Supporting Information

Tuning the Electrochemical Redox Potentials of Catechol with Boronic Acid Derivatives

Zachary M. Robole, Kira L. Rahn, Bryan J. Lampkin, Robbyn K. Anand, Brett VanVeller*

*Department of Chemistry, Iowa State University, Ames, Iowa 50011, United States

Contents

<table>
<thead>
<tr>
<th>Contents</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cyclic Voltammetry Data</td>
<td>S2</td>
</tr>
<tr>
<td>Computational Data</td>
<td>S4</td>
</tr>
</tbody>
</table>
Cyclic Voltammetry Data

**Figure S1:** CV scan of 3a (red) and (dashed)

**Figure S2:** CV scan of 3b (red) and (dashed)
Figure S3: CV scan of 3c (red) and di-p-fluorophenyl borinic acid (dashed)

Figure S4: CV scan of 12 (red) and 2-carboxyphenylboronic acid (dashed)
Computational Data

![Chemical structure](image)

Table S1. Reported NBO natural charges and electrostatic potential, CHELPG.

<table>
<thead>
<tr>
<th>R</th>
<th>NBO Natural Charges</th>
<th>CHELPG electrostatic charges</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>O</td>
<td>B</td>
</tr>
<tr>
<td>NMMe2</td>
<td>-0.32</td>
<td>0.83</td>
</tr>
<tr>
<td>tBu</td>
<td>-0.29</td>
<td>0.75</td>
</tr>
<tr>
<td>OMe</td>
<td>-0.3</td>
<td>0.77</td>
</tr>
<tr>
<td>Et</td>
<td>-0.32</td>
<td>0.83</td>
</tr>
<tr>
<td>H</td>
<td>-0.37</td>
<td>0.66</td>
</tr>
<tr>
<td>F</td>
<td>-0.35</td>
<td>0.68</td>
</tr>
<tr>
<td>COOH</td>
<td>-0.24</td>
<td>0.42</td>
</tr>
<tr>
<td>CN</td>
<td>-0.26</td>
<td>0.43</td>
</tr>
<tr>
<td>NO₂</td>
<td>-0.27</td>
<td>0.51</td>
</tr>
<tr>
<td>11</td>
<td>-0.28</td>
<td>0.67</td>
</tr>
<tr>
<td>12</td>
<td>-0.33</td>
<td>0.73</td>
</tr>
</tbody>
</table>

R  NMMe2

<table>
<thead>
<tr>
<th></th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.0667</td>
<td>3.0176</td>
<td>-0.6939</td>
</tr>
<tr>
<td>C</td>
<td>0.0746</td>
<td>2.9958</td>
<td>0.7196</td>
</tr>
<tr>
<td>C</td>
<td>0.1111</td>
<td>4.1768</td>
<td>1.4472</td>
</tr>
<tr>
<td>C</td>
<td>0.1347</td>
<td>5.3992</td>
<td>0.7448</td>
</tr>
<tr>
<td>C</td>
<td>0.1219</td>
<td>5.4205</td>
<td>-0.6467</td>
</tr>
</tbody>
</table>
C  0.0872  4.2202  -1.3857
H  0.1195  4.1548   2.5318
H  0.1620  6.3307   1.2999
H  0.1395  6.3686  -1.1736
H  0.0784  4.2309  -2.4705
O  0.0426  1.7370   1.1901
O  0.0401  1.7738  -1.2025
C  1.3391  -0.1517  -0.0397
C  2.4053   0.0539  -0.9269
C  1.5252  -1.1980   0.8791
C  3.5693  -0.7177  -0.9146
H  2.3294   0.8512  -1.6606
C  2.6784  -1.9794   0.9241
H  0.7401  -1.4195   1.5986
C  3.7347  -1.7700   0.0098
H  4.3467  -0.4927  -1.6332
H  2.7468  -2.7602   1.6704
C  -1.3848  -0.0580  -0.0321
C  -1.6587  -1.0230  -1.0159
C  -2.4086   0.1384   0.9054
C  -2.8576  -1.7304  -1.0798
H  -0.9038  -1.2453  -1.7668
C  -3.6170  -0.5617   0.8754
H  -2.2576   0.8613   1.7018
C  -3.8837  -1.5094  -0.1343
H  -2.9880  -2.4584  -1.8699
H  -4.3515  -0.3587   1.6440
B  0.0076   0.7760  -0.0215
N  4.8730  -2.5861   0.0030
N  -5.1111  -2.1803  -0.2120
C  5.1454  -3.4031  1.1792
H  6.0416  -3.9953  0.9968
H  5.3050  -2.8037  2.0891
H  4.3266  -4.0994  1.3705
C  6.0496  -2.1244  -0.7229
H  6.8237  -2.8889  -0.6620
H  5.8221  -1.9724  -1.7798
H  6.4586  -1.1838  -0.3220
C  -5.1917  -3.3801  -1.0362
H  -4.5181  -4.1808  -0.6931
H  -6.2137  -3.7571  -1.0102
H  -4.9520  -3.1574  -2.0777
C  -5.9780  -2.1697   0.9596
H  -6.2520  -1.1492   1.2343
H  -6.8983  -2.7025   0.7217
H  -5.5171  -2.6487   1.8376

Energy  -1138.10646677

R  tBu

<table>
<thead>
<tr>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-0.0343</td>
<td>3.2283</td>
</tr>
<tr>
<td>C</td>
<td>-0.0056</td>
<td>3.2364</td>
</tr>
<tr>
<td>C</td>
<td>-0.0056</td>
<td>4.4317</td>
</tr>
<tr>
<td>C</td>
<td>-0.0399</td>
<td>5.6387</td>
</tr>
<tr>
<td>C</td>
<td>-0.0725</td>
<td>5.6307</td>
</tr>
<tr>
<td>C</td>
<td>-0.0700</td>
<td>4.4154</td>
</tr>
<tr>
<td>H</td>
<td>0.0188</td>
<td>4.4320</td>
</tr>
<tr>
<td>H</td>
<td>-0.0418</td>
<td>6.5820</td>
</tr>
<tr>
<td>Atom</td>
<td>X</td>
<td>Y</td>
</tr>
<tr>
<td>------</td>
<td>-----</td>
<td>-----</td>
</tr>
<tr>
<td>H</td>
<td>-0.0996</td>
<td>6.5677</td>
</tr>
<tr>
<td>H</td>
<td>-0.0938</td>
<td>4.4033</td>
</tr>
<tr>
<td>O</td>
<td>0.0200</td>
<td>1.9856</td>
</tr>
<tr>
<td>O</td>
<td>-0.0191</td>
<td>1.9721</td>
</tr>
<tr>
<td>C</td>
<td>1.3618</td>
<td>0.1181</td>
</tr>
<tr>
<td>C</td>
<td>2.3648</td>
<td>0.2718</td>
</tr>
<tr>
<td>C</td>
<td>1.6201</td>
<td>-0.8396</td>
</tr>
<tr>
<td>C</td>
<td>3.5424</td>
<td>-0.4769</td>
</tr>
<tr>
<td>H</td>
<td>2.2194</td>
<td>0.9973</td>
</tr>
<tr>
<td>C</td>
<td>2.8007</td>
<td>-1.5869</td>
</tr>
<tr>
<td>H</td>
<td>0.8798</td>
<td>-1.0167</td>
</tr>
<tr>
<td>C</td>
<td>3.7948</td>
<td>-1.4262</td>
</tr>
<tr>
<td>H</td>
<td>4.2755</td>
<td>-0.3106</td>
</tr>
<tr>
<td>H</td>
<td>2.9333</td>
<td>-2.3048</td>
</tr>
<tr>
<td>C</td>
<td>-1.3593</td>
<td>0.1182</td>
</tr>
<tr>
<td>C</td>
<td>-1.6424</td>
<td>-0.8101</td>
</tr>
<tr>
<td>C</td>
<td>-2.3331</td>
<td>0.2356</td>
</tr>
<tr>
<td>C</td>
<td>-2.8180</td>
<td>-1.5559</td>
</tr>
<tr>
<td>H</td>
<td>-0.9235</td>
<td>-0.9569</td>
</tr>
<tr>
<td>C</td>
<td>-3.5143</td>
<td>-0.5174</td>
</tr>
<tr>
<td>H</td>
<td>-2.1695</td>
<td>0.9363</td>
</tr>
<tr>
<td>C</td>
<td>-3.7895</td>
<td>-1.4309</td>
</tr>
<tr>
<td>H</td>
<td>-2.9770</td>
<td>-2.2496</td>
</tr>
<tr>
<td>H</td>
<td>-4.2218</td>
<td>-0.3748</td>
</tr>
<tr>
<td>B</td>
<td>0.0012</td>
<td>1.0073</td>
</tr>
<tr>
<td>C</td>
<td>5.1936</td>
<td>-3.2174</td>
</tr>
<tr>
<td>H</td>
<td>6.1399</td>
<td>-3.7637</td>
</tr>
<tr>
<td>H</td>
<td>5.1570</td>
<td>-2.7026</td>
</tr>
<tr>
<td>H</td>
<td>4.3847</td>
<td>-3.9528</td>
</tr>
<tr>
<td>C</td>
<td>-6.0109</td>
<td>-1.9952</td>
</tr>
<tr>
<td></td>
<td>X</td>
<td>Y</td>
</tr>
<tr>
<td>------</td>
<td>-------</td>
<td>-------</td>
</tr>
<tr>
<td>H</td>
<td>-6.9089</td>
<td>-2.6134</td>
</tr>
<tr>
<td>H</td>
<td>-5.5329</td>
<td>-2.2374</td>
</tr>
<tr>
<td>H</td>
<td>-6.3307</td>
<td>-0.9500</td>
</tr>
<tr>
<td>C</td>
<td>-5.0788</td>
<td>-2.2701</td>
</tr>
<tr>
<td>C</td>
<td>-4.7212</td>
<td>-3.7751</td>
</tr>
<tr>
<td>H</td>
<td>-5.6309</td>
<td>-4.3817</td>
</tr>
<tr>
<td>H</td>
<td>-4.0873</td>
<td>-4.0444</td>
</tr>
<tr>
<td>H</td>
<td>-4.1894</td>
<td>-4.0450</td>
</tr>
<tr>
<td>C</td>
<td>-5.8520</td>
<td>-1.9399</td>
</tr>
<tr>
<td>H</td>
<td>-5.2571</td>
<td>-2.1555</td>
</tr>
<tr>
<td>H</td>
<td>-6.7692</td>
<td>-2.5348</td>
</tr>
<tr>
<td>H</td>
<td>-6.1305</td>
<td>-0.8824</td>
</tr>
<tr>
<td>C</td>
<td>5.1072</td>
<td>-2.2314</td>
</tr>
<tr>
<td>C</td>
<td>6.3093</td>
<td>-1.2622</td>
</tr>
<tr>
<td>H</td>
<td>7.2504</td>
<td>-1.8213</td>
</tr>
<tr>
<td>H</td>
<td>6.3286</td>
<td>-0.5607</td>
</tr>
<tr>
<td>H</td>
<td>6.2685</td>
<td>-0.6806</td>
</tr>
<tr>
<td>C</td>
<td>5.2134</td>
<td>-3.0430</td>
</tr>
<tr>
<td>H</td>
<td>6.1464</td>
<td>-3.6154</td>
</tr>
<tr>
<td>H</td>
<td>4.3812</td>
<td>-3.7474</td>
</tr>
<tr>
<td>H</td>
<td>5.2019</td>
<td>-2.3938</td>
</tr>
</tbody>
</table>

Energy: -1184.69157879

R Ome

<table>
<thead>
<tr>
<th></th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.3368</td>
<td>2.7468</td>
<td>0.6623</td>
</tr>
<tr>
<td>C</td>
<td>0.3160</td>
<td>2.6864</td>
<td>-0.7492</td>
</tr>
<tr>
<td>C</td>
<td>0.4864</td>
<td>3.8325</td>
<td>-1.5120</td>
</tr>
<tr>
<td>C</td>
<td>0.6879</td>
<td>5.0584</td>
<td>-0.8458</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
</tr>
<tr>
<td>C</td>
<td>0.7141</td>
<td>5.1170</td>
<td>0.5446</td>
</tr>
<tr>
<td>C</td>
<td>0.5374</td>
<td>3.9522</td>
<td>1.3189</td>
</tr>
<tr>
<td>H</td>
<td>0.4663</td>
<td>3.7811</td>
<td>-2.5955</td>
</tr>
<tr>
<td>H</td>
<td>0.8248</td>
<td>5.9633</td>
<td>-1.4280</td>
</tr>
<tr>
<td>H</td>
<td>0.8712</td>
<td>6.0674</td>
<td>1.0431</td>
</tr>
<tr>
<td>H</td>
<td>0.5550</td>
<td>3.9926</td>
<td>2.4028</td>
</tr>
<tr>
<td>O</td>
<td>0.1171</td>
<td>1.4279</td>
<td>-1.1818</td>
</tr>
<tr>
<td>O</td>
<td>0.1402</td>
<td>1.5322</td>
<td>1.2064</td>
</tr>
<tr>
<td>C</td>
<td>-1.4583</td>
<td>-0.1918</td>
<td>0.0992</td>
</tr>
<tr>
<td>C</td>
<td>-2.4779</td>
<td>0.2339</td>
<td>0.9697</td>
</tr>
<tr>
<td>C</td>
<td>-1.7945</td>
<td>-1.2400</td>
<td>-0.7687</td>
</tr>
<tr>
<td>C</td>
<td>-3.7454</td>
<td>-0.3438</td>
<td>0.9768</td>
</tr>
<tr>
<td>H</td>
<td>-2.2699</td>
<td>1.0404</td>
<td>1.6657</td>
</tr>
<tr>
<td>C</td>
<td>-3.0613</td>
<td>-1.8346</td>
<td>-0.7925</td>
</tr>
<tr>
<td>H</td>
<td>-1.0455</td>
<td>-1.6211</td>
<td>-1.4581</td>
</tr>
<tr>
<td>C</td>
<td>-4.0460</td>
<td>-1.3830</td>
<td>0.0903</td>
</tr>
<tr>
<td>H</td>
<td>-4.5145</td>
<td>-0.0016</td>
<td>1.6615</td>
</tr>
<tr>
<td>H</td>
<td>-3.2616</td>
<td>-2.6395</td>
<td>-1.4883</td>
</tr>
<tr>
<td>C</td>
<td>1.2468</td>
<td>-0.5339</td>
<td>0.0969</td>
</tr>
<tr>
<td>C</td>
<td>1.3412</td>
<td>-1.5149</td>
<td>1.1041</td>
</tr>
<tr>
<td>C</td>
<td>2.3043</td>
<td>-0.4964</td>
<td>-0.8188</td>
</tr>
<tr>
<td>C</td>
<td>2.4176</td>
<td>-2.3896</td>
<td>1.1989</td>
</tr>
<tr>
<td>H</td>
<td>0.5454</td>
<td>-1.6006</td>
<td>1.8395</td>
</tr>
<tr>
<td>C</td>
<td>3.3990</td>
<td>-1.3710</td>
<td>-0.7559</td>
</tr>
<tr>
<td>H</td>
<td>2.2806</td>
<td>0.2378</td>
<td>-1.6179</td>
</tr>
<tr>
<td>C</td>
<td>3.4582</td>
<td>-2.3219</td>
<td>0.2634</td>
</tr>
<tr>
<td>H</td>
<td>2.4700</td>
<td>-3.1340</td>
<td>1.9866</td>
</tr>
<tr>
<td>H</td>
<td>4.1856</td>
<td>-1.2967</td>
<td>-1.4959</td>
</tr>
<tr>
<td>B</td>
<td>0.0046</td>
<td>0.5138</td>
<td>0.0554</td>
</tr>
<tr>
<td>O</td>
<td>4.4790</td>
<td>-3.2258</td>
<td>0.4306</td>
</tr>
</tbody>
</table>
O  -5.3198  -1.8924   0.1629
C  -5.6767  -2.9515  -0.7229
H  -6.7144  -3.1923  -0.4983
H  -5.5948  -2.6406 -1.7692
H  -5.0548  -3.8367  -0.5568
C   5.5692  -3.1921  -0.4881
H   6.2550  -3.9745  -0.1674
H   5.2359  -3.3984 -1.5101
H   6.0826  -2.2258  -0.4613

Energy -1099.21659453

R  Et

X     Y     Z
C  0.1507  2.7825 -0.7777
C  0.1318  2.8771  0.6311
C  0.1961  4.1106  1.2620
C  0.2770  5.2687  0.4624
C  0.2923  5.1756 -0.9263
C  0.2286  3.9211 -1.5659
H  0.1834  4.1772  2.3446
H  0.3271  6.2414  0.9397
H  0.3545  6.0760 -1.5280
H  0.2406  3.8425 -2.6477
O   0.0470  1.6604  1.2017
O   0.0858  1.4999 -1.1823
C  1.3113  -0.3543  0.1689
C  2.3136  -0.3669 -0.8145
C  1.4964  -1.2145  1.2672
C  3.4404  -1.1889 -0.7138
<table>
<thead>
<tr>
<th></th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>2.2076</td>
<td>0.2823</td>
<td>-1.6779</td>
</tr>
<tr>
<td>C</td>
<td>2.6198</td>
<td>-2.0333</td>
<td>1.3862</td>
</tr>
<tr>
<td>H</td>
<td>0.7434</td>
<td>-1.2465</td>
<td>2.0507</td>
</tr>
<tr>
<td>C</td>
<td>3.5998</td>
<td>-2.0258</td>
<td>0.3902</td>
</tr>
<tr>
<td>H</td>
<td>4.1940</td>
<td>-1.1747</td>
<td>-1.4955</td>
</tr>
<tr>
<td>H</td>
<td>2.7317</td>
<td>-2.6807</td>
<td>2.2507</td>
</tr>
<tr>
<td>C</td>
<td>-1.4012</td>
<td>-0.1963</td>
<td>0.0966</td>
</tr>
<tr>
<td>C</td>
<td>-1.6961</td>
<td>-1.1654</td>
<td>-0.8803</td>
</tr>
<tr>
<td>C</td>
<td>-2.3901</td>
<td>0.0401</td>
<td>1.0651</td>
</tr>
<tr>
<td>C</td>
<td>-2.9099</td>
<td>-1.8532</td>
<td>-0.8993</td>
</tr>
<tr>
<td>H</td>
<td>-0.9585</td>
<td>-1.3897</td>
<td>-1.6468</td>
</tr>
<tr>
<td>C</td>
<td>-3.6075</td>
<td>-0.6480</td>
<td>1.0646</td>
</tr>
<tr>
<td>H</td>
<td>-2.2007</td>
<td>0.7800</td>
<td>1.8364</td>
</tr>
<tr>
<td>C</td>
<td>-3.8741</td>
<td>-1.5980</td>
<td>0.0792</td>
</tr>
<tr>
<td>H</td>
<td>-3.1048</td>
<td>-2.5907</td>
<td>-1.6720</td>
</tr>
<tr>
<td>H</td>
<td>-4.3479</td>
<td>-0.4413</td>
<td>1.8316</td>
</tr>
<tr>
<td>B</td>
<td>0.0085</td>
<td>0.6160</td>
<td>0.0736</td>
</tr>
<tr>
<td>C</td>
<td>-5.2133</td>
<td>-2.3582</td>
<td>0.0698</td>
</tr>
<tr>
<td>H</td>
<td>-5.5232</td>
<td>-2.5472</td>
<td>1.0763</td>
</tr>
<tr>
<td>H</td>
<td>-5.9549</td>
<td>-1.7682</td>
<td>-0.4269</td>
</tr>
<tr>
<td>C</td>
<td>-5.0391</td>
<td>-3.6957</td>
<td>-0.6734</td>
</tr>
<tr>
<td>H</td>
<td>-5.9202</td>
<td>-4.2900</td>
<td>-0.5496</td>
</tr>
<tr>
<td>H</td>
<td>-4.8795</td>
<td>-3.5071</td>
<td>-1.7145</td>
</tr>
<tr>
<td>H</td>
<td>-4.1965</td>
<td>-4.2194</td>
<td>-0.2726</td>
</tr>
<tr>
<td>C</td>
<td>4.8390</td>
<td>-2.9322</td>
<td>0.5102</td>
</tr>
<tr>
<td>H</td>
<td>5.6903</td>
<td>-2.3396</td>
<td>0.7728</td>
</tr>
<tr>
<td>H</td>
<td>4.6700</td>
<td>-3.6690</td>
<td>1.2675</td>
</tr>
<tr>
<td>C</td>
<td>5.0962</td>
<td>-3.6312</td>
<td>-0.8377</td>
</tr>
<tr>
<td>H</td>
<td>5.4828</td>
<td>-2.9218</td>
<td>-1.5393</td>
</tr>
<tr>
<td>H</td>
<td>5.8058</td>
<td>-4.4203</td>
<td>-0.7006</td>
</tr>
<tr>
<td></td>
<td>X</td>
<td>Y</td>
<td>Z</td>
</tr>
<tr>
<td>---</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
</tr>
<tr>
<td>C</td>
<td>-2.1065</td>
<td>0.0200</td>
<td>-0.7058</td>
</tr>
<tr>
<td>C</td>
<td>-2.1065</td>
<td>-0.0195</td>
<td>0.7058</td>
</tr>
<tr>
<td>C</td>
<td>-3.2973</td>
<td>-0.0365</td>
<td>1.4167</td>
</tr>
<tr>
<td>C</td>
<td>-4.5084</td>
<td>-0.0173</td>
<td>0.6957</td>
</tr>
<tr>
<td>C</td>
<td>-4.5084</td>
<td>0.0183</td>
<td>-0.6957</td>
</tr>
<tr>
<td>C</td>
<td>-3.2973</td>
<td>0.0373</td>
<td>-1.4167</td>
</tr>
<tr>
<td>H</td>
<td>-3.2913</td>
<td>-0.0647</td>
<td>2.5011</td>
</tr>
<tr>
<td>H</td>
<td>-5.4487</td>
<td>-0.0312</td>
<td>1.2363</td>
</tr>
<tr>
<td>H</td>
<td>-5.4487</td>
<td>0.0323</td>
<td>-1.2363</td>
</tr>
<tr>
<td>H</td>
<td>-3.2913</td>
<td>0.0654</td>
<td>-2.5011</td>
</tr>
<tr>
<td>O</td>
<td>-0.8519</td>
<td>-0.0367</td>
<td>1.1943</td>
</tr>
<tr>
<td>O</td>
<td>-0.8519</td>
<td>0.0370</td>
<td>-1.1943</td>
</tr>
<tr>
<td>C</td>
<td>1.0112</td>
<td>1.3580</td>
<td>0.0506</td>
</tr>
<tr>
<td>C</td>
<td>0.8990</td>
<td>2.3696</td>
<td>-0.9168</td>
</tr>
<tr>
<td>C</td>
<td>1.9295</td>
<td>1.5831</td>
<td>1.0929</td>
</tr>
<tr>
<td>C</td>
<td>1.6572</td>
<td>3.5429</td>
<td>-0.8536</td>
</tr>
<tr>
<td>H</td>
<td>0.2016</td>
<td>2.2336</td>
<td>-1.7375</td>
</tr>
<tr>
<td>C</td>
<td>2.6860</td>
<td>2.7526</td>
<td>1.1745</td>
</tr>
<tr>
<td>H</td>
<td>2.0580</td>
<td>0.8252</td>
<td>1.8617</td>
</tr>
<tr>
<td>C</td>
<td>2.5543</td>
<td>3.7408</td>
<td>0.1955</td>
</tr>
<tr>
<td>H</td>
<td>1.5465</td>
<td>4.3025</td>
<td>-1.6217</td>
</tr>
<tr>
<td>H</td>
<td>3.3812</td>
<td>2.8943</td>
<td>1.9965</td>
</tr>
<tr>
<td>H</td>
<td>3.1439</td>
<td>4.6500</td>
<td>0.2508</td>
</tr>
<tr>
<td>C</td>
<td>1.0108</td>
<td>-1.3582</td>
<td>-0.0506</td>
</tr>
</tbody>
</table>

Energy

H  4.1788  -4.0372  -1.2098
<table>
<thead>
<tr>
<th></th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.0052</td>
<td>2.4317</td>
<td>-0.7057</td>
</tr>
<tr>
<td>C</td>
<td>-0.0028</td>
<td>2.4317</td>
<td>0.7058</td>
</tr>
<tr>
<td>C</td>
<td>-0.0029</td>
<td>3.6220</td>
<td>1.4173</td>
</tr>
<tr>
<td>C</td>
<td>0.0005</td>
<td>4.8329</td>
<td>0.6960</td>
</tr>
<tr>
<td>C</td>
<td>0.0042</td>
<td>4.8329</td>
<td>-0.6959</td>
</tr>
<tr>
<td>C</td>
<td>0.0064</td>
<td>3.6221</td>
<td>-1.4173</td>
</tr>
<tr>
<td>H</td>
<td>-0.0066</td>
<td>3.6159</td>
<td>2.5020</td>
</tr>
<tr>
<td>H</td>
<td>-0.0006</td>
<td>5.7731</td>
<td>1.2367</td>
</tr>
<tr>
<td>H</td>
<td>0.0062</td>
<td>5.7732</td>
<td>-1.2366</td>
</tr>
<tr>
<td>H</td>
<td>0.0101</td>
<td>3.6159</td>
<td>-2.5019</td>
</tr>
<tr>
<td>O</td>
<td>-0.0108</td>
<td>1.1760</td>
<td>1.1944</td>
</tr>
<tr>
<td>O</td>
<td>0.0119</td>
<td>1.1760</td>
<td>-1.1945</td>
</tr>
<tr>
<td>C</td>
<td>1.3588</td>
<td>-0.6845</td>
<td>0.0174</td>
</tr>
<tr>
<td>C</td>
<td>2.3617</td>
<td>-0.5446</td>
<td>-0.9539</td>
</tr>
</tbody>
</table>

Energy: -870.10116843
<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>1.5945</td>
<td>-1.6253</td>
<td>1.0357</td>
</tr>
<tr>
<td>C</td>
<td>3.5424</td>
<td>-1.2946</td>
<td>-0.9252</td>
</tr>
<tr>
<td>H</td>
<td>2.2191</td>
<td>0.1696</td>
<td>-1.7578</td>
</tr>
<tr>
<td>C</td>
<td>2.7654</td>
<td>-2.3824</td>
<td>1.0995</td>
</tr>
<tr>
<td>H</td>
<td>0.8451</td>
<td>-1.7781</td>
<td>1.8072</td>
</tr>
<tr>
<td>C</td>
<td>3.7156</td>
<td>-2.1973</td>
<td>0.1080</td>
</tr>
<tr>
<td>H</td>
<td>4.3097</td>
<td>-1.1812</td>
<td>-1.6825</td>
</tr>
<tr>
<td>H</td>
<td>2.9395</td>
<td>-3.1016</td>
<td>1.8916</td>
</tr>
<tr>
<td>C</td>
<td>-1.3595</td>
<td>-0.6832</td>
<td>-0.0175</td>
</tr>
<tr>
<td>C</td>
<td>-1.5962</td>
<td>-1.6236</td>
<td>-1.0359</td>
</tr>
<tr>
<td>C</td>
<td>-2.3622</td>
<td>-0.5424</td>
<td>0.9540</td>
</tr>
<tr>
<td>C</td>
<td>-2.7678</td>
<td>-2.3796</td>
<td>-1.0996</td>
</tr>
<tr>
<td>H</td>
<td>-0.8471</td>
<td>-1.7770</td>
<td>-1.8075</td>
</tr>
<tr>
<td>C</td>
<td>-3.5435</td>
<td>-1.2914</td>
<td>0.9253</td>
</tr>
<tr>
<td>H</td>
<td>-2.2187</td>
<td>0.1715</td>
<td>1.7580</td>
</tr>
<tr>
<td>C</td>
<td>-3.7177</td>
<td>-2.1938</td>
<td>-0.1080</td>
</tr>
<tr>
<td>H</td>
<td>-2.9427</td>
<td>-3.0985</td>
<td>-1.8919</td>
</tr>
<tr>
<td>H</td>
<td>-4.3107</td>
<td>-1.1774</td>
<td>1.6827</td>
</tr>
<tr>
<td>B</td>
<td>0.0001</td>
<td>0.2110</td>
<td>0.0000</td>
</tr>
<tr>
<td>F</td>
<td>4.8687</td>
<td>-2.9390</td>
<td>0.1536</td>
</tr>
<tr>
<td>F</td>
<td>-4.8715</td>
<td>-2.9344</td>
<td>-0.1535</td>
</tr>
</tbody>
</table>

Energy: -1068.64330750
<table>
<thead>
<tr>
<th>Element</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.0001</td>
<td>5.0904</td>
<td>0.6961</td>
</tr>
<tr>
<td>C</td>
<td>-0.0002</td>
<td>3.8804</td>
<td>1.4179</td>
</tr>
<tr>
<td>H</td>
<td>0.0003</td>
<td>3.8739</td>
<td>-2.5023</td>
</tr>
<tr>
<td>H</td>
<td>-0.0002</td>
<td>6.0308</td>
<td>-1.2364</td>
</tr>
<tr>
<td>H</td>
<td>0.0001</td>
<td>6.0308</td>
<td>1.2364</td>
</tr>
<tr>
<td>H</td>
<td>-0.0003</td>
<td>3.8739</td>
<td>2.5023</td>
</tr>
<tr>
<td>O</td>
<td>0.0019</td>
<td>1.4328</td>
<td>-1.1939</td>
</tr>
<tr>
<td>O</td>
<td>-0.0019</td>
<td>1.4328</td>
<td>1.1939</td>
</tr>
<tr>
<td>C</td>
<td>-1.3423</td>
<td>-0.4360</td>
<td>-0.0081</td>
</tr>
<tr>
<td>C</td>
<td>-2.0804</td>
<td>-0.6803</td>
<td>1.1626</td>
</tr>
<tr>
<td>C</td>
<td>-1.8042</td>
<td>-1.0378</td>
<td>-1.1931</td>
</tr>
<tr>
<td>C</td>
<td>-3.2171</td>
<td>-1.4815</td>
<td>1.1649</td>
</tr>
<tr>
<td>H</td>
<td>-1.7622</td>
<td>-0.2232</td>
<td>2.0933</td>
</tr>
<tr>
<td>C</td>
<td>-2.9383</td>
<td>-1.8394</td>
<td>-1.2207</td>
</tr>
<tr>
<td>H</td>
<td>-1.2666</td>
<td>-0.8702</td>
<td>-2.1208</td>
</tr>
<tr>
<td>C</td>
<td>-3.6538</td>
<td>-2.0685</td>
<td>-0.0331</td>
</tr>
<tr>
<td>H</td>
<td>-3.7706</td>
<td>-1.6534</td>
<td>2.0809</td>
</tr>
<tr>
<td>H</td>
<td>-3.2765</td>
<td>-2.2882</td>
<td>-2.1475</td>
</tr>
<tr>
<td>C</td>
<td>1.3423</td>
<td>-0.4360</td>
<td>0.0081</td>
</tr>
<tr>
<td>C</td>
<td>1.8042</td>
<td>-1.0378</td>
<td>1.1931</td>
</tr>
<tr>
<td>C</td>
<td>2.0804</td>
<td>-0.6803</td>
<td>-1.1626</td>
</tr>
<tr>
<td>C</td>
<td>2.9383</td>
<td>-1.8394</td>
<td>1.2207</td>
</tr>
<tr>
<td>H</td>
<td>1.2666</td>
<td>-0.8702</td>
<td>2.1208</td>
</tr>
<tr>
<td>C</td>
<td>3.2172</td>
<td>-1.4815</td>
<td>-1.1649</td>
</tr>
<tr>
<td>H</td>
<td>1.7622</td>
<td>-0.2232</td>
<td>-2.0933</td>
</tr>
<tr>
<td>C</td>
<td>3.6538</td>
<td>-2.0685</td>
<td>0.0331</td>
</tr>
<tr>
<td>H</td>
<td>3.2765</td>
<td>-2.2882</td>
<td>2.1475</td>
</tr>
<tr>
<td>H</td>
<td>3.7706</td>
<td>-1.6534</td>
<td>-2.0809</td>
</tr>
<tr>
<td>B</td>
<td>0.0000</td>
<td>0.4846</td>
<td>0.0000</td>
</tr>
<tr>
<td>C</td>
<td>-4.8204</td>
<td>-2.8910</td>
<td>-0.0459</td>
</tr>
</tbody>
</table>
N  -5.7663 -3.5587  -0.0564
C   4.8204 -2.8910  0.0459
N   5.7664 -3.5587  0.0564

Energy  -1054.65383344

R  NO2

<table>
<thead>
<tr>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.0005</td>
<td>3.0100</td>
</tr>
<tr>
<td>C    -0.0005</td>
<td>3.0100</td>
<td>-0.7048</td>
</tr>
<tr>
<td>C    -0.0018</td>
<td>4.1983</td>
<td>-1.4181</td>
</tr>
<tr>
<td>C    -0.0011</td>
<td>5.4079</td>
<td>-0.6961</td>
</tr>
<tr>
<td>C     0.0011</td>
<td>5.4079</td>
<td>0.6961</td>
</tr>
<tr>
<td>C     0.0018</td>
<td>4.1983</td>
<td>1.4181</td>
</tr>
<tr>
<td>H    -0.0031</td>
<td>4.1916</td>
<td>-2.5025</td>
</tr>
<tr>
<td>H    -0.0019</td>
<td>6.3483</td>
<td>-1.2363</td>
</tr>
<tr>
<td>H     0.0018</td>
<td>6.3483</td>
<td>1.2363</td>
</tr>
<tr>
<td>H     0.0031</td>
<td>4.1916</td>
<td>2.5025</td>
</tr>
<tr>
<td>O     0.0002</td>
<td>1.7501</td>
<td>-1.1935</td>
</tr>
<tr>
<td>O    -0.0002</td>
<td>1.7501</td>
<td>1.1935</td>
</tr>
<tr>
<td>C    -1.3397</td>
<td>-0.1187</td>
<td>-0.0068</td>
</tr>
<tr>
<td>C    -2.0641</td>
<td>-0.3781</td>
<td>1.1705</td>
</tr>
<tr>
<td>C    -1.8128</td>
<td>-0.7047</td>
<td>-1.1963</td>
</tr>
<tr>
<td>C    -3.1998</td>
<td>-1.1795</td>
<td>1.1760</td>
</tr>
<tr>
<td>H    -1.7363</td>
<td>0.0679</td>
<td>2.1027</td>
</tr>
<tr>
<td>C    -2.9466</td>
<td>-1.5059</td>
<td>-1.2237</td>
</tr>
<tr>
<td>H    -1.2853</td>
<td>-0.5237</td>
<td>-2.1267</td>
</tr>
<tr>
<td>C    -3.6298</td>
<td>-1.7371</td>
<td>-0.0282</td>
</tr>
<tr>
<td>H    -3.7508</td>
<td>-1.3703</td>
<td>2.0868</td>
</tr>
<tr>
<td>H    -3.3036</td>
<td>-1.9476</td>
<td>-2.1439</td>
</tr>
</tbody>
</table>
### Energy

-1279.25013130

### 2-Carboxyphenylboronic Acid

**BAC**

```
\[
\begin{array}{ccc}
  & \text{X} & \text{Y} & \text{Z} \\
\text{C} & -2.1237 & -0.0704 & -0.7029 \\
\text{C} & -2.1237 & -0.0704 & 0.7029 \\
\text{C} & -3.3024 & -0.1791 & 1.4206 \\
\end{array}
\]
```
<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-4.5046</td>
<td>-0.2905</td>
<td>0.6967</td>
</tr>
<tr>
<td>C</td>
<td>-4.5046</td>
<td>-0.2905</td>
<td>-0.6966</td>
</tr>
<tr>
<td>C</td>
<td>-3.3024</td>
<td>-0.1791</td>
<td>-1.4206</td>
</tr>
<tr>
<td>H</td>
<td>-3.2957</td>
<td>-0.1789</td>
<td>2.5047</td>
</tr>
<tr>
<td>H</td>
<td>-5.4417</td>
<td>-0.3770</td>
<td>1.2354</td>
</tr>
<tr>
<td>H</td>
<td>-5.4417</td>
<td>-0.3770</td>
<td>-1.2353</td>
</tr>
<tr>
<td>H</td>
<td>-3.2958</td>
<td>-0.1789</td>
<td>-2.5047</td>
</tr>
<tr>
<td>O</td>
<td>-0.8561</td>
<td>0.0314</td>
<td>1.1772</td>
</tr>
<tr>
<td>O</td>
<td>-0.8561</td>
<td>0.0314</td>
<td>-1.1772</td>
</tr>
<tr>
<td>C</td>
<td>1.4314</td>
<td>-0.5644</td>
<td>0.0000</td>
</tr>
<tr>
<td>C</td>
<td>1.7802</td>
<td>-1.9157</td>
<td>0.0000</td>
</tr>
<tr>
<td>C</td>
<td>2.4568</td>
<td>0.3865</td>
<td>0.0000</td>
</tr>
<tr>
<td>C</td>
<td>3.1299</td>
<td>-2.2815</td>
<td>0.0000</td>
</tr>
<tr>
<td>H</td>
<td>1.0169</td>
<td>-2.6880</td>
<td>0.0000</td>
</tr>
<tr>
<td>C</td>
<td>3.8078</td>
<td>0.0447</td>
<td>0.0000</td>
</tr>
<tr>
<td>C</td>
<td>4.1389</td>
<td>-1.3099</td>
<td>0.0000</td>
</tr>
<tr>
<td>H</td>
<td>3.4041</td>
<td>-3.3314</td>
<td>0.0000</td>
</tr>
<tr>
<td>H</td>
<td>4.5771</td>
<td>0.8090</td>
<td>0.0000</td>
</tr>
<tr>
<td>H</td>
<td>5.1794</td>
<td>-1.6150</td>
<td>0.0000</td>
</tr>
<tr>
<td>C</td>
<td>1.8722</td>
<td>1.7600</td>
<td>0.0000</td>
</tr>
<tr>
<td>O</td>
<td>0.5447</td>
<td>1.6888</td>
<td>0.0000</td>
</tr>
<tr>
<td>O</td>
<td>2.4907</td>
<td>2.8147</td>
<td>0.0000</td>
</tr>
<tr>
<td>B</td>
<td>0.0352</td>
<td>0.2336</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

Energy -826.47675189

Benzoxaborole 11
<table>
<thead>
<tr>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>1.9828</td>
<td>0.0180</td>
</tr>
<tr>
<td>C</td>
<td>1.9828</td>
<td>0.0179</td>
</tr>
<tr>
<td>C</td>
<td>3.1457</td>
<td>-0.2291</td>
</tr>
<tr>
<td>C</td>
<td>4.3286</td>
<td>-0.4837</td>
</tr>
<tr>
<td>C</td>
<td>4.3285</td>
<td>-0.4836</td>
</tr>
<tr>
<td>C</td>
<td>3.1456</td>
<td>-0.2288</td>
</tr>
<tr>
<td>H</td>
<td>3.1405</td>
<td>-0.2270</td>
</tr>
<tr>
<td>H</td>
<td>5.2482</td>
<td>-0.6816</td>
</tr>
<tr>
<td>H</td>
<td>5.2481</td>
<td>-0.6814</td>
</tr>
<tr>
<td>H</td>
<td>3.1404</td>
<td>-0.2265</td>
</tr>
<tr>
<td>O</td>
<td>0.7486</td>
<td>0.2747</td>
</tr>
<tr>
<td>O</td>
<td>0.7485</td>
<td>0.2749</td>
</tr>
<tr>
<td>C</td>
<td>-1.5605</td>
<td>-0.2664</td>
</tr>
<tr>
<td>C</td>
<td>-1.8824</td>
<td>-1.6278</td>
</tr>
<tr>
<td>C</td>
<td>-2.6036</td>
<td>0.6664</td>
</tr>
<tr>
<td>C</td>
<td>-3.2190</td>
<td>-2.0364</td>
</tr>
<tr>
<td>H</td>
<td>-1.0968</td>
<td>-2.3792</td>
</tr>
<tr>
<td>C</td>
<td>-3.9432</td>
<td>0.2777</td>
</tr>
<tr>
<td>C</td>
<td>-4.2463</td>
<td>-1.0858</td>
</tr>
<tr>
<td>H</td>
<td>-3.4662</td>
<td>-3.0933</td>
</tr>
<tr>
<td>H</td>
<td>-4.7422</td>
<td>1.0138</td>
</tr>
<tr>
<td>H</td>
<td>-5.2818</td>
<td>-1.4101</td>
</tr>
<tr>
<td>C</td>
<td>-2.3766</td>
<td>2.6365</td>
</tr>
<tr>
<td>H</td>
<td>-2.3769</td>
<td>2.6366</td>
</tr>
<tr>
<td>O</td>
<td>-0.6282</td>
<td>1.9502</td>
</tr>
<tr>
<td>B</td>
<td>-0.1735</td>
<td>0.5504</td>
</tr>
<tr>
<td>-----</td>
<td>---------</td>
<td>--------</td>
</tr>
<tr>
<td>Energy</td>
<td>-752.39300831</td>
<td></td>
</tr>
</tbody>
</table>