1.15927  -0.02186  -2.15562
  6   0.05728  -0.07563  -2.86238
  6   1.27205  -0.10658  -2.13014
  6   1.25044  -0.08318  -0.70496
  6   2.49303  -0.11532   0.02252
  6   2.48441  -0.09250   1.46265
  6   3.71790  -0.16908  -0.67481
  6   4.95490  -0.20099   0.03682
  6   4.95745  -0.17913   1.45865
  6   3.72083  -0.12489   2.17152
  6   6.18759  -0.25459  -0.67417
  6   6.17752  -0.27583  -2.07541
  6   4.97764  -0.24569  -2.79953
  6   3.73733  -0.19202  -2.10217
  1   7.12327  -0.31683  -2.61421
  6   7.40744  -0.28560   0.07228
  1   8.34667  -0.32657  -0.47613
  6   6.18212  -0.21065   2.16734
  6   7.40254  -0.26422   1.43446
  1  -0.59484   0.90606   1.78509
  1   0.36806   0.02369   4.12406
  6   3.73061  -0.10308   3.59000
  6   6.16063  -0.18781   3.59188
  6   4.98480  -0.13619   4.27735
  1   7.11000  -0.21257   4.12407
  1   8.33989  -0.28817   1.98775
  1   2.50259  -0.03222   5.36423
  1   4.97739  -0.11907   5.36567
  1  -2.09502   0.00200  -2.71107
  1  -2.11790   0.04200  -0.24268
  6   2.51605  -0.16122  -2.82992
  6   4.95836  -0.26721  -4.22911
  6   3.78434  -0.23770  -4.92025
  6   2.53180  -0.18405  -4.24532
  6   1.29571  -0.15196  -4.95358
  6   0.10643  -0.09997  -4.29214
  1   1.32280  -0.17027  -6.04177
  1  -0.83309  -0.07572  -4.84117
  1   3.78816  -0.25474  -6.00889
  1   5.90881  -0.30832  -4.75780
  1  -0.65880  -0.85853   1.81392
Energy      -1221.688769          (Hartree)
Frequencies cm-1:
    48.277    58.734   103.731   119.410   125.215   183.193   187.538   256.007   265.481   275.372
```

275.821	314.003	316.320	324.757	332.095	337.404	386.953	399.108	421.127	427.953
456.781	475.860	478.322	480.789	491.500	509.134	526.113	532.570	539.545	560.546
562.711	563.093	585.711	614.352	616.733	642.160	646.113	653.846	665.482	691.533
714.899	718.780	737.416	750.586	753.556	767.526	780.483	783.588	798.223	801.468
807.701	820.125	840.223	841.011	858.297	864.400	871.426	885.678	902.256	906.359
924.389	939.867	977.588	983.846	985.630	988.176	992.799	996.390	997.132	1054.983
1077.398	1092.614	1135.607	1164.935	1168.709	1178.670	1184.194	1190.627	1205.221	1213.320
1213.681	1229.509	1243.360	1253.848	1261.217	1269.669	1270.640	1292.446	1303.041	1306.127
1335.670	1343.046	1372.169	1375.438	1387.899	1398.687	1416.201	1425.237	1439.225	1449.629
1456.876	1461.332	1469.399	1470.849	1483.018	1489.588	1513.382	1533.248	1553.958	1555.668
1567.552	1576.780	1602.970	1618.092	1642.201	1646.346	1664.418	1673.555	1687.808	1694.334
3048.019	3073.493	3132.338	3132.849	3136.706	3142.927	3143.527	3161.602	3161.954	3162.348
3162.639	3165.758	3166.048	3190.077	3190.358					

C96H24 circumcircumcoronene

Atom	X	Y	X	(Angstrom)
6	8.47008	1.71710	-0.00014	
6	8.63431	0.37787	-0.00019	
6	7.50334	-0.52863	-0.00017	
6	6.18581	0.04141	-0.00013	
6	6.01265	1.45272	-0.00010	
6	7.15370	2.32387	-0.00009	
6	4.71387	2.00735	-0.00006	
6	3.57371	1.14795	-0.00007	
6	3.74515	-0.25140	-0.00009	
6	5.05873	-0.81028	-0.00011	
6	2.26482	1.70554	-0.00004	
6	1.13608	0.85557	-0.00005	
6	1.30919	-0.55602	-0.00006	
6	2.60915	-1.10845	-0.00007	
6	2.78103	-2.52073	-0.00006	
6	1.65459	-3.36901	-0.00002	
6	0.34465	-2.81384	-0.00002	
6	0.17283	-1.41171	-0.00004	
6	-0.79294	-3.66881	0.00001	
6	-0.61836	-5.08555	0.00007	
6	0.69078	-5.63975	0.00008	
6	1.82779	-4.78591	0.00002	
6	4.09515	-3.07834	-0.00008	
6	4.26459	-4.48045	-0.00004	
6	3.12855	-5.33602	0.00002	
6	3.29388	-6.76185	0.00009	
6	2.17992	-7.58021	0.00017	
6	0.86434	-7.05428	0.00016	
6	-1.13608	-0.85557	-0.00005	
6	-2.26482	-1.70555	-0.00004	
6	-2.09032	-3.11753	-0.00001	
6	-3.23133	-3.97585	0.00002	
6	-3.05707	-5.37747	0.00009	
6	-1.74834	-5.93346	0.00012	
6	-1.56390	-7.35692	0.00021	
6	-0.28557	-7.88227	0.00024	
6	-0.17283	1.41171	-0.00004	
6	-1.30919	0.55602	-0.00005	
6	-2.60915	1.10845	-0.00007	
6	-3.74515	0.25140	-0.00009	
6	-3.57371	-1.14795	-0.00007	
6	-4.71387	-2.00735	-0.00006	
6	-4.53897	-3.41814	-0.00001	
6	-0.34465	2.81384	-0.00002	
6	-1.65459	3.36901	-0.00002	
6	-2.78103	2.52073	-0.00006	
6	-4.09515	3.07834	-0.00007	
6	-5.22982	2.22145	-0.00012	
6	-5.05873	0.81028	-0.00011	
6	-6.18581	-0.04141	-0.00013	
6	-6.01265	-1.45272	-0.00009	
6	-7.50334	0.52863	-0.00018	
6	-7.65496	1.90256	-0.00019	
6	-6.54148	2.77881	-0.00015	
6	-6.68364	4.18844	-0.00013	
6	-5.58964	5.03306	-0.00006	
6	-4.26459	4.48045	-0.00004	
6	-3.12855	5.33602	0.00002	
6	-1.82779	4.78591	0.00003	
6	0.79294	3.66881	0.00001	
6	0.61836	5.08555	0.00007	
6	-0.69078	5.63975	0.00009	
6	-0.86434	7.05428	0.00016	
6	-2.17992	7.58021	0.00017	
6	-3.29388	6.76185	0.00009	
6	-4.64430	7.28807	0.00007	
6	-5.72235	6.47616	-0.00001	
6	2.09032	3.11753	-0.00001	
6	-5.67766	-4.27570	0.00003	

```
  6  -6.96940  -3.69387  -0.00002
  6  -7.15370  -2.32387  -0.00008
  6  -8.47008  -1.71710  -0.00014
  6  -8.63431  -0.37787  -0.00019
  6   4.53897   3.41814  -0.00001
  6   3.23133   3.97585   0.00002
  6   3.05707   5.37747   0.00009
  6   1.74834   5.93346   0.00012
  6   1.56390   7.35692   0.00021
  6   0.28557   7.88227   0.00024
  6  -5.47499  -5.67811   0.00011
  6  -4.20952  -6.23373   0.00015
  6   5.22982  -2.22145  -0.00011
  6   6.96940   3.69387  -0.00002
  6   5.67766   4.27570   0.00003
  6   5.47499   5.67811   0.00011
  6   4.20952   6.23373   0.00015
  6   3.98979   7.66598   0.00025
  6   2.74720   8.19368   0.00028
  6  -3.98979  -7.66598   0.00025
  6  -2.74720  -8.19368   0.00028
  6   4.64430  -7.28807   0.00007
  6   5.72235  -6.47616  -0.00001
  6   5.58964  -5.03306  -0.00006
  6   6.68364  -4.18844  -0.00013
  6   6.54148  -2.77881  -0.00015
  6   7.65496  -1.90256  -0.00019
  1  -7.83996  -4.34979   0.00000
  1   2.31174  -8.66170   0.00024
  1  -0.15142  -8.96348   0.00032
  1  -2.60601  -9.27296   0.00035
  1  -4.86474  -8.31409   0.00029
  1  -6.34689  -6.33227   0.00015
  1   8.65763  -2.32974  -0.00024
  1   4.76888  -8.36931   0.00012
  1   6.72781  -6.89376  -0.00004
  1   7.68736  -4.61317  -0.00017
  1  -9.33521  -2.37844  -0.00014
  1  -9.63300   0.05566  -0.00024
  1  -7.68736   4.61317  -0.00018
  1  -8.65763   2.32974  -0.00025
  1  -6.72781   6.89376  -0.00004
  1  -4.76888   8.36931   0.00012
  1  -2.31174   8.66170   0.00024
  1   0.15142   8.96348   0.00032
  1   2.60601   9.27296   0.00036
  1   4.86474   8.31409   0.00029
  1   6.34689   6.33227   0.00015
  1   7.83996   4.34979   0.00000
  1   9.63300  -0.05566  -0.00024
  1   9.33521   2.37844  -0.00014
Energy      -3652.903482          (Hartree)
Frequencies cm-1:
    11.326    21.701    26.662    43.813    55.250    64.314    70.201    80.622    84.696   123.865
   126.507   127.005   128.715   131.151   169.784   172.511   183.693   194.259   194.400   201.693
   205.993   208.709   209.576   210.523   234.581   236.487   237.691   238.391   254.292   270.857
   281.282   282.108   300.008   300.307   300.914   302.559   310.546   313.367   315.196   316.129
   317.100   340.783   354.829   367.265   367.809   368.602   382.683   383.461   385.409   395.439
   404.301   407.741   408.761   409.610   409.806   413.744   420.123   421.997   427.633   427.901
   443.066   444.043   448.139   448.765   450.018   450.043   453.180   484.617   504.066   504.531
   508.147   508.483   516.884   517.549   526.365   526.484   546.298   546.840   553.016   556.237
   557.032   557.220   557.644   560.832   566.213   570.269   572.591   573.865   588.286   592.207
   594.004   594.028   594.449   596.971   600.226   602.147   605.939   607.305   609.913   612.293
   612.710   612.803   614.091   630.550   631.585   638.254   639.059   639.247   651.692   652.216
   660.861   660.973   661.294   670.863   671.158   671.292   678.900   679.590   685.937   689.505
   689.972   699.095   713.007   715.849   717.279   719.277   719.740   731.927   732.111   732.512
   739.196   739.298   744.178   756.913   757.305   757.701   757.936   758.246   776.317   780.304
   780.795   783.754   784.124   789.939   792.532   798.286   798.362   801.722   805.329   805.525
   808.722   809.126   809.617   810.884   811.015   812.489   817.719   818.261   821.033   822.411
   825.987   826.565   841.037   841.273   873.715   874.235   882.469   892.614   893.904   895.180
   895.604   903.179   904.629   914.030   914.686   921.664   932.266   932.403   938.091   938.111
   941.765   941.845   956.136   971.156   972.489   987.122   992.381  1001.938  1001.945  1002.223
  1002.227  1018.476  1018.478  1056.256  1064.243  1064.886  1066.632  1067.004  1070.394  1104.148
  1106.030  1108.416  1111.042  1112.947  1128.135  1153.056  1155.351  1167.743  1172.090  1188.063
  1191.940  1201.170  1203.729  1204.849  1206.124  1206.682  1222.410  1223.216  1224.280  1226.126
  1227.811  1244.016  1247.404  1248.829  1250.028  1250.388  1254.668  1257.228  1261.123  1277.185
  1307.344  1308.678  1308.732  1310.041  1316.983  1319.212  1320.903  1326.348  1327.661  1332.104
  1333.509  1353.780  1354.659  1363.784  1369.326  1380.343  1381.074  1383.233  1383.907  1390.434
  1392.445  1402.603  1403.412  1410.799  1411.511  1411.605  1412.514  1415.090  1416.351  1426.755
  1427.544  1427.861  1433.322  1438.293  1438.615  1440.474  1440.712  1441.236  1441.891  1445.186
  1446.328  1451.489  1455.079  1455.896  1456.628  1457.765  1458.425  1461.520  1473.101  1476.121
  1478.526  1480.576  1489.119  1491.788  1499.886  1500.926  1508.038  1510.314  1512.157  1516.204
  1516.758  1519.126  1527.718  1528.263  1531.343  1537.207  1541.728  1541.758  1558.461  1558.799
  1561.189  1563.408  1568.916  1570.912  1582.840  1591.726  1610.621  1623.303  1629.398  1629.603
  1639.111  1645.779  1645.809  1647.815  1648.219  1659.457  1661.782  1667.075  1668.171  1668.662
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 1673.399  1680.295  1682.096  1685.009  1692.522  1698.597  1701.198  1706.926  1708.569  1710.730
 3122.559  3122.559  3126.069  3126.072  3126.901  3126.920  3141.825  3141.829  3166.474  3166.477
 3169.724  3169.738  3172.811  3172.820  3188.165  3188.180  3207.709  3207.713  3210.334  3210.343
 3215.906  3215.922  3241.339  3241.352

Complex R:P
Atom    X         Y         X   (Angstrom)
 6   6.57199   3.80739   1.46619
 6   7.87112   3.37253   1.30377
 6   8.16341   1.99496   1.25703
 6   7.10075   1.06629   1.40017
 6   5.76177   1.52864   1.56720
 6   5.50710   2.90663   1.59671
 6   4.68813   0.57396   1.67310
 6   4.96844  -0.80718   1.63124
 6   6.30807  -1.26889   1.45853
 6   7.37152  -0.33316   1.32150
 6   9.48496   1.50721   1.01356
 6   9.73265   0.17094   0.90743
 6   8.68740  -0.78544   1.05954
 6   4.10682   3.44242   1.75119
 6   3.02080   2.40010   1.82612
 6   3.32821   1.03009   1.79529
 6   2.27394   0.07527   1.88093
 6   2.56454  -1.32231   1.84603
 6   3.91060  -1.76197   1.72143
 6   4.19564  -3.15449   1.65314
 6   5.51947  -3.57886   1.47447
 6   6.57477  -2.66389   1.36742
 6   7.91524  -3.08785   1.10121
 6   8.92581  -2.18641   0.94604
 6   0.57413  -4.54821  -1.02621
 6   0.25913  -3.15551  -1.03312
 6  -1.08404  -2.72974  -0.84061
 6  -2.11324  -3.69044  -0.62849
 6  -1.79836  -5.08344  -0.62505
 6  -0.45536  -5.50751  -0.82165
 6  -1.39171  -1.35015  -0.81521
 6  -2.72431  -0.92441  -0.56228
 6  -3.74757  -1.87926  -0.36039
 6  -3.43920  -3.26764  -0.39725
 6  -3.02501   0.46449  -0.48168
 6  -4.34700   0.88853  -0.21508
 6  -5.37809  -0.07446  -0.02924
 6  -5.07901  -1.45077  -0.09797
 6  -6.71269   0.35436   0.24198
 6  -7.00979   1.74214   0.32514
 6  -5.97922   2.70474   0.14586
 6  -4.64371   2.27710  -0.12337
 6  -3.61773   3.23040  -0.28864
 6  -3.91500   4.62361  -0.18886
 6  -5.23804   5.04499   0.07115
 6  -6.27183   4.08341   0.23989
 6  -7.61689   4.50469   0.51189
 6  -8.60981   3.55813   0.68188
 6  -8.34226   2.16959   0.59791
 6  -2.28512   2.80489  -0.54847
 6  -1.99033   1.42605  -0.65225
 6  -6.11041  -2.41642   0.10827
 6  -7.43197  -1.99019   0.36892
 6  -7.73404  -0.60251   0.43447
 6  -9.07356  -0.16300   0.70640
 6  -9.34896   1.18927   0.78021
 6  -0.35615  -0.38824  -0.97649
 6  -0.65690   0.99925  -0.90384
 6   0.37717   1.95457  -1.02924
 6   0.07735   3.34282  -0.93531
 6  -1.24591   3.76629  -0.69848
 6  -1.54442   5.15886  -0.59404
 6  -2.87832   5.58347  -0.34581
 6  -5.80297  -3.80361   0.06458
 6  -4.46933  -4.23205  -0.17889
 6   1.28824  -2.20103  -1.17571
 6   0.98115  -0.81218  -1.14255
 6   2.02407   0.15079  -1.23948
 6   1.72185   1.52721  -1.19340
 6   2.77046   2.49201  -1.28654
 6   2.46498   3.87907  -1.24085
 6   1.12355   4.30699  -1.05109
 6   0.82507   5.68564  -0.95937
 6  -0.51158   6.11244  -0.73390
 6  -4.15833  -5.61008  -0.19244
 6  -2.81968  -6.03610  -0.40941
 6   1.91365  -4.96910  -1.18104
 6   2.94999  -4.00630  -1.32640
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6   2.64214  -2.62702  -1.31251
6   3.68359  -1.66413  -1.39854
6   3.37945  -0.27706  -1.35766
6   4.41733   0.67833  -1.43639
6   4.11141   2.06692  -1.40789
6   2.22621  -6.36842  -1.12858
6   1.21216  -7.29220  -0.94750
6  -0.13769  -6.89784  -0.79068
6  -1.18313  -7.83242  -0.58532
6  -2.49290  -7.43422  -0.40017
6  -3.56840  -8.38113  -0.18341
6  -4.84042  -7.97688   0.01543
6  -5.20031  -6.57326   0.02760
6  -6.49468  -6.14302   0.24884
6  -6.83157  -4.76711   0.27854
6  -8.15075  -4.31321   0.52427
6  -8.46282  -2.96776   0.57477
6  -9.80611  -2.49172   0.83766
6 -10.09292  -1.17452   0.89977
6   3.61671  -6.75859  -1.24252
6   4.59914  -5.84230  -1.38240
6   4.31675  -4.42373  -1.42789
6   5.32027  -3.47437  -1.50097
6   5.04001  -2.08821  -1.49384
6   6.06441  -1.11049  -1.53761
6   5.78010   0.24193  -1.53116
1  -8.93652  -5.05133   0.68346
1   1.45537  -8.35407  -0.91226
1  -0.93988  -8.89479  -0.56977
1  -3.32024  -9.44142  -0.18374
1  -5.63190  -8.70677   0.17664
1  -7.28149  -6.87894   0.41312
6   6.81758   1.25152  -1.59198
1   7.10461  -1.44039  -1.55822
1   3.85176  -7.82124  -1.20772
1   5.63918  -6.15717  -1.46022
1   6.36219  -3.79427  -1.54340
1 -10.58749  -3.23475   0.98820
1 -11.10933  -0.83992   1.10159
6  -7.87753   5.92755   0.60089
1  -9.62905   3.88332   0.89038
1 -10.36737   1.51697   0.98893
1  10.29099   2.23054   0.90149
1  10.74132  -0.18991   0.71021
1   9.94017  -2.52547   0.73947
1   8.11120  -4.15650   1.02210
1   5.72497  -4.64617   1.38753
6   1.68582   2.80886   1.91729
1   3.89355   4.11375   0.90358
1   8.68294   4.09035   1.19660
1   6.35569   4.87563   1.48511
6   0.65670   1.88977   1.98127
1   1.45926   3.87531   1.90966
1  -0.37976   2.22676   2.01608
6   0.92687   0.50789   1.97867
6  -0.11440  -0.47148   2.04284
6   0.16907  -1.80357   2.02958
1  -1.14799  -0.12621   2.08137
1  -0.63401  -2.53913   2.06775
6   1.51306  -2.26722   1.92653
6   1.82345  -3.65554   1.86112
6   3.11001  -4.08269   1.71770
1   1.00427  -4.37324   1.89335
1   3.33161  -5.14571   1.62132
6  -6.89678   6.84003   0.43914
1  -8.89877   6.24500   0.80618
1  -7.11481   7.90430   0.51093
6  -5.52836   6.44745   0.16862
6  -4.51129   7.36968   0.00863
6  -3.17556   6.97402  -0.24656
1  -4.73646   8.43345   0.08326
6  -2.12311   7.90972  -0.40192
6  -0.82124   7.51125  -0.63661
1  -2.35175   8.97288  -0.32925
6   0.26482   8.45843  -0.78818
6   1.53443   8.05342  -1.00077
1   0.02766   9.51924  -0.72491
1   2.33457   8.78333  -1.11121
6   1.88167   6.64913  -1.08939
6   3.18010   6.21915  -1.28558
6   3.51115   4.84272  -1.35736
1   3.97793   6.95542  -1.38220
6   4.84507   4.38861  -1.49890
6   5.15935   3.04206  -1.51549
1   5.64523   5.12475  -1.57783
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6	6.52424	2.56804	-1.60646
1	7.85453	0.91509	-1.60573
1	7.31912	3.31031	-1.64799
1	4.06359	4.06618	2.66037

Energy -4874.677948 (Hartree)

Frequencies cm-1:

10.393	20.353	23.898	27.149	39.018	44.106	47.318	56.315	63.377	74.890
75.249	80.819	90.890	102.649	120.019	127.142	130.392	136.350	136.984	147.277
165.617	169.137	177.821	184.173	186.143	190.079	195.027	195.946	200.429	204.205
209.856	210.349	216.949	218.245	221.539	223.352	237.384	245.015	253.982	254.450
258.008	258.611	271.054	271.859	276.561	283.733	290.251	296.681	297.631	300.015
300.804	303.147	308.760	315.775	318.203	319.012	321.086	323.015	327.328	330.135
343.586	346.252	356.016	362.435	364.982	368.111	368.730	375.189	383.970	388.310
388.869	395.581	397.668	400.248	409.274	409.375	409.790	413.126	413.368	420.861
422.043	427.727	428.457	430.224	430.920	434.621	443.237	443.966	447.378	449.700
452.372	453.925	456.794	457.829	478.341	480.677	484.285	488.109	492.461	503.870
504.329	507.175	507.954	517.021	517.381	518.583	528.478	529.605	531.653	534.763
539.230	545.137	546.095	554.835	556.429	556.846	557.468	558.904	560.293	564.168
566.670	567.991	570.511	571.856	572.888	575.998	585.816	589.530	591.023	593.404
593.793	595.324	599.274	600.516	603.678	606.401	610.152	612.377	612.640	612.791
613.060	615.045	621.385	622.387	629.092	631.087	637.611	637.995	638.116	645.064
645.588	650.951	651.131	653.756	659.118	660.563	661.327	668.130	668.507	669.832
670.337	671.331	678.553	678.775	682.599	686.149	687.822	691.418	698.118	700.639
705.941	713.810	715.098	716.990	718.097	718.305	718.336	721.100	726.252	729.405
730.281	739.948	748.295	752.693	753.120	753.986	756.606	757.417	757.933	762.047
769.952	775.905	776.438	780.052	782.577	782.974	783.990	786.483	786.960	788.937
791.251	795.649	795.870	799.471	801.916	802.814	804.514	805.780	807.068	809.626
809.880	810.307	810.595	813.342	815.004	817.859	818.069	820.959	821.880	828.610
830.312	840.175	840.408	843.767	857.245	870.496	872.213	874.990	879.862	881.162
881.305	883.813	894.311	894.788	895.420	900.917	903.168	905.845	908.348	913.648
918.834	920.534	920.998	924.108	933.743	935.210	937.573	937.778	938.439	940.975
956.563	970.981	971.398	976.057	982.081	983.166	985.933	989.026	992.535	992.606
993.972	995.374	999.659	1001.018	1001.372	1007.126	1011.681	1019.578	1055.897	1056.660
1063.976	1064.981	1066.357	1067.111	1070.661	1077.388	1093.810	1104.357	1105.436	1108.872
1110.626	1111.278	1127.562	1135.549	1152.853	1154.277	1165.934	1166.151	1171.285	1173.316
1179.675	1184.860	1185.954	1189.021	1190.657	1199.377	1201.853	1203.277	1203.682	1206.389
1206.976	1210.343	1215.493	1220.612	1221.192	1222.429	1225.623	1226.620	1230.703	1240.929
1243.856	1245.366	1247.157	1249.175	1250.197	1254.017	1254.515	1256.060	1259.674	1262.559
1266.459	1268.387	1275.415	1292.140	1303.518	1305.509	1307.221	1308.097	1308.938	1310.791
1314.086	1319.268	1319.621	1323.855	1326.704	1331.355	1332.621	1336.184	1344.119	1352.272
1354.163	1362.578	1368.359	1373.357	1376.609	1378.436	1379.191	1380.503	1381.582	1389.267
1390.145	1390.559	1398.586	1400.398	1401.217	1408.488	1409.112	1409.973	1411.725	1411.852
1414.428	1416.892	1423.911	1425.144	1425.958	1426.569	1432.983	1436.282	1436.766	1437.321
1438.045	1439.466	1439.833	1440.694	1443.775	1444.610	1448.880	1450.534	1453.091	1453.828
1454.993	1455.788	1456.982	1457.337	1459.131	1461.761	1468.034	1471.770	1472.496	1473.913
1478.525	1478.757	1482.154	1487.770	1489.089	1490.648	1497.812	1499.614	1508.514	1509.357
1510.138	1512.636	1514.769	1515.682	1518.459	1526.200	1528.376	1528.741	1532.229	1535.617
1539.120	1539.986	1551.777	1555.687	1557.211	1558.022	1560.570	1561.665	1565.982	1566.952
1568.428	1575.726	1582.390	1589.628	1602.009	1607.527	1617.451	1621.753	1626.113	1627.381
1637.992	1640.822	1644.001	1644.647	1645.568	1645.809	1647.420	1657.610	1659.437	1662.174
1663.649	1665.586	1666.571	1669.323	1671.940	1677.007	1679.457	1682.842	1683.830	1689.862
1693.916	1699.587	1701.253	1706.671	1708.689	1711.473	3054.200	3083.001	3140.508	3143.685
3145.949	3146.708	3149.386	3150.543	3151.298	3152.664	3153.121	3154.184	3154.725	3157.492
3157.504	3162.214	3162.567	3166.037	3167.580	3171.325	3175.915	3176.437	3180.692	3183.572
3185.475	3189.516	3191.333	3193.789	3195.271	3196.059	3196.281	3201.313	3204.088	3208.120
3210.084	3212.206	3220.363	3233.530	3247.088					

Syn addition TS

Atom	X	Y	X (Angstrom)
6	0.74361	8.60137	-0.53468
6	-0.33843	7.63902	-0.46675
6	-0.01926	6.25097	-0.66328
6	1.31990	5.84837	-0.90340
6	2.37541	6.82606	-0.93831
6	2.01800	8.21923	-0.75477
6	3.67775	6.41850	-1.13198
6	4.02048	5.04816	-1.28655
6	2.97742	4.07402	-1.27107
6	1.62851	4.48150	-1.08813
6	5.35592	4.61889	-1.41253
6	5.68582	3.27253	-1.48766
6	4.64584	2.29034	-1.44765
6	3.29640	2.69595	-1.35562
6	2.25562	1.71514	-1.30943
6	2.57672	0.34091	-1.34495
6	3.94152	-0.06578	-1.38801
6	4.97208	0.90552	-1.44369
6	1.54911	-0.63725	-1.26857
6	1.88185	-2.02357	-1.25559
6	3.23717	-2.42144	-1.23628
6	4.26896	-1.43743	-1.28213
6	5.62932	-1.82750	-1.16852
6	5.90663	-3.17935	-0.72507
6	4.92778	-4.19486	-1.00455
6	3.57503	-3.80596	-1.16258

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6   2.54558  -4.78335  -1.16808
6   2.87927  -6.17423  -1.09073
6   4.26049  -6.53437  -1.03134
6   5.23687  -5.57827  -0.96216
6   1.18604  -4.38419  -1.16105
6   0.85202  -2.99872  -1.18434
6   6.33092   0.49032  -1.44827
6   6.62962  -0.86720  -1.29783
6   0.90436   2.12072  -1.16738
6  -0.12176   1.14794  -1.08343
6   0.19903  -0.23521  -1.15473
6  -0.82984  -1.21378  -1.05317
6  -0.50265  -2.59280  -1.08578
6   7.35693   1.49758  -1.52955
6   7.05145   2.81625  -1.55596
6   0.58992   3.50407  -1.03320
6  -1.04864   5.28370  -0.59879
6  -0.74109   3.90350  -0.78918
6  -1.77401   2.92486  -0.69542
6  -1.46601   1.55275  -0.85649
6  -2.49302   0.57446  -0.73999
6  -2.17591  -0.80837  -0.85576
6  -2.38666   5.68381  -0.32891
6  -3.41656   4.70963  -0.23457
6  -3.10908   3.32595  -0.41503
6  -4.12804   2.35621  -0.29748
6  -3.81983   0.97637  -0.45667
6  -4.84251  -0.00262  -0.30264
6  -4.52873  -1.37384  -0.41704
6  -3.19173  -1.78027  -0.68646
6  -2.86478  -3.16481  -0.73405
6  -1.52837  -3.56997  -0.94152
6  -1.19512  -4.95728  -0.93122
6   0.16198  -5.35916  -1.04417
6   1.85626  -7.12238  -1.01389
6   0.50275  -6.74720  -0.97138
6  -0.54121  -7.69916  -0.81798
6  -1.86111  -7.32002  -0.69629
6  -2.20836  -5.92499  -0.73313
6  -3.55468  -5.51958  -0.54500
6  -3.88471  -4.14426  -0.53377
6  -5.22601  -3.73698  -0.29713
6  -5.54993  -2.35519  -0.23110
6  -6.24380  -4.71623  -0.09873
6  -5.88935  -6.08740  -0.13659
6  -4.58745  -6.49823  -0.34176
6  -4.21029  -7.89697  -0.34699
6  -2.92797  -8.28289  -0.50991
6  -5.46603   2.75993  -0.00075
6  -6.48819   1.78236   0.13661
6  -6.17931   0.40239  -0.00856
6  -7.19201  -0.57024   0.15441
6  -6.87650  -1.95092   0.04380
6  -7.89597  -2.94408   0.22874
6  -7.56792  -4.28446   0.15025
6  -4.74195   5.10646   0.05318
6  -5.76889   4.12949   0.16934
6  -7.11442   4.52602   0.47088
6  -8.10045   3.56446   0.59393
6  -7.82275   2.18569   0.43772
6  -8.82103   1.19077   0.58180
6  -8.53399  -0.15427   0.45052
6  -9.54326  -1.18046   0.61297
6  -9.24318  -2.49206   0.50862
6  -1.64242   8.01308  -0.21698
6  -2.69208   7.06270  -0.13544
6  -4.02797   7.43385   0.14175
6  -5.04081   6.49685   0.23919
6  -6.40973   6.86493   0.53515
6  -7.38479   5.93825   0.64359
6   5.77238  -2.94028   1.34818
6   4.41889  -3.34452   1.68730
6   3.40295  -2.37323   1.78310
6   3.72661  -0.96629   1.75161
6   5.11569  -0.57692   1.67537
6   6.13187  -1.55244   1.57562
6   2.04869  -2.77720   1.89773
6   1.72006  -4.15730   1.92544
6   2.76165  -5.10475   1.90820
6   4.07569  -4.70555   1.80344
6   2.72490  -0.01014   1.83871
6   1.33464  -0.41006   1.93269
6   1.01017  -1.79379   1.94597
6  -0.34537  -2.20609   2.00909
6  -0.64763  -3.61057   1.99052
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  6   0.33773  -4.54227   1.95475
  6   3.05994   1.40024   1.82252
  6   4.42212   1.79007   1.74940
  6   5.45518   0.79819   1.70532
  6   6.81682   1.19536   1.67281
  6   7.81248   0.20365   1.62835
  6   7.47478  -1.13293   1.56452
  6  -1.34956  -1.22764   2.06688
  6  -1.02207   0.11586   2.07624
  6   0.30851   0.54022   2.00973
  6   0.60833   2.01647   2.05552
  6   2.06034   2.38474   1.88233
  6   2.41713   3.73256   1.82413
  6   3.74342   4.12201   1.73720
  6   4.76684   3.16643   1.71826
  6   6.15668   3.53579   1.67277
  6   7.13316   2.59746   1.66651
  1  -8.34436  -5.03498   0.29675
  1   2.11374  -8.17993  -0.95540
  1  -0.28145  -8.75714  -0.77954
  1  -2.66342  -9.33926  -0.50092
  1  -4.99610  -8.63683  -0.20493
  1  -6.66815  -6.83428   0.01583
  1   7.67328  -1.17444  -1.24247
  1   4.52064  -7.59142  -1.00324
  1   6.28165  -5.87457  -0.86805
  1   6.95464  -3.48658  -0.75591
  1 -10.01565  -3.24784   0.64059
  1 -10.56181  -0.86275   0.83032
  1  -9.12069   3.86993   0.82571
  1  -9.84053   1.50014   0.81148
  1   6.40287   4.59657   1.64586
  1   8.18296   2.88671   1.63403
  1   8.85914   0.50602   1.62091
  1   8.25756  -1.88899   1.49470
  1   6.55044  -3.67823   1.55642
  1   0.00505   2.53764   1.29669
  1   3.99713   5.17965   1.67731
  1   1.63089   4.48823   1.84253
  1  -1.81272   0.86590   2.11907
  1  -2.39396  -1.53768   2.09427
  1  -1.69547  -3.91221   1.99390
  1   0.09535  -5.60452   1.92746
  1   2.51189  -6.16389   1.95042
  1   4.86725  -5.45114   1.76786
  1  -8.40759   6.23532   0.87035
  1  -6.63309   7.92160   0.67240
  1  -4.25868   8.48881   0.28823
  1  -1.87737   9.06679  -0.06825
  1   0.49860   9.65313  -0.39656
  1   2.81689   8.95798  -0.79902
  1   4.47469   7.16234  -1.15596
  1   6.15091   5.36518  -1.42972
  1   8.39540   1.16928  -1.54589
  1   7.83963   3.56676  -1.59964
  1   0.27381   2.40272   3.03355
Energy      -4874.661507          (Hartree)
Frequencies cm-1:
  -513.400    18.033    21.303    27.840    33.673    41.242    47.002    57.869    66.523    72.512
    76.773    86.402    93.389   117.804   120.644   124.193   129.006   132.857   135.052   142.523
   154.740   161.824   170.786   174.970   176.719   187.784   193.809   194.294   196.645   198.058
   208.936   211.127   213.261   216.450   218.869   226.038   228.638   240.860   247.458   250.422
   253.249   257.147   270.869   276.369   280.798   284.997   290.855   296.960   298.961   301.325
   302.572   304.763   311.813   313.697   318.153   319.019   320.154   325.366   327.393   329.400
   345.575   349.851   357.674   359.367   367.629   368.201   372.900   375.163   381.215   385.784
   395.149   395.913   403.015   403.911   409.072   409.482   411.229   412.385   414.665   420.527
   422.785   423.958   427.305   429.575   432.035   434.871   442.344   444.615   447.939   448.210
   452.036   452.327   453.044   458.393   479.164   483.324   484.081   495.881   496.865   504.092
   505.073   506.589   506.870   508.955   516.909   517.379   522.384   525.698   535.635   539.443
   540.664   545.350   546.646   550.369   555.061   556.380   557.082   557.184   559.911   566.067
   566.698   568.509   570.665   572.828   573.098   575.076   583.741   587.153   591.275   593.009
   595.066   596.103   597.532   598.596   601.641   603.759   609.146   610.519   611.598   613.095
   614.167   615.562   617.898   619.454   628.173   632.908   636.891   637.202   638.308   645.680
   649.480   651.070   651.875   655.920   657.124   658.283   662.790   664.115   666.065   668.356
   669.837   672.550   678.613   678.960   680.676   683.145   684.187   691.626   693.436   695.205
   699.098   708.706   710.343   714.400   717.643   717.921   718.791   721.550   722.836   723.204
   724.532   730.082   742.115   744.238   746.965   749.573   751.021   757.534   758.229   761.384
   762.749   771.652   776.117   777.596   780.438   781.306   784.498   784.983   785.317   788.746
   789.228   792.548   795.376   798.937   799.489   800.758   803.985   804.389   806.475   809.070
   809.287   809.636   810.625   816.512   817.720   819.190   821.069   821.786   823.228   831.216
   833.992   839.914   840.369   841.349   859.990   865.420   867.834   871.570   875.154   878.062
   879.472   883.825   889.116   895.369   897.997   899.912   908.052   908.749   910.529   913.507
   919.419   921.867   922.783   926.964   928.228   932.964   938.350   946.894   949.282   958.576
   963.433   966.349   970.036   972.167   974.718   975.835   981.635   986.248   988.984   993.060
   995.965   996.657  1004.600  1008.815  1009.052  1015.916  1021.738  1037.198  1056.678  1059.272
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1065.029	1065.257	1066.837	1068.987	1073.172	1073.717	1090.919	1103.969	1104.989	1108.255
1110.543	1113.055	1127.861	1141.975	1152.776	1155.014	1163.373	1169.426	1172.507	1178.630
1178.807	1180.071	1183.733	1188.367	1195.038	1197.253	1199.763	1201.286	1202.227	1205.065
1205.484	1210.823	1218.678	1219.839	1221.167	1223.969	1225.607	1226.639	1230.187	1240.078
1240.951	1241.985	1247.027	1249.850	1251.281	1251.684	1252.348	1254.051	1257.089	1258.416
1261.276	1267.006	1270.916	1271.510	1282.251	1302.421	1305.288	1305.964	1307.509	1308.252
1314.296	1317.866	1322.197	1323.888	1325.040	1328.803	1331.449	1336.494	1339.502	1346.759
1348.214	1352.940	1356.940	1361.395	1366.093	1372.884	1375.729	1377.482	1378.215	1386.502
1390.043	1390.306	1393.408	1398.018	1399.594	1402.913	1404.745	1405.976	1407.882	1409.761
1410.494	1413.035	1417.649	1423.466	1424.452	1426.963	1427.574	1428.050	1432.760	1433.964
1435.480	1437.181	1438.950	1440.129	1443.905	1444.685	1447.044	1449.963	1451.435	1452.599
1454.250	1456.340	1456.961	1459.108	1462.797	1465.483	1467.532	1469.569	1471.396	1474.256
1475.132	1476.920	1477.977	1481.499	1483.983	1488.072	1494.926	1497.065	1504.093	1506.099
1508.258	1512.465	1512.790	1518.121	1522.425	1526.357	1528.872	1531.987	1534.197	1535.381
1538.158	1544.641	1551.049	1552.540	1555.842	1558.758	1562.543	1563.923	1567.400	1569.209
1577.533	1579.881	1586.334	1589.759	1595.479	1605.457	1615.676	1621.216	1621.818	1626.676
1628.376	1631.005	1636.787	1637.391	1640.771	1644.675	1646.886	1647.223	1653.981	1655.548
1658.824	1660.308	1665.008	1667.206	1669.318	1673.558	1677.883	1678.992	1682.210	1690.952
1697.803	1698.462	1703.603	1704.328	1708.312	1711.140	3042.360	3085.759	3123.979	3127.451
3132.700	3136.851	3147.940	3148.439	3154.366	3155.910	3157.131	3158.867	3167.584	3168.114
3168.982	3169.069	3171.675	3172.100	3173.363	3179.327	3183.348	3183.841	3194.505	3199.078
3199.947	3199.956	3200.120	3203.701	3206.758	3214.279	3218.475	3218.753	3221.307	3226.425
3230.719	3234.063	3241.834	3243.995	3259.330					

Syn adduct R:P

Atom	X	Y	X (Angstrom)
6	4.13582	-4.69439	1.78060
6	4.45614	-3.34236	1.62209
6	3.44711	-2.38165	1.75885
6	2.09760	-2.79283	1.90682
6	1.77828	-4.17463	1.94472
6	2.82426	-5.10929	1.92495
6	3.75964	-0.96507	1.72453
6	5.15363	-0.56581	1.66601
6	6.17657	-1.52235	1.54397
6	5.82530	-2.93072	1.14721
6	1.05181	-1.81536	1.95748
6	1.36639	-0.42992	1.93331
6	2.75751	-0.02134	1.82829
6	3.08024	1.39546	1.81850
6	4.43889	1.79596	1.75414
6	5.48071	0.81117	1.72026
6	6.84055	1.21879	1.70409
6	7.83930	0.23814	1.67306
6	7.50704	-1.10591	1.58603
6	7.14553	2.62730	1.69524
6	6.16244	3.55584	1.68757
6	4.77338	3.17513	1.72284
6	3.74336	4.12180	1.73616
6	2.41988	3.72156	1.82191
6	2.07322	2.37103	1.87922
6	0.62352	1.99295	2.05676
6	0.33572	0.51324	2.01349
6	-0.30099	-2.23666	2.02633
6	-1.31080	-1.26567	2.08260
6	-0.99172	0.08005	2.08715
6	-0.59485	-3.64515	2.01270
6	0.39481	-4.56903	1.97958
6	5.93651	-3.05107	-0.51649
6	4.97387	-4.10588	-0.97612
6	3.62568	-3.73202	-1.15460
6	3.26211	-2.34643	-1.21090
6	4.28189	-1.34227	-1.25406
6	5.64133	-1.70215	-1.10804
6	3.93204	0.01750	-1.39053
6	2.56074	0.40228	-1.34808
6	1.55160	-0.59034	-1.26450
6	1.90887	-1.97318	-1.24642
6	4.94808	1.00441	-1.45739
6	4.59971	2.38671	-1.46140
6	3.24548	2.77049	-1.36046
6	2.21866	1.77246	-1.31236
6	5.62362	3.38143	-1.50411
6	6.99397	2.94513	-1.58020
6	7.31810	1.62913	-1.55769
6	6.30737	0.61091	-1.46904
6	6.62362	-0.74879	-1.28586
6	2.90528	4.14178	-1.27192
6	3.93327	5.13285	-1.29168
6	5.27267	4.72551	-1.42215
6	1.55017	4.52739	-1.08293
6	0.52797	3.53378	-1.02523
6	0.86454	2.15509	-1.16439
6	-0.14669	1.16469	-1.07849
6	0.19562	-0.21098	-1.15071

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6  -2.50727   0.55335  -0.72829
6  -2.16817  -0.82455  -0.84657
6  -0.81826  -1.20768  -1.04581
6  -0.46965  -2.58217  -1.08212
6   0.89075  -2.96795  -1.18318
6   2.61280  -4.72257  -1.19204
6   1.24432  -4.34405  -1.17572
6   0.23572  -5.33680  -1.06613
6  -1.12427  -4.95675  -0.94142
6  -1.47850  -3.57481  -0.94010
6  -2.82164  -3.19102  -0.72928
6  -3.16911  -1.81363  -0.67707
6  -3.82657  -4.18736  -0.53351
6  -3.47578  -5.55796  -0.55499
6  -2.12434  -5.94229  -0.75015
6  -1.75751  -7.33145  -0.73054
6  -0.43213  -7.69087  -0.86752
6   0.59795  -6.72277  -1.01733
6   1.95305  -7.07793  -1.08273
6   2.96930  -6.10811  -1.14790
6   5.31294  -5.46318  -1.00276
6   4.34613  -6.44459  -1.11117
6  -3.84024   0.93362  -0.44393
6  -4.84796  -0.06251  -0.29049
6  -4.51276  -1.42843  -0.40660
6  -5.51808  -2.42555  -0.22321
6  -5.17289  -3.80213  -0.29448
6  -6.17618  -4.79805  -0.10070
6  -5.80182  -6.16227  -0.14722
6  -4.49324  -6.55276  -0.35755
6  -4.09610  -7.94501  -0.37490
6  -2.80855  -8.31103  -0.54728
6  -3.16636   3.29370  -0.40244
6  -4.17020   2.30703  -0.28451
6  -5.51485   2.68924   0.01242
6  -6.52096   1.69576   0.14965
6  -6.19013   0.32071   0.00368
6  -7.18779  -0.66841   0.16534
6  -6.85109  -2.04265   0.05240
6  -7.85557  -3.05268   0.23427
6  -7.50731  -4.38697   0.15072
6  -1.13843   5.28505  -0.58925
6  -2.48308   5.66332  -0.31852
6  -3.49644   4.67270  -0.22252
6  -4.82813   5.04790   0.06501
6  -5.83975   4.05380   0.18211
6  -7.19053   4.42871   0.48338
6  -8.16163   3.45045   0.60684
6  -7.86186   2.07766   0.45075
6  -8.84480   1.06597   0.59412
6  -8.53681  -0.27351   0.46170
6  -9.53008  -1.31574   0.62240
6  -9.20968  -2.62224   0.51543
6  -5.14977   6.43234   0.24978
6  -6.52385   6.77837   0.54602
6  -7.48398   5.83584   0.65535
6  -4.15161   7.38657   0.15057
6  -2.81125   7.03728  -0.12696
6   1.21912   5.88922  -0.89921
6  -0.12485   6.26933  -0.65716
6  -0.46760   7.65312  -0.46276
6  -1.77624   8.00554  -0.21197
6   3.56686   6.49916  -1.13602
6   2.25975   6.88489  -0.93931
6   1.87858   8.27266  -0.75763
6   0.59872   8.63356  -0.53532
1  -8.27240  -5.14961   0.29431
1   2.22772  -8.13219  -1.04829
1  -0.15780  -8.74566  -0.84393
1  -2.52888  -9.36358  -0.54797
1  -4.87042  -8.69736  -0.23514
1  -6.56916  -6.92166   0.00136
1   7.67166  -1.03301  -1.19966
1   4.62960  -7.49607  -1.11467
1   6.35967  -5.74788  -0.89524
1   6.97636  -3.33898  -0.72050
1  -9.97058  -3.38989   0.64593
1 -10.55356  -1.01476   0.84062
1  -9.18675   3.73963   0.83841
1  -9.86926   1.35888   0.82373
1   6.39927   4.61866   1.65667
1   8.19332   2.92474   1.67182
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1	8.88479	0.54435	1.68813
1	8.29687	-1.85386	1.50646
1	6.57439	-3.64011	1.52399
1	0.01319	2.50929	1.30011
1	3.98868	5.18141	1.67591
1	1.62779	4.47107	1.84123
1	-1.78700	0.82512	2.13185
1	-2.35313	-1.58237	2.11310
1	-1.64110	-3.95239	2.01719
1	0.16018	-5.63311	1.95516
1	2.58936	-6.17102	1.98328
1	4.92919	-5.43687	1.71927
1	-8.51147	6.11640	0.88218
1	-6.76433	7.83130	0.68299
1	-4.39987	8.43767	0.29625
1	-2.02873	9.05545	-0.06481
1	0.33617	9.68135	-0.39915
1	2.66458	9.02490	-0.80587
1	4.35119	7.25624	-1.16374
1	6.05647	5.48358	-1.44116
1	8.36141	1.31652	-1.57558
1	7.77204	3.70593	-1.62522
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Energy -4874.670467 (Hartree)

Frequencies cm-1:

18.012	20.642	25.057	31.902	39.266	47.738	55.358	66.690	71.193	76.681
86.005	96.737	111.316	119.217	120.549	129.496	131.872	135.493	142.848	147.128
159.750	168.423	171.315	173.989	186.487	192.521	194.058	195.417	197.300	206.595
210.903	212.530	216.375	217.601	224.498	230.732	240.300	245.238	250.016	253.357
257.724	270.746	274.544	279.324	284.708	291.039	296.899	298.382	301.997	304.755
306.005	312.216	313.366	316.501	319.557	320.012	324.283	325.357	330.614	345.102
351.491	358.103	359.889	366.214	367.245	372.460	378.973	381.659	387.945	395.248
399.551	404.169	404.886	408.541	409.288	411.099	411.560	414.190	419.156	421.351
422.667	426.707	429.760	433.900	436.420	442.122	444.416	448.022	448.283	450.943
452.419	454.770	458.151	481.413	482.790	485.642	495.388	497.482	500.600	504.117
505.215	507.246	510.778	515.422	517.299	519.562	524.615	536.542	538.403	540.802
543.657	546.270	549.940	553.971	555.711	556.131	556.937	559.313	565.317	565.650
567.188	568.590	570.038	571.307	573.256	582.367	585.602	589.872	591.010	594.471
596.597	598.068	599.130	601.305	603.091	606.610	609.173	611.080	613.061	614.625
617.906	618.601	621.331	626.945	630.744	634.864	636.828	638.406	639.560	650.245
650.645	651.586	654.751	658.008	659.590	662.852	663.972	666.815	668.446	670.500
674.072	675.495	678.614	680.778	683.122	686.224	691.750	694.203	695.614	699.038
703.778	709.073	710.676	714.946	716.032	717.541	719.226	720.982	723.787	725.611
726.433	732.433	740.896	747.043	748.750	751.012	757.264	757.543	758.776	764.759
770.952	773.770	775.593	777.482	781.171	782.971	784.507	785.440	787.719	789.649
790.634	791.656	794.153	799.173	800.231	802.980	804.012	804.800	806.779	809.466
810.176	811.126	812.676	817.766	819.345	822.972	823.403	825.240	826.941	834.309
835.513	839.738	841.079	845.194	859.991	865.846	868.728	874.621	877.298	879.648
882.849	891.681	892.425	895.263	898.650	900.718	906.893	911.232	911.963	916.323
916.826	922.799	924.862	930.782	931.274	935.372	938.060	949.293	956.010	957.832
962.630	968.291	969.184	971.561	972.375	974.371	983.030	988.470	989.498	992.684
994.157	1004.914	1006.066	1007.964	1018.057	1023.168	1033.847	1051.025	1057.826	1061.778
1065.836	1066.537	1069.488	1072.855	1085.597	1094.311	1098.129	1101.655	1106.921	1109.214
1121.367	1135.561	1149.162	1150.569	1156.257	1161.704	1163.592	1169.478	1176.170	1178.691
1179.966	1185.800	1188.283	1194.841	1196.102	1197.956	1200.001	1200.165	1203.899	1205.305
1206.943	1215.206	1219.037	1221.155	1223.108	1225.637	1229.941	1231.769	1232.812	1236.571
1239.060	1244.583	1247.518	1248.471	1250.461	1251.525	1253.572	1255.684	1257.163	1259.919
1262.363	1267.595	1268.461	1269.624	1281.039	1292.931	1300.122	1305.654	1307.026	1309.837
1311.694	1312.408	1317.284	1318.703	1325.034	1325.749	1329.000	1329.949	1334.770	1339.165
1345.427	1348.061	1349.407	1354.203	1362.489	1369.441	1370.560	1371.836	1377.044	1378.205
1379.779	1384.144	1388.655	1392.343	1396.610	1397.917	1401.297	1402.462	1404.433	1406.241
1406.653	1409.620	1411.080	1415.930	1420.321	1424.108	1427.059	1431.129	1432.532	1433.258
1433.748	1435.184	1437.395	1440.207	1442.949	1443.282	1444.776	1445.690	1449.149	1451.006
1452.224	1454.838	1456.840	1459.435	1460.183	1462.658	1466.963	1470.556	1471.330	1471.553
1473.977	1479.115	1479.668	1482.521	1486.236	1487.363	1494.187	1494.892	1503.549	1505.408
1506.944	1510.556	1512.628	1517.460	1521.463	1523.167	1529.786	1530.100	1531.455	1536.945
1540.662	1549.393	1551.418	1554.231	1555.001	1557.579	1561.320	1564.717	1570.525	1573.786
1578.117	1585.445	1586.968	1590.952	1598.838	1610.655	1612.228	1614.220	1621.764	1625.764
1631.658	1632.892	1637.375	1639.713	1640.655	1643.630	1645.730	1652.486	1653.959	1655.262
1658.286	1660.250	1664.373	1671.614	1674.205	1677.001	1680.278	1680.466	1685.415	1691.113
1697.181	1703.179	1704.363	1707.872	1709.936	1710.761	3042.232	3088.006	3102.364	3117.392
3121.905	3127.831	3129.272	3132.145	3139.124	3143.989	3147.710	3149.463	3150.523	3155.919
3159.077	3166.840	3168.868	3174.658	3177.982	3181.654	3184.503	3190.001	3190.278	3191.540
3197.481	3205.575	3210.205	3215.418	3216.536	3217.847	3219.093	3220.466	3225.377	3233.399
3236.006	3246.680	3249.943	3258.113	3259.794					

Gauche addition TS

Atom	X	Y	X (Angstrom)
6	12.17802	-0.22998	-0.36956
6	12.34884	1.14133	-0.42896
6	11.24646	1.99112	-0.60004
6	9.95410	1.41687	-0.71429
6	9.79024	0.00484	-0.65829
6	10.91257	-0.81388	-0.47997
6	8.46575	-0.56320	-0.81342

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6   7.36365   0.26612  -0.96089
6   7.51950   1.70273  -0.96258
6   8.81516   2.26749  -0.87344
6  11.38446   3.42096  -0.66371
6  10.30369   4.22420  -0.82086
6   8.98073   3.67672  -0.92366
6  10.77931  -2.31570  -0.38370
6   9.39737  -2.85909  -0.66289
6   8.30584  -2.00446  -0.85509
6   7.01743  -2.55544  -1.10758
6   5.89082  -1.69608  -1.28654
6   6.04992  -0.29088  -1.18323
6   4.92678   0.55362  -1.27375
6   5.06902   1.95693  -0.96624
6   6.39139   2.54330  -1.06350
6   6.57835   3.93759  -1.13485
6   7.84133   4.48947  -1.07258
6   0.36287   4.10828   0.79815
6  -0.20893   2.80402   0.74216
6  -1.60553   2.65042   0.53449
6  -2.43407   3.79745   0.38607
6  -1.86210   5.10312   0.45597
6  -0.46480   5.25433   0.65965
6  -2.17418   1.35551   0.46529
6  -3.56683   1.20265   0.23757
6  -4.38961   2.34408   0.08862
6  -3.82023   3.64459   0.16758
6  -4.13600  -0.09932   0.15366
6  -5.52129  -0.25145  -0.08200
6  -6.34792   0.89820  -0.22804
6  -5.78466   2.18877  -0.14170
6  -7.74626   0.74387  -0.46446
6  -8.31111  -0.55788  -0.55787
6  -7.48555  -1.70600  -0.41648
6  -6.08652  -1.55279  -0.17617
6  -5.26521  -2.69167  -0.03743
6  -5.83231  -3.99845  -0.14202
6  -7.21682  -4.14789  -0.37961
6  -8.04550  -2.99946  -0.51510
6  -9.45206  -3.14459  -0.75604
6 -10.24424  -2.01864  -0.88875
6  -9.70828  -0.71146  -0.79602
6  -3.87274  -2.54024   0.20227
6  -3.31003  -1.24691   0.30008
6  -6.61458   3.34078  -0.28721
6  -8.00036   3.18586  -0.51624
6  -8.56680   1.88551  -0.60672
6  -9.97343   1.72111  -0.84252
6 -10.50901   0.45028  -0.93115
6  -1.34845   0.20615   0.62284
6  -1.91640  -1.09358   0.54014
6  -1.09338  -2.23616   0.68112
6  -1.66016  -3.53863   0.57143
6  -3.04177  -3.68943   0.33480
6  -3.60799  -4.99395   0.22293
6  -5.00230  -5.14466  -0.01302
6  -6.04565   4.64081  -0.20197
6  -4.65099   4.79604   0.02224
6   0.61590   1.66101   0.89760
6   0.03774   0.35726   0.85364
6   0.85762  -0.79048   1.02721
6   0.29550  -2.08345   0.92723
6   1.12978  -3.23826   1.05449
6   0.56830  -4.53564   0.92581
6  -0.82611  -4.69007   0.69100
6  -1.38759  -5.98133   0.57117
6  -2.78006  -6.13340   0.34087
6  -4.08362   6.08864   0.10085
6  -2.68868   6.24256   0.31551
6   1.76033   4.25868   0.97439
6   2.59262   3.11254   1.08935
6   2.01251   1.80907   1.07906
6   2.83050   0.65708   1.28378
6   2.25268  -0.63647   1.27648
6   3.07608  -1.78091   1.41180
6   2.51389  -3.08428   1.29327
6   2.33347   5.57225   1.01703
6   1.50213   6.68682   0.90088
6   0.11084   6.56195   0.72035
6  -0.74493   7.68739   0.58756
6  -2.10491   7.55307   0.39064
6  -2.98543   8.69581   0.25209
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6  -6.28373   7.07525  -0.25365
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  6 -10.78248   2.91612  -0.97619
  6   3.75324   5.67939   1.17635
  6   4.54857   4.56890   1.25304
  6   4.00064   3.25767   1.19617
  6   4.82384   2.08438   1.11559
  6   4.23697   0.79806   1.41074
  6   5.02657  -0.33855   1.59155
  6   4.47777  -1.62122   1.59933
  1  -8.89686   6.48838  -0.67246
  1   1.94040   7.68381   0.94409
  1  -0.30808   8.68456   0.64178
  1  -2.54333   9.68882   0.31746
  1  -4.95524   9.42247  -0.04757
  1  -6.92085   7.95371  -0.35705
  6   5.29847  -2.80239   1.69828
  1   6.10885  -0.22686   1.67201
  1   4.19201   6.67412   1.23687
  1   5.62734   4.67313   1.36198
  1   5.88290   2.20145   1.34601
  1 -10.87295   5.03456  -0.98835
  1 -11.84985   2.79041  -1.15063
  6  -9.98856  -4.48667  -0.85359
  1 -11.31255  -2.13523  -1.07037
  1 -11.57755   0.33139  -1.10988
  1  12.38387   3.84471  -0.58019
  1  10.41854   5.30604  -0.86771
  1   7.96937   5.56923  -1.13516
  1   5.70399   4.57828  -1.23742
  1   4.22394   2.59550  -1.22457
  6   9.20309  -4.24356  -0.71472
  1  11.08070  -2.62787   0.63109
  1  13.34427   1.57366  -0.34099
  1  13.04476  -0.87654  -0.23427
  6   7.95575  -4.78881  -0.95762
  1  10.05840  -4.90115  -0.56132
  1   7.83016  -5.86978  -0.99709
  6   6.83934  -3.96242  -1.16089
  6   5.52688  -4.49260  -1.40400
  6   4.45645  -3.67424  -1.56118
  1   5.40577  -5.57469  -1.43684
  1   3.45911  -4.08648  -1.70887
  6   4.60298  -2.24980  -1.50024
  6   3.49974  -1.38022  -1.61783
  6   3.65741  -0.01946  -1.50122
  1   2.50713  -1.80625  -1.76292
  1   2.78849   0.63578  -1.55208
  6  -9.20173  -5.57651  -0.72741
  1 -11.05671  -4.59562  -1.03443
  1  -9.62674  -6.57578  -0.80731
  6  -7.77800  -5.46376  -0.48606
  6  -6.95776  -6.57063  -0.35921
  6  -5.56781  -6.44837  -0.12511
  1  -7.38941  -7.56781  -0.44474
  6  -4.71454  -7.57503  -0.00250
  6  -3.35872  -7.44346   0.22154
  1  -5.14802  -8.57099  -0.09297
  6  -2.47560  -8.58741   0.33885
  6  -1.15119  -8.44307   0.55149
  1  -2.91468  -9.57947   0.24530
  1  -0.50661  -9.31704   0.63182
  6  -0.53695  -7.13577   0.67985
  6   0.81560  -6.97227   0.89755
  6   1.40690  -5.68656   1.02790
  1   1.45550  -7.85137   0.97476
  6   2.78871  -5.50497   1.25222
  6   3.35101  -4.24249   1.39009
  1   3.43058  -6.38365   1.31952
  6   4.76578  -4.04187   1.59993
  1   6.37335  -2.67171   1.81945
  1   5.40733  -4.92082   1.64412
  1  11.49434  -2.78343  -1.07885
Energy      -4874.608573          (Hartree)
Frequencies cm-1:
  -561.747     8.935    13.523    18.478    23.409    28.238    32.647    33.857    41.800    53.945
    59.614    67.939    72.461    76.716    86.113    90.725   101.413   116.261   125.737   128.696
   132.381   135.224   139.020   151.541   158.167   171.935   176.487   189.123   191.855   194.855
   195.812   198.533   207.451   208.798   212.390   214.632   220.853   237.383   238.646   243.193
   246.245   254.549   266.616   271.373   272.085   276.124   280.312   287.273   292.692   300.211
   302.122   304.215   304.359   310.202   313.776   317.185   318.467   319.283   321.073   324.484
   334.804   340.952   350.774   356.949   363.255   367.949   369.498   372.231   379.231   383.344
   391.659   396.198   398.050   403.566   406.368   407.642   409.952   411.372   412.829   414.899
```

420.447	422.304	425.062	429.856	431.713	433.547	442.974	444.608	445.870	449.476
451.873	452.571	453.273	459.621	475.091	483.216	485.110	488.137	496.036	504.293
505.734	506.402	508.332	509.994	517.309	518.344	522.729	527.273	535.088	535.476
540.240	546.570	547.982	551.247	555.882	556.990	558.787	559.300	561.514	564.865
566.396	568.089	569.047	569.608	571.431	577.016	584.186	588.754	592.968	593.863
594.982	596.666	597.170	601.244	602.858	603.630	609.365	611.426	612.310	613.005
614.965	616.256	617.780	620.025	631.721	633.225	639.117	639.629	640.063	648.803
650.498	653.027	654.370	656.652	659.366	661.343	662.790	669.965	670.413	671.036
673.757	679.679	680.682	684.965	687.235	689.331	692.095	696.471	711.074	714.202
716.982	717.358	720.669	721.031	722.153	728.945	730.540	731.077	736.368	737.256
738.147	739.773	748.649	750.275	752.176	755.509	757.852	758.632	760.260	763.665
769.493	776.332	776.795	780.092	783.591	785.163	785.679	790.253	791.994	792.987
795.995	798.000	801.757	803.952	805.530	805.628	806.610	807.214	807.701	808.009
810.415	812.169	815.276	817.913	818.959	820.445	821.095	821.956	822.547	824.613
841.545	841.893	843.051	850.809	863.957	870.145	870.956	875.359	878.017	882.794
883.873	891.851	895.053	895.977	900.010	903.130	910.985	911.093	916.063	917.550
919.107	922.119	924.068	930.840	936.371	936.435	938.328	941.475	956.249	969.087
971.187	971.572	975.624	977.763	980.373	987.079	988.533	989.018	991.053	993.560
999.585	1000.059	1002.009	1002.231	1004.389	1010.530	1010.880	1039.559	1056.462	1059.464
1064.533	1066.194	1067.213	1068.906	1073.487	1073.952	1091.960	1103.865	1104.520	1109.412
1110.910	1112.769	1127.610	1143.333	1153.593	1154.925	1163.233	1170.621	1171.041	1180.180
1181.091	1183.560	1187.518	1190.662	1195.775	1198.567	1199.866	1201.055	1203.745	1206.682
1208.857	1209.826	1219.943	1220.179	1222.990	1224.754	1225.348	1227.730	1229.543	1239.495
1240.822	1243.942	1245.901	1248.701	1250.084	1252.141	1253.418	1254.246	1255.936	1261.032
1265.714	1270.275	1271.673	1273.598	1286.509	1302.568	1304.696	1305.725	1308.027	1308.899
1313.878	1316.664	1321.328	1324.364	1326.110	1328.270	1329.563	1337.341	1341.550	1347.684
1349.302	1351.682	1360.051	1363.738	1365.673	1374.514	1375.231	1377.028	1378.151	1386.546
1390.253	1392.977	1393.378	1397.861	1399.957	1403.437	1404.991	1407.757	1408.951	1410.451
1411.841	1412.992	1416.241	1423.865	1425.604	1427.809	1428.492	1431.895	1432.784	1434.160
1435.296	1437.523	1438.438	1439.225	1442.801	1443.892	1448.903	1450.246	1452.562	1454.447
1454.885	1455.473	1457.293	1458.553	1461.831	1464.523	1466.947	1468.157	1471.548	1473.028
1477.008	1478.009	1478.779	1482.139	1484.112	1487.652	1495.599	1497.011	1504.055	1505.842
1507.178	1511.725	1511.995	1517.487	1522.391	1525.764	1527.897	1530.898	1533.988	1535.391
1537.817	1546.552	1551.279	1554.591	1556.958	1559.297	1562.121	1564.369	1566.010	1569.305
1575.786	1580.121	1584.193	1588.932	1595.569	1605.823	1616.243	1618.843	1621.071	1623.677
1626.441	1633.319	1635.845	1638.017	1639.389	1644.657	1645.534	1646.636	1654.985	1657.344
1660.910	1662.051	1665.353	1667.448	1670.248	1670.769	1676.539	1681.039	1681.388	1691.318
1697.948	1698.977	1701.937	1703.124	1707.467	1710.947	3015.096	3081.149	3124.600	3133.230
3138.639	3141.122	3145.993	3150.542	3153.405	3153.627	3158.113	3158.757	3168.192	3170.910
3171.001	3174.493	3174.636	3174.791	3177.919	3178.605	3180.903	3182.434	3183.079	3185.572
3186.411	3188.088	3189.729	3194.425	3198.305	3198.607	3202.435	3202.653	3207.360	3208.398
3216.366	3219.771	3222.822	3226.554	3234.596					

Gauche adduct R-P

Atom	X	Y	X	(Angstrom)
6	12.27293	-0.11162	-0.35924	
6	12.42079	1.25149	-0.54777	
6	11.30196	2.06961	-0.75359	
6	10.01588	1.47288	-0.77115	
6	9.87726	0.07016	-0.59216	
6	11.01345	-0.71725	-0.37705	
6	8.55752	-0.52907	-0.69063	
6	7.44321	0.26549	-0.85632	
6	7.56735	1.71029	-0.93453	
6	8.85678	2.29359	-0.95241	
6	11.41532	3.49263	-0.94603	
6	10.31942	4.26624	-1.12676	
6	8.99701	3.69608	-1.12550	
6	10.89138	-2.20233	-0.12334	
6	9.54303	-2.79700	-0.46139	
6	8.43521	-1.97795	-0.70086	
6	7.17213	-2.56600	-0.98639	
6	6.02981	-1.73772	-1.21521	
6	6.14403	-0.32989	-1.10196	
6	5.00603	0.47348	-1.20486	
6	5.08264	1.90932	-0.76617	
6	6.42861	2.52375	-1.03283	
6	6.58290	3.89760	-1.23370	
6	7.84323	4.47464	-1.28754	
6	0.34662	4.09317	0.78311	
6	-0.22461	2.79437	0.69707	
6	-1.62268	2.64509	0.50179	
6	-2.45113	3.79471	0.38393	
6	-1.87863	5.09767	0.48400	
6	-0.48229	5.24301	0.68573	
6	-2.19625	1.35090	0.41975	
6	-3.58817	1.20401	0.20021	
6	-4.41096	2.35027	0.07151	
6	-3.84041	3.64701	0.17133	
6	-4.16259	-0.09623	0.10858	
6	-5.54945	-0.24250	-0.12318	
6	-6.37435	0.91156	-0.25391	
6	-5.80800	2.20008	-0.15227	
6	-7.77323	0.76304	-0.48461	
6	-8.34162	-0.53663	-0.59085	

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6  -7.51914  -1.68772  -0.46223
6  -6.11874  -1.54021  -0.22388
6  -5.30120  -2.68356  -0.08930
6  -5.87386  -3.98838  -0.19665
6  -7.25857  -4.13175  -0.43689
6  -8.08352  -2.97887  -0.56788
6  -9.48972  -3.11834  -0.80774
6 -10.27962  -1.98795  -0.92955
6  -9.74027  -0.68452  -0.82500
6  -3.91015  -2.53819   0.15241
6  -3.34179  -1.24680   0.25061
6  -6.63722   3.35482  -0.27187
6  -8.02500   3.20540  -0.49570
6  -8.59309   1.90844  -0.60556
6 -10.00188   1.74944  -0.83618
6 -10.53969   0.48150  -0.94127
6  -1.37339   0.19625   0.57015
6  -1.94733  -1.09906   0.49201
6  -1.13086  -2.24706   0.64312
6  -1.70445  -3.54824   0.53691
6  -3.08470  -3.69259   0.29104
6  -3.65603  -4.99349   0.17970
6  -5.05011  -5.13796  -0.06448
6  -6.06686   4.65249  -0.16233
6  -4.67162   4.80198   0.05763
6   0.60447   1.64314   0.82844
6   0.01432   0.34062   0.79602
6   0.82310  -0.80872   0.98541
6   0.25335  -2.10089   0.89899
6   1.07983  -3.26085   1.04845
6   0.51400  -4.55412   0.92378
6  -0.87867  -4.70268   0.67171
6  -1.44576  -5.99177   0.55270
6  -2.83454  -6.13732   0.30861
6  -4.10336   6.09297   0.16631
6  -2.70839   6.24185   0.37929
6   1.74942   4.23851   0.95129
6   2.58652   3.09195   1.00680
6   1.99568   1.78262   0.98569
6   2.80760   0.62349   1.21409
6   2.21688  -0.65982   1.24333
6   3.02994  -1.80950   1.41896
6   2.46062  -3.11289   1.30791
6   2.32164   5.54778   1.04097
6   1.47965   6.67318   0.96923
6   0.09383   6.55147   0.78686
6  -0.76553   7.68001   0.69028
6  -2.12585   7.54982   0.49067
6  -3.00686   8.69516   0.38639
6  -4.33408   8.55345   0.18474
6  -4.94966   7.24845   0.06065
6  -6.30620   7.08725  -0.15272
6  -6.89833   5.80649  -0.27192
6  -8.28597   5.62872  -0.49460
6  -8.85318   4.37345  -0.60752
6 -10.27059   4.17976  -0.83617
6 -10.81011   2.94758  -0.94492
6   3.72858   5.65077   1.19516
6   4.53192   4.52547   1.20393
6   3.98742   3.23906   1.08493
6   4.84426   2.02435   0.86730
6   4.20968   0.74984   1.34180
6   4.97803  -0.36524   1.60736
6   4.41886  -1.65683   1.64421
1  -8.92052   6.51132  -0.57543
1   1.91884   7.66736   1.04809
1  -0.32962   8.67542   0.77422
1  -2.56513   9.68621   0.47794
1  -4.97787   9.42858   0.11158
1  -6.94356   7.96809  -0.23014
6   5.23143  -2.83447   1.78092
1   6.06180  -0.26426   1.68658
1   4.17309   6.63980   1.29308
1   5.61284   4.63182   1.28850
1   5.83869   2.14999   1.31183
1 -10.89836   5.06591  -0.91659
1 -11.87849   2.82610  -1.11630
6 -10.03072  -4.45729  -0.91364
1 -11.34870  -2.10032  -1.10935
1 -11.60933   0.36674  -1.11625
1  12.41153   3.93238  -0.94078
1  10.41582   5.34147  -1.27010
1   7.94592   5.54725  -1.44552
1   5.69469   4.51996  -1.33423
1   4.27908   2.49142  -1.23394
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  6   9.38840  -4.18662  -0.50120
  1  11.09185  -2.38546   0.94670
  1  13.41268   1.70076  -0.53390
  1  13.15352  -0.73201  -0.19401
  6   8.16378  -4.76926  -0.77642
  1  10.25551  -4.81872  -0.31099
  1   8.06970  -5.85376  -0.80624
  6   7.03303  -3.97775  -1.02608
  6   5.74158  -4.54564  -1.30998
  6   4.65883  -3.75899  -1.51897
  1   5.65123  -5.63092  -1.33386
  1   3.67788  -4.19818  -1.69739
  6   4.76513  -2.32589  -1.47261
  6   3.65301  -1.48795  -1.64142
  6   3.77548  -0.11633  -1.50865
  1   2.67569  -1.93293  -1.82784
  1   2.88957   0.51435  -1.58112
  6  -9.24756  -5.55078  -0.79190
  1 -11.09904  -4.56172  -1.09607
  1  -9.67608  -6.54811  -0.87712
  6  -7.82464  -5.44385  -0.54728
  6  -7.00861  -6.55549  -0.41873
  6  -5.62115  -6.43913  -0.17804
  1  -7.44466  -7.55055  -0.50664
  6  -4.77281  -7.57100  -0.04714
  6  -3.41987  -7.44582   0.18799
  1  -5.21102  -8.56479  -0.13884
  6  -2.54334  -8.59447   0.31833
  6  -1.22139  -8.45661   0.54668
  1  -2.98669  -9.58441   0.22244
  1  -0.58232  -9.33363   0.63758
  6  -0.60099  -7.15169   0.67833
  6   0.74704  -6.99525   0.91431
  6   1.34587  -5.70965   1.04705
  1   1.38133  -7.87713   1.00532
  6   2.72035  -5.53580   1.29360
  6   3.28925  -4.27074   1.43216
  1   3.35644  -6.41686   1.38123
  6   4.69614  -4.07554   1.67566
  1   6.30274  -2.70687   1.93148
  1   5.33372  -4.95571   1.74429
  1  11.67484  -2.73367  -0.68387
Energy      -4874.620294          (Hartree)
Frequencies cm-1:
     9.776    16.192    19.328    24.751    28.145    32.930    36.322    44.147    54.684    61.064
    68.114    73.009    79.168    85.881    92.885   102.339   115.618   123.823   129.246   132.529
   135.270   138.179   146.187   156.892   172.800   176.175   189.207   190.546   195.216   196.061
   196.402   204.967   208.311   213.631   215.918   220.642   237.747   239.565   242.551   246.130
   255.193   265.897   269.664   272.932   274.858   280.071   289.477   293.107   298.985   302.030
   304.505   305.251   311.009   313.533   316.680   318.427   320.104   322.549   326.817   333.918
   340.480   353.919   358.003   366.042   367.260   371.365   373.925   378.612   384.771   394.312
   396.154   401.738   405.780   406.347   408.101   409.798   411.638   413.709   414.460   419.098
   421.973   425.287   429.832   433.532   436.382   442.739   444.714   446.686   450.040   451.983
   453.587   455.146   460.612   478.958   483.472   485.733   491.834   498.012   502.169   504.033
   507.306   508.167   510.990   516.049   517.653   520.524   526.827   535.199   536.848   539.414
   545.028   548.017   550.028   555.996   557.151   558.269   559.111   561.400   564.109   568.436
   568.811   569.448   571.065   571.634   577.237   580.970   588.215   592.521   593.200   595.014
   596.716   599.353   601.613   603.208   603.957   609.258   610.008   611.060   612.624   614.604
   615.392   618.056   623.416   631.080   634.292   636.695   639.474   640.352   646.177   651.380
   652.639   654.721   659.245   660.537   662.979   664.920   669.410   670.580   673.553   674.445
   679.813   683.035   684.538   686.325   689.000   693.589   695.155   708.474   713.377   715.881
   719.447   720.713   721.528   723.935   724.219   728.951   730.472   732.631   735.782   737.049
   737.691   741.620   746.121   747.671   754.250   757.564   758.960   760.106   763.777   767.837
   773.713   777.259   778.603   780.866   783.597   785.706   788.684   789.935   791.831   795.568
   799.032   801.235   801.998   804.040   806.084   806.741   807.666   810.292   810.496   811.706
   813.042   814.799   816.168   818.240   820.654   821.586   822.150   824.349   829.670   838.998
   842.225   843.041   846.074   853.954   861.661   872.427   877.028   878.561   881.156   884.881
   886.094   892.908   895.274   896.120   900.184   906.071   912.028   916.264   917.464   918.000
   923.359   926.000   930.417   936.388   936.718   937.336   938.053   938.604   958.158   967.699
   969.513   970.324   972.297   982.521   984.004   986.817   987.393   989.087   989.779   991.781
   993.124   997.779  1006.255  1008.989  1009.993  1011.574  1046.969  1052.458  1060.967  1063.084
  1066.428  1067.845  1070.477  1073.285  1084.961  1095.768  1101.015  1103.680  1108.821  1110.096
  1123.689  1137.224  1151.718  1154.377  1162.017  1163.151  1170.404  1174.427  1176.592  1180.056
  1182.935  1190.626  1195.750  1196.563  1199.475  1200.966  1201.981  1204.618  1208.724  1209.636
  1213.039  1216.719  1222.165  1223.023  1224.100  1227.855  1230.199  1233.209  1235.631  1240.373
  1243.478  1244.646  1246.785  1249.247  1251.043  1252.072  1252.774  1255.578  1256.290  1259.300
  1265.754  1268.478  1269.434  1270.868  1284.580  1294.943  1301.740  1306.951  1308.321  1310.495
  1312.562  1313.715  1318.865  1320.671  1324.430  1326.793  1328.819  1329.983  1336.857  1340.068
  1345.999  1347.078  1351.307  1356.323  1362.766  1370.082  1371.524  1374.405  1375.826  1380.382
  1382.017  1385.685  1388.224  1393.184  1396.706  1397.885  1403.188  1404.092  1404.946  1405.861
  1407.325  1411.055  1413.716  1414.085  1420.610  1425.678  1427.547  1430.759  1433.843  1434.526
  1437.116  1438.214  1438.733  1439.244  1443.072  1444.362  1446.120  1448.592  1449.534  1451.347
  1453.907  1454.804  1456.708  1458.795  1460.544  1462.076  1465.266  1469.605  1470.796  1472.190
  1475.668  1478.352  1478.552  1483.461  1487.056  1487.367  1494.839  1495.232  1504.608  1505.954
  1507.361  1509.659  1512.996  1516.711  1521.768  1524.694  1529.039  1530.244  1531.598  1538.275
```

1539.839	1550.277	1552.984	1555.300	1557.862	1561.083	1562.854	1565.062	1569.171	1573.669
1577.929	1583.860	1585.904	1590.255	1598.076	1610.881	1613.471	1615.343	1620.205	1625.897
1631.803	1633.303	1636.271	1639.216	1643.204	1643.952	1645.483	1653.342	1655.227	1657.795
1659.621	1661.080	1663.608	1668.989	1673.660	1675.475	1680.220	1681.218	1688.973	1692.027
1696.899	1701.438	1705.291	1706.332	1709.893	1711.361	3016.911	3087.280	3117.129	3117.989
3123.185	3135.724	3153.215	3154.816	3156.916	3158.703	3163.184	3163.505	3167.703	3168.961
3170.313	3172.693	3173.293	3173.834	3175.665	3176.087	3177.012	3178.014	3182.506	3182.762
3188.728	3190.362	3194.242	3196.893	3197.352	3200.941	3203.154	3203.845	3206.834	3210.232
3211.043	3217.785	3225.066	3229.857	3234.174					

Anti addition TS

Atom	X	Y	X	(Angstrom)
6	4.94816	-2.02610	-1.44382	
6	5.76222	-0.89607	-1.22285	
6	7.14443	-1.08180	-0.99676	
6	7.68046	-2.39132	-0.93944	
6	6.83531	-3.51452	-1.15132	
6	5.47541	-3.30003	-1.43615	
6	8.01576	0.05537	-0.83297	
6	7.46719	1.37855	-1.00669	
6	6.08159	1.55573	-1.20985	
6	5.20351	0.42114	-1.08290	
6	9.07013	-2.58033	-0.66059	
6	9.92208	-1.45653	-0.47448	
6	9.37267	-0.12220	-0.59256	
6	10.25384	1.02438	-0.51268	
6	9.72464	2.32659	-0.73162	
6	8.32810	2.50260	-0.98471	
6	7.80216	3.80350	-1.20707	
6	6.42354	3.94773	-1.44208	
6	5.58149	2.85633	-1.42192	
6	8.69561	4.92715	-1.17252	
6	10.01831	4.76402	-0.92606	
6	10.57849	3.45917	-0.69586	
6	11.94334	3.26703	-0.43918	
6	12.44714	1.99669	-0.22138	
6	11.62196	0.86947	-0.25139	
6	12.21530	-0.49192	0.02600	
6	11.28255	-1.65801	-0.20296	
6	9.59416	-3.89622	-0.57049	
6	10.95865	-4.06080	-0.29522	
6	11.77952	-2.96064	-0.11815	
6	8.71116	-5.01461	-0.76915	
6	7.39766	-4.83252	-1.05156	
6	4.83577	0.47032	1.04176	
6	4.24739	1.75936	1.19617	
6	2.83997	1.90146	1.05356	
6	2.01940	0.74534	0.91655	
6	2.59813	-0.55569	1.00907	
6	4.00498	-0.70239	1.16817	
6	1.77250	-1.70599	0.94359	
6	0.36721	-1.56554	0.74111	
6	-0.20688	-0.26998	0.64110	
6	0.61901	0.88739	0.74848	
6	2.34389	-2.99897	1.06130	
6	1.51811	-4.15559	0.95649	
6	0.12772	-4.01651	0.74694	
6	-0.45086	-2.71299	0.64219	
6	2.09518	-5.46317	1.04875	
6	3.52421	-5.56037	1.23633	
6	4.30482	-4.45678	1.33884	
6	3.74560	-3.13055	1.26576	
6	4.54625	-1.98534	1.29894	
6	-0.69470	-5.16799	0.63889	
6	-0.11517	-6.46883	0.74216	
6	1.27676	-6.58082	0.94351	
6	-2.09448	-5.02842	0.42758	
6	-2.67284	-3.72821	0.32454	
6	-1.84719	-2.57265	0.43328	
6	-2.42149	-1.28275	0.33703	
6	-1.60034	-0.12897	0.44829	
6	-4.06010	-3.58743	0.11563	
6	-4.63904	-2.28974	0.01771	
6	-3.82200	-1.14189	0.13155	
6	-4.40041	0.15383	0.04511	
6	-3.57952	1.30933	0.17139	
6	-2.18094	1.16854	0.37071	
6	-1.36551	2.31758	0.50542	
6	0.03504	2.17753	0.69717	
6	2.24668	3.19400	1.04761	
6	0.85094	3.33543	0.85474	
6	0.26399	4.62902	0.81742	
6	-1.13328	4.77164	0.60782	
6	-1.95136	3.61299	0.45075	
6	-3.34089	3.75230	0.24584	

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6  -4.15872   2.59824   0.10210
6  -3.92666   5.05256   0.18521
6  -3.11427   6.19888   0.34011
6  -1.71802   6.05876   0.55601
6  -0.88827   7.21934   0.72218
6   0.46749   7.06771   0.93582
6   1.08199   5.78875   0.98935
6   2.46482   5.62227   1.20130
6   3.05994   4.36141   1.22987
6   5.03429   2.93335   1.37700
6   4.46772   4.17516   1.41754
6  -5.79195   0.29417  -0.15935
6  -6.37135   1.59200  -0.23868
6  -5.55914   2.73735  -0.10497
6  -6.14246   4.03818  -0.17531
6  -5.32463   5.19154  -0.02894
6  -5.90874   6.49061  -0.09543
6  -5.07227   7.62309   0.06184
6  -3.71261   7.50312   0.27741
6  -2.84871   8.65426   0.44501
6  -1.52229   8.52097   0.65527
6  -6.03759  -2.14723  -0.19053
6  -6.61147  -0.86125  -0.28064
6  -8.01680  -0.71910  -0.48923
6  -8.59382   0.57698  -0.57509
6  -7.77555   1.73287  -0.44776
6  -8.35043   3.02156  -0.52411
6  -7.53282   4.17581  -0.38669
6  -8.11079   5.48806  -0.45859
6  -7.30358   6.60071  -0.31409
6  -4.88618  -4.74519   0.00750
6  -6.28548  -4.60182  -0.20236
6  -6.86314  -3.30724  -0.30290
6  -8.25326  -3.16440  -0.50995
6  -8.83097  -1.86772  -0.60549
6 -10.24206  -1.71619  -0.81460
6 -10.78978  -0.44891  -0.89998
6  -9.99702   0.71836  -0.78395
6 -10.54695   2.02249  -0.86239
6  -9.76409   3.15417  -0.73696
6 -10.31581   4.49219  -0.81052
6  -9.53915   5.58842  -0.67946
6  -9.07598  -4.33466  -0.61716
6 -10.49685  -4.14782  -0.82770
6 -11.04466  -2.91765  -0.92160
6  -8.50017  -5.58869  -0.51595
6  -7.11107  -5.75901  -0.30764
6  -2.91482  -6.17399   0.32174
6  -4.31158  -6.03247   0.11161
6  -5.15279  -7.19304   0.00737
6  -6.50936  -7.03912  -0.19677
6  -0.96487  -7.60272   0.63464
6  -2.32367  -7.48053   0.43105
6  -3.19999  -8.63093   0.32331
6  -4.52762  -8.49593   0.12535
1  -7.74799   7.59456  -0.36922
1   3.08731   6.50624   1.34045
1   1.09170   7.95224   1.06400
1  -0.89142   9.40001   0.77873
1  -3.30312   9.64264   0.39482
1  -5.51994   8.61572   0.01074
1   5.62756  -2.09857   1.39602
1   5.09354   5.05550   1.55640
1   6.11447   2.82311   1.47420
1   5.89640   0.36354   1.27918
1  -9.97569   6.58427  -0.73850
1 -11.38762   4.59191  -0.97453
1 -11.86284  -0.33987  -1.05748
1 -11.61983   2.12933  -1.02241
1  10.68731   5.62237  -0.89902
1   8.28160   5.91923  -1.34668
1   6.01602   4.94426  -1.60582
1   4.50880   2.99001  -1.55935
1   4.15614   0.55856  -1.35924
1  12.54930  -0.51620   1.07769
1  12.60534   4.13086  -0.41425
1  13.51037   1.86529  -0.02303
1  12.83864  -3.10725   0.09092
1  11.36912  -5.06674  -0.22464
1   9.12858  -6.01730  -0.69150
1   6.73705  -5.68432  -1.20775
1   4.82383  -4.15892  -1.59046
1   3.88008  -1.87959  -1.60353
1 -12.11592  -2.80130  -1.07867
1 -11.12073  -5.03687  -0.90603
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  1  -9.13120  -6.47409  -0.59356
  1  -7.14305  -7.92280  -0.27226
  1  -5.16678  -9.37441   0.05128
  1  -2.75283  -9.61991   0.41114
  1  -0.52312  -8.59565   0.71842
  1   1.71874  -7.57436   1.01851
  1   5.38347  -4.54985   1.46418
  1   3.96460  -6.55476   1.29514
  1  13.11757  -0.62516  -0.59181
Energy      -4874.601912          (Hartree)
Frequencies cm-1:
  -535.355     7.948    11.387    16.901    21.859    23.569    28.729    32.530    43.760    47.125
    55.411    64.240    68.575    72.182    84.847    86.351   101.886   105.683   117.550   126.879
   129.493   129.830   133.696   136.631   161.046   171.260   175.577   185.956   190.980   194.455
   195.596   196.999   205.183   208.969   210.597   214.393   214.988   233.932   236.420   239.622
   245.695   253.627   265.281   268.578   269.675   271.703   281.183   284.854   291.028   300.433
   301.828   302.729   303.995   309.460   312.635   317.017   317.107   317.891   318.958   319.611
   332.950   338.709   349.481   355.020   361.644   366.884   368.527   369.364   379.245   383.239
   390.073   394.613   396.267   403.240   404.351   406.784   410.133   410.186   411.279   412.987
   419.599   420.388   424.272   429.361   430.739   432.791   442.669   444.277   445.456   449.343
   450.449   452.156   452.824   459.446   470.335   482.297   484.844   488.839   495.306   503.698
   504.704   506.805   508.738   509.215   517.337   518.031   522.176   525.411   532.758   535.068
   542.076   546.318   548.212   550.555   554.856   556.744   558.329   558.987   561.509   564.577
   565.594   567.516   569.361   570.337   570.510   574.192   583.973   587.898   592.870   593.309
   594.566   595.879   596.290   599.319   600.763   603.886   608.788   610.623   611.573   612.264
   614.650   616.254   617.225   618.358   631.194   633.209   638.563   639.555   639.763   648.402
   650.658   653.425   653.586   656.578   658.754   660.644   662.328   669.612   670.389   670.740
   675.399   679.503   680.004   684.053   686.725   688.718   692.119   695.331   710.889   714.070
   717.016   717.843   720.358   721.025   722.883   729.536   729.825   730.656   736.381   737.273
   741.929   743.115   751.974   752.215   753.016   756.140   757.195   758.724   760.663   765.810
   773.866   776.227   777.735   780.320   782.900   784.396   785.288   787.499   790.080   793.140
   795.567   799.441   800.379   801.393   802.975   804.674   805.704   806.860   807.387   809.474
   809.794   811.501   812.014   817.600   817.926   818.645   819.543   821.759   822.664   824.645
   841.309   841.677   844.788   851.162   855.049   865.763   870.652   873.315   878.618   883.333
   884.197   887.611   892.805   894.015   894.877   896.112   903.984   912.040   918.973   920.052
   921.713   923.872   924.908   927.022   930.437   935.712   937.871   942.968   946.722   957.769
   968.020   969.934   971.040   974.633   978.626   985.498   985.863   989.217   992.878   993.096
   994.001   996.705   997.861  1002.420  1002.736  1004.903  1009.546  1020.287  1055.850  1058.288
  1064.267  1064.803  1067.153  1067.552  1072.946  1073.677  1091.733  1102.823  1104.444  1108.311
  1109.976  1111.815  1126.852  1143.938  1152.630  1153.752  1161.779  1168.187  1169.596  1177.664
  1180.326  1182.205  1185.097  1188.620  1193.072  1196.781  1198.586  1199.803  1202.172  1203.848
  1206.700  1207.759  1216.290  1219.641  1220.751  1221.706  1223.993  1225.431  1230.251  1237.988
  1242.489  1243.642  1245.056  1247.469  1249.083  1251.308  1251.386  1253.341  1254.134  1261.909
  1262.823  1270.897  1271.338  1273.553  1286.712  1303.102  1305.335  1306.278  1307.090  1307.960
  1313.645  1315.802  1318.789  1321.584  1323.821  1327.186  1328.444  1338.503  1342.418  1347.035
  1348.225  1353.257  1358.348  1362.980  1363.483  1373.658  1375.666  1376.483  1377.160  1385.426
  1389.079  1391.416  1393.945  1396.385  1399.485  1402.747  1404.869  1405.644  1408.311  1409.330
  1411.406  1411.847  1417.479  1421.914  1425.421  1426.956  1429.983  1432.503  1433.467  1434.593
  1434.808  1436.010  1437.329  1438.478  1441.114  1442.655  1447.428  1449.592  1451.931  1453.183
  1454.709  1455.220  1456.225  1457.142  1462.268  1464.469  1466.589  1467.738  1468.967  1471.466
  1475.581  1475.787  1477.584  1482.162  1483.281  1486.557  1494.115  1496.173  1502.623  1504.825
  1506.417  1510.874  1511.682  1516.438  1519.867  1524.771  1526.608  1530.030  1532.802  1533.769
  1536.018  1544.060  1549.501  1552.082  1556.741  1559.016  1560.352  1562.811  1564.287  1568.208
  1574.322  1580.321  1583.184  1587.916  1594.368  1606.731  1615.090  1619.327  1621.853  1625.362
  1626.349  1633.406  1635.626  1636.822  1640.093  1644.638  1645.940  1646.896  1654.584  1656.814
  1659.404  1661.494  1665.059  1666.905  1669.807  1670.370  1675.819  1679.439  1681.687  1687.838
  1694.458  1697.449  1697.709  1703.011  1708.129  1711.585  3038.918  3066.970  3114.046  3116.930
  3122.238  3128.165  3130.327  3139.308  3142.458  3144.994  3154.936  3160.439  3165.585  3165.714
  3166.582  3166.852  3168.154  3168.646  3168.840  3172.195  3173.599  3175.983  3179.193  3179.823
  3182.843  3183.890  3184.387  3186.331  3187.627  3189.043  3190.325  3192.077  3195.411  3198.979
  3200.766  3205.816  3208.568  3209.829  3220.450

 Anti adduct R-P
 Atom    X         Y         X   (Angstrom)
  6   3.46573  -5.60802   1.30040
  6   4.25535  -4.50668   1.39129
  6   3.70551  -3.18284   1.29769
  6   2.31550  -3.04051   1.07970
  6   1.47769  -4.19307   0.98787
  6   2.04285  -5.50023   1.10267
  6   0.09036  -4.04342   0.76798
  6  -0.47600  -2.73376   0.64452
  6   0.35346  -1.59051   0.73001
  6   1.75751  -1.74065   0.93653
  6  -1.86647  -2.58362   0.42872
  6  -2.42965  -1.28768   0.31932
  6  -1.59984  -0.14184   0.42300
  6  -0.20662  -0.29353   0.61340
  6   0.63456   0.85900   0.71088
  6   0.05012   2.15912   0.67844
  6  -1.34894   2.30650   0.48915
  6  -2.17262   1.16165   0.34420
  6  -1.92960   3.60433   0.45142
  6  -1.10939   4.75664   0.63534
  6   0.28289   4.60452   0.85523
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6   0.86535   3.30814   0.86549
6   2.02578   0.70788   0.85847
6   2.85898   1.86747   1.01771
6   2.26292   3.15769   1.06398
6   3.07554   4.31384   1.29274
6   2.47656   5.58749   1.29377
6   1.10359   5.76034   1.06660
6  -3.56754   1.31150   0.14583
6  -4.14081   2.60596   0.08253
6  -3.31921   3.75289   0.24152
6  -3.89902   5.05680   0.19548
6  -3.08325   6.19796   0.37632
6  -1.69097   6.04901   0.60388
6  -0.86091   7.20316   0.80607
6   0.49133   7.04307   1.03565
6  -3.82945  -1.13743   0.11007
6  -4.39738   0.16128   0.01767
6  -5.78808   0.31125  -0.18937
6  -6.35928   1.61399  -0.26897
6  -5.54026   2.75394  -0.12757
6  -6.11640   4.05769  -0.19002
6  -5.29396   5.20524  -0.02625
6  -4.65587  -2.27989   0.00104
6  -6.05082  -2.12803  -0.21248
6  -6.61504  -0.83707  -0.31008
6  -8.01925  -0.68550  -0.52319
6  -8.58673   0.61372  -0.61254
6  -7.76091   1.76418  -0.48135
6  -8.32828   3.05714  -0.55494
6  -7.50561   4.20474  -0.40671
6  -9.74099   3.19904  -0.77271
6 -10.53000   2.07331  -0.90448
6  -9.98855   0.76450  -0.82575
6 -10.78861  -0.39558  -0.94327
6 -10.24990  -1.66789  -0.85272
6  -8.84183  -1.82840  -0.63839
6  -8.27408  -3.12995  -0.53464
6  -6.88587  -3.28248  -0.32113
6  -4.08776  -3.58330   0.11107
6  -4.92237  -4.73377   0.00882
6  -6.31992  -4.58039  -0.20930
6  -7.15478  -5.73136  -0.31003
6  -8.53930  -5.55220  -0.52626
6  -9.10522  -4.29275  -0.63859
6 -10.52291  -4.09686  -0.85644
6 -11.06118  -2.86268  -0.95830
6  -2.70316  -3.73420   0.32780
6  -5.87241   6.50830  -0.07947
6  -7.26515   6.62779  -0.30792
6  -8.07652   5.52115  -0.47004
6  -9.50275   5.63139  -0.69892
6 -10.28475   4.54051  -0.84190
6  -0.74009  -5.18687   0.66888
6  -2.13776  -5.03742   0.44681
6  -2.96757  -6.17720   0.34705
6  -4.35931  -6.02584   0.12712
6  -5.21129  -7.18095   0.02728
6  -6.56344  -7.01741  -0.18570
6  -5.03403   7.63411   0.10361
6  -3.67656   7.50520   0.33158
6   2.59754  -0.60367   0.96565
6   1.21185  -6.61600   1.00446
6  -0.17183  -6.49285   0.79075
6  -1.03382  -7.62240   0.68727
6  -2.38715  -7.48984   0.47257
6  -3.27355  -8.63383   0.36790
6  -4.59787  -8.48889   0.15971
6  -2.81264   8.64970   0.53374
6  -1.48948   8.50772   0.75976
6   4.46468   4.12169   1.50117
6   5.03049   2.86512   1.41738
6   4.25485   1.72943   1.14941
6   4.88547   0.40746   0.81162
6   3.99868  -0.76824   1.12009
6   4.51971  -2.03058   1.31553
6   5.15784   0.38434  -0.79165
6   5.78123  -0.94191  -1.12739
6   7.15816  -1.10055  -0.92424
6   8.01580   0.05479  -0.73529
6   7.44649   1.37447  -0.93808
6   6.06642   1.53802  -1.11469
6   8.30531   2.49897  -0.99907
6   9.70688   2.34249  -0.75558
6  10.24538   1.05600  -0.48370
6   9.36966  -0.10249  -0.52576
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  6  11.61425   0.91810  -0.22908
  6  12.43449   2.04981  -0.25564
  6  11.92158   3.30604  -0.52731
  6  10.55438   3.47926  -0.78132
  6   7.76976   3.78301  -1.28351
  6   8.66071   4.91406  -1.31527
  6   9.98409   4.76986  -1.07127
  6   9.94989  -1.43179  -0.43996
  6  11.31240  -1.60994  -0.17552
  6  12.20901  -0.42822   0.11235
  6   9.12529  -2.56518  -0.67287
  6   7.73033  -2.39608  -0.94218
  6   5.55918   2.80205  -1.42039
  6   6.39343   3.90409  -1.51668
  6   9.67996  -3.87012  -0.63910
  6  11.04712  -4.01372  -0.36828
  6  11.84154  -2.90303  -0.14350
  6   8.82337  -5.00048  -0.89219
  6   7.50837  -4.83774  -1.16886
  6   6.91217  -3.52682  -1.20662
  6   5.55472  -3.32813  -1.49050
  6   5.00217  -2.05814  -1.44021
  1  -7.70411   7.62449  -0.35422
  1   3.10065   6.46356   1.46949
  1   1.11586   7.92207   1.19589
  1  -0.85783   9.38139   0.91359
  1  -3.26371   9.64028   0.49941
  1  -5.47729   8.62930   0.06583
  1   5.59988  -2.15707   1.40775
  1   5.09326   4.98948   1.69376
  1   6.11038   2.75391   1.51690
  1   5.87141   0.30168   1.28448
  1  -9.93315   6.63015  -0.75312
  1 -11.35506   4.64724  -1.01114
  1 -11.86035  -0.27945  -1.10447
  1 -11.60163   2.18703  -1.06791
  1  10.64909   5.63154  -1.09165
  1   8.23995   5.89397  -1.53633
  1   5.97589   4.88459  -1.74096
  1   4.48289   2.92513  -1.54193
  1   4.17624   0.50041  -1.27100
  1  12.45285  -0.43400   1.18893
  1  12.57913   4.17347  -0.54666
  1  13.50003   1.93293  -0.06083
  1  12.90385  -3.03267   0.06033
  1  11.48110  -5.01209  -0.34061
  1   9.26521  -5.99543  -0.86106
  1   6.86976  -5.69695  -1.36927
  1   4.92188  -4.18883  -1.70174
  1   3.92997  -1.93068  -1.59042
  1 -12.13079  -2.73886  -1.12035
  1 -11.15322  -4.98148  -0.93327
  1  -9.17749  -6.43265  -0.60108
  1  -7.20476  -7.89579  -0.25802
  1  -5.24444  -9.36207   0.08786
  1  -2.83524  -9.62574   0.46630
  1  -0.60074  -8.61796   0.78342
  1   1.64566  -7.61176   1.09488
  1   5.33303  -4.60624   1.51909
  1   3.89904  -6.60442   1.37274
  1  13.16068  -0.55337  -0.42552
Energy      -4874.619054          (Hartree)
Frequencies cm-1:
     7.830    12.986    18.945    22.658    24.628    29.407    34.061    40.535    44.451    56.010
    65.906    70.869    73.477    83.812    94.219   101.572   106.864   114.342   127.694   129.689
   130.590   134.385   141.001   161.892   171.546   174.156   183.452   188.261   194.162   195.089
   196.942   204.813   208.274   210.757   215.461   218.216   234.529   236.712   239.022   247.405
   253.919   264.387   265.681   270.549   272.160   282.253   287.041   292.200   298.913   301.696
   304.019   304.257   310.762   313.115   316.701   317.385   317.747   321.380   323.019   334.165
   341.331   353.274   357.309   366.115   367.721   369.556   370.696   378.444   384.265   393.896
   395.942   399.115   405.179   406.787   407.759   409.381   410.193   412.068   413.303   418.545
   421.375   424.087   430.034   432.443   435.502   442.600   444.313   447.732   449.550   450.823
   453.743   455.357   460.403   475.469   484.325   485.806   492.402   497.346   500.148   503.398
   506.785   508.857   509.762   516.270   517.937   519.805   525.122   534.955   536.944   542.501
   545.169   547.765   551.622   554.747   556.555   557.330   558.915   561.374   565.523   567.085
   568.405   568.971   570.677   572.874   574.417   580.836   587.267   592.037   593.353   594.032
   596.997   598.073   600.373   601.320   604.188   608.822   609.290   611.237   612.830   614.862
   616.239   616.916   623.793   630.150   635.510   636.642   639.330   640.182   647.777   652.545
   653.038   654.000   658.128   660.578   662.045   664.823   669.443   670.635   672.440   677.893
   680.360   682.860   684.132   686.836   688.481   693.880   694.768   710.455   713.693   716.080
   719.521   720.617   721.701   725.562   729.657   729.778   731.043   735.624   737.428   739.539
   744.066   745.382   749.943   751.933   755.766   758.321   759.255   761.043   765.843   772.415
   775.666   777.307   779.344   784.051   786.566   787.726   788.684   790.266   793.955   796.122
   798.880   802.063   803.497   804.162   804.928   806.235   808.086   809.875   811.806   812.308
   812.889   815.354   817.683   819.143   819.909   820.890   823.123   824.206   828.016   841.315
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842.510 848.035 852.223 857.766 863.645 869.329 874.145 878.089 882.217 884.524
885.695 890.379 895.940 896.263 897.079 898.129 906.205 913.153 918.089 919.016
923.606 924.033 928.100 933.517 935.589 937.990 939.266 939.954 957.555 968.908
970.087 973.414 981.361 983.504 984.116 986.006 987.563 990.735 991.309 993.853
994.135 995.712 1000.773 1003.429 1004.275 1013.341 1049.406 1052.564 1059.756 1062.637
1066.192 1066.562 1070.489 1073.326 1086.376 1094.660 1101.118 1103.626 1108.198 1109.653
1123.164 1139.816 1151.708 1153.699 1160.307 1162.499 1169.685 1175.496 1179.106 1181.223
1182.323 1188.241 1193.774 1197.372 1198.073 1198.713 1201.773 1203.233 1207.649 1209.112
1213.335 1215.759 1220.886 1221.572 1223.654 1226.068 1230.056 1231.818 1235.281 1238.845
1243.067 1244.105 1246.165 1249.873 1250.397 1250.966 1252.866 1253.312 1258.233 1261.083
1264.004 1268.627 1271.781 1273.679 1290.683 1297.392 1301.670 1305.186 1307.232 1311.265
1311.487 1312.797 1318.029 1319.399 1322.978 1326.001 1329.940 1330.251 1338.400 1339.160
1345.232 1346.237 1352.187 1356.778 1360.603 1369.301 1370.642 1372.609 1375.034 1378.295
1381.207 1384.160 1387.571 1393.541 1395.581 1396.750 1402.992 1404.531 1405.437 1406.699
1406.922 1410.691 1414.417 1415.304 1419.469 1423.997 1427.809 1429.809 1432.850 1433.743
1436.004 1437.366 1438.959 1441.809 1442.290 1443.116 1445.114 1447.807 1451.351 1451.851
1452.237 1453.206 1455.941 1458.331 1459.714 1460.707 1465.197 1468.751 1469.979 1470.486
1474.819 1477.520 1478.821 1482.310 1482.986 1486.271 1493.515 1494.373 1503.749 1504.479
1506.918 1509.963 1512.624 1516.003 1521.335 1522.976 1528.436 1528.727 1530.771 1536.526
1539.073 1548.696 1552.269 1555.248 1556.682 1558.792 1561.847 1564.797 1568.168 1574.364
1578.439 1585.039 1586.251 1589.004 1596.617 1609.918 1612.165 1614.745 1620.003 1625.630
1630.795 1636.190 1636.540 1640.096 1643.955 1644.886 1645.734 1653.488 1656.888 1657.324
1660.184 1660.489 1664.714 1666.985 1675.322 1676.309 1680.437 1683.043 1688.102 1690.478
1693.425 1700.789 1701.734 1706.592 1709.678 1710.459 3033.007 3063.929 3126.611 3129.173
3129.293 3135.448 3137.602 3138.312 3141.963 3145.023 3148.657 3149.242 3153.742 3158.388
3162.239 3167.546 3168.008 3169.605 3170.294 3171.516 3173.641 3174.175 3175.741 3175.856
3178.066 3178.652 3180.204 3182.774 3183.217 3184.532 3192.269 3193.826 3196.890 3198.726
3200.768 3207.062 3214.748 3218.250 3232.640

System 4:

C18H13 1-H-pyrenyl-C2H2
Atom X Y X (Angstrom)
6 0.09668 -0.03334 -0.10469
6 0.01235 -0.07954 1.39519
6 1.35478 -0.04478 2.10038
6 2.56784 0.02330 1.35254
6 2.54443 0.05996 -0.07636
6 1.25221 0.02958 -0.76477
6 1.41848 -0.07826 3.47387
6 2.65191 -0.03825 4.15129
6 3.83985 0.02915 3.45897
6 3.81538 0.05536 2.03073
6 3.73371 0.12204 -0.76828
6 4.96671 0.14576 -0.09031
6 5.02728 0.11645 1.28295
6 6.38097 0.11806 1.97734
6 6.28649 0.16178 3.48069
6 5.13214 0.09548 4.14308
1 0.49633 -0.13166 4.05170
1 2.66714 -0.05640 5.24003
1 5.89375 0.17203 -0.66192
1 3.71888 0.14782 -1.85679
1 6.96742 0.98154 1.62601
1 7.23283 0.21298 4.01651
1 5.11865 0.10287 5.23251
1 -0.60129 0.76737 1.74545
1 -0.84591 -0.05349 -0.64979
1 1.26860 0.06096 -1.85360
1 -0.52963 -0.99188 1.69538
6 7.13488 -1.15708 1.58865
6 8.28936 -1.17196 0.97452
1 6.62786 -2.08354 1.86919
1 8.96200 -0.40357 0.60703
Energy -689.734779 (Hartree)
Frequencies cm-1:
32.497 76.480 97.487 101.306 182.380 202.629 220.666 290.957 316.635 333.037
365.354 410.019 442.103 464.376 469.034 477.867 495.027 507.661 549.978 558.710
604.007 654.152 668.054 668.677 713.953 739.551 748.799 782.678 798.201 825.815
828.866 867.645 871.672 884.271 924.221 949.464 953.949 967.102 971.641 983.611
989.946 1005.918 1017.205 1034.649 1046.065 1142.539 1150.206 1154.551 1200.235 1209.479
1233.439 1236.162 1253.390 1256.417 1262.840 1279.149 1297.034 1315.622 1342.183 1385.542
1397.383 1418.048 1433.332 1456.608 1459.337 1493.233 1517.605 1579.570 1667.885 1674.377
1675.552 1711.516 1753.379 1762.670 3036.901 3044.405 3077.839 3139.159 3140.804 3159.404
3161.219 3163.373 3165.504 3177.604 3192.284 3207.593 3247.797

CComplex R:P
Atom X Y X (Angstrom)
6 -3.45860 4.23002 -0.71600
6 -2.08576 3.85263 -0.60543
6 -1.72912 2.50406 -0.87132
6 -2.73520 1.55250 -1.21311
6 -4.08044 1.95973 -1.32745
6 -4.41292 3.32208 -1.07377

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  6  -0.37535   2.09599  -0.75614
  6  -0.02489   0.72520  -0.94985
  6  -1.03877  -0.23462  -1.24778
  6  -2.38775   0.17931  -1.38481
  6  -5.07061   0.98552  -1.64203
  6  -4.74161  -0.32747  -1.81366
  6  -3.39147  -0.77667  -1.68437
  6  -3.03053  -2.13270  -1.83509
  6  -1.72205  -2.55585  -1.68589
  6  -0.70023  -1.59731  -1.39249
  6   0.65383  -2.00877  -1.26591
  6   1.65811  -1.05704  -0.98729
  6   1.31082   0.31804  -0.82251
  6   2.32264   1.27439  -0.50067
  6   1.97140   2.62300  -0.27406
  6   0.61561   3.03361  -0.39666
  6   0.24666   4.39247  -0.12901
  6  -1.08052   4.77098  -0.23114
  6   1.29131   5.32319   0.24541
  6   2.58048   4.93631   0.34622
  6   2.98316   3.56818   0.09527
  6   4.29719   3.15002   0.21384
  6   4.67064   1.80769  -0.00951
  6   3.67441   0.86239  -0.36972
  6   4.02274  -0.51162  -0.55168
  6   3.01073  -1.46770  -0.86419
  6   5.35959  -0.92739  -0.38283
  6   6.34728   0.04520  -0.04441
  6   6.01837   1.35640   0.13522
  6   3.35055  -2.83736  -1.02066
  6   4.71453  -3.22411  -0.85625
  6   5.67722  -2.30801  -0.54607
  6   1.00551  -3.38958  -1.41334
  6   2.33088  -3.77209  -1.29496
  6  -1.33911  -3.94507  -1.81052
  6  -0.05307  -4.33809  -1.68328
  6  -0.92816   1.55766   2.14874
  6  -1.92513   0.63498   1.91676
  6  -1.58635  -0.75060   1.83681
  6  -0.22761  -1.14457   1.93219
  6   0.77423  -0.16887   2.20885
  6   0.40892   1.15409   2.32322
  6   0.11675  -2.52261   1.75484
  6   1.52513  -2.91337   1.82092
  6   2.49176  -2.03361   2.08246
  6   2.21979  -0.58536   2.37974
  6  -2.60103  -1.73527   1.63944
  6  -2.23199  -3.04359   1.44255
  6  -0.87767  -3.43361   1.48050
  6  -4.05991  -1.33907   1.83045
  6  -4.29329   0.13161   1.55695
  6  -3.31203   1.02962   1.65400
  1  -1.17397   2.62066   2.16260
  1  -2.12289  -4.67375  -2.01292
  1  -3.80552  -2.86430  -2.06865
  1  -1.35982   5.80408  -0.02303
  1   2.59627  -4.82355  -1.40870
  1   0.21600  -5.38872  -1.78323
  1   1.17431   1.90851   2.50691
  1   3.35281   5.65108   0.62636
  1   1.00792   6.35570   0.44448
  1   5.06559   3.86992   0.49636
  1  -5.51337  -1.05845  -2.05336
  1  -6.10665   1.30826  -1.73442
  1  -5.45537   3.62660  -1.15572
  1  -3.72968   5.26466  -0.51085
  1   4.97320  -4.27502  -0.97626
  1   6.71213  -2.62154  -0.41813
  1   7.37821  -0.28406   0.07504
  1   6.78346   2.08441   0.40059
  1  -0.61595  -4.47665   1.30893
  1  -3.00328  -3.79531   1.27974
  1  -4.29479  -1.50795   2.89820
  1  -5.31696   0.43706   1.34563
  1  -3.51053   2.09268   1.50690
  1   1.76240  -3.95570   1.61017
  1   3.53672  -2.34632   2.08409
  1   2.85796   0.04424   1.74328
  1   2.52878  -0.37640   3.41916
  6  -5.00298  -2.21563   1.02368
  6  -5.94692  -2.95909   1.54178
  1  -4.84277  -2.19271  -0.05357
  1  -6.28927  -3.14843   2.55464
Energy      -2291.126021          (Hartree)
Frequencies cm-1:
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30.213	37.523	44.240	48.727	57.719	63.127	75.036	90.462	108.819	115.779
123.557	144.898	161.025	171.710	175.200	179.392	195.073	206.081	214.915	225.857
236.209	249.736	263.332	264.833	274.610	278.347	284.979	296.499	297.369	324.479
328.413	330.814	340.103	351.880	368.800	372.444	377.318	379.256	381.328	382.721
384.129	385.124	409.789	434.043	435.089	446.665	464.601	466.293	476.306	477.950
482.574	489.398	491.235	496.910	515.551	526.106	531.266	532.744	533.706	551.606
553.921	555.927	556.430	560.270	567.260	570.555	573.096	582.254	604.509	607.188
608.719	626.803	633.182	634.995	638.036	638.664	643.598	646.646	649.381	664.881
673.072	693.115	702.540	706.017	709.441	714.049	723.266	729.067	730.956	740.359
755.272	757.813	758.923	764.500	780.008	789.454	797.251	798.188	801.231	803.240
803.674	809.423	815.695	817.517	820.233	826.531	841.948	842.770	848.159	858.130
859.222	863.327	869.027	869.526	880.308	890.686	895.755	901.043	909.185	911.701
936.637	937.894	946.889	947.644	957.392	967.293	973.651	978.839	979.200	980.850
991.016	991.539	992.062	994.179	994.558	1004.171	1005.749	1010.434	1048.542	1048.818
1081.615	1084.656	1090.833	1121.552	1123.179	1131.928	1140.732	1143.229	1153.186	1155.975
1184.736	1189.662	1192.691	1196.753	1202.289	1205.508	1207.170	1214.893	1218.807	1230.971
1232.381	1238.668	1247.115	1250.723	1257.139	1257.803	1260.503	1264.094	1273.364	1278.194
1289.879	1291.329	1294.542	1314.696	1316.043	1328.117	1336.203	1340.861	1345.809	1347.127
1375.584	1377.524	1382.361	1403.530	1409.078	1414.271	1416.107	1418.655	1421.559	1423.273
1432.105	1444.367	1445.578	1449.409	1449.479	1455.142	1455.552	1457.064	1459.403	1459.580
1468.601	1483.173	1492.261	1503.234	1517.824	1519.685	1523.544	1528.880	1536.524	1541.063
1546.980	1549.518	1563.327	1577.287	1577.453	1619.822	1635.759	1656.242	1661.842	1666.150
1671.921	1673.218	1676.948	1679.702	1681.955	1693.505	1698.880	1707.665	1712.116	1716.353
1750.952	1765.574	2992.601	3035.423	3123.362	3124.538	3128.868	3133.189	3136.001	3137.694
3141.626	3143.585	3149.829	3150.580	3154.348	3155.028	3158.829	3159.478	3159.973	3168.226
3181.705	3181.882	3186.535	3188.160	3198.176	3205.247	3206.161	3213.956	3221.630	3225.598
3244.544									

Crowded-cis addition TS

Atom	X	Y	X	(Angstrom)
6	-3.64614	0.96467	1.66027	
6	-2.20961	1.04558	1.93110	
6	-1.46122	-0.16819	2.01643	
6	-2.11604	-1.43936	1.95132	
6	-3.62443	-1.47040	2.16487	
6	-4.30297	-0.19409	1.70809	
6	-0.04750	-0.10259	2.12349	
6	0.60174	1.16042	2.23820	
6	-0.15521	2.30963	2.17181	
6	-1.54896	2.25442	2.00159	
6	-1.35116	-2.57820	1.88866	
6	0.05828	-2.51296	1.93220	
6	0.71481	-1.31389	2.07921	
6	2.17556	-1.22846	2.12236	
6	2.81526	-0.06883	2.27722	
6	2.09966	1.23947	2.45727	
6	-4.35297	-2.69671	1.65452	
6	-4.08620	-3.42708	0.59750	
6	-0.55417	1.75381	-0.98326	
6	-1.92589	2.09879	-1.09506	
6	-2.32211	3.45917	-1.01089	
6	-1.34245	4.44845	-0.78640	
6	-0.00051	4.12835	-0.66755	
6	0.41235	2.76226	-0.78427	
6	-2.90975	1.07867	-1.25348	
6	-4.27268	1.42339	-1.37653	
6	-4.64396	2.80009	-1.31848	
6	-3.71097	3.77624	-1.12971	
6	-0.15518	0.38346	-1.03440	
6	-1.14047	-0.63768	-1.15569	
6	-2.51684	-0.29238	-1.24817	
6	-3.49690	-1.30524	-1.36606	
6	-4.86257	-0.92840	-1.49150	
6	-5.23612	0.38574	-1.50339	
6	1.78490	2.41603	-0.65246	
6	2.18243	1.06280	-0.73689	
6	1.20420	0.04231	-0.92875	
6	1.60111	-1.32825	-0.96884	
6	0.62544	-2.34163	-1.09416	
6	-0.75214	-1.99761	-1.17482	
6	-1.74024	-3.01878	-1.29180	
6	-3.09582	-2.67259	-1.36879	
6	1.02487	-3.71597	-1.09306	
6	-0.00206	-4.72546	-1.20542	
6	-1.30963	-4.39187	-1.30816	
6	2.36738	-4.03750	-0.96141	
6	3.35556	-3.04200	-0.82248	
6	2.96952	-1.67475	-0.83092	
6	3.94745	-0.65594	-0.62823	
6	3.54785	0.71295	-0.57115	
6	4.50739	1.72337	-0.29685	
6	4.08852	3.06765	-0.21022	
6	2.76239	3.42824	-0.38540	
6	2.31466	4.79981	-0.27645	
6	1.01215	5.13010	-0.41298	

6	5.29699	-1.00543	-0.41551
6	6.24476	0.02761	-0.15358
6	5.86755	1.33676	-0.09365
6	5.66596	-2.38348	-0.43824
6	4.73659	-3.36078	-0.63548
1	-2.11530	3.17881	1.89510
1	-2.07137	-5.16610	-1.39285
1	-3.80756	-3.41622	-1.72526
1	-1.65421	5.49012	-0.70561
1	2.66920	-5.08520	-0.95344
1	0.30508	-5.77039	-1.20761
1	0.34159	3.27997	2.21920
1	3.06286	5.56658	-0.08125
1	0.69310	6.16797	-0.32977
1	4.82996	3.83801	0.00270
1	-5.61144	-1.71492	-1.57253
1	-6.28661	0.65760	-1.59734
1	-5.69816	3.05714	-1.41264
1	-4.01099	4.82169	-1.07295
1	5.03161	-4.40917	-0.63895
1	6.71210	-2.64168	-0.28146
1	7.28496	-0.25090	0.00900
1	6.60243	2.11323	0.11312
1	0.63933	-3.43165	1.85047
1	-1.83491	-3.54889	1.80970
1	-3.75186	-1.49199	3.26514
1	-5.36634	-0.24768	1.48204
1	-4.15442	1.88648	1.37579
1	2.73271	-2.15667	1.99173
1	3.90515	-0.03867	2.27992
1	2.53484	1.99498	1.78480
1	2.28498	1.60194	3.48445
1	-5.21734	-2.98860	2.26665
1	-4.60424	-4.31834	0.24845

Energy -2291.117587 (Hartree)

Frequencies cm-1:

-469.408	35.331	40.298	44.717	58.236	62.937	75.420	101.769	107.762	113.661
137.510	146.399	159.101	164.080	180.584	184.013	193.905	200.744	204.838	216.509
221.169	260.617	265.606	267.333	273.699	277.915	284.539	287.212	297.071	319.074
324.360	334.425	339.592	364.762	369.129	375.450	378.534	381.042	383.245	384.735
386.915	400.483	413.117	428.325	445.664	451.854	463.877	469.253	473.140	475.962
485.188	487.123	489.568	500.663	519.305	524.768	531.701	532.839	533.729	547.500
554.889	556.443	557.815	564.204	570.604	573.372	580.943	584.496	601.755	605.956
610.390	624.581	630.280	637.167	638.266	641.183	645.241	646.879	651.128	657.442
672.227	692.000	698.405	701.895	703.028	707.727	711.992	716.869	729.001	739.453
754.077	754.811	758.148	763.234	785.942	790.179	796.810	797.437	803.420	803.840
806.128	811.696	817.134	817.886	824.900	827.691	840.813	846.284	848.405	853.140
854.856	856.398	861.229	868.780	882.701	895.176	899.824	907.399	909.315	919.654
935.819	938.327	946.045	949.969	960.226	963.500	967.976	973.512	973.999	986.850
988.506	989.157	994.116	998.177	998.493	999.827	1004.204	1005.546	1047.129	1049.274
1078.674	1081.947	1088.786	1122.907	1125.590	1131.115	1144.137	1146.160	1148.160	1152.970
1182.515	1187.046	1195.624	1198.227	1199.664	1210.489	1211.811	1214.019	1222.018	1232.049
1232.287	1249.237	1250.385	1251.392	1257.772	1258.907	1259.462	1269.075	1270.562	1279.176
1285.090	1290.974	1301.566	1314.482	1327.891	1330.309	1340.924	1346.064	1349.625	1349.807
1365.977	1371.717	1377.641	1400.704	1406.717	1413.364	1414.130	1416.856	1422.076	1423.419
1429.024	1441.379	1446.196	1447.408	1449.302	1450.359	1453.016	1455.933	1458.800	1462.336
1471.968	1480.243	1487.763	1493.134	1510.459	1515.336	1519.427	1526.280	1535.789	1537.520
1546.584	1552.807	1563.805	1570.734	1576.312	1614.071	1636.919	1640.167	1657.876	1660.169
1664.229	1667.746	1669.379	1671.861	1678.733	1685.025	1691.359	1696.048	1708.438	1729.966
1746.301	1757.149	2975.981	3014.491	3098.061	3107.523	3125.139	3135.431	3136.425	3140.253
3142.375	3145.122	3145.527	3146.329	3155.098	3155.235	3159.804	3160.155	3170.065	3172.703
3177.427	3186.716	3191.759	3199.808	3201.367	3203.396	3207.192	3213.586	3216.588	3227.827
3232.929									

Crowded-cis adduct R-P

Atom	X	Y	X (Angstrom)
6	-3.64453	0.67785	1.74528
6	-2.19931	0.77360	1.95520
6	-1.42676	-0.42897	1.98992
6	-2.05365	-1.70516	1.86740
6	-3.57358	-1.81103	1.94024
6	-4.27589	-0.49423	1.68293
6	-0.01368	-0.34163	2.10790
6	0.61325	0.93298	2.24854
6	-0.16400	2.06758	2.20899
6	-1.56058	1.99024	2.05390
6	-1.26672	-2.83235	1.81692
6	0.13677	-2.74837	1.89033
6	0.77077	-1.53512	2.04440
6	2.23041	-1.42066	2.07407
6	2.84886	-0.25211	2.24726
6	2.10819	1.03466	2.47562
6	-4.16719	-2.96635	1.14711
6	-4.04832	-3.27757	-0.14241
6	-0.54871	1.88228	-0.92828

```
  6  -1.90596   2.26809  -1.00492
  6  -2.26372   3.63926  -0.86368
  6  -1.26662   4.58766  -0.62255
  6   0.07532   4.22521  -0.53047
  6   0.44628   2.85863  -0.69911
  6  -2.92304   1.27737  -1.15871
  6  -4.28389   1.66974  -1.21988
  6  -4.61437   3.06746  -1.11844
  6  -3.65427   4.00373  -0.93675
  6  -0.18893   0.49373  -1.02161
  6  -1.18521  -0.48682  -1.13975
  6  -2.57431  -0.10143  -1.19390
  6  -3.59072  -1.06157  -1.24647
  6  -4.92410  -0.65506  -1.33963
  6  -5.27115   0.68249  -1.33561
  6   1.81564   2.47479  -0.58304
  6   2.18262   1.11325  -0.72013
  6   1.18259   0.12032  -0.93447
  6   1.55199  -1.24751  -1.01371
  6   0.54793  -2.24371  -1.13135
  6  -0.82610  -1.87591  -1.17773
  6  -1.81065  -2.87928  -1.21142
  6  -3.28877  -2.54418  -1.24592
  6   0.92226  -3.62286  -1.14152
  6  -0.10212  -4.59949  -1.19604
  6  -1.42638  -4.22682  -1.22996
  6   2.28094  -3.97401  -1.05515
  6   3.28084  -3.00558  -0.93494
  6   2.91805  -1.62579  -0.90850
  6   3.91619  -0.63728  -0.69259
  6   3.54209   0.73362  -0.58193
  6   4.52735   1.71740  -0.28143
  6   4.13881   3.05801  -0.13901
  6   2.81098   3.45181  -0.28890
  6   2.40300   4.82590  -0.12991
  6   1.10648   5.19236  -0.24820
  6   5.26757  -1.01783  -0.51045
  6   6.23730  -0.01290  -0.22884
  6   5.88526   1.29930  -0.11427
  6   5.61183  -2.39907  -0.58001
  6   4.66202  -3.35370  -0.78489
  1  -2.14621   2.90707   1.98897
  1  -2.19971  -4.99395  -1.26045
  1  -3.67496  -2.94084  -2.20140
  1  -1.54596   5.63391  -0.49766
  1   2.55641  -5.02869  -1.06109
  1   0.17489  -5.65258  -1.20627
  1   0.31222   3.04634   2.28141
  1   3.17116   5.56641   0.08771
  1   0.81216   6.23356  -0.12626
  1   4.89522   3.80770   0.09362
  1  -5.70167  -1.41659  -1.39211
  1  -6.31714   0.97984  -1.39637
  1  -5.66429   3.35237  -1.17180
  1  -3.91472   5.05682  -0.84205
  1   4.93556  -4.40721  -0.81908
  1   6.65586  -2.68037  -0.45076
  1   7.27442  -0.31699  -0.09505
  1   6.63614   2.05569   0.10837
  1   0.73420  -3.65594   1.80960
  1  -1.73571  -3.80708   1.69297
  1  -3.79304  -2.04687   2.99863
  1  -5.34978  -0.53963   1.51190
  1  -4.18981   1.61130   1.60621
  1   2.80445  -2.33328   1.90934
  1   3.93778  -0.19944   2.23281
  1   2.52938   1.82667   1.83657
  1   2.28297   1.35742   3.51804
  1  -4.78374  -3.64528   1.73899
  1  -4.56607  -4.18019  -0.47203
Energy      -2291.190223          (Hartree)
Frequencies cm-1:
    30.978    34.883    41.397    58.209    68.867    77.332    98.774   110.519   122.154   148.363
   151.479   158.975   168.650   179.990   185.267   197.379   205.304   215.513   225.553   245.417
   260.655   268.223   271.649   278.550   286.267   288.675   295.466   311.036   323.695   335.541
   337.344   351.586   366.149   369.424   376.523   380.510   383.486   386.733   390.856   399.623
   412.065   422.258   439.625   455.776   459.893   465.214   473.075   475.433   476.816   482.687
   486.705   510.578   515.941   520.040   521.080   531.956   533.774   541.220   550.156   552.987
   554.716   559.183   564.825   573.547   575.157   582.956   592.933   597.964   610.694   616.246
   624.017   629.919   634.617   638.092   641.226   652.511   657.678   661.093   670.226   688.317
   698.399   701.749   703.965   710.846   715.141   716.073   724.415   741.068   748.368   757.554
   762.149   767.907   776.833   788.288   794.417   796.469   799.819   801.491   805.543   808.029
   812.747   817.446   820.628   824.971   838.904   844.366   845.956   849.071   853.567   861.368
   863.564   867.894   871.341   882.852   890.361   895.944   902.745   905.225   938.720   940.935
   949.895   962.056   966.353   967.957   970.101   971.864   973.243   978.908   983.743   987.326
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 995.206 995.454 996.940 998.169 1001.249 1017.861 1039.469 1044.717 1069.604 1075.203
1094.303 1116.255 1122.588 1127.984 1142.793 1150.331 1152.151 1154.310 1169.160 1182.095
1186.772 1194.649 1200.584 1202.480 1207.486 1215.435 1220.195 1228.121 1234.348 1235.122
1243.947 1245.773 1255.765 1257.467 1258.175 1262.637 1276.111 1277.344 1280.874 1286.294
1298.018 1303.510 1310.735 1316.432 1324.363 1328.649 1332.755 1342.838 1347.865 1353.726
1361.644 1366.960 1375.347 1378.612 1385.113 1394.012 1403.205 1409.044 1411.794 1415.740
1429.029 1430.077 1435.046 1437.825 1445.611 1450.562 1452.927 1453.327 1454.971 1456.756
1458.860 1468.476 1480.596 1483.347 1497.431 1512.376 1514.330 1522.805 1527.975 1531.233
1536.085 1555.189 1572.969 1579.002 1580.358 1591.409 1611.155 1627.097 1630.759 1641.032
1650.895 1659.415 1664.293 1664.978 1668.142 1676.854 1678.031 1690.440 1708.619 1750.119
1759.408 1764.094 3015.605 3025.648 3051.469 3059.581 3118.598 3123.033 3127.874 3134.360
3135.155 3136.634 3136.900 3136.941 3142.710 3154.093 3157.599 3160.612 3160.919 3166.480
3169.686 3179.844 3180.148 3181.508 3181.843 3183.266 3193.395 3217.016 3226.177 3234.553
3244.522

Extended-cis addition TS
Atom   X   Y   X   (Angstrom)
 6 -9.46533   0.48255   0.45750
 6 -8.89502 -0.75215   0.14596
 6 -7.47277 -0.90064   0.13872
 6 -6.64710   0.22413   0.44184
 6 -7.26029   1.48051   0.77122
 6 -8.65500   1.59202   0.77240
 6 -6.41010   2.61063   1.11496
 6 -5.06549   2.52195   1.08372
 6 -4.33614   1.27769   0.65300
 6 -5.22586   0.07738   0.42092
 6 -6.86173 -2.16443 -0.16675
 6 -5.46720 -2.28158 -0.15230
 6 -4.65954 -1.16696   0.14431
 6 -9.78325 -1.92000 -0.17941
 6 -9.06011 -3.19473 -0.48859
 6 -7.71508 -3.30035 -0.48044
 6 -3.26097   0.94096   1.66189
 6 -2.07145   0.50634   1.36497
 6 -1.65071   0.33392 -0.89280
 6 -0.85352 -0.84357 -0.81785
 6   0.55590 -0.72454 -0.58545
 6   1.16023   0.56897 -0.49726
 6   0.36035   1.74463 -0.65334
 6 -1.04876   1.62805 -0.87750
 6   2.56590   0.68856 -0.26408
 6   3.17377   1.98297 -0.18426
 6   2.37648   3.15737 -0.34392
 6   0.96893   3.03837 -0.58054
 6   3.36677 -0.48361 -0.11367
 6   4.77313 -0.36353   0.12435
 6   5.37824   0.92768   0.20908
 6   4.57728   2.10282   0.05269
 6   6.78929   1.04136   0.44871
 6   7.56914 -0.12670   0.59964
 6   6.98338 -1.41353   0.51616
 6   5.57472 -1.53645   0.27568
 6   4.97021 -2.83142   0.18525
 6   5.77150 -4.00484   0.33547
 6   7.17340 -3.85964   0.57685
 6   7.75934 -2.60999   0.66424
 6   3.56415 -2.95189 -0.05706
 6   2.76325 -1.77807 -0.20488
 6   5.18039   3.40342   0.13185
 6   6.59431   3.48821   0.37374
 6   7.36604   2.35521   0.52624
 6   4.37984   4.55608 -0.02862
 6   2.98770   4.45256 -0.26605
 6   1.36021 -1.89898 -0.44578
 6   2.15968   5.61159 -0.43270
 6   0.80134   5.49481 -0.66077
 6   0.17025   4.21306 -0.73854
 6 -1.23328   4.07136 -0.96290
 6 -1.82241   2.82029 -1.02625
 6   0.76195 -3.20079 -0.54621
 6 -0.64790 -3.28745 -0.79922
 6 -1.42383 -2.15170 -0.93146
 6   2.95737 -4.24825 -0.15284
 6   1.56675 -4.35332 -0.39744
 6   5.14617 -5.28722   0.23880
 6   3.78875 -5.40604   0.00275
 1 -9.12438   2.54200   1.01980
 1 -2.49498 -2.23595 -1.12576
 1   4.83926   5.54043   0.03063
 1   1.11076 -5.33813 -0.47240
 1 -1.09774 -4.27532 -0.88593
 1 -10.54712   0.59845   0.46286
 1   8.43669   2.43696   0.70919
 1   7.04728   4.47696   0.43431

1	8.63793	-0.03793	0.78216
1	-2.90132	2.72120	-1.17358
1	-1.83670	4.97007	-1.08019
1	0.18552	6.38449	-0.78543
1	2.62671	6.59361	-0.37539
1	3.32599	-6.38912	-0.06941
1	5.76429	-6.17651	0.35501
1	7.77665	-4.75931	0.69121
1	8.82840	-2.51436	0.84801
1	-4.99811	-3.23895	-0.36798
1	-3.57423	-1.28459	0.17503
1	-3.86192	1.52370	-0.34723
1	-4.42272	3.35699	1.35656
1	-6.91098	3.53406	1.40761
1	-7.21842	-4.24343	-0.70878
1	-9.69943	-4.04353	-0.72338
1	-10.47888	-2.09641	0.67501
1	-10.43244	-1.65196	-1.04638
1	-1.11051	0.18728	1.60046
1	-2.71494	0.23768	-1.11749
1	-3.57430	1.06305	2.70727

Energy -2291.057650 (Hartree)

Frequencies cm-1:

-363.437	10.085	13.083	17.483	21.755	34.571	43.265	56.282	67.988	77.875
88.821	100.126	104.719	108.817	128.545	166.134	172.975	181.379	185.370	189.308
211.854	230.027	247.105	250.990	264.672	277.388	285.582	293.865	296.911	318.945
327.091	328.443	339.474	350.938	358.483	365.191	370.760	372.256	380.222	382.941
384.431	388.047	410.370	427.404	443.689	447.203	464.379	467.756	471.404	473.026
482.058	485.734	490.205	498.397	510.420	526.518	531.870	532.617	533.447	552.208
555.719	557.374	558.354	560.117	566.515	570.569	572.739	582.624	605.055	606.886
608.499	622.928	633.474	638.499	641.280	642.886	644.286	650.825	658.144	664.937
672.538	694.380	703.170	704.605	707.236	724.717	733.018	740.187	741.072	742.928
757.650	760.393	761.598	784.397	793.268	798.273	800.051	803.865	805.471	813.701
814.197	820.956	824.888	827.179	827.390	833.338	840.469	842.802	850.608	852.678
857.256	863.012	868.341	869.445	871.171	881.247	889.574	901.378	926.322	929.765
937.552	938.558	945.986	948.435	949.783	966.381	973.779	974.431	974.733	979.812
990.782	998.656	1000.963	1002.687	1004.929	1008.264	1025.755	1029.806	1046.755	1049.297
1081.162	1086.337	1097.486	1120.735	1123.433	1130.912	1141.610	1145.674	1154.909	1159.591
1182.457	1185.838	1191.788	1195.199	1204.246	1207.029	1213.520	1217.034	1219.481	1228.460
1232.498	1238.843	1246.702	1249.306	1254.545	1257.687	1259.694	1264.497	1270.018	1279.780
1281.700	1290.363	1306.117	1311.740	1319.668	1331.882	1339.823	1344.124	1346.654	1347.884
1364.655	1369.937	1388.713	1401.781	1403.766	1411.290	1416.145	1418.417	1421.189	1424.594
1438.098	1439.439	1442.629	1446.148	1448.372	1451.832	1457.134	1459.825	1460.271	1462.950
1467.903	1479.694	1486.489	1486.551	1513.978	1517.243	1519.679	1523.795	1535.194	1537.693
1544.605	1549.851	1560.841	1574.173	1581.636	1614.808	1635.928	1643.116	1658.745	1666.012
1668.405	1670.061	1673.201	1675.735	1679.262	1683.893	1691.062	1697.388	1710.513	1713.592
1765.374	1772.177	3021.271	3055.600	3071.888	3109.617	3119.241	3125.080	3131.807	3132.001
3135.599	3135.865	3142.885	3143.625	3148.327	3149.107	3149.413	3149.974	3155.303	3160.848
3172.248	3201.191	3218.123	3220.552	3224.798	3225.821	3230.331	3240.639	3241.200	3247.590
3252.386									

Extended-cis adduct R-P

Atom	X	Y	X (Angstrom)
6	3.17319	-5.48790	-0.33652
6	2.51513	-4.21648	-0.31700
6	3.31339	-3.03985	-0.19223
6	4.72797	-3.14905	-0.09399
6	5.34666	-4.42281	-0.11779
6	4.52912	-5.58343	-0.24019
6	2.69463	-1.75954	-0.16797
6	1.28169	-1.65343	-0.26654
6	0.49267	-2.83855	-0.39836
6	1.12692	-4.09420	-0.41929
6	0.65546	-0.37433	-0.23669
6	1.46716	0.80559	-0.12587
6	2.86320	0.69333	-0.03926
6	3.48682	-0.58735	-0.05208
6	0.84483	2.10953	-0.13053
6	1.65981	3.27391	-0.05007
6	3.08134	3.15224	0.04721
6	3.68277	1.87307	0.05509
6	3.89411	4.31923	0.13137
6	5.28114	4.18378	0.22633
6	5.89305	2.93202	0.23691
6	5.08869	1.75796	0.14779
6	4.90642	-0.69560	0.04120
6	5.70566	0.46982	0.14510
6	1.06514	4.56170	-0.06415
6	1.91121	5.72427	0.01820
6	3.25583	5.60945	0.11269
6	7.12230	0.35359	0.23769
6	7.90640	1.56116	0.33378
6	7.32399	2.78184	0.33194
6	-0.54803	2.24747	-0.21687
6	-1.11268	3.52356	-0.22503

```
  6  -0.32915   4.66253  -0.15525
  6  -0.74549  -0.28610  -0.32808
  6  -1.47064   1.04299  -0.26321
  6   7.71066  -0.90920   0.22578
  6   6.94163  -2.07757   0.11845
  6   5.52433  -1.97193   0.02361
  6  -0.91339  -2.70111  -0.50976
  6  -1.50198  -1.45637  -0.47287
  6   6.76578  -4.50206  -0.01987
  6   7.53266  -3.38074   0.09451
  6  -2.34029   1.07153   0.98034
  6  -3.66943   1.04569   1.02638
  6  -4.61773   0.94237  -0.15099
  6  -5.70797  -0.08106   0.14336
  6  -7.08398   0.22160  -0.08009
  6  -7.48570   1.52716  -0.49739
  6  -6.46191   2.56017  -0.66115
  6  -5.16507   2.30735  -0.49446
  6  -8.07228  -0.77501   0.13984
  6  -9.44699  -0.47614  -0.09575
  6  -9.79342   0.78744  -0.51458
  6  -8.82140   1.78770  -0.70565
  6  -7.67561  -2.06781   0.60397
  6  -6.34300  -2.31752   0.84185
  6  -5.36706  -1.32739   0.61511
  6  -8.70363  -3.08695   0.82686
  6  -9.99627  -2.85283   0.60549
  6 -10.51582  -1.53219   0.11101
  1  -9.12982   2.78384  -1.01907
  1  -2.58582  -1.37076  -0.55464
  1   5.89928   5.07938   0.28911
  1   0.51760  -4.99248  -0.51657
  1  -1.52265  -3.59620  -0.62306
  1 -10.84216   1.02218  -0.69442
  1   8.98886   1.46456   0.40420
  1   7.92967   3.68421   0.39918
  1   8.79525  -0.99274   0.29607
  1  -2.19740   3.61320  -0.27115
  1  -0.79164   5.64826  -0.16550
  1   1.43737   6.70466   0.00272
  1   3.88639   6.49503   0.17272
  1   2.56160  -6.38399  -0.42872
  1   5.01377  -6.55863  -0.25780
  1   7.23180  -5.48627  -0.04027
  1   8.61640  -3.45799   0.16674
  1  -6.03815  -3.29597   1.20998
  1  -4.32117  -1.54850   0.82730
  1  -4.05591   0.58580  -1.03232
  1  -4.42461   3.09525  -0.62624
  1  -6.80005   3.56120  -0.92725
  1  -8.36885  -4.05988   1.18505
  1 -10.73414  -3.63503   0.77843
  1 -11.26667  -1.15205   0.82297
  1 -11.05176  -1.69315  -0.83965
  1  -1.77420   1.13391   1.91082
  1  -2.10488   1.13370  -1.15932
  1  -4.16521   1.10512   1.99666
Energy      -2291.155022          (Hartree)
Frequencies cm-1:
     1.721    16.370    23.003    32.538    43.496    50.252    60.836    71.502    78.921    96.041
   100.398   110.293   113.845   162.042   167.572   178.658   189.361   192.607   208.782   228.561
   241.176   256.264   260.973   272.628   275.497   288.890   293.503   316.175   324.252   326.804
   336.541   350.797   362.596   364.217   367.764   376.226   377.651   383.423   386.171   400.216
   414.715   420.579   443.993   452.571   462.696   467.613   470.997   473.957   476.165   483.731
   487.407   499.885   511.128   519.705   522.059   528.621   533.502   548.632   550.710   553.366
   556.532   560.538   568.510   569.430   574.373   577.895   590.790   606.028   614.956   616.973
   623.817   633.209   634.316   638.537   643.007   653.972   660.293   663.435   673.297   677.604
   698.026   703.330   711.579   723.883   729.613   736.790   742.121   746.259   755.016   759.354
   765.184   783.160   786.224   793.637   795.933   798.365   808.072   810.913   811.688   813.372
   820.668   823.501   827.004   828.426   835.782   845.366   847.146   853.963   862.715   864.415
   867.104   872.841   880.439   887.325   909.012   917.663   918.955   938.196   939.792   949.598
   950.678   969.752   971.983   977.499   977.755   979.729   981.491   991.245   992.319   993.887
   999.134  1005.647  1014.344  1017.917  1028.088  1030.322  1042.350  1046.962  1073.215  1090.775
  1106.813  1111.513  1122.951  1127.249  1146.591  1152.593  1155.348  1159.353  1169.474  1182.464
  1190.541  1194.953  1202.120  1205.040  1206.690  1213.347  1215.499  1228.969  1234.520  1240.099
  1241.661  1243.047  1254.327  1255.650  1257.912  1259.108  1262.823  1268.249  1275.503  1280.172
  1282.449  1295.171  1301.918  1308.540  1316.424  1320.619  1330.496  1335.780  1339.504  1345.342
  1358.397  1360.682  1366.706  1384.994  1385.776  1398.539  1401.731  1403.832  1412.229  1415.116
  1424.847  1425.401  1435.348  1439.274  1443.134  1447.165  1451.704  1453.496  1457.437  1460.406
  1462.497  1466.882  1480.303  1488.600  1496.466  1511.723  1517.745  1520.244  1526.512  1529.270
  1535.142  1554.614  1576.742  1579.163  1582.827  1589.377  1610.132  1624.726  1630.429  1639.606
  1649.239  1661.099  1673.057  1675.284  1677.293  1677.693  1679.742  1692.448  1712.931  1753.321
  1764.851  1771.931  3014.386  3042.616  3066.197  3075.157  3120.121  3126.163  3126.564  3130.453
  3139.207  3147.334  3150.428  3151.811  3154.801  3165.597  3165.706  3170.286  3186.277  3188.101
  3190.668  3194.479  3197.039  3200.862  3203.013  3205.558  3206.733  3207.756  3224.755  3227.279
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3234.246

Trans addition TS

Atom	X	Y	X	(Angstrom)
6	9.21463	0.58266	-1.28056	
6	8.13503	-0.45508	-1.03892	
6	6.76397	-0.15040	-1.28491	
6	6.37765	1.13446	-1.77776	
6	7.41443	2.13977	-2.02235	
6	8.70549	1.89871	-1.79875	
6	5.04563	1.39349	-2.01291	
6	4.06053	0.41941	-1.75883	
6	4.39452	-0.82269	-1.27167	
6	5.76588	-1.13213	-1.04084	
6	6.15283	-2.42909	-0.58333	
6	5.11983	-3.44919	-0.40521	
6	3.82591	-3.18812	-0.58851	
6	3.30335	-1.81181	-0.91540	
6	8.46783	-1.70887	-0.58026	
6	7.48629	-2.69406	-0.36225	
6	2.51583	-1.34720	0.32043	
6	2.78641	-0.29478	1.04759	
6	1.25066	-0.02071	2.92338	
6	0.94255	1.32776	2.59096	
6	-0.20933	1.60279	1.81499	
6	-1.06208	0.53998	1.40768	
6	-0.76728	-0.78862	1.79192	
6	0.38791	-1.06168	2.58803	
6	-2.22292	0.81706	0.62667	
6	-3.06988	-0.23031	0.22857	
6	-2.76946	-1.57442	0.60687	
6	-1.62391	-1.85001	1.38744	
6	-1.32853	-3.20117	1.76368	
6	-2.17141	-4.22267	1.35578	
6	-3.32104	-3.96913	0.57931	
6	-3.62362	-2.63349	0.20239	
6	-4.78445	-2.35538	-0.58070	
6	-5.63387	-3.40807	-0.98118	
6	-5.30846	-4.74106	-0.59296	
6	-4.20043	-5.01163	0.15474	
6	-4.23332	0.04805	-0.55333	
6	-5.08714	-1.01128	-0.95603	
6	-6.24320	-0.73108	-1.73252	
6	-7.08177	-1.82062	-2.12201	
6	-6.78857	-3.10229	-1.76093	
6	0.66360	-2.43057	2.94776	
6	-0.14614	-3.44311	2.55951	
6	-0.51658	2.94623	1.44427	
6	-1.67914	3.22346	0.66210	
6	-2.52934	2.16369	0.25388	
6	-3.68055	2.43966	-0.51671	
6	-4.53537	1.37738	-0.92364	
6	1.77876	2.41128	2.98085	
6	1.48360	3.69705	2.62404	
6	0.32965	4.00098	1.84813	
6	-0.00153	5.33615	1.46430	
6	-1.11099	5.60486	0.72050	
6	-1.98795	4.55963	0.29327	
6	-3.14176	4.81264	-0.47595	
6	-3.98370	3.79066	-0.88260	
6	-5.70390	1.64986	-1.70523	
6	-5.98183	3.02543	-2.06007	
6	-5.17214	4.03371	-1.67183	
6	-6.52567	0.60355	-2.09074	
1	7.78575	-3.68334	-0.01943	
1	1.55779	-2.63373	3.53540	
1	2.10042	-0.22053	3.57590	
1	-3.37450	5.84091	-0.75345	
1	-1.94455	-5.25019	1.64056	
1	0.08104	-4.47125	2.83746	
1	9.51410	-1.94821	-0.39117	
1	-6.87172	3.22958	-2.65343	
1	-5.39958	5.06288	-1.94592	
1	-7.41477	0.81335	-2.68533	
1	2.66762	2.19380	3.57153	
1	2.13327	4.51502	2.93104	
1	0.65575	6.14414	1.78161	
1	-1.34997	6.62921	0.43872	
1	-3.96712	-6.03583	0.44164	
1	-5.96822	-5.54817	-0.90740	
1	-7.43847	-3.92096	-2.06579	
1	-7.96740	-1.60425	-2.71723	
1	4.74838	2.36951	-2.39382	
1	3.01169	0.65955	-1.92992	
1	2.58749	-1.88489	-1.75099	

1	3.07817	-3.96827	-0.45012
1	5.44864	-4.44961	-0.12555
1	7.08736	3.10873	-2.39840
1	9.44984	2.67099	-1.98862
1	9.76468	0.75756	-0.34047
1	9.95233	0.17845	-1.99315
1	1.68142	-1.99755	0.60343
1	3.51732	0.50525	0.99192

Energy -2291.082311 (Hartree)

Frequencies cm-1:

-272.422	9.572	14.987	19.458	24.794	41.499	48.839	56.647	72.361	91.502
97.657	104.715	110.870	120.005	136.267	147.789	170.771	180.269	183.888	191.526
194.513	240.938	250.060	252.258	263.665	277.772	285.474	286.555	296.592	314.277
321.114	327.585	339.495	361.886	363.794	369.355	371.223	376.367	380.548	382.547
384.516	398.600	423.905	435.555	446.070	447.990	463.945	469.077	471.720	476.434
488.750	489.502	497.876	500.685	513.303	525.941	531.814	533.285	534.114	555.391
555.575	558.506	559.329	562.468	567.758	570.097	576.214	582.337	603.038	604.767
608.527	629.215	633.347	638.788	639.340	642.828	645.607	650.088	659.019	671.703
679.787	693.688	700.979	703.618	706.832	727.081	730.567	735.069	740.027	740.148
757.573	760.482	766.848	787.922	798.368	803.422	804.376	805.749	810.814	813.644
819.439	825.906	827.669	828.494	828.970	829.755	842.198	854.453	858.294	861.015
863.327	868.047	869.190	872.920	880.064	895.761	908.499	911.305	912.613	921.017
937.722	938.071	938.770	948.383	953.353	969.474	971.799	982.746	983.890	994.049
995.375	996.417	999.608	1005.103	1005.454	1005.968	1007.053	1019.615	1024.297	1037.819
1049.024	1081.595	1086.482	1120.695	1123.453	1129.643	1141.879	1144.899	1156.098	1158.587
1182.524	1184.642	1191.678	1195.808	1205.422	1210.226	1213.684	1215.105	1218.854	1232.669
1232.972	1241.850	1247.236	1249.204	1253.668	1259.416	1263.122	1266.252	1270.462	1279.869
1282.009	1288.220	1288.993	1313.793	1325.776	1331.330	1340.507	1343.253	1346.439	1358.047
1367.941	1370.650	1397.022	1405.226	1406.801	1412.075	1415.414	1418.068	1420.689	1427.344
1440.025	1440.387	1443.371	1446.522	1448.280	1453.001	1456.412	1458.982	1462.402	1464.807
1468.116	1479.609	1487.231	1493.981	1514.516	1518.691	1521.013	1523.957	1535.052	1537.304
1545.909	1549.239	1562.725	1574.954	1581.953	1617.268	1635.265	1644.905	1658.033	1665.304
1668.732	1672.157	1676.402	1676.801	1678.597	1683.918	1691.163	1695.165	1708.310	1720.033
1760.491	1770.908	3020.065	3039.869	3085.367	3106.608	3149.862	3150.332	3151.288	3154.645
3155.494	3164.833	3165.308	3173.461	3180.293	3180.847	3183.971	3184.558	3194.241	3194.585
3195.689	3207.578	3207.899	3210.022	3212.827	3215.353	3216.746	3218.280	3218.431	3221.373
3244.589									

Trans adduct R-P

Atom	X	Y	X (Angstrom)
6	9.46793	0.51478	-0.09976
6	8.36806	-0.50590	-0.32185
6	7.07708	-0.09913	-0.77067
6	6.79659	1.27653	-1.03920
6	7.85803	2.26667	-0.84399
6	9.07471	1.92998	-0.41810
6	5.54123	1.63521	-1.47793
6	4.52897	0.67114	-1.64793
6	4.75963	-0.66020	-1.38932
6	6.05467	-1.06852	-0.95772
6	6.34370	-2.44830	-0.72569
6	5.30030	-3.43961	-0.98739
6	4.07107	-3.09294	-1.36658
6	3.61911	-1.65552	-1.48703
6	8.60395	-1.84181	-0.09216
6	7.60287	-2.80933	-0.30013
6	2.58202	-1.44431	-0.39073
6	2.73615	-0.63772	0.65030
6	1.71232	-0.41298	1.75921
6	1.28908	1.04202	1.65578
6	0.02015	1.39380	1.17150
6	-0.97495	0.38560	0.89327
6	-0.68813	-0.99560	1.16339
6	0.57098	-1.39297	1.64804
6	-2.24197	0.76085	0.41973
6	-3.24376	-0.22301	0.18010
6	-2.97215	-1.59027	0.44848
6	-1.70083	-1.97466	0.95110
6	-1.44081	-3.35142	1.23565
6	-2.44681	-4.30818	1.00358
6	-3.69976	-3.94786	0.50075
6	-3.97278	-2.57510	0.22078
6	-5.24663	-2.19249	-0.28256
6	-6.24446	-3.17146	-0.51225
6	-5.94775	-4.53625	-0.22988
6	-4.73093	-4.91099	0.25676
6	-4.52529	0.16318	-0.31368
6	-5.52136	-0.81876	-0.54910
6	-6.79916	-0.43103	-1.04460
6	-7.78219	-1.44693	-1.26812
6	-7.51309	-2.75855	-1.01223
6	0.80467	-2.74396	1.93784
6	-0.16555	-3.70350	1.74369
6	-0.29857	2.76566	0.97267
6	-1.58107	3.14004	0.46307

```
  6  -2.54778   2.14709   0.18404
  6  -3.81930   2.52247  -0.30695
  6  -4.81182   1.52811  -0.56407
  6   2.20519   2.04589   1.97309
  6   1.90162   3.38492   1.78895
  6   0.65699   3.76969   1.27534
  6   0.31714   5.15022   1.04543
  6  -0.89098   5.50394   0.54904
  6  -1.88964   4.51309   0.24227
  6  -3.14613   4.86172  -0.25837
  6  -4.11418   3.89831  -0.53619
  6  -6.09379   1.90606  -1.05653
  6  -6.35467   3.30559  -1.29127
  6  -5.41777   4.24844  -1.04307
  6  -7.05667   0.92609  -1.29015
  1   7.82770  -3.86086  -0.12770
  1   1.79002  -3.03497   2.30028
  1   2.22111  -0.56236   2.72653
  1  -3.37567   5.91308  -0.43090
  1  -2.24010  -5.35559   1.22181
  1   0.03973  -4.74819   1.97078
  1   9.58855  -2.16045   0.24882
  1  -7.33576   3.58687  -1.67047
  1  -5.63131   5.30117  -1.22017
  1  -8.03628   1.22086  -1.66588
  1   3.18301   1.76484   2.36369
  1   2.63460   4.15113   2.03670
  1   1.06459   5.90755   1.27724
  1  -1.13463   6.55056   0.37449
  1  -4.52061  -5.95759   0.47059
  1  -6.72074  -5.28247  -0.40721
  1  -8.27386  -3.51860  -1.18360
  1  -8.75785  -1.14649  -1.64623
  1   5.32606   2.68183  -1.68881
  1   3.53557   0.98826  -1.96334
  1   3.11251  -1.52341  -2.45800
  1   3.31478  -3.85460  -1.55382
  1   5.56809  -4.48948  -0.87150
  1   7.61598   3.30624  -1.06400
  1   9.83995   2.69321  -0.28401
  1   9.79933   0.46467   0.95131
  1  10.34552   0.24066  -0.70787
  1   1.67901  -2.05019  -0.48404
  1   3.63973  -0.03263   0.73338
Energy      -2291.154644          (Hartree)
Frequencies cm-1:
    10.370    14.104    18.658    22.746    39.189    52.135    61.480    79.694    84.670    98.851
   106.849   125.520   130.150   155.704   168.401   182.263   188.911   190.719   213.251   236.106
   245.288   251.913   260.739   267.208   275.983   287.103   294.773   304.188   310.215   320.189
   331.712   346.760   363.911   366.075   369.874   374.350   380.031   383.313   385.580   397.248
   404.986   419.823   440.877   447.269   459.033   465.740   471.824   472.578   475.857   482.737
   489.614   502.625   510.568   520.495   523.317   531.795   531.939   541.022   553.459   555.031
   559.114   562.228   569.380   574.353   577.165   585.850   595.696   602.739   608.347   609.656
   624.339   631.316   637.852   639.122   642.885   656.918   667.451   670.766   676.332   690.901
   699.891   703.225   705.298   725.153   728.230   730.849   739.420   744.418   756.109   761.209
   773.380   783.924   787.665   798.164   799.565   804.239   809.027   810.474   817.613   821.135
   826.372   826.989   830.010   833.296   838.738   848.924   852.358   857.221   861.531   867.471
   867.558   872.855   882.520   898.933   906.708   915.916   920.593   927.024   937.851   946.138
   951.822   968.774   970.902   974.117   981.289   983.155   985.477   986.642   996.231   996.596
  1000.578  1002.763  1007.814  1008.174  1011.218  1032.785  1033.232  1050.407  1060.799  1074.936
  1094.963  1110.562  1122.891  1131.690  1151.514  1153.650  1154.861  1160.902  1173.993  1184.328
  1190.368  1196.135  1203.020  1207.542  1209.468  1213.175  1217.253  1225.493  1234.634  1238.732
  1241.796  1242.384  1250.674  1255.342  1259.551  1262.736  1266.937  1269.201  1279.138  1280.787
  1283.443  1293.865  1303.762  1313.971  1318.377  1326.412  1334.273  1340.344  1345.418  1350.160
  1360.599  1360.867  1366.926  1379.639  1389.427  1397.149  1402.423  1406.553  1408.368  1415.423
  1427.129  1432.070  1438.164  1441.820  1445.840  1450.032  1454.432  1457.058  1459.936  1461.929
  1466.076  1471.735  1483.450  1492.239  1497.993  1513.029  1521.602  1521.752  1530.164  1531.590
  1536.207  1555.195  1578.673  1581.954  1582.808  1591.330  1613.672  1625.454  1631.446  1641.123
  1651.931  1661.552  1669.130  1676.501  1676.657  1679.857  1680.260  1690.851  1710.074  1756.844
  1765.187  1770.683  3030.157  3035.144  3046.633  3087.512  3123.581  3131.450  3140.669  3145.967
  3148.753  3149.209  3152.174  3152.963  3156.811  3159.013  3159.534  3167.742  3179.423  3190.292
  3190.452  3200.954  3214.957  3215.016  3217.853  3218.484  3221.710  3227.216  3233.817  3241.995
  3256.293
```

System 5:

```
 C18H15   1-H-6-ethyl-pyrenyl radical
 Atom    X         Y         X   (Angstrom)
  6  -0.07083  -0.13278  -0.04933
  6  -0.00378   0.01739   1.40537
  6   1.27338  -0.04879   2.04278
  6   2.46488  -0.16707   1.26592
  6   2.40690  -0.00488  -0.23749
  6   1.02801  -0.20992  -0.80050
```

6	1.34732	-0.03871	3.46027
6	0.15754	0.10278	4.23271
6	-1.05213	0.19900	3.58329
6	-1.13639	0.14086	2.18016
6	2.61965	-0.18826	4.09673
6	2.68256	-0.18892	5.55987
6	1.59736	-0.03977	6.31837
6	0.21939	0.14785	5.74732
6	3.66641	-0.33875	1.91341
6	3.74456	-0.35174	3.32062
6	2.83684	1.46430	-0.61246
6	4.24715	1.78371	-0.26952
1	-1.96628	0.30038	4.16806
1	-2.11263	0.17893	1.69891
1	4.57737	-0.45285	1.32700
1	4.71181	-0.48810	3.80211
1	3.12119	-0.69344	-0.71274
1	0.95076	-0.33549	-1.88024
1	-1.06088	-0.21015	-0.49756
1	-0.45160	-0.62258	6.16174
1	1.68224	-0.04491	7.40406
1	3.66373	-0.31979	6.01497
1	-0.17984	1.11637	6.09401
1	2.67473	1.58386	-1.69511
1	4.50320	2.22186	0.68860
1	2.14073	2.13624	-0.09307
1	5.05509	1.41579	-0.89594

Energy -690.975373 (Hartree)

Frequencies cm-1:

48.026	76.786	88.926	126.104	171.684	193.437	215.889	277.538	303.682	323.830
339.213	382.642	414.065	448.139	465.520	466.989	479.118	496.888	512.667	524.286
535.475	568.780	600.526	651.554	666.811	674.607	716.004	737.550	771.441	782.497
806.446	825.153	829.289	859.600	861.636	902.693	942.781	950.304	960.013	971.519
976.278	987.498	1004.858	1006.611	1022.665	1077.832	1086.080	1148.168	1149.613	1154.835
1202.428	1213.168	1238.683	1252.590	1254.126	1254.911	1264.043	1281.753	1290.973	1321.873
1336.464	1362.338	1396.096	1411.512	1424.668	1436.532	1459.050	1462.682	1487.359	1489.989
1511.494	1517.952	1579.707	1672.656	1675.034	1679.925	1755.842	1765.685	3020.947	3028.110
3050.612	3068.134	3090.366	3138.190	3148.269	3153.997	3155.029	3160.051	3170.202	3173.568
3177.507	3192.344	3341.963							

Complex R:P

Atom	X	Y	X (Angstrom)
6	-3.23043	1.17815	1.64713
6	-1.86809	0.71686	1.92026
6	-1.59338	-0.68300	1.83012
6	-2.65238	-1.62100	1.61372
6	-4.09509	-1.15548	1.78320
6	-4.24557	0.32380	1.52245
6	-0.25069	-1.13295	1.92090
6	0.79165	-0.20380	2.20798
6	0.48425	1.13261	2.33605
6	-0.83302	1.59403	2.16298
6	-2.32784	-2.93865	1.39257
6	-0.99043	-3.38419	1.43287
6	0.03956	-2.52087	1.72444
6	1.43015	-2.97077	1.78621
6	2.43266	-2.13487	2.05498
6	2.22028	-0.68087	2.36850
6	-5.11883	-2.00579	1.00247
6	-5.45417	-3.29469	1.67209
6	-2.67030	1.64432	-1.22335
6	-1.64208	2.56988	-0.87617
6	-1.96639	3.92614	-0.60754
6	-3.32878	4.33788	-0.72272
6	-4.30405	3.45424	-1.08525
6	-4.00466	2.08470	-1.34024
6	-0.29962	2.12757	-0.75466
6	0.71260	3.03901	-0.38685
6	0.37589	4.40561	-0.11568
6	-0.94065	4.81772	-0.22424
6	0.01799	0.74925	-0.95281
6	-1.01775	-0.18375	-1.26025
6	-2.35620	0.26336	-1.39765
6	-3.38225	-0.66707	-1.70090
6	-4.72239	-0.18685	-1.82063
6	-5.01899	1.13414	-1.65108
6	2.05681	2.59395	-0.25757
6	2.37599	1.23799	-0.48914
6	1.34272	0.30887	-0.82203
6	1.65732	-1.07327	-0.99467
6	0.63170	-1.99814	-1.28549
6	-0.71129	-1.55284	-1.41572
6	-1.75408	-2.48381	-1.72380
6	-3.05198	-2.02872	-1.87043
6	0.95151	-3.38548	-1.44471

6	-0.12765	-4.30520	-1.73196
6	-1.40281	-3.88006	-1.86343
6	2.26669	-3.80093	-1.32426
6	3.30700	-2.89385	-1.03599
6	2.99905	-1.51770	-0.86885
6	4.03238	-0.58876	-0.54455
6	3.71638	0.79206	-0.35359
6	4.73341	1.71018	0.01879
6	4.39178	3.06002	0.24831
6	3.08932	3.51153	0.12351
6	2.71914	4.88810	0.37919
6	1.44095	5.30772	0.27096
6	5.35774	-1.03823	-0.37224
6	6.36662	-0.09291	-0.01952
6	6.06868	1.22441	0.16872
6	5.64313	-2.42471	-0.54581
6	4.66039	-3.31478	-0.86893
1	-1.03388	2.66601	2.18487
1	-2.20211	-4.58739	-2.08049
1	-3.84383	-2.73807	-2.11518
1	-1.19530	5.85656	-0.01323
1	2.50673	-4.85734	-1.44786
1	0.11661	-5.36074	-1.84335
1	1.28130	1.85086	2.52992
1	3.50683	5.58158	0.66935
1	1.18219	6.34592	0.47386
1	5.17566	3.75875	0.54068
1	-5.51115	-0.90136	-2.05362
1	-6.04698	1.48263	-1.74098
1	-5.33829	3.78482	-1.16990
1	-3.57501	5.37840	-0.51625
1	4.89393	-4.37055	-0.99732
1	6.66942	-2.76425	-0.41528
1	7.38811	-0.44876	0.10418
1	6.84940	1.93088	0.44590
1	-0.77167	-4.43423	1.24469
1	-3.11995	-3.66446	1.21353
1	-4.33242	-1.29422	2.85787
1	-5.24809	0.68802	1.29782
1	-3.37969	2.25084	1.51026
1	1.62381	-4.02002	1.56603
1	3.46352	-2.49024	2.05343
1	2.87954	-0.07005	1.73495
1	2.54277	-0.49474	3.40827
1	-6.03654	-1.39775	0.87446
1	-5.48370	-3.34509	2.75749
1	-4.72803	-2.18676	-0.00619
1	-5.94449	-4.08993	1.11773

Energy -2292.363777 (Hartree)

Frequencies cm-1:

30.206	38.574	44.604	56.666	59.199	74.180	89.286	106.503	112.607	120.165
126.164	146.057	162.536	172.470	175.782	183.127	194.629	206.748	212.582	221.348
234.320	252.107	262.539	264.571	268.425	278.030	284.544	294.111	296.401	300.300
309.604	327.723	331.308	339.353	357.581	368.509	374.009	377.928	380.740	381.915
383.937	384.916	402.438	412.096	433.581	437.435	445.708	463.220	463.521	476.399
478.065	485.235	488.654	491.578	508.171	514.185	519.885	525.104	530.407	532.021
533.670	546.366	552.844	555.629	556.660	560.454	564.880	569.785	574.285	581.055
602.722	604.118	607.830	627.976	633.065	635.081	637.682	639.388	643.722	647.558
650.531	662.537	671.177	691.829	701.481	706.121	710.666	714.835	724.149	730.943
736.628	740.060	757.410	757.500	761.114	779.214	792.396	793.760	799.051	801.484
804.052	804.693	808.842	810.787	819.351	821.998	824.766	841.376	845.829	850.236
855.701	857.684	860.402	862.866	868.551	874.107	876.789	887.077	901.484	904.098
915.080	936.851	937.916	943.857	947.386	959.718	965.600	969.749	977.885	980.535
984.290	992.207	995.039	996.193	997.220	999.762	1002.231	1005.628	1007.618	1048.194
1050.322	1081.790	1084.568	1106.663	1111.743	1122.358	1124.569	1131.796	1144.545	1146.156
1152.842	1159.555	1186.035	1191.139	1195.215	1198.852	1200.383	1207.147	1212.880	1212.960
1214.874	1221.348	1234.243	1235.076	1249.642	1252.210	1254.365	1257.491	1260.525	1261.158
1274.022	1281.952	1289.290	1290.712	1292.243	1317.527	1326.076	1336.521	1341.935	1346.012
1346.563	1348.031	1365.867	1376.096	1377.674	1385.871	1400.553	1409.376	1415.085	1416.475
1417.736	1423.041	1424.128	1432.243	1444.907	1447.231	1449.692	1450.157	1453.476	1455.685
1456.856	1458.089	1460.099	1470.250	1483.803	1491.755	1493.288	1499.581	1503.409	1512.072
1520.233	1523.319	1529.334	1537.083	1541.130	1547.682	1550.258	1564.495	1576.388	1578.654
1620.405	1636.483	1655.515	1661.839	1666.143	1670.772	1674.028	1675.758	1679.507	1682.373
1693.525	1698.354	1706.692	1711.169	1750.527	1765.530	2965.013	2986.974	3027.053	3128.422
3131.175	3134.568	3135.137	3138.173	3138.464	3140.302	3143.561	3145.178	3145.381	3145.516
3145.781	3151.506	3161.765	3162.819	3163.665	3166.760	3169.180	3170.240	3176.503	3180.735
3188.367	3203.341	3207.474	3207.601	3210.424	3223.024	3293.025			

Gauche Addition TS

Atom	X	Y	X (Angstrom)
6	2.22493	-3.52629	1.77300
6	3.04237	-2.27324	1.53606
6	2.44154	-0.98468	1.62335
6	1.03172	-0.85413	1.82115
6	0.21345	-2.06410	1.91256

```
6   0.74581  -3.28641   1.87994
6   0.48000   0.40365   1.89428
6   1.28678   1.55673   1.84029
6   2.65023   1.47461   1.67870
6   3.24320   0.18325   1.52127
6   4.64593   0.04449   1.29880
6   5.47630   1.24824   1.27973
6   4.98219   2.45152   1.57117
6   3.52578   2.70714   1.86769
6   4.39243  -2.36422   1.28444
6   5.19041  -1.21358   1.15893
6   3.04786   3.95681   1.08785
6   3.53793   4.00792  -0.31712
6   2.15960   2.80129  -1.79237
6   2.57673   1.43461  -1.73463
6   1.62897   0.42869  -1.42740
6   0.28345   0.77935  -1.13227
6  -0.08243   2.14303  -1.05436
6   0.85518   3.15714  -1.41966
6  -0.68336  -0.23743  -0.89044
6  -1.99493   0.11019  -0.52601
6  -2.35768   1.48562  -0.39634
6  -1.40914   2.49647  -0.67736
6  -1.79898   3.87333  -0.60315
6  -3.08838   4.19940  -0.20993
6  -4.04256   3.20754   0.09401
6  -3.67883   1.83829  -0.01472
6  -4.64377   0.81839   0.24604
6  -5.95600   1.16889   0.62792
6  -6.29322   2.54945   0.74518
6  -5.37875   3.52747   0.48680
6  -2.96368  -0.90964  -0.27486
6  -4.28299  -0.55656   0.11075
6  -5.24421  -1.57385   0.35693
6  -6.56342  -1.18406   0.74350
6  -6.90217   0.13059   0.87408
6   0.41802   4.52933  -1.38653
6  -0.82641   4.87329  -0.97728
6   2.01019  -0.94555  -1.46752
6   1.03161  -1.96568  -1.26521
6  -0.31442  -1.61453  -0.99221
6  -1.27872  -2.62296  -0.77249
6  -2.60850  -2.27082  -0.41142
6   3.91788   1.04647  -2.00515
6   4.29706  -0.26617  -1.96608
6   3.35136  -1.29790  -1.72057
6   3.70718  -2.68071  -1.75768
6   2.77407  -3.65776  -1.58651
6   1.40404  -3.33279  -1.33387
6   0.42276  -4.32325  -1.12774
6  -0.89671  -3.99854  -0.85566
6  -3.58356  -3.28837  -0.15604
6  -3.17416  -4.67054  -0.28393
6  -1.90695  -5.00464  -0.61051
6  -4.86798  -2.92552   0.21557
1   6.26047  -1.31577   0.97962
1   1.12858   5.30066  -1.68239
1   2.74668   3.48892  -2.39721
1   0.71466  -5.37326  -1.17885
1  -3.38020   5.24806  -0.15119
1  -1.12682   5.91940  -0.93994
1   4.85282  -3.34823   1.19327
1  -3.92047  -5.44226  -0.10172
1  -1.61543  -6.05093  -0.69154
1  -5.60935  -3.70132   0.40683
1   4.65196   1.82056  -2.22416
1   5.33507  -0.54305  -2.14551
1   4.74937  -2.93858  -1.94204
1   3.05711  -4.70898  -1.63530
1  -5.65568   4.57706   0.57137
1  -7.30843   2.81133   1.03967
1  -7.91320   0.40962   1.16685
1  -7.30034  -1.96353   0.93003
1  -0.59939   0.51038   2.00535
1   0.80704   2.52684   1.96302
1   3.45540   2.96261   2.94051
1   5.63921   3.32206   1.60319
1   6.53957   1.11984   1.07622
1  -0.86625  -1.92967   1.99052
1   0.10368  -4.16420   1.93943
1   2.42700  -4.24953   0.96716
1   2.57481  -3.99926   2.70791
1   1.94844   4.02640   1.10142
1   3.41391   4.85047   1.62656
1   4.43576   3.44873  -0.56990
```

```
  1   3.40383   4.94996  -0.84701
Energy      -2292.341298          (Hartree)
Frequencies cm-1:
  -477.042    21.772    33.081    40.866    47.807    57.973    68.255    82.733    91.529   104.207
   129.658   143.754   147.081   155.961   177.042   183.216   188.441   197.847   208.672   210.297
   225.926   251.772   259.278   262.800   266.837   278.063   287.389   290.328   294.750   318.143
   325.688   330.910   339.534   364.584   366.675   370.498   373.877   378.394   381.954   384.007
   388.372   397.249   411.314   430.504   432.062   446.475   461.093   464.035   473.281   473.434
   483.113   487.216   488.156   506.113   512.455   522.266   523.667   530.079   532.000   547.187
   552.665   553.578   557.424   560.928   564.202   569.479   573.702   579.509   595.702   599.435
   601.877   608.760   624.526   628.294   635.613   637.620   640.588   645.784   647.058   664.861
   666.674   685.360   689.745   699.050   704.189   715.337   715.798   727.184   729.237   735.927
   754.103   759.073   760.984   773.092   787.298   791.973   796.879   800.638   801.032   803.367
   804.645   806.628   812.028   819.761   820.785   824.125   826.380   836.073   845.399   848.430
   851.208   858.111   860.479   866.072   867.846   876.691   902.360   905.718   908.288   915.073
   933.683   936.915   942.975   945.765   948.036   970.559   974.135   974.977   976.506   982.915
   983.190   990.953   992.378   994.316   997.351  1001.423  1004.939  1008.137  1019.046  1025.255
  1047.137  1080.874  1085.186  1101.619  1120.134  1123.328  1125.878  1131.897  1144.677  1150.504
  1156.220  1164.432  1183.099  1191.495  1195.413  1196.962  1202.892  1203.763  1207.622  1210.066
  1221.054  1229.989  1238.469  1246.762  1248.456  1251.475  1252.242  1257.312  1258.816  1268.199
  1271.304  1279.747  1281.964  1291.136  1292.508  1312.486  1322.774  1327.020  1339.921  1343.006
  1347.033  1353.802  1362.776  1366.661  1377.434  1387.751  1399.437  1402.523  1408.435  1413.509
  1416.661  1418.241  1421.532  1434.263  1438.228  1441.991  1446.180  1447.706  1452.315  1455.258
  1458.625  1459.863  1462.281  1468.488  1476.796  1487.108  1489.990  1491.792  1494.897  1510.325
  1517.369  1519.906  1523.828  1534.058  1535.528  1543.986  1548.218  1562.308  1573.384  1579.825
  1611.697  1631.867  1635.110  1657.705  1659.269  1665.276  1667.436  1669.289  1674.998  1675.308
  1680.216  1687.926  1695.353  1710.525  1751.902  1760.674  3003.505  3019.025  3024.500  3052.246
  3066.135  3134.373  3144.244  3154.025  3155.361  3156.110  3159.471  3160.036  3162.470  3175.722
  3178.898  3179.374  3181.796  3184.491  3184.780  3193.408  3194.227  3198.065  3199.126  3199.824
  3200.287  3203.830  3207.817  3212.846  3225.896  3226.330  3272.334

 Gauche Adduct R-P
 Atom    X         Y         X   (Angstrom)
  6  -5.42685   3.53671   0.52874
  6  -4.08240   3.21514   0.15516
  6  -3.72767   1.84181  -0.00255
  6  -4.70582   0.83081   0.21022
  6  -6.02745   1.18346   0.57801
  6  -6.35613   2.56131   0.73044
  6  -2.40097   1.48511  -0.37378
  6  -1.42707   2.49682  -0.59075
  6  -1.80102   3.86881  -0.43831
  6  -3.11588   4.19870  -0.06500
  6  -0.09448   2.14887  -0.96198
  6   0.25842   0.76343  -1.09383
  6  -0.71477  -0.23270  -0.89063
  6  -2.04697   0.11886  -0.53270
  6   1.62802   0.39442  -1.35969
  6   1.97693  -0.98377  -1.41084
  6   0.97956  -1.99185  -1.23297
  6  -0.36072  -1.62308  -0.98056
  6   1.33811  -3.36906  -1.28244
  6   0.35672  -4.34102  -1.07470
  6  -0.96978  -3.99897  -0.82131
  6  -1.33728  -2.62399  -0.76271
  6  -3.02635  -0.89585  -0.30754
  6  -2.67710  -2.26308  -0.43394
  6   3.32407  -1.37154  -1.62087
  6   3.66080  -2.76934  -1.65603
  6   2.71377  -3.72441  -1.51060
  6  -3.65790  -3.27199  -0.20044
  6  -3.25970  -4.65415  -0.30531
  6  -1.98376  -4.99768  -0.59251
  6   2.62696   1.37234  -1.53093
  6   3.93865   0.96169  -1.77490
  6   4.28854  -0.37633  -1.79863
  6   0.85755   3.16710  -1.17665
  6   2.28194   2.85151  -1.59105
  6  -4.95693  -2.90294   0.13858
  6  -5.32628  -1.55659   0.27543
  6  -4.35096  -0.54123   0.05676
  6  -0.82123   4.85958  -0.68475
  6   0.45854   4.50698  -1.04983
  6  -6.98564   0.15008   0.78380
  6  -6.65293  -1.16416   0.63923
  6   3.30536   3.77628  -0.87580
  6   3.17380   3.92752   0.64337
  6   3.70197   2.75441   1.49764
  6   2.80240   1.52426   1.53184
  6   3.36902   0.21089   1.47445
  6   4.76433   0.02399   1.24144
  6   5.60680   1.19976   1.02770
  6   5.12838   2.43916   1.12835
  6   2.54002  -0.92936   1.64611
  6   3.10591  -2.23547   1.60915
```

6	4.45777	-2.37333	1.38429
6	5.28335	-1.25237	1.19899
6	1.13331	-0.75427	1.84033
6	0.61758	0.52097	1.87935
6	1.44913	1.64985	1.74688
6	0.27855	-1.93677	1.95083
6	0.77382	-3.17527	1.93830
6	2.24497	-3.46066	1.83384
1	6.34893	-1.38961	1.01672
1	1.18254	5.29652	-1.24090
1	2.34917	3.11321	-2.66511
1	0.63688	-5.39476	-1.10981
1	-3.38447	5.24858	0.04797
1	-1.09652	5.90841	-0.58953
1	4.89191	-3.37257	1.34367
1	-4.01574	-5.41919	-0.13620
1	-1.69362	-6.04559	-0.65519
1	-5.70409	-3.67738	0.31089
1	4.71596	1.70323	-1.93568
1	5.32611	-0.66491	-1.96154
1	4.70478	-3.03729	-1.81280
1	2.97265	-4.78198	-1.55206
1	-5.69109	4.58607	0.64723
1	-7.37534	2.82246	1.01186
1	-8.00005	0.43185	1.06219
1	-7.39666	-1.94257	0.80027
1	-0.45752	0.66098	1.99851
1	0.99245	2.63671	1.81073
1	3.73051	3.13602	2.53608
1	5.78795	3.29612	0.97948
1	6.65635	1.02577	0.78840
1	-0.79695	-1.76873	2.02199
1	0.10604	-4.03285	2.00808
1	2.42280	-4.17089	1.00981
1	2.57862	-3.96675	2.75688
1	2.13211	4.14659	0.90761
1	3.76100	4.81293	0.93048
1	4.32287	3.44723	-1.11821
1	3.20632	4.77581	-1.31971

Energy -2292.410074 (Hartree)

Frequencies cm-1:

26.031	30.695	43.651	58.746	70.492	72.450	96.592	105.699	131.945	137.821
154.113	159.252	161.245	173.628	187.007	192.030	199.526	221.168	228.691	253.094
258.279	268.318	274.605	276.471	285.448	289.936	295.795	314.387	322.881	326.273
335.703	361.098	365.189	371.315	373.181	377.537	378.958	382.858	389.142	399.032
406.130	410.921	431.643	438.952	453.590	463.587	468.229	475.516	479.863	481.618
483.011	507.486	511.037	516.037	518.724	527.427	531.886	537.066	546.275	550.224
552.387	553.171	559.545	573.102	573.861	582.183	582.865	595.775	598.073	605.958
618.086	625.425	633.609	637.714	639.343	649.948	659.908	661.520	667.392	678.706
691.000	698.894	702.036	709.713	719.479	724.393	731.586	732.544	751.358	755.225
763.065	768.191	784.388	789.703	791.602	797.511	801.412	803.416	806.293	811.934
816.316	819.499	821.679	825.506	826.652	831.935	848.767	850.746	852.091	853.902
861.827	865.415	870.681	875.917	884.028	909.678	919.324	925.141	931.191	936.889
939.187	943.563	963.970	965.549	969.320	974.085	975.849	978.578	984.556	987.534
991.038	998.572	1003.046	1004.366	1005.883	1006.931	1023.944	1042.342	1068.000	1082.800
1088.204	1105.820	1123.481	1128.177	1134.354	1150.550	1154.690	1156.803	1158.590	1173.887
1186.737	1191.306	1195.139	1201.513	1205.479	1207.771	1212.790	1222.756	1226.872	1234.168
1236.735	1238.903	1244.096	1250.862	1253.048	1258.866	1261.487	1264.046	1272.706	1278.382
1280.727	1286.823	1292.497	1304.763	1311.021	1314.531	1320.044	1330.536	1334.909	1343.009
1349.238	1358.519	1361.262	1366.281	1375.064	1384.316	1389.545	1398.864	1399.155	1407.016
1409.979	1413.794	1417.634	1427.247	1429.357	1436.329	1437.162	1444.781	1448.593	1453.714
1455.104	1455.485	1461.479	1461.843	1470.349	1475.294	1482.330	1496.321	1512.762	1516.689
1518.308	1525.016	1527.094	1529.098	1534.617	1537.717	1555.521	1577.488	1579.048	1580.791
1590.918	1612.209	1625.981	1628.637	1637.930	1651.593	1663.114	1667.419	1671.473	1674.128
1676.680	1678.864	1691.588	1710.631	1749.997	1765.997	2980.374	2999.598	3017.197	3043.484
3093.569	3104.082	3111.868	3130.403	3132.111	3133.444	3138.802	3140.371	3142.126	3146.755
3151.600	3157.076	3168.107	3169.679	3175.503	3176.604	3177.547	3183.727	3196.162	3196.967
3200.717	3203.699	3211.701	3223.072	3239.858	3244.375	3261.397			

Syn addition TS

Atom	X	Y	X (Angstrom)
6	0.48479	1.20944	2.27587
6	0.88563	-0.10393	2.19287
6	-0.09698	-1.12187	2.01388
6	-1.47423	-0.77717	1.94840
6	-1.84620	0.60057	2.00352
6	-0.87232	1.56147	2.16328
6	-3.26503	0.94650	1.92774
6	-4.21833	0.01591	1.94135
6	-3.95021	-1.47067	1.94863
6	-2.46707	-1.80517	1.90703
6	0.29033	-2.49637	1.94749
6	-0.68595	-3.46568	1.93778
6	-2.04823	-3.11665	1.97885
6	2.34852	-0.46764	2.33476

```
  6   2.66143  -1.91194   2.06211
  6   1.71320  -2.83611   1.91420
  6  -4.83620  -2.09042   0.80571
  6  -4.28413  -3.16010  -0.06778
  6  -3.09791  -2.13729  -1.84104
  6  -1.76907  -2.55450  -1.64672
  6  -0.76416  -1.59873  -1.31629
  6  -1.10709  -0.23229  -1.17144
  6  -2.46264   0.17441  -1.30832
  6  -3.45138  -0.76517  -1.68939
  6  -0.09715   0.73329  -0.90844
  6  -0.45292   2.10405  -0.71246
  6  -1.81393   2.49684  -0.77055
  6  -2.81841   1.54088  -1.10600
  6   1.25038   0.34141  -0.82976
  6   2.26409   1.31393  -0.57224
  6   1.90884   2.66249  -0.34585
  6   0.54208   3.05501  -0.40239
  6   2.92394   3.62222  -0.03385
  6   4.24892   3.22124   0.02505
  6   4.62657   1.88123  -0.19701
  6   3.62519   0.91853  -0.49555
  6   3.97906  -0.45607  -0.66151
  6   5.32674  -0.85556  -0.53907
  6   6.31847   0.13431  -0.27019
  6   5.98491   1.44615  -0.10566
  6   2.96400  -1.42885  -0.90391
  6   1.60286  -1.03274  -0.97783
  6   0.16900   4.40821  -0.11895
  6   1.21775   5.35444   0.19641
  6   2.51613   4.98585   0.22945
  6  -1.16837   4.76986  -0.15650
  6  -2.17550   3.84195  -0.49027
  6   0.59638  -1.99933  -1.20341
  6  -3.55601   4.20815  -0.56623
  6  -4.50615   3.30249  -0.93331
  6  -4.16532   1.94661  -1.22504
  6  -5.13476   0.99270  -1.63419
  6  -4.78514  -0.30810  -1.87937
  6   0.95645  -3.37837  -1.34298
  6  -0.09417  -4.32917  -1.61273
  6  -1.37984  -3.93207  -1.77836
  6   3.30957  -2.80059  -1.03758
  6   2.29083  -3.74921  -1.25211
  6   5.64962  -2.23737  -0.67716
  6   4.68369  -3.17011  -0.91971
  1  -1.15856   2.61421   2.18547
  1  -2.15473  -4.66317  -2.00927
  1  -3.77853  -2.79375  -2.38040
  1  -1.44960   5.80017   0.06279
  1   2.56172  -4.79990  -1.35865
  1   0.17651  -5.37942  -1.70955
  1   1.23214   1.99213   2.40593
  1   3.29206   5.71360   0.46242
  1   0.93095   6.38402   0.40584
  1   5.02075   3.95424   0.26024
  1  -5.53812  -1.02753  -2.20314
  1  -6.16699   1.31701  -1.75717
  1  -5.55063   3.60208  -1.00737
  1  -3.83109   5.23777  -0.34171
  1   4.94776  -4.22169  -1.02105
  1   6.69225  -2.53830  -0.58579
  1   7.35746  -0.18212  -0.19087
  1   6.75326   2.18791   0.10658
  1  -0.39899  -4.51652   1.92685
  1  -2.78755  -3.90964   2.08175
  1  -4.33356  -1.88060   2.89805
  1  -5.26853   0.30945   1.90433
  1  -3.52065   2.00600   1.87305
  1   1.97123  -3.87852   1.73038
  1   3.71541  -2.18416   1.99332
  1   2.94932   0.17166   1.67339
  1   2.67283  -0.23017   3.36355
  1  -5.78029  -2.43696   1.26098
  1  -3.38842  -3.70893   0.18669
  1  -5.12565  -1.25492   0.14931
  1  -5.00952  -3.68950  -0.68530
Energy      -2292.345593          (Hartree)
Frequencies cm-1:
  -482.787    36.083    41.700    48.503    56.948    60.754    76.116    82.420    85.704   104.044
   122.573   141.761   162.134   171.601   177.584   187.660   200.695   208.933   213.299   234.118
   237.683   251.136   263.170   267.413   275.819   278.274   291.089   297.159   304.922   324.629
   329.916   336.259   339.898   353.697   367.492   369.935   376.206   381.881   382.824   385.821
   387.770   388.599   424.344   427.999   433.508   447.058   463.861   466.448   474.370   479.917
   485.667   487.650   490.124   505.212   511.065   523.576   526.317   530.745   531.950   536.759
```

553.154	555.555	557.724	563.302	565.496	570.843	572.598	575.113	581.449	599.789
603.104	609.687	624.081	629.129	635.318	638.571	640.903	646.260	648.882	654.236
672.435	678.356	690.963	700.112	704.740	708.511	711.376	719.905	729.660	735.391
749.927	755.506	759.259	766.685	770.683	776.790	789.434	791.493	797.003	801.251
803.806	808.198	809.994	815.423	816.893	820.750	824.034	828.202	842.686	845.470
856.003	857.028	862.555	869.152	877.866	888.261	890.088	897.120	899.123	913.308
937.210	938.357	940.874	944.374	948.006	951.767	973.266	977.960	981.740	985.223
987.354	991.545	993.976	994.891	997.438	999.367	1001.670	1004.175	1008.637	1025.552
1047.986	1080.721	1086.327	1090.146	1120.532	1124.755	1125.543	1130.989	1142.365	1153.407
1156.753	1161.498	1182.708	1185.905	1191.014	1196.934	1200.953	1204.651	1207.612	1218.522
1222.333	1227.339	1237.761	1243.157	1247.228	1249.324	1252.467	1256.569	1260.111	1267.236
1270.135	1278.523	1284.756	1288.914	1311.225	1311.782	1325.355	1325.999	1337.894	1340.855
1346.543	1348.641	1359.619	1366.701	1384.912	1399.884	1401.751	1407.293	1412.830	1416.390
1418.968	1419.594	1425.140	1435.182	1435.961	1442.591	1445.211	1447.555	1451.383	1455.320
1456.693	1459.495	1462.187	1467.667	1474.648	1485.258	1488.753	1489.599	1509.780	1516.823
1520.813	1522.893	1525.082	1533.655	1535.891	1543.274	1549.009	1561.065	1572.426	1581.724
1609.809	1631.018	1632.746	1655.273	1659.065	1662.220	1666.059	1669.139	1675.073	1678.075
1678.502	1689.281	1694.320	1712.815	1757.280	1768.436	3020.099	3025.554	3048.174	3067.365
3124.196	3134.678	3135.439	3136.057	3137.666	3140.952	3144.803	3149.150	3153.789	3156.875
3158.136	3158.602	3159.229	3160.212	3162.663	3163.834	3186.890	3189.291	3192.090	3193.988
3195.800	3198.601	3210.746	3218.514	3225.753	3232.770	3321.413			

Syn Adduct R-P

Atom	X	Y	X	(Angstrom)
6	4.63751	-3.24676	-0.95662	
6	3.26769	-2.84744	-1.05331	
6	2.94876	-1.46587	-0.89509	
6	3.98481	-0.52413	-0.64810	
6	5.33048	-0.95397	-0.54764	
6	5.62428	-2.33802	-0.71028	
6	1.59332	-1.03696	-0.95233	
6	0.55698	-1.98398	-1.16550	
6	0.89012	-3.36460	-1.32351	
6	2.23611	-3.76630	-1.26466	
6	-0.80300	-1.56222	-1.21832	
6	-1.11141	-0.16603	-1.07889	
6	-0.08311	0.76237	-0.85989	
6	1.27300	0.33524	-0.78958	
6	-2.48007	0.28147	-1.17145	
6	-2.77674	1.66473	-1.02181	
6	-1.73206	2.59623	-0.73730	
6	-0.39130	2.15506	-0.67332	
6	-2.04263	3.96549	-0.49229	
6	-1.01397	4.85860	-0.18295	
6	0.31529	4.44505	-0.12581	
6	0.63604	3.07816	-0.37637	
6	2.31101	1.28115	-0.53571	
6	1.99493	2.64376	-0.31193	
6	-4.11653	2.12179	-1.10939	
6	-4.40075	3.51338	-0.87604	
6	-3.41587	4.38926	-0.56813	
6	3.03237	3.57502	-0.01740	
6	2.67346	4.95170	0.22424	
6	1.38624	5.36207	0.17688	
6	-3.52565	-0.62378	-1.40028	
6	-4.82933	-0.14250	-1.54844	
6	-5.12848	1.20035	-1.40075	
6	-1.82290	-2.51042	-1.41751	
6	-3.28125	-2.10848	-1.53669	
6	4.35402	3.13836	0.03788	
6	4.69296	1.79478	-0.17905	
6	3.66233	0.85449	-0.46788	
6	-0.16384	-4.28388	-1.54794	
6	-1.47115	-3.85718	-1.60131	
6	6.34583	0.01044	-0.28120	
6	6.04403	1.32763	-0.10417	
6	-4.22251	-2.95745	-0.61341	
6	-4.85224	-2.33896	0.65328	
6	-3.99919	-1.52759	1.67948	
6	-2.51745	-1.86126	1.70006	
6	-1.54087	-0.83600	1.89602	
6	-1.92465	0.53727	1.98491	
6	-3.33211	0.88604	1.79005	
6	-4.26694	-0.04303	1.59992	
6	-0.16620	-1.17863	2.00189	
6	0.80683	-0.16240	2.23250	
6	0.39613	1.14731	2.33721	
6	-0.96007	1.49658	2.20587	
6	0.23014	-2.54682	1.87610	
6	-0.73381	-3.51254	1.70331	
6	-2.09655	-3.17033	1.64546	
6	1.65369	-2.88299	1.90288	
6	2.59365	-1.96002	2.10264	
6	2.27233	-0.51729	2.37130	
1	-1.25015	2.54736	2.24444	

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  1  -2.25802  -4.58535  -1.79706
  1  -3.56512  -2.37079  -2.57183
  1  -1.25535   5.90386   0.01031
  1   2.47721  -4.82234  -1.38654
  1   0.07666  -5.33566  -1.69416
  1   1.13759   1.93114   2.49313
  1   3.47238   5.65682   0.44812
  1   1.13102   6.40377   0.36530
  1   5.14417   3.85523   0.26080
  1  -5.62741  -0.84742  -1.78098
  1  -6.15478   1.55019  -1.50114
  1  -5.43649   3.84372  -0.94044
  1  -3.64098   5.43762  -0.37924
  1   4.87665  -4.30199  -1.07856
  1   6.66180  -2.66072  -0.63594
  1   7.37824  -0.33007  -0.21675
  1   6.83013   2.05183   0.10299
  1  -0.43617  -4.55593   1.61042
  1  -2.83180  -3.96902   1.55938
  1  -4.38858  -1.82873   2.67075
  1  -5.30480   0.24886   1.43938
  1  -3.58646   1.94663   1.76943
  1   1.92229  -3.92122   1.70988
  1   3.64965  -2.23088   2.06981
  1   2.86439   0.11874   1.69704
  1   2.60487  -0.26748   3.39409
  1  -5.30938  -3.18906   1.18030
  1  -3.66934  -3.85999  -0.33733
  1  -5.68938  -1.69385   0.35705
  1  -5.07295  -3.30079  -1.22027
Energy      -2292.408043          (Hartree)
Frequencies cm-1:
    34.427    41.913    52.140    60.743    65.377    88.082   106.338   125.960   130.553   139.037
   158.871   159.883   171.167   184.099   185.236   194.086   208.480   214.063   233.315   242.887
   257.430   271.305   272.174   277.003   282.678   286.590   289.396   299.834   319.251   330.120
   333.851   347.999   365.315   371.322   372.268   376.746   381.186   382.528   388.136   392.200
   404.165   412.059   425.659   445.247   458.725   462.357   467.651   472.197   475.847   481.469
   491.162   503.614   504.199   511.560   519.060   528.068   531.072   535.237   550.353   553.201
   555.750   557.168   561.978   571.209   573.593   574.259   585.879   597.707   599.662   612.768
   618.794   624.544   633.327   637.818   639.148   650.187   657.586   659.019   662.988   679.644
   684.365   698.170   701.038   704.631   707.480   719.493   724.730   740.863   750.968   754.391
   757.259   763.495   773.716   786.034   792.400   796.971   798.704   802.499   805.249   808.407
   810.240   813.527   818.915   821.280   826.271   838.628   842.858   846.475   853.810   856.010
   862.831   866.256   868.346   873.511   881.482   899.573   903.489   911.432   929.024   936.478
   939.974   946.462   965.794   969.114   972.419   975.256   977.784   978.640   982.468   987.535
   991.857   996.362   999.706  1000.223  1006.763  1013.975  1026.247  1047.861  1063.584  1078.343
  1090.955  1114.275  1122.218  1128.696  1139.179  1150.682  1154.122  1156.689  1159.963  1174.610
  1185.986  1193.671  1197.601  1200.545  1205.607  1211.323  1213.985  1221.385  1230.884  1234.827
  1238.890  1244.036  1252.499  1254.817  1255.380  1260.238  1261.144  1264.759  1267.023  1278.970
  1281.172  1288.457  1295.520  1301.239  1311.076  1317.810  1319.958  1331.970  1340.569  1344.100
  1347.826  1350.390  1361.424  1368.547  1375.866  1385.977  1391.206  1398.923  1401.560  1406.441
  1410.679  1414.941  1419.642  1427.608  1431.681  1436.130  1440.766  1445.805  1447.719  1454.524
  1455.181  1455.966  1458.566  1460.850  1471.874  1482.724  1485.253  1498.600  1512.230  1518.049
  1520.200  1522.868  1528.544  1530.247  1533.388  1536.431  1554.495  1578.616  1578.754  1579.559
  1591.809  1611.709  1628.000  1630.923  1642.140  1651.746  1664.061  1664.757  1666.665  1671.030
  1678.464  1679.810  1691.543  1711.320  1764.948  1771.057  2985.552  3016.051  3032.580  3052.563
  3083.484  3088.107  3108.155  3131.200  3137.737  3142.185  3142.542  3146.506  3156.848  3157.000
  3159.525  3159.620  3160.332  3160.575  3164.361  3165.186  3180.714  3184.336  3187.718  3191.186
  3194.353  3196.110  3197.384  3205.008  3211.364  3212.617  3221.553
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