Table S1. Total C-C spin-spin coupling constants (J) and contributions to J from PSO, DSO, FC, and SD terms (Hz) for molecules RCCH and RCCR.

<table>
<thead>
<tr>
<th></th>
<th>Molecules RCCH</th>
<th></th>
<th>Molecules RCCR</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1(^1)J(C-C)</td>
<td>PSO</td>
<td>DSO</td>
<td>FC</td>
</tr>
<tr>
<td>R = H</td>
<td>6.0858</td>
<td>0.0198</td>
<td>178.0831</td>
<td>8.0813</td>
</tr>
<tr>
<td>CH₃</td>
<td>6.1326</td>
<td>0.0773</td>
<td>178.5274</td>
<td>7.9619</td>
</tr>
<tr>
<td>NH₂</td>
<td>7.429</td>
<td>0.114</td>
<td>210.8327</td>
<td>7.9413</td>
</tr>
<tr>
<td>OH</td>
<td>8.9391</td>
<td>0.1413</td>
<td>232.818</td>
<td>8.253</td>
</tr>
<tr>
<td>F</td>
<td>10.8607</td>
<td>0.1654</td>
<td>258.8027</td>
<td>8.8629</td>
</tr>
</tbody>
</table>

| R = H   | 6.0858         | 0.0198 | 178.0831       | 8.0813 | 192.27 |
| CH₃    | 6.2404         | 0.1341 | 180.8851       | 7.9225 | 195.1821 |
| NH₂    | 8.404          | 0.2066 | 253.7466       | 7.77   | 270.1272 |
| OH     | 11.4892        | 0.2555 | 313.5668       | 8.6679 | 333.9794 |
| F      | 14.6835        | 0.3049 | 394.1132       | 9.7456 | 418.8472 |

a) Data extracted electronically from output files.
Table S2. Total B-N, N-H, and B-H spin-spin coupling constants (J) and contributions to J from PSO, DSO, FC, and SD terms (Hz) for molecules RBNH, HBNR, and RBNR

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<thead>
<tr>
<th>Molecules</th>
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</tr>
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<td>-1.859</td>
</tr>
<tr>
<td>CH₃</td>
<td>-1.6018</td>
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<tr>
<td>NH₂</td>
<td>-1.0363</td>
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<td>OH</td>
<td>-1.9201</td>
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<tr>
<td>F</td>
<td>-2.3965</td>
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</table>

<table>
<thead>
<tr>
<th>$^1$J(N-H)</th>
<th>R = H</th>
<th>CH₃</th>
<th>NH₂</th>
<th>OH</th>
<th>F</th>
</tr>
</thead>
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<tr>
<td>-0.873</td>
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<td>-0.5743</td>
<td>-111.9132</td>
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<tr>
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<tr>
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<table>
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<tr>
<th>$^2$J(B-H)</th>
<th>R = H</th>
<th>CH₃</th>
<th>NH₂</th>
<th>OH</th>
<th>F</th>
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## Molecules HBNR

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<th>DSO</th>
<th>FC</th>
<th>SD</th>
<th>J</th>
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<tbody>
<tr>
<td>R = H</td>
<td>-1.859</td>
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<td>-84.9195</td>
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<tr>
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<table>
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<th></th>
<th>$^1$J(B-H)</th>
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<td>R = H</td>
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<tr>
<td>$^1J(B-N)$</td>
<td>PSO</td>
<td>DSO</td>
<td>FC</td>
<td>SD</td>
<td>J</td>
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<tr>
<td>R = H</td>
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a) Data extracted electronically from output files.