Unusual chalcogen-boron ring compounds: the molecular structure of 1,4-B₄S₂(NMe₂)₄ determined by gas-phase electron diffraction and related molecules by quantum chemical calculations

Derek A. Wann, Heather E. Robertson, George Bramham, Andrew E. A. Bull, Nicholas C. Norman, Christopher A. Russell and David W. H. Rankin

Electronic Supplementary Information

Table S1. Nozzle-to-film distances / mm, sample and nozzle temperatures / K, weighting functions / nm⁻¹, scale factors, correlation parameters and electron wavelengths / pm used in the electron diffraction study of 1,4-B₄S₂(NMe₂)₄.

<table>
<thead>
<tr>
<th>Nozzle-to-film distance&lt;sup&gt;a&lt;/sup&gt;</th>
<th>253.6</th>
<th>92.7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample temperature</td>
<td>415</td>
<td>433</td>
</tr>
<tr>
<td>Nozzle temperature</td>
<td>428</td>
<td>453</td>
</tr>
<tr>
<td>Δs</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>s&lt;sub&gt;min&lt;/sub&gt;</td>
<td>20</td>
<td>90</td>
</tr>
<tr>
<td>s&lt;sub&gt;W&lt;/sub&gt;&lt;sup&gt;1&lt;/sup&gt;</td>
<td>40</td>
<td>110</td>
</tr>
<tr>
<td>s&lt;sub&gt;W&lt;/sub&gt;&lt;sup&gt;2&lt;/sup&gt;</td>
<td>112</td>
<td>310</td>
</tr>
<tr>
<td>s&lt;sub&gt;max&lt;/sub&gt;</td>
<td>120</td>
<td>320</td>
</tr>
<tr>
<td>Scale factor&lt;sup&gt;b&lt;/sup&gt;</td>
<td>0.924(5)</td>
<td>0.842(25)</td>
</tr>
<tr>
<td>Correlation parameter</td>
<td>0.497</td>
<td>0.346</td>
</tr>
<tr>
<td>Electron wavelength</td>
<td>6.18</td>
<td>6.18</td>
</tr>
</tbody>
</table>

<sup>a</sup> Determined by reference to the scattering pattern of benzene. <sup>b</sup> Values in parentheses are the estimated standard deviations.
<table>
<thead>
<tr>
<th>Atom pair</th>
<th>$r_a$ (pm)</th>
<th>$u_{\text{exp.}}$</th>
<th>$r_a - r_e$ (pm)</th>
<th>$u_{\text{calc.}}$</th>
<th>Restraint</th>
</tr>
</thead>
<tbody>
<tr>
<td>u2</td>
<td>C(12)–H(23)</td>
<td>110.1(3)</td>
<td>8.9(1)</td>
<td>0.4</td>
<td>7.4</td>
</tr>
<tr>
<td>u1</td>
<td>C(11)–H(20)</td>
<td>110.1(3)</td>
<td>8.9(3)</td>
<td>0.4</td>
<td>7.4(7)</td>
</tr>
<tr>
<td>u5</td>
<td>C(11)–H(21)</td>
<td>110.1(3)</td>
<td>9.1(tied to u1)</td>
<td>0.4</td>
<td>7.5</td>
</tr>
<tr>
<td>u6</td>
<td>C(12)–H(24)</td>
<td>110.1(3)</td>
<td>9.1(tied to u1)</td>
<td>0.4</td>
<td>7.5</td>
</tr>
<tr>
<td>u3</td>
<td>C(12)–H(22)</td>
<td>110.1(3)</td>
<td>9.1(tied to u1)</td>
<td>0.4</td>
<td>7.5</td>
</tr>
<tr>
<td>u4</td>
<td>C(11)–H(19)</td>
<td>110.1(3)</td>
<td>9.1(tied to u1)</td>
<td>0.4</td>
<td>7.5</td>
</tr>
<tr>
<td>u7</td>
<td>B(3)–N(7)</td>
<td>140.9(5)</td>
<td>5.4(tied to u9)</td>
<td>0.1</td>
<td>4.5</td>
</tr>
<tr>
<td>u8</td>
<td>N(7)–C(12)</td>
<td>146.4(2)</td>
<td>5.7(tied to u1)</td>
<td>0.1</td>
<td>4.7</td>
</tr>
<tr>
<td>u9</td>
<td>N(7)–C(11)</td>
<td>146.4(2)</td>
<td>5.7(2)</td>
<td>0.1</td>
<td>4.7(5)</td>
</tr>
<tr>
<td>u10</td>
<td>B(3)–B(4)</td>
<td>173.6(8)</td>
<td>6.3(6)</td>
<td>0.3</td>
<td>5.9(6)</td>
</tr>
<tr>
<td>u15</td>
<td>H(20)...H(21)</td>
<td>178.2(8)</td>
<td>11.9(fixed)</td>
<td>0.0</td>
<td>11.9</td>
</tr>
<tr>
<td>u14</td>
<td>H(19)...H(21)</td>
<td>178.2(8)</td>
<td>11.9(fixed)</td>
<td>0.0</td>
<td>11.9</td>
</tr>
<tr>
<td>u13</td>
<td>H(19)...H(20)</td>
<td>178.2(8)</td>
<td>11.9(fixed)</td>
<td>0.0</td>
<td>11.9</td>
</tr>
<tr>
<td>u11</td>
<td>H(22)...H(23)</td>
<td>178.2(8)</td>
<td>11.9(fixed)</td>
<td>0.0</td>
<td>11.9</td>
</tr>
<tr>
<td>u16</td>
<td>H(23)...H(24)</td>
<td>178.2(8)</td>
<td>11.9(fixed)</td>
<td>0.0</td>
<td>11.9</td>
</tr>
<tr>
<td>u12</td>
<td>H(22)...H(24)</td>
<td>178.3(8)</td>
<td>11.9(fixed)</td>
<td>0.1</td>
<td>11.9</td>
</tr>
<tr>
<td>u17</td>
<td>S(1)...B(4)</td>
<td>186.0(2)</td>
<td>5.8(2)</td>
<td>0.1</td>
<td>5.6</td>
</tr>
<tr>
<td>u19</td>
<td>N(7)...H(22)</td>
<td>211.1(7)</td>
<td>12.0(1)</td>
<td>–0.1</td>
<td>9.9</td>
</tr>
<tr>
<td>u25</td>
<td>N(7)...H(24)</td>
<td>211.1(7)</td>
<td>12.0(5)</td>
<td>–0.1</td>
<td>9.9(10)</td>
</tr>
<tr>
<td>u22</td>
<td>N(7)...H(20)</td>
<td>211.1(7)</td>
<td>12.0(tied to u23)</td>
<td>–0.1</td>
<td>10.0</td>
</tr>
<tr>
<td>u20</td>
<td>N(7)...H(23)</td>
<td>211.1(7)</td>
<td>12.0(tied to u23)</td>
<td>–0.1</td>
<td>10.0</td>
</tr>
<tr>
<td>u21</td>
<td>N(7)...H(21)</td>
<td>211.1(7)</td>
<td>12.1(tied to u23)</td>
<td>–0.1</td>
<td>10.1</td>
</tr>
<tr>
<td>u18</td>
<td>N(7)...H(19)</td>
<td>211.1(7)</td>
<td>12.1(tied to u23)</td>
<td>–0.1</td>
<td>10.0</td>
</tr>
<tr>
<td>u26</td>
<td>N(7)...H(22)</td>
<td>239.0(42)</td>
<td>27.9(1)</td>
<td>5.2</td>
<td>27.9</td>
</tr>
<tr>
<td>u24</td>
<td>C(11)...C(12)</td>
<td>240.6(4)</td>
<td>5.5(7)</td>
<td>–0.7</td>
<td>6.9</td>
</tr>
<tr>
<td>u27</td>
<td>B(3)...C(12)</td>
<td>250.0(4)</td>
<td>5.3(tied to u24)</td>
<td>–0.3</td>
<td>6.6</td>
</tr>
<tr>
<td>u28</td>
<td>B(3)...C(11)</td>
<td>255.8(6)</td>
<td>5.1(tied to u24)</td>
<td>–0.4</td>
<td>6.4</td>
</tr>
<tr>
<td>u29</td>
<td>B(3)...H(23)</td>
<td>260.5(12)</td>
<td>18.8(tied to u40)</td>
<td>2.0</td>
<td>14.2</td>
</tr>
<tr>
<td>u32</td>
<td>C(12)...H(19)</td>
<td>260.9(21)</td>
<td>26.8(tied to u40)</td>
<td>0.1</td>
<td>20.2</td>
</tr>
<tr>
<td>u33</td>
<td>C(11)...H(22)</td>
<td>262.2(21)</td>
<td>23.3(tied to u40)</td>
<td>–0.4</td>
<td>17.6</td>
</tr>
<tr>
<td>u26</td>
<td>H(21)...H(24)</td>
<td>263.7(38)</td>
<td>29.3(1)</td>
<td>4.4</td>
<td>29.3</td>
</tr>
<tr>
<td>u30</td>
<td>B(3)...H(25)</td>
<td>265.9(26)</td>
<td>25.8(tied to u40)</td>
<td>5.5</td>
<td>19.5</td>
</tr>
<tr>
<td>u34</td>
<td>B(3)...H(20)</td>
<td>271.4(13)</td>
<td>19.1(tied to u40)</td>
<td>3.2</td>
<td>14.4</td>
</tr>
<tr>
<td>u36</td>
<td>C(11)...H(24)</td>
<td>271.7(17)</td>
<td>23.8(tied to u40)</td>
<td>–0.5</td>
<td>18.0</td>
</tr>
<tr>
<td>u31</td>
<td>S(1)...H(29)</td>
<td>273.8(12)</td>
<td>27.8(tied to u40)</td>
<td>10.0</td>
<td>21.0</td>
</tr>
<tr>
<td>u35</td>
<td>C(12)...H(21)</td>
<td>273.9(18)</td>
<td>16.9(tied to u24)</td>
<td>–0.3</td>
<td>21.2</td>
</tr>
<tr>
<td>u38</td>
<td>B(3)...N(8)</td>
<td>279.4(13)</td>
<td>10.1(tied to u40)</td>
<td>–0.3</td>
<td>7.7</td>
</tr>
<tr>
<td>u42</td>
<td>B(3)...B(6)</td>
<td>279.7(11)</td>
<td>12.4(tied to u40)</td>
<td>–2.0</td>
<td>9.4</td>
</tr>
<tr>
<td>u40</td>
<td>S(1)...N(8)</td>
<td>282.3(5)</td>
<td>9.3(3)</td>
<td>0.1</td>
<td>7.0</td>
</tr>
<tr>
<td>u37</td>
<td>H(23)...H(25)</td>
<td>283.8(63)</td>
<td>41.5(1)</td>
<td>3.6</td>
<td>41.5</td>
</tr>
<tr>
<td>u39</td>
<td>N(7)...H(25)</td>
<td>286.2(27)</td>
<td>34.8(1)</td>
<td>6.0</td>
<td>26.3</td>
</tr>
<tr>
<td>u44</td>
<td>H(19)...H(24)</td>
<td>298.7(23)</td>
<td>36.5(1)</td>
<td>–2.5</td>
<td>36.5</td>
</tr>
</tbody>
</table>

*Table S2. Interatomic distances ($r_a$ / pm), refined and calculated amplitudes of vibration ($u / pm$) and distance corrections ($r_a - r_e$) for the SARACEN-restrained GED structure of 1,4-B₄S₂(NMe₂)₄.¹,*
<p>| u48  | B(3)...B(5) | 302.8(19) | 15.6 (tied to u49) | –1.6 | 13.5 | — |
| u46  | S(1)...B(3) | 302.8(7)  | 11.5 (tied to u48) | –0.4 | 8.7  | — |
| u41  | H(23)...H(27) | 303.2(32) | 49.7 (fixed) | 5.1 | 49.7 | — |
| u45  | H(21)...H(22) | 304.1(22) | 36.9 (fixed) | –2.7 | 36.9 | — |
| u43  | C(12)...H(25) | 305.8(42) | 45.3 (tied to u40) | 3.7 | 34.2 | — |
| u50  | B(3)...H(22) | 317.7(10) | 17.4 (1) | –1.8 | 15.1 | — |
| u47  | B(3)...C(13) | 318.7(19) | 13.7 (tied to u49) | 0.0 | 11.8 | — |
| u49  | S(1)...C(14) | 322.3(8)  | 12.7 (4) | 0.4 | 11.0 | 11.0(1) |
| u52  | B(3)...H(19) | 322.9(11) | 21.8 (tied to u40) | –2.4 | 16.4 | — |
| u51  | B(3)...H(24) | 323.0(9)  | 17.0 (tied to u49) | –1.7 | 14.7 | — |
| u53  | B(3)...H(21) | 326.0(10) | 21.4 (tied to u75) | –2.4 | 16.4 | — |
| u54  | C(12)...H(20) | 333.2(7)  | 13.5 (tied to u75) | –3.3 | 10.3 | — |
| u71  | S(1)...H(23) | 349.7(54) | 61.6 (fixed) | 4.2 | 61.6 | — |
| u57  | C(12)...C(13) | 358.0(26) | 34.1 (tied to u75) | 0.3 | 26.1 | — |
| u60  | N(7)...C(13) | 359.0(17) | 24.5 (tied to u75) | –0.1 | 18.8 | — |
| u58  | C(12)...H(27) | 363.0(32) | 60.3 (tied to u67) | 1.4 | 45.7 | — |
| u64  | H(20)...H(24) | 372.3(21) | 20.1 (fixed) | –3.0 | 20.1 | — |
| u66  | S(1)...H(23) | 380.3(18) | 35.7 (tied to u75) | 4.8 | 27.4 | — |
| u71  | S(1)...H(30) | 387.7(23) | 37.9 (tied to u75) | –3.1 | 29.1 | — |
| u67  | S(1)...S(2) | 388.6(9)  | 12.4 (7) | –1.3 | 9.4  | 9.4(9) |
| u70  | B(3)...H(26) | 389.6(34) | 30.9 (tied to u67) | –2.3 | 23.4 | — |
| u69  | B(3)...H(27) | 390.9(15) | 30.4 (tied to u75) | –2.2 | 23.3 | — |
| u72  | S(1)...H(28) | 396.4(16) | 36.9 (tied to u75) | –3.8 | 28.3 | — |
| u68  | C(11)...H(25) | 398.0(22) | 39.9 (tied to u75) | 5.6 | 30.5 | — |
| u73  | N(7)...H(27) | 402.2(25) | 45.9 (tied to u75) | –1.2 | 35.1 | — |
| u65  | H(21)...H(25) | 402.3(29) | 40.8 (fixed) | 9.0 | 40.8 | — |
| u78  | B(3)...N(10) | 407.7(6)  | 14.9 (tied to u75) | –3.2 | 11.4 | — |
| u75  | S(1)...N(7) | 408.4(12) | 18.4 (4) | –1.1 | 14.1 | 14.1(14) |
| u74  | H(22)...H(25) | 410.8(43) | 35.1 (fixed) | –0.6 | 35.1 | — |
| u77  | H(20)...H(23) | 415.9(14) | 13.4 (fixed) | –3.7 | 13.4 | — |
| u76  | B(3)...C(14) | 416.6(12) | 10.5 (tied to u75) | –1.3 | 8.1  | — |
| u81  | B(3)...N(9) | 417.9(13) | 28.2 (tied to u75) | –2.6 | 21.6 | — |
| u79  | S(1)...C(13) | 419.3(5)  | 9.8 (tied to u75) | –1.2 | 7.5  | — |
| u82  | B(3)...H(41) | 432.8(21) | 33.5 (tied to u75) | 4.4 | 25.7 | — |
| u86  | S(1)...C(12) | 439.6(12) | 26.4 (tied to u75) | –0.7 | 20.2 | — |
| u80  | H(20)...H(25) | 440.9(33) | 37.2 (fixed) | 5.8 | 37.2 | — |
| u83  | B(3)...H(29) | 442.1(17) | 19.2 (tied to u75) | 0.9 | 14.7 | — |
| u85  | S(1)...H(25) | 443.8(12) | 18.6 (tied to u75) | 0.2 | 14.2 | — |
| u84  | N(7)...H(26) | 444.1(25) | 32.1 (tied to u75) | –3.5 | 24.6 | — |
| u87  | H(22)...H(27) | 457.8(31) | 48.8 (fixed) | –2.6 | 48.8 | — |
| u88  | C(12)...H(26) | 458.4(29) | 36.2 (tied to u75) | –4.0 | 27.7 | — |</p>
<table>
<thead>
<tr>
<th>Bond Lengths (Å)</th>
<th>Bond Distance (Å)</th>
<th>Bond Angle (°)</th>
<th>Torsion Angle (°)</th>
<th>Supplementary Material (ESI) for Dalton Transactions</th>
</tr>
</thead>
<tbody>
<tr>
<td>B(3)...H(28)</td>
<td>472.2(25)</td>
<td>22.2(tied to u75)</td>
<td>–3.0 17.0</td>
<td>—</td>
</tr>
<tr>
<td>B(3)...H(32)</td>
<td>472.7(25)</td>
<td>30.6(fixed)</td>
<td>–0.1 30.6</td>
<td>—</td>
</tr>
<tr>
<td>B(3)...C(18)</td>
<td>474.8(9)</td>
<td>15.0(tied to u93)</td>
<td>–3.6 15.9</td>
<td>—</td>
</tr>
<tr>
<td>S(1)...H(22)</td>
<td>476.0(33)</td>
<td>49.3(0)</td>
<td>–1.9 38.3</td>
<td>—</td>
</tr>
<tr>
<td>S(1)...H(26)</td>
<td>476.5(9)</td>
<td>15.2(tied to u93)</td>
<td>–2.7 16.1</td>
<td>—</td>
</tr>
<tr>
<td>B(3)...H(30)</td>
<td>478.2(12)</td>
<td>15.5(tied to u93)</td>
<td>–3.1 16.4</td>
<td>—</td>
</tr>
<tr>
<td>H(19)...H(25)</td>
<td>479.9(25)</td>
<td>32.1(fixed)</td>
<td>0.6 32.1</td>
<td>—</td>
</tr>
<tr>
<td>S(1)...H(27)</td>
<td>480.2(9)</td>
<td>15.7(fixed)</td>
<td>–2.4 15.7</td>
<td>—</td>
</tr>
<tr>
<td>B(3)...H(34)</td>
<td>484.8(37)</td>
<td>44.2(tied to u112)</td>
<td>2.5 34.3</td>
<td>—</td>
</tr>
<tr>
<td>C(11)...C(13)</td>
<td>485.0(15)</td>
<td>22.4(11)</td>
<td>–1.2 23.7</td>
<td>—</td>
</tr>
<tr>
<td>N(7)...C(14)</td>
<td>496.4(11)</td>
<td>12.8(tied to u93)</td>
<td>–2.2 13.6</td>
<td>—</td>
</tr>
<tr>
<td>C(12)...H(30)</td>
<td>497.0(26)</td>
<td>46.0(tied to u112)</td>
<td>14.2 36.7</td>
<td>—</td>
</tr>
<tr>
<td>B(3)...C(15)</td>
<td>496.6(15)</td>
<td>24.5(tied to u93)</td>
<td>–3.5 26.0</td>
<td>—</td>
</tr>
<tr>
<td>C(11)...H(27)</td>
<td>501.2(27)</td>
<td>37.1(tied to u93)</td>
<td>–2.5 39.4</td>
<td>—</td>
</tr>
<tr>
<td>N(7)...N(9)</td>
<td>512.9(22)</td>
<td>46.2(tied to u112)</td>
<td>–3.8 35.9</td>
<td>—</td>
</tr>
<tr>
<td>B(3)...H(38)</td>
<td>515.1(17)</td>
<td>25.8(tied to u112)</td>
<td>–1.3 20.0</td>
<td>—</td>
</tr>
<tr>
<td>H(20)...H(41)</td>
<td>504.9(37)</td>
<td>36.7(fixed)</td>
<td>14.2 36.7</td>
<td>—</td>
</tr>
<tr>
<td>B(3)...C(16)</td>
<td>503.3(17)</td>
<td>33.7(tied to u112)</td>
<td>–3.0 26.1</td>
<td>—</td>
</tr>
<tr>
<td>C(12)...H(29)</td>
<td>525.2(27)</td>
<td>37.1(tied to u93)</td>
<td>–2.5 39.4</td>
<td>—</td>
</tr>
<tr>
<td>H(21)...H(27)</td>
<td>527.3(38)</td>
<td>48.0(fixed)</td>
<td>1.5 48.0</td>
<td>—</td>
</tr>
<tr>
<td>C(12)...H(29)</td>
<td>529.5(26)</td>
<td>38.9(tied to u112)</td>
<td>–1.2 30.1</td>
<td>—</td>
</tr>
<tr>
<td>B(3)...H(42)</td>
<td>530.1(20)</td>
<td>46.4(tied to u112)</td>
<td>–6.4 36.0</td>
<td>—</td>
</tr>
<tr>
<td>S(1)...H(24)</td>
<td>530.3(14)</td>
<td>30.0(tied to u112)</td>
<td>–4.3 23.3</td>
<td>—</td>
</tr>
<tr>
<td>S(1)...C(11)</td>
<td>531.0(19)</td>
<td>22.0(7)</td>
<td>–2.5 17.0</td>
<td>17.0(17)</td>
</tr>
<tr>
<td>B(3)...H(35)</td>
<td>533.0(24)</td>
<td>57.3(tied to u112)</td>
<td>–3.3 44.5</td>
<td>—</td>
</tr>
<tr>
<td>N(7)...H(29)</td>
<td>534.7(17)</td>
<td>23.8(tied to u112)</td>
<td>–1.2 18.5</td>
<td>—</td>
</tr>
<tr>
<td>N(7)...H(30)</td>
<td>535.9(19)</td>
<td>31.4(tied to u112)</td>
<td>–2.1 24.4</td>
<td>—</td>
</tr>
<tr>
<td>N(7)...N(10)</td>
<td>534.9(6)</td>
<td>12.8(tied to u112)</td>
<td>–5.2 9.9</td>
<td>—</td>
</tr>
<tr>
<td>H(20)...H(32)</td>
<td>535.7(45)</td>
<td>61.3(fixed)</td>
<td>6.8 61.3</td>
<td>—</td>
</tr>
<tr>
<td>N(7)...H(30)</td>
<td>535.9(19)</td>
<td>31.4(tied to u112)</td>
<td>–2.1 24.4</td>
<td>—</td>
</tr>
<tr>
<td>B(3)...H(40)</td>
<td>537.9(19)</td>
<td>32.9(0)</td>
<td>3.3 25.5</td>
<td>—</td>
</tr>
<tr>
<td>B(3)...H(34)</td>
<td>555.3(47)</td>
<td>59.6(tied to u137)</td>
<td>1.3 49.8</td>
<td>—</td>
</tr>
<tr>
<td>N(7)...H(34)</td>
<td>555.3(47)</td>
<td>59.6(tied to u137)</td>
<td>1.3 49.8</td>
<td>—</td>
</tr>
<tr>
<td>N(7)...H(28)</td>
<td>557.8(31)</td>
<td>19.6(tied to u137)</td>
<td>–4.8 16.4</td>
<td>—</td>
</tr>
<tr>
<td>C(12)...H(28)</td>
<td>559.5(18)</td>
<td>29.7(tied to u137)</td>
<td>–5.2 24.8</td>
<td>—</td>
</tr>
<tr>
<td>H(22)...H(26)</td>
<td>557.9(32)</td>
<td>28.8(fixed)</td>
<td>–9.0 28.8</td>
<td>—</td>
</tr>
<tr>
<td>C(11)...H(26)</td>
<td>561.2(26)</td>
<td>38.2(tied to u137)</td>
<td>–4.6 32.0</td>
<td>—</td>
</tr>
<tr>
<td>S(1)...H(19)</td>
<td>562.2(33)</td>
<td>38.3(tied to u137)</td>
<td>–2.6 32.0</td>
<td>—</td>
</tr>
<tr>
<td>H(20)...H(31)</td>
<td>563.5(64)</td>
<td>78.8(fixed)</td>
<td>2.9 78.8</td>
<td>—</td>
</tr>
<tr>
<td>N(7)...H(32)</td>
<td>565.4(24)</td>
<td>56.9(tied to u112)</td>
<td>–2.3 44.2</td>
<td>—</td>
</tr>
<tr>
<td>H(21)...H(26)</td>
<td>567.4(30)</td>
<td>44.5(fixed)</td>
<td>–1.5 44.5</td>
<td>—</td>
</tr>
<tr>
<td>S(1)...H(41)</td>
<td>569.5(26)</td>
<td>34.3(tied to u137)</td>
<td>3.8 28.7</td>
<td>—</td>
</tr>
<tr>
<td>H(3)...H(37)</td>
<td>569.6(15)</td>
<td>32.5(tied to u112)</td>
<td>–5.7 27.2</td>
<td>—</td>
</tr>
<tr>
<td>C(12)...H(34)</td>
<td>576.1(46)</td>
<td>74.4(tied to u160)</td>
<td>2.0 60.0</td>
<td>—</td>
</tr>
<tr>
<td>N(7)...C(16)</td>
<td>579.0(30)</td>
<td>51.8(tied to u112)</td>
<td>–4.1 43.3</td>
<td>—</td>
</tr>
<tr>
<td>u139</td>
<td>N(7)...C(15)</td>
<td>584.0(20)</td>
<td>51.1 (tied to u137)</td>
<td>−5.2</td>
</tr>
<tr>
<td>u140</td>
<td>H(20)...H(27)</td>
<td>584.7(30)</td>
<td>51.7 (tied to u112)</td>
<td>−4.8</td>
</tr>
<tr>
<td>u141</td>
<td>N(7)...H(35)</td>
<td>588.2(45)</td>
<td>75.7(1)</td>
<td>−2.8</td>
</tr>
<tr>
<td>u142</td>
<td>N(7)...C(18)</td>
<td>589.2(34)</td>
<td>76.0 (tied to u160)</td>
<td>−4.3</td>
</tr>
<tr>
<td>u143</td>
<td>H(19)...H(27)</td>
<td>589.9(33)</td>
<td>44.0 (fixed)</td>
<td>−5.5</td>
</tr>
<tr>
<td>u144</td>
<td>B(3)...H(33)</td>
<td>591.5(18)</td>
<td>29.7 (tied to u137)</td>
<td>−7.4</td>
</tr>
<tr>
<td>u145</td>
<td>N(7)...H(35)</td>
<td>592.0(10)</td>
<td>17.7(9)</td>
<td>−5.8</td>
</tr>
<tr>
<td>u146</td>
<td>N(7)...H(31)</td>
<td>594.8(19)</td>
<td>31.7 (tied to u137)</td>
<td>−8.6</td>
</tr>
<tr>
<td>u147</td>
<td>H(20)...H(26)</td>
<td>593.8(41)</td>
<td>44.0 (fixed)</td>
<td>−3.5</td>
</tr>
<tr>
<td>u148</td>
<td>H(20)...H(27)</td>
<td>594.0(33)</td>
<td>44.0 (fixed)</td>
<td>−5.5</td>
</tr>
<tr>
<td>u149</td>
<td>H(20)...H(27)</td>
<td>596.4(40)</td>
<td>47.2 (fixed)</td>
<td>−3.3</td>
</tr>
<tr>
<td>u150</td>
<td>H(19)...H(32)</td>
<td>596.8(33)</td>
<td>75.9 (fixed)</td>
<td>−3.3</td>
</tr>
<tr>
<td>u151</td>
<td>B(3)...H(39)</td>
<td>597.5(58)</td>
<td>94.5 (fixed)</td>
<td>−3.3</td>
</tr>
<tr>
<td>u152</td>
<td>H(20)...H(41)</td>
<td>598.6(19)</td>
<td>31.7 (fixed)</td>
<td>−8.6</td>
</tr>
<tr>
<td>u153</td>
<td>C(11)...H(31)</td>
<td>607.1(46)</td>
<td>91.5 (tied to u160)</td>
<td>−3.3</td>
</tr>
<tr>
<td>u154</td>
<td>C(11)...H(32)</td>
<td>607.8(45)</td>
<td>94.5 (fixed)</td>
<td>−3.3</td>
</tr>
<tr>
<td>u155</td>
<td>H(19)...H(35)</td>
<td>613.4(40)</td>
<td>47.2 (fixed)</td>
<td>−3.3</td>
</tr>
<tr>
<td>u156</td>
<td>H(19)...H(35)</td>
<td>614.8(94)</td>
<td>89.8 (fixed)</td>
<td>−3.3</td>
</tr>
<tr>
<td>u157</td>
<td>C(11)...C(15)</td>
<td>620.3(26)</td>
<td>66.5 (tied to u160)</td>
<td>−5.0</td>
</tr>
<tr>
<td>u158</td>
<td>C(12)...H(35)</td>
<td>625.8(39)</td>
<td>94.1 (tied to u160)</td>
<td>−4.1</td>
</tr>
<tr>
<td>u159</td>
<td>H(19)...H(34)</td>
<td>632.4(94)</td>
<td>73.2 (fixed)</td>
<td>−3.3</td>
</tr>
<tr>
<td>u160</td>
<td>N(7)...H(38)</td>
<td>633.3(20)</td>
<td>23.5 (tied to u160)</td>
<td>−6.2</td>
</tr>
<tr>
<td>u161</td>
<td>C(11)...C(14)</td>
<td>638.8(11)</td>
<td>17.6 (tied to u160)</td>
<td>−4.0</td>
</tr>
<tr>
<td>u162</td>
<td>C(11)...H(35)</td>
<td>639.9(75)</td>
<td>88.4 (tied to u160)</td>
<td>−1.6</td>
</tr>
<tr>
<td>u163</td>
<td>C(11)...H(34)</td>
<td>641.0(78)</td>
<td>54.6 (tied to u192)</td>
<td>−1.1</td>
</tr>
<tr>
<td>u164</td>
<td>C(11)...H(34)</td>
<td>642.0(24)</td>
<td>30.5 (fixed)</td>
<td>−10.0</td>
</tr>
<tr>
<td>u165</td>
<td>H(19)...H(41)</td>
<td>643.2(24)</td>
<td>30.5 (fixed)</td>
<td>−10.0</td>
</tr>
<tr>
<td>u166</td>
<td>N(7)...H(35)</td>
<td>645.2(15)</td>
<td>26.6 (tied to u160)</td>
<td>−3.6</td>
</tr>
<tr>
<td>u167</td>
<td>H(20)...H(34)</td>
<td>648.4(99)</td>
<td>58.7 (fixed)</td>
<td>0.5</td>
</tr>
<tr>
<td>u168</td>
<td>H(19)...H(41)</td>
<td>648.6(34)</td>
<td>40.1 (fixed)</td>
<td>−2.9</td>
</tr>
<tr>
<td>u169</td>
<td>H(19)...H(41)</td>
<td>648.8(58)</td>
<td>63.9 (tied to u160)</td>
<td>−4.6</td>
</tr>
<tr>
<td>u170</td>
<td>N(7)...H(42)</td>
<td>652.0(16)</td>
<td>45.2 (tied to u160)</td>
<td>−9.7</td>
</tr>
<tr>
<td>u171</td>
<td>N(7)...H(42)</td>
<td>652.6(6)</td>
<td>15.4(7)</td>
<td>−6.8</td>
</tr>
<tr>
<td>u172</td>
<td>N(7)...H(38)</td>
<td>652.6(6)</td>
<td>15.4(7)</td>
<td>−6.8</td>
</tr>
<tr>
<td>u173</td>
<td>H(22)...H(31)</td>
<td>660.2(41)</td>
<td>85.7 (fixed)</td>
<td>−3.6</td>
</tr>
<tr>
<td>u174</td>
<td>H(20)...H(40)</td>
<td>662.5(25)</td>
<td>29.4 (tied to u192)</td>
<td>−10.4</td>
</tr>
<tr>
<td>u175</td>
<td>H(22)...H(31)</td>
<td>669.2(22)</td>
<td>27.1(1)</td>
<td>0.7</td>
</tr>
<tr>
<td>u176</td>
<td>C(12)...H(32)</td>
<td>672.4(27)</td>
<td>59.0 (tied to u160)</td>
<td>−5.2</td>
</tr>
<tr>
<td>u177</td>
<td>C(12)...H(32)</td>
<td>673.6(20)</td>
<td>47.6 (tied to u192)</td>
<td>−7.2</td>
</tr>
<tr>
<td>u178</td>
<td>C(12)...H(31)</td>
<td>674.0(28)</td>
<td>66.0 (tied to u192)</td>
<td>−6.3</td>
</tr>
<tr>
<td>u179</td>
<td>C(12)...H(29)</td>
<td>676.4(17)</td>
<td>22.0 (tied to u160)</td>
<td>−3.3</td>
</tr>
<tr>
<td>u180</td>
<td>N(7)...H(36)</td>
<td>677.2(28)</td>
<td>40.6 (tied to u192)</td>
<td>−10.9</td>
</tr>
<tr>
<td>u181</td>
<td>N(7)...H(36)</td>
<td>678.4(22)</td>
<td>24.4 (tied to u192)</td>
<td>−4.2</td>
</tr>
<tr>
<td>u182</td>
<td>H(20)...H(33)</td>
<td>678.9(44)</td>
<td>59.4 (fixed)</td>
<td>−3.2</td>
</tr>
<tr>
<td>u183</td>
<td>H(20)...H(33)</td>
<td>679.0(39)</td>
<td>45.1 (fixed)</td>
<td>−3.4</td>
</tr>
<tr>
<td>u184</td>
<td>H(20)...H(38)</td>
<td>680.4(34)</td>
<td>33.4 (fixed)</td>
<td>2.0</td>
</tr>
<tr>
<td>u185</td>
<td>H(22)...H(32)</td>
<td>683.8(27)</td>
<td>64.0 (fixed)</td>
<td>−5.5</td>
</tr>
<tr>
<td>u186</td>
<td>N(7)...H(33)</td>
<td>684.4(19)</td>
<td>39.3 (tied to u192)</td>
<td>−9.8</td>
</tr>
<tr>
<td>u187</td>
<td>H(21)...H(32)</td>
<td>685.2(33)</td>
<td>55.1 (fixed)</td>
<td>−8.9</td>
</tr>
<tr>
<td>u</td>
<td>C(11)...H(40)</td>
<td>687.3(36)</td>
<td>38.3(tied to u_192)</td>
<td>−9.8</td>
</tr>
<tr>
<td>u</td>
<td>C(11)...H(28)</td>
<td>695.6(17)</td>
<td>18.5(tied to u_192)</td>
<td>−6.4</td>
</tr>
<tr>
<td>u</td>
<td>N(7)...H(37)</td>
<td>704.9(14)</td>
<td>24.0(tied to u_192)</td>
<td>−9.0</td>
</tr>
<tr>
<td>u</td>
<td>C(11)...H(42)</td>
<td>705.4(24)</td>
<td>44.2(tied to u_160)</td>
<td>−11.7</td>
</tr>
<tr>
<td>u</td>
<td>H(21)...H(31)</td>
<td>706.1(48)</td>
<td>74.1(fixed)</td>
<td>−11.6</td>
</tr>
<tr>
<td>u</td>
<td>C(11)...H(28)</td>
<td>705.6(17)</td>
<td>18.5(tied to u_192)</td>
<td>−6.4</td>
</tr>
<tr>
<td>u</td>
<td>H(21)...H(30)</td>
<td>711.9(43)</td>
<td>33.0(fixed)</td>
<td>−3.3</td>
</tr>
<tr>
<td>u</td>
<td>C(11)...H(42)</td>
<td>719.1(9)</td>
<td>16.8(15)</td>
<td>−7.8</td>
</tr>
<tr>
<td>u</td>
<td>N(7)...H(39)</td>
<td>720.9(19)</td>
<td>24.3(tied to u_192)</td>
<td>−5.1</td>
</tr>
<tr>
<td>u</td>
<td>C(11)...H(33)</td>
<td>724.1(25)</td>
<td>51.0(tied to u_192)</td>
<td>−10.4</td>
</tr>
<tr>
<td>u</td>
<td>H(20)...H(29)</td>
<td>726.0(27)</td>
<td>26.1(fixed)</td>
<td>−4.6</td>
</tr>
<tr>
<td>u</td>
<td>H(20)...H(30)</td>
<td>735.8(21)</td>
<td>27.3(fixed)</td>
<td>−2.5</td>
</tr>
<tr>
<td>u</td>
<td>C(11)...H(38)</td>
<td>735.7(20)</td>
<td>55.8(fixed)</td>
<td>−7.3</td>
</tr>
<tr>
<td>u</td>
<td>H(19)...H(38)</td>
<td>740.4(73)</td>
<td>72.3(fixed)</td>
<td>−9.8</td>
</tr>
<tr>
<td>u</td>
<td>H(21)...H(39)</td>
<td>741.6(61)</td>
<td>51.6(fixed)</td>
<td>−14.5</td>
</tr>
<tr>
<td>u</td>
<td>C(11)...H(36)</td>
<td>748.3(53)</td>
<td>49.1(tied to u_192)</td>
<td>−11.9</td>
</tr>
<tr>
<td>u</td>
<td>C(11)...H(33)</td>
<td>754.1(25)</td>
<td>54.1(fixed)</td>
<td>−14.4</td>
</tr>
<tr>
<td>u</td>
<td>C(12)...C(17)</td>
<td>757.9(12)</td>
<td>16.0(tied to u_192)</td>
<td>−8.7</td>
</tr>
<tr>
<td>u</td>
<td>H(19)...H(37)</td>
<td>761.7(28)</td>
<td>19.8(fixed)</td>
<td>−10.7</td>
</tr>
<tr>
<td>u</td>
<td>H(20)...H(36)</td>
<td>763.1(28)</td>
<td>46.0(fixed)</td>
<td>−9.0</td>
</tr>
<tr>
<td>u</td>
<td>H(19)...H(38)</td>
<td>763.2(34)</td>
<td>46.5(fixed)</td>
<td>−7.1</td>
</tr>
<tr>
<td>u</td>
<td>H(19)...H(37)</td>
<td>770.7(20)</td>
<td>45.8(tied to u_192)</td>
<td>−12.0</td>
</tr>
<tr>
<td>u</td>
<td>C(12)...H(33)</td>
<td>771.0(33)</td>
<td>68.3(fixed)</td>
<td>−11.5</td>
</tr>
<tr>
<td>u</td>
<td>C(12)...H(42)</td>
<td>771.0(20)</td>
<td>39.4(tied to u_192)</td>
<td>−11.2</td>
</tr>
<tr>
<td>u</td>
<td>H(22)...H(38)</td>
<td>776.1(33)</td>
<td>41.0(fixed)</td>
<td>−5.9</td>
</tr>
<tr>
<td>u</td>
<td>C(11)...H(39)</td>
<td>776.3(16)</td>
<td>28.0(tied to u_192)</td>
<td>−9.6</td>
</tr>
<tr>
<td>u</td>
<td>C(11)...H(37)</td>
<td>781.1(11)</td>
<td>20.1(tied to u_192)</td>
<td>−10.7</td>
</tr>
<tr>
<td>u</td>
<td>C(11)...H(42)</td>
<td>781.9(34)</td>
<td>41.6(fixed)</td>
<td>−18.2</td>
</tr>
<tr>
<td>u</td>
<td>C(12)...H(40)</td>
<td>794.6(22)</td>
<td>27.9(tied to u_192)</td>
<td>−13.2</td>
</tr>
<tr>
<td>u</td>
<td>H(21)...H(38)</td>
<td>803.6(23)</td>
<td>29.8(fixed)</td>
<td>−11.2</td>
</tr>
<tr>
<td>u</td>
<td>H(21)...H(37)</td>
<td>804.7(22)</td>
<td>30.3(tied to u_192)</td>
<td>−10.7</td>
</tr>
<tr>
<td>u</td>
<td>H(21)...H(33)</td>
<td>821.2(26)</td>
<td>51.6(fixed)</td>
<td>−18.3</td>
</tr>
<tr>
<td>u</td>
<td>H(23)...H(39)</td>
<td>822.9(24)</td>
<td>27.4(fixed)</td>
<td>−9.0</td>
</tr>
<tr>
<td>u</td>
<td>H(19)...H(39)</td>
<td>823.8(22)</td>
<td>52.0(fixed)</td>
<td>−12.7</td>
</tr>
<tr>
<td>u</td>
<td>C(12)...H(39)</td>
<td>836.1(14)</td>
<td>21.5(tied to u_192)</td>
<td>−12.1</td>
</tr>
<tr>
<td>u</td>
<td>H(19)...H(37)</td>
<td>840.1(23)</td>
<td>37.5(fixed)</td>
<td>−15.4</td>
</tr>
<tr>
<td>u</td>
<td>H(21)...H(36)</td>
<td>847.4(49)</td>
<td>49.1(fixed)</td>
<td>−19.6</td>
</tr>
<tr>
<td>u</td>
<td>H(21)...H(37)</td>
<td>850.1(24)</td>
<td>35.4(fixed)</td>
<td>−15.1</td>
</tr>
<tr>
<td>( u_{226} )</td>
<td>H(21)...H(39)</td>
<td>852.8(29)</td>
<td>35.5(fixed)</td>
<td>-15.7</td>
</tr>
<tr>
<td>( u_{228} )</td>
<td>H(22)...H(37)</td>
<td>860.2(38)</td>
<td>36.5(fixed)</td>
<td>-13.9</td>
</tr>
<tr>
<td>( u_{229} )</td>
<td>H(24)...H(33)</td>
<td>868.5(21)</td>
<td>44.8(fixed)</td>
<td>-17.2</td>
</tr>
<tr>
<td>( u_{230} )</td>
<td>H(22)...H(39)</td>
<td>877.1(16)</td>
<td>38.9(fixed)</td>
<td>-13.6</td>
</tr>
<tr>
<td>( u_{231} )</td>
<td>H(24)...H(39)</td>
<td>915.1(19)</td>
<td>23.3(fixed)</td>
<td>-15.9</td>
</tr>
</tbody>
</table>

*a* Estimated standard deviations, as obtained in the least-squares refinement, are given in parentheses. *b* Amplitudes not refined were fixed at the values obtained using the force field calculated at the RHF/6-31G* level.
<table>
<thead>
<tr>
<th></th>
<th>$p_1$</th>
<th>$p_2$</th>
<th>$p_3$</th>
<th>$p_4$</th>
<th>$p_5$</th>
<th>$p_6$</th>
<th>$p_7$</th>
<th>$p_8$</th>
<th>$p_9$</th>
<th>$p_{10}$</th>
<th>$p_{11}$</th>
<th>$p_{12}$</th>
<th>$p_{13}$</th>
<th>$u_1$</th>
<th>$u_2$</th>
<th>$u_3$</th>
<th>$u_4$</th>
<th>$u_5$</th>
<th>$u_6$</th>
<th>$k_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$p_1$</td>
<td>100</td>
<td>100</td>
<td>-84</td>
<td>-59</td>
<td>-64</td>
<td>68</td>
<td>-52</td>
<td>57</td>
<td>-57</td>
<td>-56</td>
<td>53</td>
<td>-56</td>
<td>53</td>
<td>100</td>
<td>100</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$p_2$</td>
<td>100</td>
<td>100</td>
<td>-84</td>
<td>-59</td>
<td>-64</td>
<td>68</td>
<td>-52</td>
<td>57</td>
<td>-57</td>
<td>-56</td>
<td>53</td>
<td>-56</td>
<td>53</td>
<td>100</td>
<td>100</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table S3. Least-squares correlation matrix ($\times 100$) for 1,4-B$_4$S$_2$(NM$_2$)$_4$.\(^a\)

\(^a\) Only elements with absolute values $\geq 50\%$ are shown.
Table S4. GED coordinates (in Å) for 1,4-B₄S₂(NMe₂)₄.

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>S(1)</td>
<td>0.000</td>
<td>0.000</td>
<td>-1.949</td>
</tr>
<tr>
<td>S(2)</td>
<td>0.000</td>
<td>0.000</td>
<td>1.949</td>
</tr>
<tr>
<td>B(3)</td>
<td>1.332</td>
<td>0.458</td>
<td>0.736</td>
</tr>
<tr>
<td>B(4)</td>
<td>1.332</td>
<td>-0.458</td>
<td>-0.736</td>
</tr>
<tr>
<td>B(5)</td>
<td>-1.332</td>
<td>0.458</td>
<td>-0.736</td>
</tr>
<tr>
<td>B(6)</td>
<td>-1.332</td>
<td>-0.458</td>
<td>0.736</td>
</tr>
<tr>
<td>N(7)</td>
<td>2.324</td>
<td>1.376</td>
<td>1.129</td>
</tr>
<tr>
<td>N(8)</td>
<td>2.324</td>
<td>-1.376</td>
<td>-1.129</td>
</tr>
<tr>
<td>N(9)</td>
<td>-2.324</td>
<td>1.376</td>
<td>-1.129</td>
</tr>
<tr>
<td>N(10)</td>
<td>-2.324</td>
<td>-1.376</td>
<td>1.129</td>
</tr>
<tr>
<td>C(11)</td>
<td>2.299</td>
<td>2.222</td>
<td>2.321</td>
</tr>
<tr>
<td>C(12)</td>
<td>3.397</td>
<td>1.775</td>
<td>0.219</td>
</tr>
<tr>
<td>C(13)</td>
<td>3.397</td>
<td>-1.775</td>
<td>-0.219</td>
</tr>
<tr>
<td>C(14)</td>
<td>2.299</td>
<td>-2.222</td>
<td>-2.321</td>
</tr>
<tr>
<td>C(15)</td>
<td>-3.397</td>
<td>1.775</td>
<td>-0.219</td>
</tr>
<tr>
<td>C(16)</td>
<td>-2.299</td>
<td>2.222</td>
<td>-2.321</td>
</tr>
<tr>
<td>C(17)</td>
<td>-3.397</td>
<td>-1.775</td>
<td>0.219</td>
</tr>
<tr>
<td>C(18)</td>
<td>-2.299</td>
<td>-2.222</td>
<td>2.321</td>
</tr>
<tr>
<td>H(19)</td>
<td>2.288</td>
<td>3.282</td>
<td>2.036</td>
</tr>
<tr>
<td>H(20)</td>
<td>1.404</td>
<td>2.012</td>
<td>2.920</td>
</tr>
<tr>
<td>H(21)</td>
<td>3.186</td>
<td>2.036</td>
<td>2.940</td>
</tr>
<tr>
<td>H(22)</td>
<td>3.319</td>
<td>2.843</td>
<td>-0.017</td>
</tr>
<tr>
<td>H(23)</td>
<td>3.336</td>
<td>1.204</td>
<td>-0.716</td>
</tr>
<tr>
<td>H(24)</td>
<td>4.376</td>
<td>1.589</td>
<td>0.679</td>
</tr>
<tr>
<td>H(25)</td>
<td>3.336</td>
<td>-1.204</td>
<td>0.716</td>
</tr>
<tr>
<td>H(26)</td>
<td>3.319</td>
<td>-2.843</td>
<td>0.017</td>
</tr>
<tr>
<td>H(27)</td>
<td>4.376</td>
<td>-1.589</td>
<td>-0.679</td>
</tr>
<tr>
<td>H(28)</td>
<td>2.288</td>
<td>-3.282</td>
<td>-2.036</td>
</tr>
<tr>
<td>H(29)</td>
<td>1.404</td>
<td>-2.012</td>
<td>-2.920</td>
</tr>
<tr>
<td>H(30)</td>
<td>3.186</td>
<td>-2.036</td>
<td>-2.940</td>
</tr>
<tr>
<td>H(31)</td>
<td>-3.319</td>
<td>2.843</td>
<td>0.017</td>
</tr>
<tr>
<td>H(32)</td>
<td>-3.336</td>
<td>1.204</td>
<td>0.716</td>
</tr>
<tr>
<td>H(33)</td>
<td>-4.376</td>
<td>1.589</td>
<td>-0.679</td>
</tr>
<tr>
<td>H(34)</td>
<td>-1.404</td>
<td>2.012</td>
<td>-2.920</td>
</tr>
<tr>
<td>H(35)</td>
<td>-2.288</td>
<td>3.282</td>
<td>-2.036</td>
</tr>
<tr>
<td>H(36)</td>
<td>-3.186</td>
<td>2.036</td>
<td>-2.940</td>
</tr>
<tr>
<td>H(37)</td>
<td>-3.319</td>
<td>-2.843</td>
<td>-0.017</td>
</tr>
<tr>
<td>H(38)</td>
<td>-3.336</td>
<td>-1.204</td>
<td>-0.716</td>
</tr>
<tr>
<td>H(39)</td>
<td>-4.376</td>
<td>-1.589</td>
<td>0.679</td>
</tr>
<tr>
<td>H(40)</td>
<td>-3.186</td>
<td>-2.036</td>
<td>2.940</td>
</tr>
<tr>
<td>H(41)</td>
<td>-1.404</td>
<td>-2.012</td>
<td>2.920</td>
</tr>
<tr>
<td>H(42)</td>
<td>-2.288</td>
<td>-3.282</td>
<td>2.036</td>
</tr>
</tbody>
</table>
Table S5. Calculated coordinates [MP2(full)/6-311++G**] for 1,4-B\textsubscript{4}S\textsubscript{2}(NMe\textsubscript{2})\textsubscript{4}.

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>S(1)</td>
<td>0.000</td>
<td>0.000</td>
<td>-1.956</td>
</tr>
<tr>
<td>S(2)</td>
<td>0.000</td>
<td>0.000</td>
<td>1.956</td>
</tr>
<tr>
<td>B(3)</td>
<td>1.336</td>
<td>0.415</td>
<td>0.742</td>
</tr>
<tr>
<td>B(4)</td>
<td>1.336</td>
<td>-0.415</td>
<td>-0.742</td>
</tr>
<tr>
<td>B(5)</td>
<td>-1.336</td>
<td>0.415</td>
<td>-0.742</td>
</tr>
<tr>
<td>B(6)</td>
<td>-1.336</td>
<td>-0.415</td>
<td>0.742</td>
</tr>
<tr>
<td>N(7)</td>
<td>2.317</td>
<td>1.356</td>
<td>1.101</td>
</tr>
<tr>
<td>N(8)</td>
<td>2.317</td>
<td>-1.356</td>
<td>-1.101</td>
</tr>
<tr>
<td>N(9)</td>
<td>-2.317</td>
<td>1.356</td>
<td>-1.101</td>
</tr>
<tr>
<td>N(10)</td>
<td>-2.317</td>
<td>-1.356</td>
<td>1.101</td>
</tr>
<tr>
<td>C(11)</td>
<td>2.367</td>
<td>2.097</td>
<td>2.353</td>
</tr>
<tr>
<td>C(12)</td>
<td>3.420</td>
<td>1.700</td>
<td>0.216</td>
</tr>
<tr>
<td>C(13)</td>
<td>3.420</td>
<td>-1.700</td>
<td>-0.216</td>
</tr>
<tr>
<td>C(14)</td>
<td>2.367</td>
<td>-2.097</td>
<td>-2.353</td>
</tr>
<tr>
<td>C(15)</td>
<td>-3.420</td>
<td>1.700</td>
<td>-0.216</td>
</tr>
<tr>
<td>C(16)</td>
<td>-2.367</td>
<td>2.097</td>
<td>-2.353</td>
</tr>
<tr>
<td>C(17)</td>
<td>-3.420</td>
<td>-1.700</td>
<td>0.216</td>
</tr>
<tr>
<td>C(18)</td>
<td>-2.367</td>
<td>-2.097</td>
<td>2.353</td>
</tr>
<tr>
<td>H(19)</td>
<td>2.415</td>
<td>3.174</td>
<td>2.150</td>
</tr>
<tr>
<td>H(20)</td>
<td>1.479</td>
<td>1.890</td>
<td>2.950</td>
</tr>
<tr>
<td>H(21)</td>
<td>3.259</td>
<td>1.819</td>
<td>2.930</td>
</tr>
<tr>
<td>H(22)</td>
<td>3.418</td>
<td>2.778</td>
<td>0.009</td>
</tr>
<tr>
<td>H(23)</td>
<td>3.323</td>
<td>1.162</td>
<td>-0.728</td>
</tr>
<tr>
<td>H(24)</td>
<td>4.384</td>
<td>1.445</td>
<td>0.676</td>
</tr>
<tr>
<td>H(25)</td>
<td>3.323</td>
<td>-1.162</td>
<td>0.728</td>
</tr>
<tr>
<td>H(26)</td>
<td>3.418</td>
<td>-2.778</td>
<td>-0.009</td>
</tr>
<tr>
<td>H(27)</td>
<td>4.384</td>
<td>-1.445</td>
<td>-0.676</td>
</tr>
<tr>
<td>H(28)</td>
<td>2.415</td>
<td>-3.174</td>
<td>-2.150</td>
</tr>
<tr>
<td>H(29)</td>
<td>1.479</td>
<td>-1.890</td>
<td>-2.950</td>
</tr>
<tr>
<td>H(30)</td>
<td>3.259</td>
<td>-1.819</td>
<td>-2.930</td>
</tr>
<tr>
<td>H(31)</td>
<td>-3.418</td>
<td>2.778</td>
<td>-0.009</td>
</tr>
<tr>
<td>H(32)</td>
<td>-3.323</td>
<td>1.162</td>
<td>0.728</td>
</tr>
<tr>
<td>H(33)</td>
<td>-4.384</td>
<td>1.445</td>
<td>-0.676</td>
</tr>
<tr>
<td>H(34)</td>
<td>-1.479</td>
<td>1.890</td>
<td>-2.950</td>
</tr>
<tr>
<td>H(35)</td>
<td>-2.415</td>
<td>3.174</td>
<td>-2.150</td>
</tr>
<tr>
<td>H(36)</td>
<td>-3.259</td>
<td>1.819</td>
<td>-2.930</td>
</tr>
<tr>
<td>H(37)</td>
<td>-3.418</td>
<td>-2.778</td>
<td>0.009</td>
</tr>
<tr>
<td>H(38)</td>
<td>-3.323</td>
<td>-1.162</td>
<td>-0.728</td>
</tr>
<tr>
<td>H(39)</td>
<td>-4.384</td>
<td>-1.445</td>
<td>0.676</td>
</tr>
<tr>
<td>H(40)</td>
<td>-3.259</td>
<td>-1.819</td>
<td>2.930</td>
</tr>
<tr>
<td>H(41)</td>
<td>-1.479</td>
<td>-1.890</td>
<td>2.950</td>
</tr>
<tr>
<td>H(42)</td>
<td>-2.415</td>
<td>-3.174</td>
<td>2.150</td>
</tr>
</tbody>
</table>

Energy = –1432.02121 Hartrees (corrected for ZPE).
**Figure S1.** Experimental and difference (experimental minus theoretical) molecular-scattering intensities for 1,4-B₄S₂(NMe₂)₄.