

**Structural data for [DADMB]YCl(THF)<sub>2</sub> (2)****Table 1.** Atomic coordinates and  $B_{iso}/B_{eq}$  for [DADMB]YCl(THF)<sub>2</sub> (2)

| atom  | x           | y           | z          | $B_{eq}$ |
|-------|-------------|-------------|------------|----------|
| Y(1)  | -0.47592(4) | -0.16953(7) | -0.314     | 1.98(2)  |
| Cl(1) | -0.5616(1)  | 0.0192(2)   | -0.2802(1) | 3.74(6)  |
| Si(1) | -0.5965(1)  | -0.2571(2)  | -0.4463(1) | 2.54(6)  |
| Si(2) | -0.3271(1)  | -0.1208(3)  | -0.1972(1) | 2.50(6)  |
| O(1)  | -0.5479(3)  | -0.2782(7)  | -0.2338(3) | 2.3(2)   |
| O(2)  | -0.4191(4)  | -0.0220(5)  | -0.3875(3) | 2.6(1)   |
| N(1)  | -0.5196(4)  | -0.2906(7)  | -0.3954(3) | 2.0(2)   |
| N(2)  | -0.3630(4)  | -0.2063(6)  | -0.2618(3) | 2.1(2)   |
| C(1)  | -0.5008(5)  | -0.4060(8)  | -0.3648(4) | 2.6(2)   |
| C(2)  | -0.5551(5)  | -0.5062(8)  | -0.3533(4) | 2.1(2)   |
| C(3)  | -0.5353(5)  | -0.6090(7)  | -0.3189(5) | 2.6(2)   |
| C(4)  | -0.4615(5)  | -0.6218(8)  | -0.2908(4) | 2.3(2)   |
| C(5)  | -0.4060(5)  | -0.5302(8)  | -0.3023(4) | 2.5(2)   |
| C(6)  | -0.4230(5)  | -0.4202(8)  | -0.3392(4) | 1.0(2)   |
| C(7)  | -0.3556(5)  | -0.3379(9)  | -0.3593(4) | 1.8(2)   |
| C(8)  | -0.3229(4)  | -0.2452(7)  | -0.3177(5) | 2.1(2)   |
| C(9)  | -0.2510(5)  | -0.1905(7)  | -0.3364(4) | 2.7(2)   |
| C(10) | -0.2142(5)  | -0.2259(9)  | -0.3912(4) | 2.3(2)   |
| C(11) | -0.2476(5)  | -0.3144(8)  | -0.4329(4) | 2.5(2)   |
| C(12) | -0.3187(4)  | -0.3692(8)  | -0.4175(4) | 1.7(2)   |
| C(13) | -0.3517(5)  | -0.4680(8)  | -0.4605(4) | 2.7(2)   |
| C(14) | -0.3237(5)  | -0.5464(8)  | -0.2763(4) | 2.8(2)   |
| C(15) | -0.5844(5)  | -0.3300(9)  | -0.5299(4) | 3.4(2)   |
| C(16) | -0.5749(6)  | -0.474(1)   | -0.5248(4) | 3.9(3)   |
| C(17) | -0.6579(6)  | -0.302(1)   | -0.5711(5) | 5.2(3)   |
| C(18) | -0.5121(6)  | -0.276(1)   | -0.5637(5) | 3.7(3)   |
| C(19) | -0.5994(6)  | -0.080(1)   | -0.4566(5) | 4.1(3)   |
| C(20) | -0.6955(5)  | -0.300(1)   | -0.4150(5) | 3.4(3)   |
| C(21) | -0.2539(6)  | -0.2135(9)  | -0.1476(5) | 2.7(2)   |
| C(22) | -0.1855(6)  | -0.265(1)   | -0.1884(5) | 4.0(3)   |
| C(23) | -0.2202(7)  | -0.129(1)   | -0.0932(5) | 5.1(3)   |
| C(24) | -0.2968(5)  | -0.327(1)   | -0.1155(5) | 4.0(3)   |

**Table 1.** Atomic coordinates and  $B_{\text{iso}}/B_{\text{eq}}$  for [DADMB]YCl(THF)<sub>2</sub> (2)

| atom  | x          | y          | z          | $B_{\text{eq}}$ |
|-------|------------|------------|------------|-----------------|
| C(25) | -0.4138(6) | -0.079(1)  | -0.1459(5) | 3.9(3)          |
| C(26) | -0.2831(6) | 0.0353(9)  | -0.2192(5) | 4.1(3)          |
| C(27) | -0.5204(5) | -0.3736(9) | -0.1869(4) | 2.9(2)          |
| C(28) | -0.5755(6) | -0.363(1)  | -0.1304(5) | 3.8(3)          |
| C(29) | -0.6511(7) | -0.314(2)  | -0.1618(5) | 6.9(4)          |
| C(30) | -0.6324(6) | -0.278(1)  | -0.2272(6) | 5.2(3)          |
| C(31) | -0.4125(7) | 0.1141(9)  | -0.3799(5) | 4.8(3)          |
| C(32) | -0.4296(6) | 0.1659(9)  | -0.4462(5) | 5.1(3)          |
| C(33) | -0.3955(6) | 0.0645(9)  | -0.4912(5) | 3.8(3)          |
| C(34) | -0.3862(5) | -0.0527(9) | -0.4489(5) | 2.3(2)          |
| H(1)  | -0.606     | -0.500     | -0.370     | 2.499           |
| H(2)  | -0.572     | -0.675     | -0.313     | 3.171           |
| H(3)  | -0.450     | -0.693     | -0.264     | 2.790           |
| H(4)  | -0.228     | -0.127     | -0.310     | 3.248           |
| H(5)  | -0.165     | -0.190     | -0.401     | 2.819           |
| H(6)  | -0.222     | -0.337     | -0.472     | 3.035           |
| H(7)  | -0.320     | -0.477     | -0.498     | 3.206           |
| H(8)  | -0.403     | -0.444     | -0.473     | 3.206           |
| H(9)  | -0.354     | -0.546     | -0.438     | 3.206           |
| H(10) | -0.300     | -0.618     | -0.296     | 3.323           |
| H(11) | -0.326     | -0.558     | -0.231     | 3.323           |
| H(12) | -0.294     | -0.473     | -0.286     | 3.323           |
| H(13) | -0.619     | -0.509     | -0.504     | 4.642           |
| H(14) | -0.570     | -0.509     | -0.567     | 4.642           |
| H(15) | -0.530     | -0.493     | -0.500     | 4.642           |
| H(16) | -0.702     | -0.336     | -0.550     | 6.275           |
| H(17) | -0.652     | -0.340     | -0.613     | 6.275           |
| H(18) | -0.664     | -0.213     | -0.576     | 6.275           |
| H(19) | -0.507     | -0.315     | -0.605     | 4.485           |
| H(20) | -0.518     | -0.187     | -0.569     | 4.485           |
| H(21) | -0.467     | -0.294     | -0.538     | 4.485           |
| H(22) | -0.552     | -0.053     | -0.476     | 4.891           |
| H(23) | -0.642     | -0.058     | -0.484     | 4.891           |

**Table 1.** Atomic coordinates and  $B_{\text{iso}}/B_{\text{eq}}$  for [DADMB]YCl(THF)<sub>2</sub> (2)

| atom  | x      | y      | z      | $B_{\text{eq}}$ |
|-------|--------|--------|--------|-----------------|
| H(24) | -0.605 | -0.041 | -0.416 | 4.891           |
| H(25) | -0.705 | -0.257 | -0.376 | 4.116           |
| H(26) | -0.698 | -0.389 | -0.408 | 4.116           |
| H(27) | -0.734 | -0.277 | -0.446 | 4.116           |
| H(28) | -0.205 | -0.323 | -0.220 | 4.844           |
| H(29) | -0.160 | -0.197 | -0.210 | 4.844           |
| H(30) | -0.149 | -0.307 | -0.161 | 4.844           |
| H(31) | -0.194 | -0.058 | -0.112 | 6.128           |
| H(32) | -0.184 | -0.176 | -0.068 | 6.128           |
| H(33) | -0.261 | -0.100 | -0.066 | 6.128           |
| H(34) | -0.262 | -0.369 | -0.087 | 4.750           |
| H(35) | -0.340 | -0.296 | -0.092 | 4.750           |
| H(36) | -0.314 | -0.383 | -0.148 | 4.750           |
| H(37) | -0.450 | -0.032 | -0.171 | 4.638           |
| H(38) | -0.438 | -0.155 | -0.131 | 4.638           |
| H(39) | -0.397 | -0.030 | -0.110 | 4.638           |
| H(40) | -0.265 | 0.077  | -0.181 | 4.861           |
| H(41) | -0.240 | 0.022  | -0.248 | 4.861           |
| H(42) | -0.321 | 0.086  | -0.240 | 4.861           |
| H(43) | -0.469 | -0.356 | -0.174 | 3.467           |
| H(44) | -0.523 | -0.456 | -0.205 | 3.467           |
| H(45) | -0.556 | -0.304 | -0.099 | 4.618           |
| H(46) | -0.583 | -0.443 | -0.111 | 4.618           |
| H(47) | -0.670 | -0.243 | -0.139 | 8.322           |
| H(48) | -0.689 | -0.379 | -0.162 | 8.322           |
| H(49) | -0.652 | -0.195 | -0.236 | 6.255           |
| H(50) | -0.655 | -0.337 | -0.257 | 6.255           |
| H(51) | -0.449 | 0.144  | -0.349 | 5.804           |
| H(52) | -0.362 | 0.137  | -0.366 | 5.804           |
| H(53) | -0.405 | 0.245  | -0.453 | 6.105           |
| H(54) | -0.484 | 0.175  | -0.453 | 6.105           |
| H(55) | -0.430 | 0.048  | -0.526 | 4.583           |
| H(56) | -0.347 | 0.091  | -0.508 | 4.583           |

**Table 1.** Atomic coordinates and  $B_{\text{iso}}/B_{\text{eq}}$  for [DADMB]YCl(THF)<sub>2</sub> (2)

| atom  | x      | y      | z      | $B_{\text{eq}}$ |
|-------|--------|--------|--------|-----------------|
| H(57) | -0.413 | -0.122 | -0.468 | 2.819           |
| H(58) | -0.333 | -0.073 | -0.444 | 2.819           |

$$B_{\text{eq}} = 8/3 \pi^2 (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos \gamma + 2U_{13}(aa^*cc^*)\cos \beta + 2U_{23}(bb^*cc^*)\cos \alpha)$$

**Table 2.** Anisotropic Displacement Parameters for [DADMB]YCl(THF)<sub>2</sub> (2)

| atom  | U <sub>11</sub> | U <sub>22</sub> | U <sub>33</sub> | U <sub>12</sub> | U <sub>13</sub> | U <sub>23</sub> |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Y(1)  | 0.0240(4)       | 0.0293(4)       | 0.0276(4)       | -0.0010(4)      | 0.0011(5)       | -0.0024(5)      |
| Cl(1) | 0.049(2)        | 0.040(1)        | 0.054(2)        | 0.012(1)        | 0.015(1)        | 0.001(1)        |
| Si(1) | 0.024(1)        | 0.037(2)        | 0.034(2)        | -0.001(1)       | -0.003(1)       | 0.002(1)        |
| Si(2) | 0.032(1)        | 0.038(2)        | 0.031(2)        | -0.008(1)       | 0.002(1)        | -0.007(1)       |
| O(1)  | 0.025(4)        | 0.049(4)        | 0.026(4)        | 0.008(3)        | 0.000(3)        | 0.003(3)        |
| O(2)  | 0.044(4)        | 0.027(4)        | 0.027(4)        | -0.008(3)       | 0.010(3)        | -0.005(3)       |
| N(1)  | 0.013(4)        | 0.032(4)        | 0.026(4)        | 0.001(4)        | 0.002(3)        | 0.004(3)        |
| N(2)  | 0.029(4)        | 0.030(4)        | 0.019(4)        | -0.010(4)       | 0.003(3)        | -0.004(3)       |
| C(1)  | 0.023(5)        | 0.030(5)        | 0.033(6)        | -0.002(4)       | -0.008(4)       | -0.002(4)       |
| C(2)  | 0.028(5)        | 0.026(5)        | 0.044(6)        | 0.003(5)        | -0.002(4)       | -0.003(4)       |
| C(3)  | 0.038(5)        | 0.024(4)        | 0.037(6)        | -0.013(4)       | 0.008(5)        | -0.015(6)       |
| C(4)  | 0.042(6)        | 0.018(5)        | 0.040(7)        | -0.001(4)       | -0.004(4)       | 0.004(3)        |
| C(5)  | 0.025(5)        | 0.040(6)        | 0.032(7)        | 0.010(4)        | -0.005(4)       | 0.007(4)        |
| C(6)  | 0.022(5)        | 0.022(5)        | 0.028(5)        | -0.008(4)       | 0.005(3)        | -0.002(4)       |
| C(7)  | 0.028(5)        | 0.040(6)        | 0.013(5)        | -0.002(5)       | -0.009(4)       | 0.003(4)        |
| C(8)  | 0.028(4)        | 0.021(4)        | 0.027(5)        | -0.003(3)       | -0.002(5)       | 0.005(5)        |
| C(9)  | 0.033(6)        | 0.023(5)        | 0.041(7)        | -0.005(4)       | -0.006(4)       | 0.006(4)        |
| C(10) | 0.025(5)        | 0.046(6)        | 0.040(7)        | -0.009(5)       | 0.002(4)        | 0.019(5)        |
| C(11) | 0.040(6)        | 0.042(6)        | 0.021(5)        | 0.015(5)        | -0.006(4)       | 0.001(4)        |
| C(12) | 0.017(5)        | 0.030(5)        | 0.025(6)        | 0.005(4)        | -0.004(4)       | 0.001(4)        |
| C(13) | 0.030(5)        | 0.037(6)        | 0.033(5)        | -0.001(5)       | 0.003(4)        | -0.006(4)       |
| C(14) | 0.041(6)        | 0.027(5)        | 0.043(6)        | 0.001(5)        | 0.000(5)        | 0.004(4)        |
| C(15) | 0.040(6)        | 0.043(6)        | 0.028(6)        | -0.013(5)       | -0.019(4)       | 0.000(5)        |
| C(16) | 0.054(7)        | 0.068(8)        | 0.029(6)        | 0.005(6)        | 0.003(5)        | -0.021(5)       |
| C(17) | 0.036(6)        | 0.083(9)        | 0.048(7)        | -0.009(6)       | -0.015(5)       | 0.005(6)        |
| C(18) | 0.046(7)        | 0.071(7)        | 0.035(6)        | -0.002(6)       | -0.003(5)       | -0.001(5)       |
| C(19) | 0.056(7)        | 0.061(8)        | 0.034(6)        | 0.012(6)        | -0.013(5)       | -0.007(5)       |
| C(20) | 0.022(5)        | 0.078(8)        | 0.041(7)        | -0.010(6)       | -0.006(4)       | 0.001(5)        |
| C(21) | 0.042(6)        | 0.048(6)        | 0.040(6)        | -0.018(5)       | -0.005(5)       | 0.004(5)        |
| C(22) | 0.042(7)        | 0.072(8)        | 0.033(7)        | 0.004(6)        | 0.002(5)        | 0.000(6)        |
| C(23) | 0.065(8)        | 0.079(9)        | 0.056(8)        | -0.009(7)       | -0.027(6)       | -0.007(6)       |
| C(24) | 0.038(6)        | 0.064(7)        | 0.038(6)        | -0.025(6)       | -0.004(4)       | 0.006(6)        |
| C(25) | 0.053(7)        | 0.067(8)        | 0.039(7)        | -0.005(6)       | -0.002(5)       | -0.022(6)       |

**Table 2.** Anisotropic Displacement Parameters for [DADMB]YCl(THF)<sub>2</sub> (2)

| atom  | U <sub>11</sub> | U <sub>22</sub> | U <sub>33</sub> | U <sub>12</sub> | U <sub>13</sub> | U <sub>23</sub> |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| C(26) | 0.039(6)        | 0.026(6)        | 0.080(8)        | -0.012(5)       | 0.001(5)        | -0.020(5)       |
| C(27) | 0.028(5)        | 0.048(6)        | 0.032(6)        | 0.006(5)        | 0.007(4)        | 0.007(4)        |
| C(28) | 0.032(6)        | 0.069(8)        | 0.035(7)        | 0.015(6)        | 0.007(5)        | 0.014(5)        |
| C(29) | 0.058(8)        | 0.17(2)         | 0.034(8)        | 0.023(10)       | 0.021(6)        | 0.046(8)        |
| C(30) | 0.030(6)        | 0.086(10)       | 0.074(9)        | 0.014(7)        | 0.006(6)        | 0.023(7)        |
| C(31) | 0.093(10)       | 0.030(5)        | 0.060(8)        | -0.014(6)       | 0.040(7)        | -0.021(6)       |
| C(32) | 0.069(7)        | 0.034(6)        | 0.070(8)        | -0.007(6)       | 0.022(6)        | 0.008(6)        |
| C(33) | 0.049(7)        | 0.039(6)        | 0.050(7)        | 0.008(5)        | 0.012(5)        | 0.014(5)        |
| C(34) | 0.040(6)        | 0.051(6)        | 0.025(6)        | 0.011(5)        | 0.014(4)        | -0.005(5)       |

The general temperature factor expression:

$$\exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2a*b*U_{12}hk + 2a*c*U_{13}hl + 2b*c*U_{23}kl))$$

**Table 3.** Bond Lengths (Å) for [DADMB]YCl(THF)<sub>2</sub> (2)

| atom  | atom  | distance  | atom  | atom  | distance |
|-------|-------|-----------|-------|-------|----------|
| Y(1)  | Cl(1) | 2.574(2)  | Y(1)  | O(1)  | 2.365(6) |
| Y(1)  | O(2)  | 2.388(5)  | Y(1)  | N(1)  | 2.247(7) |
| Y(1)  | N(2)  | 2.252(7)  | Y(1)  | C(1)  | 2.745(8) |
| Y(1)  | C(6)  | 2.847(8)  | Y(1)  | C(7)  | 2.884(9) |
| Y(1)  | C(8)  | 2.749(7)  | Si(1) | N(1)  | 1.726(7) |
| Si(1) | C(15) | 1.904(10) | Si(1) | C(19) | 1.88(1)  |
| Si(1) | C(20) | 1.876(9)  | Si(2) | N(2)  | 1.727(7) |
| Si(2) | C(21) | 1.895(10) | Si(2) | C(25) | 1.88(1)  |
| Si(2) | C(26) | 1.870(10) | O(1)  | C(27) | 1.48(1)  |
| O(1)  | C(30) | 1.46(1)   | O(2)  | C(31) | 1.45(1)  |
| O(2)  | C(34) | 1.429(10) | N(1)  | C(1)  | 1.41(1)  |
| N(2)  | C(8)  | 1.41(1)   | C(1)  | C(2)  | 1.43(1)  |
| C(1)  | C(6)  | 1.45(1)   | C(2)  | C(3)  | 1.34(1)  |
| C(3)  | C(4)  | 1.40(1)   | C(4)  | C(5)  | 1.38(1)  |
| C(5)  | C(6)  | 1.42(1)   | C(5)  | C(14) | 1.52(1)  |
| C(6)  | C(7)  | 1.51(1)   | C(7)  | C(8)  | 1.42(1)  |
| C(7)  | C(12) | 1.40(1)   | C(8)  | C(9)  | 1.42(1)  |
| C(9)  | C(10) | 1.35(1)   | C(10) | C(11) | 1.40(1)  |
| C(11) | C(12) | 1.39(1)   | C(12) | C(13) | 1.49(1)  |
| C(15) | C(16) | 1.53(1)   | C(15) | C(17) | 1.55(1)  |
| C(15) | C(18) | 1.53(1)   | C(21) | C(22) | 1.55(1)  |
| C(21) | C(23) | 1.55(1)   | C(21) | C(24) | 1.55(1)  |
| C(27) | C(28) | 1.51(1)   | C(28) | C(29) | 1.54(1)  |
| C(29) | C(30) | 1.44(1)   | C(31) | C(32) | 1.51(2)  |
| C(32) | C(33) | 1.53(1)   | C(33) | C(34) | 1.52(1)  |

**Table 4.** Bond Angles (°) for [DADMB]YCl(THF)<sub>2</sub> (2).

| atom  | atom | atom  | angle    | atom  | atom  | atom  | angle    |
|-------|------|-------|----------|-------|-------|-------|----------|
| Cl(1) | Y(1) | O(1)  | 83.5(2)  | N(2)  | Y(1)  | C(1)  | 99.3(2)  |
| Cl(1) | Y(1) | O(2)  | 84.3(1)  | N(2)  | Y(1)  | C(6)  | 69.7(2)  |
| Cl(1) | Y(1) | N(1)  | 116.9(2) | N(2)  | Y(1)  | C(7)  | 55.5(2)  |
| Cl(1) | Y(1) | N(2)  | 119.8(2) | N(2)  | Y(1)  | C(8)  | 30.7(2)  |
| Cl(1) | Y(1) | C(1)  | 136.0(2) | C(1)  | Y(1)  | C(6)  | 29.9(2)  |
| Cl(1) | Y(1) | C(6)  | 162.2(2) | C(1)  | Y(1)  | C(7)  | 54.9(2)  |
| Cl(1) | Y(1) | C(7)  | 167.3(2) | C(1)  | Y(1)  | C(8)  | 82.7(2)  |
| Cl(1) | Y(1) | C(8)  | 141.2(2) | C(6)  | Y(1)  | C(7)  | 30.5(2)  |
| O(1)  | Y(1) | O(2)  | 167.9(2) | C(6)  | Y(1)  | C(8)  | 54.5(2)  |
| O(1)  | Y(1) | N(1)  | 94.3(2)  | C(7)  | Y(1)  | C(8)  | 29.1(2)  |
| O(1)  | Y(1) | N(2)  | 91.8(2)  | N(1)  | Si(1) | C(15) | 112.9(4) |
| O(1)  | Y(1) | C(1)  | 75.3(2)  | N(1)  | Si(1) | C(19) | 107.0(4) |
| O(1)  | Y(1) | C(6)  | 81.1(2)  | N(1)  | Si(1) | C(20) | 115.6(4) |
| O(1)  | Y(1) | C(7)  | 107.7(2) | C(15) | Si(1) | C(19) | 107.6(5) |
| O(1)  | Y(1) | C(8)  | 112.3(2) | C(15) | Si(1) | C(20) | 108.3(4) |
| O(2)  | Y(1) | N(1)  | 91.6(2)  | C(19) | Si(1) | C(20) | 104.9(5) |
| O(2)  | Y(1) | N(2)  | 93.8(2)  | N(2)  | Si(2) | C(21) | 112.8(4) |
| O(2)  | Y(1) | C(1)  | 114.3(2) | N(2)  | Si(2) | C(25) | 106.0(4) |
| O(2)  | Y(1) | C(6)  | 111.0(2) | N(2)  | Si(2) | C(26) | 114.6(4) |
| O(2)  | Y(1) | C(7)  | 84.3(2)  | C(21) | Si(2) | C(25) | 109.9(5) |
| O(2)  | Y(1) | C(8)  | 77.3(2)  | C(21) | Si(2) | C(26) | 108.6(4) |
| N(1)  | Y(1) | N(2)  | 123.3(2) | C(25) | Si(2) | C(26) | 104.5(5) |
| N(1)  | Y(1) | C(1)  | 30.8(2)  | Y(1)  | O(1)  | C(27) | 128.6(5) |
| N(1)  | Y(1) | C(6)  | 55.9(2)  | Y(1)  | O(1)  | C(30) | 125.8(6) |
| N(1)  | Y(1) | C(7)  | 69.1(2)  | C(27) | O(1)  | C(30) | 105.1(7) |
| N(1)  | Y(1) | C(8)  | 97.6(3)  | Y(1)  | O(2)  | C(31) | 127.5(5) |
| Y(1)  | O(2) | C(34) | 125.6(5) | Y(1)  | C(7)  | C(6)  | 73.4(5)  |
| C(31) | O(2) | C(34) | 106.9(7) | Y(1)  | C(7)  | C(8)  | 70.2(5)  |
| Y(1)  | N(1) | Si(1) | 126.7(4) | Y(1)  | C(7)  | C(12) | 138.7(6) |
| Y(1)  | N(1) | C(1)  | 94.5(5)  | C(6)  | C(7)  | C(8)  | 122.3(7) |
| Si(1) | N(1) | C(1)  | 128.8(6) | C(6)  | C(7)  | C(12) | 116.7(7) |
| Y(1)  | N(2) | Si(2) | 126.0(4) | C(8)  | C(7)  | C(12) | 120.3(8) |
| Y(1)  | N(2) | C(8)  | 94.6(5)  | Y(1)  | C(8)  | N(2)  | 54.7(4)  |

**Table 4.** Bond Angles (°) for [DADMB]YCl(THF)<sub>2</sub> (2).

| atom  | atom  | atom  | angle    | atom  | atom  | atom  | angle    |
|-------|-------|-------|----------|-------|-------|-------|----------|
| Si(2) | N(2)  | C(8)  | 127.8(6) | Y(1)  | C(8)  | C(7)  | 80.7(5)  |
| Y(1)  | C(1)  | N(1)  | 54.7(4)  | Y(1)  | C(8)  | C(9)  | 136.3(5) |
| Y(1)  | C(1)  | C(2)  | 135.3(6) | N(2)  | C(8)  | C(7)  | 120.4(7) |
| Y(1)  | C(1)  | C(6)  | 79.0(5)  | N(2)  | C(8)  | C(9)  | 122.2(7) |
| N(1)  | C(1)  | C(2)  | 124.3(7) | C(7)  | C(8)  | C(9)  | 117.3(8) |
| N(1)  | C(1)  | C(6)  | 117.8(7) | C(8)  | C(9)  | C(10) | 121.7(8) |
| C(2)  | C(1)  | C(6)  | 117.7(7) | C(9)  | C(10) | C(11) | 120.7(8) |
| C(1)  | C(2)  | C(3)  | 121.5(8) | C(10) | C(11) | C(12) | 119.9(8) |
| C(2)  | C(3)  | C(4)  | 121.8(8) | C(7)  | C(12) | C(11) | 119.8(8) |
| C(3)  | C(4)  | C(5)  | 119.1(8) | C(7)  | C(12) | C(13) | 120.6(8) |
| C(4)  | C(5)  | C(6)  | 121.6(8) | C(11) | C(12) | C(13) | 119.4(8) |
| C(4)  | C(5)  | C(14) | 120.2(8) | Si(1) | C(15) | C(16) | 110.5(6) |
| C(6)  | C(5)  | C(14) | 118.2(7) | Si(1) | C(15) | C(17) | 109.5(7) |
| Y(1)  | C(6)  | C(1)  | 71.1(5)  | Si(1) | C(15) | C(18) | 110.7(6) |
| Y(1)  | C(6)  | C(5)  | 136.6(6) | C(16) | C(15) | C(17) | 108.2(8) |
| Y(1)  | C(6)  | C(7)  | 76.1(5)  | C(16) | C(15) | C(18) | 108.2(9) |
| C(1)  | C(6)  | C(5)  | 118.2(7) | C(17) | C(15) | C(18) | 109.7(8) |
| C(1)  | C(6)  | C(7)  | 123.3(7) | Si(2) | C(21) | C(22) | 112.9(7) |
| C(5)  | C(6)  | C(7)  | 117.6(7) | Si(2) | C(21) | C(23) | 110.0(7) |
| Si(2) | C(21) | C(24) | 108.3(6) | C(22) | C(21) | C(23) | 108.5(8) |
| C(22) | C(21) | C(24) | 108.9(8) | C(23) | C(21) | C(24) | 108.2(8) |
| O(1)  | C(27) | C(28) | 104.8(7) | C(27) | C(28) | C(29) | 103.2(8) |
| C(28) | C(29) | C(30) | 107.2(9) | O(1)  | C(30) | C(29) | 108.0(9) |
| O(2)  | C(31) | C(32) | 104.2(8) | C(31) | C(32) | C(33) | 103.1(8) |
| C(32) | C(33) | C(34) | 104.9(8) | O(2)  | C(34) | C(33) | 106.6(7) |

**Structural data for [DADMB]Y(OSiMe<sub>3</sub>)(THF)<sub>2</sub> (4).****Table 5.** Atomic coordinates and B<sub>iso</sub>/B<sub>eq</sub> for [DADMB]Y(OSiMe<sub>3</sub>)(THF)<sub>2</sub> (4).

| atom  | x          | y          | z           | B <sub>eq</sub> |
|-------|------------|------------|-------------|-----------------|
| Y(1)  | 0.85703(4) | 0.21349(2) | 0.09482(2)  | 1.686(9)        |
| Si(1) | 0.5669(1)  | 0.28712(8) | 0.03117(6)  | 2.05(3)         |
| Si(2) | 1.1176(1)  | 0.13056(7) | 0.19181(6)  | 2.06(3)         |
| Si(3) | 0.9591(1)  | 0.22446(8) | -0.05574(6) | 2.47(3)         |
| O(1)  | 0.9183(3)  | 0.2162(2)  | 0.0099(1)   | 2.21(7)         |
| O(2)  | 0.9301(3)  | 0.3411(2)  | 0.1082(1)   | 2.30(7)         |
| O(3)  | 0.7966(3)  | 0.0859(2)  | 0.0647(1)   | 2.29(7)         |
| N(1)  | 0.6663(3)  | 0.2496(2)  | 0.0959(2)   | 1.68(8)         |
| N(2)  | 0.9805(3)  | 0.1761(2)  | 0.1861(2)   | 1.80(8)         |
| C(1)  | 0.6432(4)  | 0.1952(2)  | 0.1394(2)   | 1.82(9)         |
| C(2)  | 0.5441(4)  | 0.1439(3)  | 0.1262(2)   | 2.4(1)          |
| C(3)  | 0.5279(4)  | 0.0868(3)  | 0.1671(2)   | 2.7(1)          |
| C(4)  | 0.6099(4)  | 0.0776(3)  | 0.2246(2)   | 2.9(1)          |
| C(5)  | 0.7078(4)  | 0.1273(3)  | 0.2410(2)   | 2.4(1)          |
| C(6)  | 0.7261(4)  | 0.1862(2)  | 0.1991(2)   | 1.71(9)         |
| C(7)  | 0.8235(4)  | 0.2444(2)  | 0.2254(2)   | 1.74(9)         |
| C(8)  | 0.9472(4)  | 0.2319(2)  | 0.2257(2)   | 1.77(10)        |
| C(9)  | 1.0323(4)  | 0.2832(3)  | 0.2637(2)   | 2.7(1)          |
| C(10) | 0.9957(5)  | 0.3414(3)  | 0.2966(2)   | 3.1(1)          |
| C(11) | 0.8747(5)  | 0.3553(3)  | 0.2941(2)   | 2.9(1)          |
| C(12) | 0.7890(4)  | 0.3067(3)  | 0.2592(2)   | 2.2(1)          |
| C(13) | 0.6576(5)  | 0.3186(3)  | 0.2604(2)   | 3.4(1)          |
| C(14) | 0.7914(5)  | 0.1192(3)  | 0.3048(2)   | 3.1(1)          |
| C(15) | 0.6609(5)  | 0.3412(3)  | -0.0145(2)  | 3.1(1)          |
| C(16) | 0.4820(5)  | 0.2136(3)  | -0.0260(2)  | 3.7(1)          |
| C(17) | 0.4532(4)  | 0.3566(3)  | 0.0524(2)   | 2.6(1)          |
| C(18) | 0.3634(5)  | 0.3844(3)  | -0.0083(3)  | 3.9(1)          |
| C(19) | 0.3795(4)  | 0.3184(3)  | 0.0957(3)   | 3.2(1)          |
| C(20) | 0.5171(5)  | 0.4272(3)  | 0.0861(3)   | 3.3(1)          |
| C(21) | 1.1081(5)  | 0.0827(3)  | 0.1139(2)   | 2.8(1)          |
| C(22) | 1.2534(4)  | 0.1950(3)  | 0.2037(3)   | 3.1(1)          |
| C(23) | 1.1493(4)  | 0.0537(3)  | 0.2552(2)   | 2.4(1)          |

**Table 5.** Atomic coordinates and  $B_{\text{iso}}/B_{\text{eq}}$  for [DADMB]Y(OSiMe<sub>3</sub>)(THF)<sub>2</sub> (4).

| atom  | x         | y          | z          | $B_{\text{eq}}$ |
|-------|-----------|------------|------------|-----------------|
| C(24) | 1.0473(5) | -0.0069(3) | 0.2443(2)  | 3.3(1)          |
| C(25) | 1.1615(5) | 0.0897(3)  | 0.3204(2)  | 3.0(1)          |
| C(26) | 1.2679(5) | 0.0116(3)  | 0.2537(3)  | 3.6(1)          |
| C(27) | 1.1044(6) | 0.1737(4)  | -0.0519(3) | 4.5(2)          |
| C(28) | 0.8452(6) | 0.1831(3)  | -0.1227(3) | 4.1(2)          |
| C(29) | 0.9823(5) | 0.3270(3)  | -0.0753(3) | 3.6(1)          |
| C(30) | 1.0491(4) | 0.3632(3)  | 0.1025(2)  | 2.6(1)          |
| C(31) | 1.0347(5) | 0.4461(3)  | 0.0800(2)  | 3.6(1)          |
| C(32) | 0.9283(5) | 0.4761(3)  | 0.1040(3)  | 4.0(1)          |
| C(33) | 0.8796(5) | 0.4075(3)  | 0.1333(2)  | 3.0(1)          |
| C(34) | 0.7783(5) | 0.0554(3)  | 0.0008(2)  | 3.3(1)          |
| C(35) | 0.6824(5) | -0.0051(3) | -0.0040(3) | 3.7(1)          |
| C(36) | 0.6744(5) | -0.0232(3) | 0.0633(3)  | 3.3(1)          |
| C(37) | 0.7762(4) | 0.0225(3)  | 0.1036(2)  | 2.6(1)          |
| H(1)  | 0.4864    | 0.1492     | 0.0874     | 2.8668          |
| H(2)  | 0.4604    | 0.0532     | 0.1561     | 3.2338          |
| H(3)  | 0.5989    | 0.0374     | 0.2526     | 3.4356          |
| H(4)  | 1.1161    | 0.2762     | 0.2659     | 3.2603          |
| H(5)  | 1.0547    | 0.3735     | 0.3222     | 3.7772          |
| H(6)  | 0.8510    | 0.3978     | 0.3162     | 3.5142          |
| H(7)  | 0.6506    | 0.3609     | 0.2872     | 4.0958          |
| H(8)  | 0.6272    | 0.2733     | 0.2760     | 4.0958          |
| H(9)  | 0.6127    | 0.3290     | 0.2189     | 4.0958          |
| H(10) | 0.8717    | 0.1123     | 0.2998     | 3.7484          |
| H(11) | 0.7872    | 0.1644     | 0.3289     | 3.7484          |
| H(12) | 0.7681    | 0.0758     | 0.3259     | 3.7484          |
| H(13) | 0.7022    | 0.3818     | 0.0108     | 3.7350          |
| H(14) | 0.7179    | 0.3072     | -0.0260    | 3.7350          |
| H(15) | 0.6104    | 0.3622     | -0.0515    | 3.7350          |
| H(16) | 0.5378    | 0.1802     | -0.0393    | 4.4608          |
| H(17) | 0.4347    | 0.2392     | -0.0617    | 4.4608          |
| H(18) | 0.4308    | 0.1843     | -0.0058    | 4.4608          |
| H(19) | 0.4068    | 0.4086     | -0.0356    | 4.6847          |

**Table 5.** Atomic coordinates and  $B_{\text{iso}}/B_{\text{eq}}$  for [DADMB]Y(OSiMe<sub>3</sub>)(THF)<sub>2</sub> (4).

| atom  | x      | y       | z       | $B_{\text{eq}}$ |
|-------|--------|---------|---------|-----------------|
| H(20) | 0.3083 | 0.4202  | 0.0028  | 4.6847          |
| H(21) | 0.3202 | 0.3414  | -0.0291 | 4.6847          |
| H(22) | 0.3241 | 0.3548  | 0.1058  | 3.7946          |
| H(23) | 0.3364 | 0.2756  | 0.0746  | 3.7946          |
| H(24) | 0.4325 | 0.3014  | 0.1334  | 3.7946          |
| H(25) | 0.5722 | 0.4115  | 0.1236  | 3.9907          |
| H(26) | 0.5597 | 0.4529  | 0.0591  | 3.9907          |
| H(27) | 0.4591 | 0.4613  | 0.0966  | 3.9907          |
| H(28) | 1.1815 | 0.0564  | 0.1142  | 3.3654          |
| H(29) | 1.0433 | 0.0468  | 0.1064  | 3.3654          |
| H(30) | 1.0945 | 0.1205  | 0.0814  | 3.3654          |
| H(31) | 1.2431 | 0.2315  | 0.1703  | 3.6820          |
| H(32) | 1.2625 | 0.2214  | 0.2428  | 3.6820          |
| H(33) | 1.3233 | 0.1648  | 0.2040  | 3.6820          |
| H(34) | 1.0652 | -0.0453 | 0.2763  | 3.9170          |
| H(35) | 1.0408 | -0.0302 | 0.2041  | 3.9170          |
| H(36) | 0.9732 | 0.0175  | 0.2459  | 3.9170          |
| H(37) | 1.0879 | 0.1144  | 0.3227  | 3.6443          |
| H(38) | 1.1793 | 0.0507  | 0.3518  | 3.6443          |
| H(39) | 1.2249 | 0.1266  | 0.3274  | 3.6443          |
| H(40) | 1.3327 | 0.0475  | 0.2616  | 4.2624          |
| H(41) | 1.2619 | -0.0112 | 0.2133  | 4.2624          |
| H(42) | 1.2823 | -0.0273 | 0.2852  | 4.2624          |
| H(43) | 1.0952 | 0.1206  | -0.0433 | 5.3693          |
| H(44) | 1.1273 | 0.1789  | -0.0912 | 5.3693          |
| H(45) | 1.1649 | 0.1956  | -0.0193 | 5.3693          |
| H(46) | 0.8344 | 0.1299  | -0.1151 | 4.9072          |
| H(47) | 0.7707 | 0.2094  | -0.1264 | 4.9072          |
| H(48) | 0.8725 | 0.1889  | -0.1607 | 4.9072          |
| H(49) | 1.0054 | 0.3297  | -0.1147 | 4.3223          |
| H(50) | 0.9093 | 0.3548  | -0.0779 | 4.3223          |
| H(51) | 1.0439 | 0.3489  | -0.0433 | 4.3223          |
| H(52) | 1.1046 | 0.3598  | 0.1422  | 3.0893          |

**Table 5.** Atomic coordinates and  $B_{\text{iso}}/B_{\text{eq}}$  for [DADMB]Y(OSiMe<sub>3</sub>)(THF)<sub>2</sub> (**4**).

| atom  | x      | y       | z       | $B_{\text{eq}}$ |
|-------|--------|---------|---------|-----------------|
| H(53) | 1.0759 | 0.3316  | 0.0727  | 3.0893          |
| H(54) | 1.0187 | 0.4484  | 0.0352  | 4.2694          |
| H(55) | 1.1053 | 0.4751  | 0.0972  | 4.2694          |
| H(56) | 0.9534 | 0.5153  | 0.1346  | 4.7645          |
| H(57) | 0.8684 | 0.4961  | 0.0701  | 4.7645          |
| H(58) | 0.9049 | 0.4091  | 0.1780  | 3.6062          |
| H(59) | 0.7939 | 0.4064  | 0.1217  | 3.6062          |
| H(60) | 0.7523 | 0.0950  | -0.0293 | 3.9175          |
| H(61) | 0.8508 | 0.0333  | -0.0060 | 3.9175          |
| H(62) | 0.6073 | 0.0138  | -0.0274 | 4.4350          |
| H(63) | 0.7041 | -0.0501 | -0.0240 | 4.4350          |
| H(64) | 0.6850 | -0.0768 | 0.0717  | 3.9379          |
| H(65) | 0.5988 | -0.0072 | 0.0707  | 3.9379          |
| H(66) | 0.8468 | -0.0084 | 0.1151  | 3.1373          |
| H(67) | 0.7539 | 0.0407  | 0.1406  | 3.1373          |

$$B_{\text{eq}} = 8/3 \pi^2 (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos \gamma + 2U_{13}(aa^*cc^*)\cos \beta + 2U_{23}(bb^*cc^*)\cos \alpha)$$

**Table 6.** Anisotropic Displacement Parameters for [DADMB]Y(OSiMe<sub>3</sub>)(THF)<sub>2</sub> (4).

| atom  | U <sub>11</sub> | U <sub>22</sub> | U <sub>33</sub> | U <sub>12</sub> | U <sub>13</sub> | U <sub>23</sub> |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Y(1)  | 0.0231(2)       | 0.0194(2)       | 0.0216(2)       | -0.0008(2)      | 0.0065(2)       | -0.0007(2)      |
| Si(1) | 0.0274(7)       | 0.0274(7)       | 0.0235(6)       | 0.0021(6)       | 0.0060(5)       | 0.0020(6)       |
| Si(2) | 0.0260(7)       | 0.0293(7)       | 0.0249(7)       | 0.0044(6)       | 0.0090(5)       | 0.0040(6)       |
| Si(3) | 0.0367(7)       | 0.0319(8)       | 0.0251(7)       | 0.0021(6)       | 0.0093(6)       | 0.0013(6)       |
| O(1)  | 0.032(2)        | 0.028(2)        | 0.026(2)        | -0.003(2)       | 0.010(1)        | 0.002(1)        |
| O(2)  | 0.032(2)        | 0.018(2)        | 0.038(2)        | -0.004(1)       | 0.012(1)        | -0.005(1)       |
| O(3)  | 0.037(2)        | 0.024(2)        | 0.024(2)        | -0.005(1)       | 0.012(1)        | -0.007(1)       |
| N(1)  | 0.027(2)        | 0.019(2)        | 0.020(2)        | 0.002(2)        | 0.007(2)        | 0.004(2)        |
| N(2)  | 0.023(2)        | 0.026(2)        | 0.021(2)        | -0.001(2)       | 0.005(2)        | -0.004(2)       |
| C(1)  | 0.025(2)        | 0.014(2)        | 0.027(2)        | 0.007(2)        | 0.007(2)        | 0.000(2)        |
| C(2)  | 0.028(3)        | 0.031(3)        | 0.029(3)        | 0.000(2)        | 0.007(2)        | -0.002(2)       |
| C(3)  | 0.031(3)        | 0.033(3)        | 0.041(3)        | -0.004(2)       | 0.018(2)        | 0.000(2)        |
| C(4)  | 0.040(3)        | 0.025(3)        | 0.040(3)        | 0.002(2)        | 0.021(2)        | 0.009(2)        |
| C(5)  | 0.035(3)        | 0.029(3)        | 0.027(3)        | 0.009(2)        | 0.013(2)        | 0.003(2)        |
| C(6)  | 0.025(2)        | 0.021(2)        | 0.022(2)        | 0.003(2)        | 0.012(2)        | 0.000(2)        |
| C(7)  | 0.033(3)        | 0.022(2)        | 0.015(2)        | 0.003(2)        | 0.009(2)        | 0.006(2)        |
| C(8)  | 0.032(2)        | 0.021(3)        | 0.018(2)        | 0.002(2)        | 0.008(2)        | 0.006(2)        |
| C(9)  | 0.032(3)        | 0.036(3)        | 0.030(3)        | 0.001(2)        | 0.002(2)        | -0.001(2)       |
| C(10) | 0.047(3)        | 0.039(3)        | 0.029(3)        | -0.003(3)       | 0.004(2)        | -0.010(2)       |
| C(11) | 0.057(3)        | 0.032(3)        | 0.030(3)        | 0.006(3)        | 0.013(2)        | -0.006(2)       |
| C(12) | 0.042(3)        | 0.026(3)        | 0.019(2)        | 0.008(2)        | 0.010(2)        | 0.001(2)        |
| C(13) | 0.046(3)        | 0.042(3)        | 0.040(3)        | 0.014(3)        | 0.011(3)        | -0.011(3)       |
| C(14) | 0.042(3)        | 0.044(3)        | 0.035(3)        | 0.005(2)        | 0.015(2)        | 0.012(3)        |
| C(15) | 0.043(3)        | 0.053(4)        | 0.026(3)        | 0.012(3)        | 0.013(2)        | 0.013(2)        |
| C(16) | 0.052(3)        | 0.050(3)        | 0.033(3)        | -0.002(3)       | -0.001(2)       | -0.010(3)       |
| C(17) | 0.028(3)        | 0.031(3)        | 0.037(3)        | 0.006(2)        | 0.011(2)        | 0.011(2)        |
| C(18) | 0.039(3)        | 0.050(4)        | 0.054(4)        | 0.014(3)        | 0.006(3)        | 0.020(3)        |
| C(19) | 0.035(3)        | 0.046(3)        | 0.049(3)        | 0.006(2)        | 0.014(3)        | 0.001(3)        |
| C(20) | 0.053(3)        | 0.025(3)        | 0.055(4)        | 0.005(2)        | 0.022(3)        | -0.001(3)       |
| C(21) | 0.044(3)        | 0.049(3)        | 0.028(3)        | 0.021(3)        | 0.015(2)        | 0.004(2)        |
| C(22) | 0.029(3)        | 0.044(3)        | 0.057(4)        | 0.002(2)        | 0.016(2)        | 0.008(3)        |
| C(23) | 0.027(3)        | 0.032(3)        | 0.026(3)        | 0.004(2)        | 0.007(2)        | 0.003(2)        |
| C(24) | 0.053(3)        | 0.037(3)        | 0.035(3)        | -0.007(3)       | 0.008(3)        | 0.007(2)        |

**Table 6.** Anisotropic Displacement Parameters for [DADMB]Y(OSiMe<sub>3</sub>)(THF)<sub>2</sub> (4).

| atom  | U <sub>11</sub> | U <sub>22</sub> | U <sub>33</sub> | U <sub>12</sub> | U <sub>13</sub> | U <sub>23</sub> |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| C(25) | 0.046(3)        | 0.051(3)        | 0.028(3)        | 0.000(3)        | 0.004(2)        | 0.011(2)        |
| C(26) | 0.052(4)        | 0.045(3)        | 0.045(3)        | 0.010(3)        | 0.013(3)        | 0.017(3)        |
| C(27) | 0.062(4)        | 0.071(4)        | 0.061(4)        | 0.029(3)        | 0.034(3)        | 0.016(3)        |
| C(28) | 0.082(5)        | 0.056(4)        | 0.036(3)        | -0.014(3)       | 0.011(3)        | -0.002(3)       |
| C(29) | 0.062(4)        | 0.042(3)        | 0.040(3)        | -0.008(3)       | 0.012(3)        | 0.008(3)        |
| C(30) | 0.034(3)        | 0.030(3)        | 0.037(3)        | -0.009(2)       | 0.007(2)        | -0.004(2)       |
| C(31) | 0.058(4)        | 0.034(3)        | 0.040(3)        | -0.016(3)       | 0.016(3)        | 0.000(2)        |
| C(32) | 0.056(4)        | 0.028(3)        | 0.070(4)        | 0.003(3)        | 0.022(3)        | 0.006(3)        |
| C(33) | 0.047(3)        | 0.021(3)        | 0.048(3)        | 0.001(2)        | 0.016(3)        | -0.002(2)       |
| C(34) | 0.060(4)        | 0.038(3)        | 0.027(3)        | -0.015(3)       | 0.013(3)        | -0.012(2)       |
| C(35) | 0.047(3)        | 0.044(4)        | 0.047(4)        | -0.017(3)       | -0.001(3)       | -0.006(3)       |
| C(36) | 0.048(3)        | 0.039(3)        | 0.048(3)        | -0.011(3)       | 0.021(3)        | -0.012(3)       |
| C(37) | 0.043(3)        | 0.023(3)        | 0.039(3)        | -0.006(2)       | 0.018(2)        | 0.000(2)        |

The general temperature factor expression:

$$\exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2a*b*U_{12}hk + 2a*c*U_{13}hl + 2b*c*U_{23}kl))$$

**Table 7.** Bond Lengths (Å) for [DADMB]Y(OSiMe<sub>3</sub>)(THF)<sub>2</sub> (4).

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| Y(1)  | O(1)  | 2.111(3) | Y(1)  | O(2)  | 2.358(3) |
| Y(1)  | O(3)  | 2.365(3) | Y(1)  | N(1)  | 2.262(3) |
| Y(1)  | N(2)  | 2.254(3) | Y(1)  | C(1)  | 2.827(4) |
| Y(1)  | C(8)  | 2.816(4) | Si(1) | N(1)  | 1.724(3) |
| Si(1) | C(15) | 1.864(5) | Si(1) | C(16) | 1.889(5) |
| Si(1) | C(17) | 1.897(5) | Si(2) | N(2)  | 1.726(4) |
| Si(2) | C(21) | 1.867(5) | Si(2) | C(22) | 1.876(5) |
| Si(2) | C(23) | 1.893(4) | Si(3) | O(1)  | 1.601(3) |
| Si(3) | C(27) | 1.856(6) | Si(3) | C(28) | 1.862(6) |
| Si(3) | C(29) | 1.861(5) | O(2)  | C(30) | 1.437(5) |
| O(2)  | C(33) | 1.448(5) | O(3)  | C(34) | 1.457(5) |
| O(3)  | C(37) | 1.436(5) | N(1)  | C(1)  | 1.400(5) |
| N(2)  | C(8)  | 1.401(5) | C(1)  | C(2)  | 1.414(6) |
| C(1)  | C(6)  | 1.431(6) | C(2)  | C(3)  | 1.370(6) |
| C(3)  | C(4)  | 1.392(7) | C(4)  | C(5)  | 1.390(6) |
| C(5)  | C(6)  | 1.414(6) | C(5)  | C(14) | 1.502(6) |
| C(6)  | C(7)  | 1.513(6) | C(7)  | C(8)  | 1.421(6) |
| C(7)  | C(12) | 1.410(6) | C(8)  | C(9)  | 1.434(6) |
| C(9)  | C(10) | 1.354(7) | C(10) | C(11) | 1.386(7) |
| C(11) | C(12) | 1.381(7) | C(12) | C(13) | 1.514(7) |
| C(17) | C(18) | 1.554(7) | C(17) | C(19) | 1.540(7) |
| C(17) | C(20) | 1.525(7) | C(23) | C(24) | 1.543(7) |
| C(23) | C(25) | 1.526(7) | C(23) | C(26) | 1.539(7) |
| C(30) | C(31) | 1.516(7) | C(31) | C(32) | 1.511(7) |
| C(32) | C(33) | 1.511(7) | C(34) | C(35) | 1.499(7) |
| C(35) | C(36) | 1.517(7) | C(36) | C(37) | 1.510(6) |

**Table 8.** Bond Angles (°) for [DADMB]Y(OSiMe<sub>3</sub>)(THF)<sub>2</sub> (**4**).

| atom  | atom  | atom  | angle    | atom  | atom  | atom  | angle    |
|-------|-------|-------|----------|-------|-------|-------|----------|
| O(1)  | Y(1)  | O(2)  | 84.9(1)  | O(1)  | Y(1)  | O(3)  | 84.9(1)  |
| O(1)  | Y(1)  | N(1)  | 120.4(1) | O(1)  | Y(1)  | N(2)  | 120.8(1) |
| O(1)  | Y(1)  | C(1)  | 141.0(1) | O(1)  | Y(1)  | C(8)  | 139.6(1) |
| O(2)  | Y(1)  | O(3)  | 169.8(1) | O(2)  | Y(1)  | N(1)  | 92.9(1)  |
| O(2)  | Y(1)  | N(2)  | 91.6(1)  | O(2)  | Y(1)  | C(1)  | 111.7(1) |
| O(2)  | Y(1)  | C(8)  | 74.4(1)  | O(3)  | Y(1)  | N(1)  | 92.4(1)  |
| O(3)  | Y(1)  | N(2)  | 93.4(1)  | O(3)  | Y(1)  | C(1)  | 76.7(1)  |
| O(3)  | Y(1)  | C(8)  | 113.8(1) | N(1)  | Y(1)  | N(2)  | 118.8(1) |
| N(1)  | Y(1)  | C(1)  | 29.4(1)  | N(1)  | Y(1)  | C(8)  | 95.3(1)  |
| N(2)  | Y(1)  | C(1)  | 94.6(1)  | N(2)  | Y(1)  | C(8)  | 29.5(1)  |
| C(1)  | Y(1)  | C(8)  | 79.3(1)  | N(1)  | Si(1) | C(15) | 106.0(2) |
| N(1)  | Si(1) | C(16) | 115.3(2) | N(1)  | Si(1) | C(17) | 113.5(2) |
| C(15) | Si(1) | C(16) | 105.0(2) | C(15) | Si(1) | C(17) | 108.2(2) |
| C(16) | Si(1) | C(17) | 108.2(2) | N(2)  | Si(2) | C(21) | 105.6(2) |
| N(2)  | Si(2) | C(22) | 116.0(2) | N(2)  | Si(2) | C(23) | 113.4(2) |
| C(21) | Si(2) | C(22) | 105.7(2) | C(21) | Si(2) | C(23) | 108.0(2) |
| C(22) | Si(2) | C(23) | 107.6(2) | O(1)  | Si(3) | C(27) | 110.4(2) |
| O(1)  | Si(3) | C(28) | 111.8(2) | O(1)  | Si(3) | C(29) | 111.9(2) |
| C(27) | Si(3) | C(28) | 108.0(3) | C(27) | Si(3) | C(29) | 107.1(3) |
| C(28) | Si(3) | C(29) | 107.4(3) | Y(1)  | O(1)  | Si(3) | 175.5(2) |
| Y(1)  | O(2)  | C(30) | 123.5(3) | Y(1)  | O(2)  | C(33) | 129.4(3) |
| C(30) | O(2)  | C(33) | 106.2(3) | Y(1)  | O(3)  | C(34) | 125.1(3) |
| Y(1)  | O(3)  | C(37) | 129.0(3) | C(34) | O(3)  | C(37) | 105.9(3) |
| Y(1)  | N(1)  | Si(1) | 123.5(2) | Y(1)  | N(1)  | C(1)  | 98.3(2)  |
| Si(1) | N(1)  | C(1)  | 128.2(3) | Y(1)  | N(2)  | Si(2) | 124.8(2) |
| Y(1)  | N(2)  | C(8)  | 98.1(2)  | Si(2) | N(2)  | C(8)  | 129.4(3) |
| Y(1)  | C(1)  | N(1)  | 52.3(2)  | Y(1)  | C(1)  | C(2)  | 135.1(3) |
| Y(1)  | C(1)  | C(6)  | 83.1(2)  | N(1)  | C(1)  | C(2)  | 123.1(4) |
| N(1)  | C(1)  | C(6)  | 120.0(4) | C(2)  | C(1)  | C(6)  | 116.7(4) |
| C(1)  | C(2)  | C(3)  | 122.6(4) | C(2)  | C(3)  | C(4)  | 120.4(4) |
| C(3)  | C(4)  | C(5)  | 119.8(4) | C(4)  | C(5)  | C(6)  | 120.5(4) |
| C(4)  | C(5)  | C(14) | 119.0(4) | C(6)  | C(5)  | C(14) | 120.5(4) |
| C(1)  | C(6)  | C(5)  | 120.0(4) | C(1)  | C(6)  | C(7)  | 123.3(4) |

**Table 8.** Bond Angles (°) for [DADMB]Y(OSiMe<sub>3</sub>)(THF)<sub>2</sub> (**4**).

| atom  | atom  | atom  | angle    | atom  | atom  | atom  | angle    |
|-------|-------|-------|----------|-------|-------|-------|----------|
| C(5)  | C(6)  | C(7)  | 116.0(4) | C(6)  | C(7)  | C(8)  | 122.7(4) |
| C(6)  | C(7)  | C(12) | 116.3(4) | C(8)  | C(7)  | C(12) | 120.3(4) |
| Y(1)  | C(8)  | N(2)  | 52.4(2)  | Y(1)  | C(8)  | C(7)  | 82.9(2)  |
| Y(1)  | C(8)  | C(9)  | 134.4(3) | N(2)  | C(8)  | C(7)  | 120.3(4) |
| N(2)  | C(8)  | C(9)  | 122.8(4) | C(7)  | C(8)  | C(9)  | 116.6(4) |
| C(8)  | C(9)  | C(10) | 121.3(4) | C(9)  | C(10) | C(11) | 121.8(5) |
| C(10) | C(11) | C(12) | 119.2(4) | C(7)  | C(12) | C(11) | 120.7(4) |
| C(7)  | C(12) | C(13) | 120.2(4) | C(11) | C(12) | C(13) | 119.0(4) |
| Si(1) | C(17) | C(18) | 110.2(3) | Si(1) | C(17) | C(19) | 111.6(3) |
| Si(1) | C(17) | C(20) | 110.4(3) | C(18) | C(17) | C(19) | 107.9(4) |
| C(18) | C(17) | C(20) | 108.1(4) | C(19) | C(17) | C(20) | 108.5(4) |
| Si(2) | C(23) | C(24) | 110.7(3) | Si(2) | C(23) | C(25) | 110.5(3) |
| Si(2) | C(23) | C(26) | 110.1(3) | C(24) | C(23) | C(25) | 109.4(4) |
| C(24) | C(23) | C(26) | 107.8(4) | C(25) | C(23) | C(26) | 108.3(4) |
| O(2)  | C(30) | C(31) | 104.2(4) | C(30) | C(31) | C(32) | 104.6(4) |
| C(31) | C(32) | C(33) | 105.7(4) | O(2)  | C(33) | C(32) | 104.7(4) |
| O(3)  | C(34) | C(35) | 105.6(4) | C(34) | C(35) | C(36) | 106.0(4) |
| C(35) | C(36) | C(37) | 104.4(4) | O(3)  | C(37) | C(36) | 105.3(4) |

**Structural data** for {[DADMB]YH(THF)}<sub>2</sub>·C<sub>6</sub>H<sub>6</sub> (6).**Table 9.** Atomic coordinates and B<sub>iso</sub>/B<sub>eq</sub> for {[DADMB]YH(THF)}<sub>2</sub>·C<sub>6</sub>H<sub>6</sub> (6).

| atom  | x          | y           | z           | B <sub>eq</sub> |
|-------|------------|-------------|-------------|-----------------|
| Y(1)  | 0.44736(4) | 0.53415(2)  | -0.10063(2) | 2.41(1)         |
| Si(1) | 0.1375(2)  | 0.46337(10) | -0.21648(9) | 4.32(4)         |
| Si(2) | 0.6749(1)  | 0.65248(8)  | -0.11310(8) | 3.03(3)         |
| O(1)  | 0.5332(3)  | 0.4632(2)   | -0.1800(2)  | 3.40(8)         |
| N(1)  | 0.2377(3)  | 0.5276(2)   | -0.1644(2)  | 2.98(9)         |
| N(2)  | 0.5135(3)  | 0.6302(2)   | -0.1492(2)  | 2.52(9)         |
| C(1)  | 0.2056(4)  | 0.5871(3)   | -0.1253(2)  | 2.6(1)          |
| C(2)  | 0.1444(4)  | 0.5789(3)   | -0.0660(3)  | 3.4(1)          |
| C(3)  | 0.1261(4)  | 0.6337(4)   | -0.0210(3)  | 3.5(1)          |
| C(4)  | 0.1721(4)  | 0.7005(3)   | -0.0324(3)  | 3.6(1)          |
| C(5)  | 0.2338(4)  | 0.7115(3)   | -0.0896(3)  | 2.9(1)          |
| C(6)  | 0.2494(4)  | 0.6545(3)   | -0.1380(2)  | 2.4(1)          |
| C(7)  | 0.2908(4)  | 0.6719(2)   | -0.2101(2)  | 2.5(1)          |
| C(8)  | 0.4190(4)  | 0.6608(2)   | -0.2134(3)  | 2.6(1)          |
| C(9)  | 0.4455(4)  | 0.6776(3)   | -0.2842(3)  | 2.8(1)          |
| C(10) | 0.3523(5)  | 0.7052(3)   | -0.3465(3)  | 3.3(1)          |
| C(11) | 0.2269(5)  | 0.7166(3)   | -0.3427(3)  | 3.7(1)          |
| C(12) | 0.1953(4)  | 0.7012(3)   | -0.2742(3)  | 2.8(1)          |
| C(13) | 0.0613(5)  | 0.7200(3)   | -0.2695(3)  | 3.9(1)          |
| C(14) | 0.2800(5)  | 0.7840(3)   | -0.1014(3)  | 4.2(1)          |
| C(15) | 0.0645(6)  | 0.4865(4)   | -0.3243(3)  | 5.1(2)          |
| C(16) | -0.0053(8) | 0.4226(5)   | -0.3706(4)  | 7.8(2)          |
| C(17) | -0.0356(6) | 0.5447(4)   | -0.3326(4)  | 6.6(2)          |
| C(18) | 0.1689(6)  | 0.5118(4)   | -0.3602(3)  | 5.3(2)          |
| C(19) | 0.0005(7)  | 0.4402(4)   | -0.1763(4)  | 7.0(2)          |
| C(20) | 0.2382(7)  | 0.3837(3)   | -0.2115(3)  | 6.0(2)          |
| C(21) | 0.6991(5)  | 0.7354(3)   | -0.0528(4)  | 4.6(1)          |
| C(22) | 0.6430(5)  | 0.7978(3)   | -0.1066(4)  | 5.1(2)          |
| C(23) | 0.8459(6)  | 0.7504(4)   | -0.0125(5)  | 8.2(2)          |
| C(24) | 0.6288(7)  | 0.7309(4)   | 0.0107(4)   | 6.6(2)          |
| C(25) | 0.7720(5)  | 0.6599(3)   | -0.1856(4)  | 4.8(2)          |
| C(26) | 0.7487(4)  | 0.5778(3)   | -0.0466(3)  | 3.6(1)          |

**Table 9.** Atomic coordinates and  $B_{\text{iso}}/B_{\text{eq}}$  for  $\{[\text{DADMB}]\text{YH}(\text{THF})\}_2\cdot\text{C}_6\text{H}_6$  (**6**).

| atom  | x         | y         | z          | $B_{\text{eq}}$ |
|-------|-----------|-----------|------------|-----------------|
| C(27) | 0.5358(7) | 0.4847(4) | -0.2578(3) | 5.6(2)          |
| C(28) | 0.6103(9) | 0.4393(4) | -0.2836(5) | 9.0(3)          |
| C(29) | 0.6473(6) | 0.3785(3) | -0.2278(4) | 5.3(2)          |
| C(30) | 0.5975(7) | 0.3948(4) | -0.1636(3) | 5.5(2)          |
| C(31) | 0.5731(7) | 0.0405(4) | -0.0341(4) | 5.1(2)          |
| C(32) | 0.4485(9) | 0.0573(4) | -0.0429(4) | 5.5(2)          |
| C(33) | 0.3737(6) | 0.0164(5) | -0.0099(4) | 5.5(2)          |
| H(1)  | 0.481(3)  | 0.560(2)  | 0.028(2)   | 2.0(8)          |
| H(2)  | 0.1147    | 0.5337    | -0.0569    | 4.0711          |
| H(3)  | 0.0824    | 0.6266    | 0.0178     | 4.1605          |
| H(4)  | 0.1607    | 0.7385    | -0.0005    | 4.3710          |
| H(5)  | 0.5302    | 0.6695    | -0.2888    | 3.3718          |
| H(6)  | 0.3738    | 0.7168    | -0.3932    | 3.9768          |
| H(7)  | 0.1626    | 0.7349    | -0.3869    | 4.4663          |
| H(8)  | 0.0550    | 0.7092    | -0.2186    | 4.6808          |
| H(9)  | -0.0019   | 0.6940    | -0.3077    | 4.6808          |
| H(10) | 0.0466    | 0.7687    | -0.2793    | 4.6808          |
| H(11) | 0.3212    | 0.7830    | -0.1420    | 5.0264          |
| H(12) | 0.3401    | 0.7997    | -0.0539    | 5.0264          |
| H(13) | 0.2078    | 0.8150    | -0.1156    | 5.0264          |
| H(14) | -0.0409   | 0.4350    | -0.4243    | 9.4085          |
| H(15) | -0.0733   | 0.4081    | -0.3498    | 9.4085          |
| H(16) | 0.0550    | 0.3854    | -0.3662    | 9.4085          |
| H(17) | -0.0706   | 0.5565    | -0.3865    | 7.9134          |
| H(18) | -0.1036   | 0.5290    | -0.3124    | 7.9134          |
| H(19) | 0.0047    | 0.5847    | -0.3041    | 7.9134          |
| H(20) | 0.2305    | 0.4754    | -0.3573    | 6.3413          |
| H(21) | 0.1299    | 0.5241    | -0.4136    | 6.3413          |
| H(22) | 0.2114    | 0.5516    | -0.3321    | 6.3413          |
| H(23) | 0.0343    | 0.4235    | -0.1240    | 8.4271          |
| H(24) | -0.0515   | 0.4805    | -0.1767    | 8.4271          |
| H(25) | -0.0511   | 0.4046    | -0.2079    | 8.4271          |
| H(26) | 0.3067    | 0.3934    | -0.2339    | 7.2028          |

**Table 9.** Atomic coordinates and  $B_{\text{iso}}/B_{\text{eq}}$  for  $\{[\text{DADMB}]\text{YH}(\text{THF})\}_2\cdot\text{C}_6\text{H}_6$  (**6**).

| atom  | x      | y      | z       | $B_{\text{eq}}$ |
|-------|--------|--------|---------|-----------------|
| H(27) | 0.2738 | 0.3700 | -0.1582 | 7.2028          |
| H(28) | 0.1857 | 0.3468 | -0.2400 | 7.2028          |
| H(29) | 0.6863 | 0.8018 | -0.1460 | 6.1768          |
| H(30) | 0.6552 | 0.8396 | -0.0764 | 6.1768          |
| H(31) | 0.5527 | 0.7905 | -0.1307 | 6.1768          |
| H(32) | 0.8548 | 0.7939 | 0.0145  | 9.8419          |
| H(33) | 0.8907 | 0.7525 | -0.0514 | 9.8419          |
| H(34) | 0.8816 | 0.7140 | 0.0237  | 9.8419          |
| H(35) | 0.6663 | 0.6946 | 0.0467  | 7.8713          |
| H(36) | 0.6372 | 0.7743 | 0.0379  | 7.8713          |
| H(37) | 0.5394 | 0.7211 | -0.0132 | 7.8713          |
| H(38) | 0.8607 | 0.6683 | -0.1582 | 5.7612          |
| H(39) | 0.7393 | 0.6976 | -0.2206 | 5.7612          |
| H(40) | 0.7648 | 0.6174 | -0.2146 | 5.7612          |
| H(41) | 0.8388 | 0.5865 | -0.0233 | 4.3469          |
| H(42) | 0.7381 | 0.5356 | -0.0762 | 4.3469          |
| H(43) | 0.7067 | 0.5734 | -0.0066 | 4.3469          |
| H(44) | 0.4499 | 0.4845 | -0.2926 | 6.6706          |
| H(45) | 0.5712 | 0.5306 | -0.2555 | 6.6706          |
| H(46) | 0.5632 | 0.4225 | -0.3341 | 10.7759         |
| H(47) | 0.6869 | 0.4624 | -0.2868 | 10.7759         |
| H(48) | 0.6094 | 0.3364 | -0.2528 | 6.3583          |
| H(49) | 0.7391 | 0.3735 | -0.2100 | 6.3583          |
| H(50) | 0.5368 | 0.3601 | -0.1590 | 6.6415          |
| H(51) | 0.6667 | 0.3969 | -0.1161 | 6.6415          |
| H(52) | 0.6247 | 0.0690 | -0.0572 | 6.1536          |
| H(53) | 0.4121 | 0.0977 | -0.0722 | 6.6126          |
| H(54) | 0.2854 | 0.0285 | -0.0163 | 6.5648          |

$$B_{\text{eq}} = 8/3 \pi^2 (U_{11}(\text{aa}^*)^2 + U_{22}(\text{bb}^*)^2 + U_{33}(\text{cc}^*)^2 + 2U_{12}(\text{aa}^*\text{bb}^*)\cos \gamma + 2U_{13}(\text{aa}^*\text{cc}^*)\cos \beta + 2U_{23}(\text{bb}^*\text{cc}^*)\cos \alpha)$$

**Table 10.** Anisotropic Displacement Parameters for {[DADMB]YH(THF)}<sub>2</sub>·C<sub>6</sub>H<sub>6</sub> (6).

| atom  | U <sub>11</sub> | U <sub>22</sub> | U <sub>33</sub> | U <sub>12</sub> | U <sub>13</sub> | U <sub>23</sub> |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Y(1)  | 0.0383(3)       | 0.0348(3)       | 0.0220(2)       | -0.0078(2)      | 0.0088(2)       | 0.0013(3)       |
| Si(1) | 0.065(1)        | 0.058(1)        | 0.0415(9)       | -0.0350(9)      | 0.0060(8)       | -0.0027(9)      |
| Si(2) | 0.0343(8)       | 0.0381(9)       | 0.0502(9)       | -0.0011(6)      | 0.0176(7)       | 0.0086(7)       |
| O(1)  | 0.074(2)        | 0.040(2)        | 0.026(2)        | 0.016(2)        | 0.011(2)        | 0.006(2)        |
| N(1)  | 0.042(2)        | 0.038(3)        | 0.027(2)        | -0.016(2)       | 0.007(2)        | 0.000(2)        |
| N(2)  | 0.038(2)        | 0.028(2)        | 0.029(2)        | 0.001(2)        | 0.013(2)        | 0.001(2)        |
| C(1)  | 0.024(2)        | 0.048(3)        | 0.022(2)        | -0.006(2)       | 0.000(2)        | 0.007(2)        |
| C(2)  | 0.033(3)        | 0.069(4)        | 0.030(3)        | -0.016(3)       | 0.007(2)        | 0.011(3)        |
| C(3)  | 0.026(3)        | 0.095(5)        | 0.023(3)        | -0.004(3)       | 0.007(2)        | 0.008(3)        |
| C(4)  | 0.028(3)        | 0.089(5)        | 0.028(3)        | -0.001(3)       | 0.009(2)        | -0.014(3)       |
| C(5)  | 0.027(2)        | 0.055(4)        | 0.027(3)        | -0.002(2)       | 0.005(2)        | -0.004(3)       |
| C(6)  | 0.029(3)        | 0.045(3)        | 0.021(2)        | -0.007(2)       | 0.006(2)        | -0.001(2)       |
| C(7)  | 0.037(3)        | 0.035(3)        | 0.024(3)        | -0.004(2)       | 0.010(2)        | 0.001(2)        |
| C(8)  | 0.048(3)        | 0.022(3)        | 0.029(3)        | -0.005(2)       | 0.018(2)        | -0.005(2)       |
| C(9)  | 0.047(3)        | 0.032(3)        | 0.032(3)        | 0.002(2)        | 0.021(2)        | 0.005(2)        |
| C(10) | 0.072(4)        | 0.038(3)        | 0.027(3)        | -0.002(3)       | 0.023(3)        | 0.005(2)        |
| C(11) | 0.045(3)        | 0.053(4)        | 0.035(3)        | 0.000(3)        | 0.011(2)        | 0.010(3)        |
| C(12) | 0.046(3)        | 0.037(3)        | 0.030(3)        | 0.000(2)        | 0.015(2)        | 0.004(2)        |
| C(13) | 0.045(3)        | 0.069(4)        | 0.041(3)        | 0.004(3)        | 0.008(2)        | 0.015(3)        |
| C(14) | 0.047(3)        | 0.053(4)        | 0.058(4)        | 0.002(3)        | 0.020(3)        | -0.021(3)       |
| C(15) | 0.066(4)        | 0.069(5)        | 0.047(4)        | -0.019(3)       | -0.007(3)       | -0.008(3)       |
| C(16) | 0.130(6)        | 0.093(6)        | 0.064(5)        | -0.041(5)       | -0.020(4)       | -0.028(4)       |
| C(17) | 0.075(5)        | 0.100(6)        | 0.070(5)        | -0.019(4)       | -0.017(4)       | 0.000(4)        |
| C(18) | 0.096(5)        | 0.077(5)        | 0.032(3)        | -0.014(4)       | 0.008(3)        | -0.003(3)       |
| C(19) | 0.088(5)        | 0.121(7)        | 0.070(5)        | -0.075(5)       | 0.011(4)        | -0.009(4)       |
| C(20) | 0.131(6)        | 0.048(4)        | 0.053(4)        | -0.032(4)       | 0.009(4)        | -0.006(3)       |
| C(21) | 0.048(3)        | 0.037(4)        | 0.077(4)        | -0.010(3)       | -0.001(3)       | -0.002(3)       |
| C(22) | 0.054(4)        | 0.042(4)        | 0.100(5)        | -0.004(3)       | 0.024(3)        | -0.001(4)       |
| C(23) | 0.063(5)        | 0.051(5)        | 0.188(8)        | -0.010(4)       | -0.039(5)       | -0.001(5)       |
| C(24) | 0.121(6)        | 0.061(4)        | 0.054(4)        | -0.002(4)       | 0.009(4)        | -0.016(4)       |
| C(25) | 0.043(3)        | 0.078(5)        | 0.083(4)        | 0.006(3)        | 0.027(3)        | 0.040(4)        |
| C(26) | 0.039(3)        | 0.047(4)        | 0.049(3)        | -0.002(3)       | 0.013(2)        | 0.006(3)        |
| C(27) | 0.129(6)        | 0.075(5)        | 0.029(3)        | 0.046(4)        | 0.034(3)        | 0.014(3)        |

**Table 10.** Anisotropic Displacement Parameters for {[DADMB]YH(THF)}<sub>2</sub>·C<sub>6</sub>H<sub>6</sub> (6).

| atom  | U <sub>11</sub> | U <sub>22</sub> | U <sub>33</sub> | U <sub>12</sub> | U <sub>13</sub> | U <sub>23</sub> |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| C(28) | 0.202(9)        | 0.071(6)        | 0.146(7)        | 0.057(6)        | 0.140(7)        | 0.052(5)        |
| C(29) | 0.075(4)        | 0.050(4)        | 0.126(6)        | 0.017(3)        | 0.066(4)        | 0.030(4)        |
| C(30) | 0.127(6)        | 0.058(5)        | 0.047(4)        | 0.047(4)        | 0.009(4)        | 0.000(3)        |
| C(31) | 0.092(5)        | 0.054(4)        | 0.060(4)        | -0.022(4)       | 0.037(4)        | -0.013(4)       |
| C(32) | 0.138(7)        | 0.058(5)        | 0.058(4)        | 0.040(5)        | 0.039(5)        | 0.014(4)        |
| C(33) | 0.053(4)        | 0.113(7)        | 0.046(4)        | 0.019(4)        | -0.002(3)       | -0.015(4)       |

The general temperature factor expression:

$$\exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2a*b*U_{12}hk + 2a*c*U_{13}hl + 2b*c*U_{23}kl))$$

**Table 11.** Bond Lengths (Å) for {[DADMB]YH(THF)}<sub>2</sub>·C<sub>6</sub>H<sub>6</sub> (6).

| atom  | atom  | distance  | atom  | atom  | distance  |
|-------|-------|-----------|-------|-------|-----------|
| Y(1)  | Y(1)  | 3.6652(8) | Y(1)  | O(1)  | 2.329(3)  |
| Y(1)  | N(1)  | 2.213(4)  | Y(1)  | N(2)  | 2.228(4)  |
| Y(1)  | C(1)  | 2.702(4)  | Si(1) | N(1)  | 1.714(4)  |
| Si(1) | C(15) | 1.900(6)  | Si(1) | C(19) | 1.865(7)  |
| Si(1) | C(20) | 1.853(7)  | Si(2) | N(2)  | 1.719(4)  |
| Si(2) | C(21) | 1.887(6)  | Si(2) | C(25) | 1.883(5)  |
| Si(2) | C(26) | 1.875(5)  | O(1)  | C(27) | 1.451(6)  |
| O(1)  | C(30) | 1.465(7)  | N(1)  | C(1)  | 1.425(6)  |
| N(2)  | C(8)  | 1.416(6)  | C(1)  | C(2)  | 1.403(6)  |
| C(1)  | C(6)  | 1.411(7)  | C(2)  | C(3)  | 1.364(8)  |
| C(3)  | C(4)  | 1.402(8)  | C(4)  | C(5)  | 1.381(6)  |
| C(5)  | C(6)  | 1.427(7)  | C(5)  | C(14) | 1.503(7)  |
| C(6)  | C(7)  | 1.511(6)  | C(7)  | C(8)  | 1.411(6)  |
| C(7)  | C(12) | 1.409(6)  | C(8)  | C(9)  | 1.405(6)  |
| C(9)  | C(10) | 1.366(6)  | C(10) | C(11) | 1.387(7)  |
| C(11) | C(12) | 1.387(6)  | C(12) | C(13) | 1.508(6)  |
| C(15) | C(16) | 1.539(9)  | C(15) | C(17) | 1.522(10) |
| C(15) | C(18) | 1.521(8)  | C(21) | C(22) | 1.537(8)  |
| C(21) | C(23) | 1.558(8)  | C(21) | C(24) | 1.531(9)  |
| C(27) | C(28) | 1.348(9)  | C(28) | C(29) | 1.502(9)  |
| C(29) | C(30) | 1.429(8)  | C(31) | C(32) | 1.340(9)  |
| C(31) | C(33) | 1.363(9)  | C(32) | C(33) | 1.369(10) |
| Y(1)  | H(1)  | 2.27(4)   | Y(1)  | H(1)  | 2.22(4)   |

**Table 12.** Bond Angles (°) for {[DADMB]YH(THF)}<sub>2</sub>·C<sub>6</sub>H<sub>6</sub> (6).

| atom  | atom  | atom  | angle     | atom  | atom  | atom  | angle     |
|-------|-------|-------|-----------|-------|-------|-------|-----------|
| Y(1)  | Y(1)  | O(1)  | 108.68(8) | Y(1)  | Y(1)  | N(1)  | 117.44(9) |
| Y(1)  | Y(1)  | N(2)  | 128.87(9) | Y(1)  | Y(1)  | C(1)  | 107.54(9) |
| O(1)  | Y(1)  | N(1)  | 100.3(1)  | O(1)  | Y(1)  | N(2)  | 91.0(1)   |
| O(1)  | Y(1)  | C(1)  | 130.5(1)  | N(1)  | Y(1)  | N(2)  | 103.9(1)  |
| N(1)  | Y(1)  | C(1)  | 31.8(1)   | N(2)  | Y(1)  | C(1)  | 91.7(1)   |
| N(1)  | Si(1) | C(15) | 112.9(2)  | N(1)  | Si(1) | C(19) | 113.9(3)  |
| N(1)  | Si(1) | C(20) | 107.1(2)  | C(15) | Si(1) | C(19) | 107.5(3)  |
| C(15) | Si(1) | C(20) | 107.6(3)  | C(19) | Si(1) | C(20) | 107.6(4)  |
| N(2)  | Si(2) | C(21) | 112.1(2)  | N(2)  | Si(2) | C(25) | 117.5(2)  |
| N(2)  | Si(2) | C(26) | 104.1(2)  | C(21) | Si(2) | C(25) | 108.3(3)  |
| C(21) | Si(2) | C(26) | 108.4(2)  | C(25) | Si(2) | C(26) | 105.8(2)  |
| Y(1)  | O(1)  | C(27) | 122.2(3)  | Y(1)  | O(1)  | C(30) | 130.0(3)  |
| C(27) | O(1)  | C(30) | 107.7(4)  | Y(1)  | N(1)  | Si(1) | 134.8(2)  |
| Y(1)  | N(1)  | C(1)  | 93.4(2)   | Si(1) | N(1)  | C(1)  | 129.0(3)  |
| Y(1)  | N(2)  | Si(2) | 117.3(2)  | Y(1)  | N(2)  | C(8)  | 114.6(3)  |
| Si(2) | N(2)  | C(8)  | 127.6(3)  | Y(1)  | C(1)  | N(1)  | 54.8(2)   |
| Y(1)  | C(1)  | C(2)  | 118.3(3)  | Y(1)  | C(1)  | C(6)  | 91.0(3)   |
| N(1)  | C(1)  | C(2)  | 120.8(5)  | N(1)  | C(1)  | C(6)  | 120.6(4)  |
| C(2)  | C(1)  | C(6)  | 118.2(5)  | C(1)  | C(2)  | C(3)  | 122.3(5)  |
| C(2)  | C(3)  | C(4)  | 119.7(4)  | C(3)  | C(4)  | C(5)  | 120.6(5)  |
| C(4)  | C(5)  | C(6)  | 119.5(5)  | C(4)  | C(5)  | C(14) | 119.4(5)  |
| C(6)  | C(5)  | C(14) | 121.0(4)  | C(1)  | C(6)  | C(5)  | 119.7(4)  |
| C(1)  | C(6)  | C(7)  | 122.0(4)  | C(5)  | C(6)  | C(7)  | 117.4(4)  |
| C(6)  | C(7)  | C(8)  | 122.2(4)  | C(6)  | C(7)  | C(12) | 116.6(4)  |
| C(8)  | C(7)  | C(12) | 121.2(4)  | N(2)  | C(8)  | C(7)  | 120.6(4)  |
| N(2)  | C(8)  | C(9)  | 122.2(4)  | C(7)  | C(8)  | C(9)  | 117.2(4)  |
| C(8)  | C(9)  | C(10) | 121.6(4)  | C(9)  | C(10) | C(11) | 121.0(4)  |
| C(10) | C(11) | C(12) | 120.0(4)  | C(7)  | C(12) | C(11) | 119.1(4)  |
| C(7)  | C(12) | C(13) | 122.3(4)  | C(11) | C(12) | C(13) | 118.5(4)  |
| Si(1) | C(15) | C(16) | 110.5(5)  | Si(1) | C(15) | C(17) | 110.0(5)  |
| Si(1) | C(15) | C(18) | 111.0(4)  | C(16) | C(15) | C(17) | 107.7(5)  |
| C(16) | C(15) | C(18) | 109.3(5)  | C(17) | C(15) | C(18) | 108.4(6)  |
| Si(2) | C(21) | C(22) | 109.3(4)  | Si(2) | C(21) | C(23) | 111.7(5)  |

**Table 12.** Bond Angles (°) for {[DADMB]YH(THF)}<sub>2</sub>·C<sub>6</sub>H<sub>6</sub> (6).

| atom  | atom  | atom  | angle    | atom  | atom  | atom  | angle     |
|-------|-------|-------|----------|-------|-------|-------|-----------|
| Si(2) | C(21) | C(24) | 110.9(4) | C(22) | C(21) | C(23) | 107.8(5)  |
| C(22) | C(21) | C(24) | 108.3(5) | C(23) | C(21) | C(24) | 108.8(6)  |
| O(1)  | C(27) | C(28) | 108.6(5) | C(27) | C(28) | C(29) | 110.0(5)  |
| C(28) | C(29) | C(30) | 105.7(5) | O(1)  | C(30) | C(29) | 107.4(5)  |
| C(32) | C(31) | C(33) | 119.8(6) | C(31) | C(32) | C(33) | 120.3(6)  |
| C(31) | C(33) | C(32) | 119.9(6) | Y(1)  | Y(1)  | H(1)  | 34.8(10)  |
| Y(1)  | Y(1)  | H(1)  | 35.8(9)  | O(1)  | Y(1)  | H(1)  | 139.9(9)  |
| O(1)  | Y(1)  | H(1)  | 75.3(9)  | N(1)  | Y(1)  | H(1)  | 111.7(8)  |
| N(1)  | Y(1)  | H(1)  | 112.5(9) | N(2)  | Y(1)  | H(1)  | 103.6(10) |
| N(2)  | Y(1)  | H(1)  | 142.8(9) | C(1)  | Y(1)  | H(1)  | 86.8(9)   |
| C(1)  | Y(1)  | H(1)  | 123.7(9) | H(1)  | Y(1)  | H(1)  | 70(1)     |

**Structural data for [DADMB]YEt(THF)<sub>2</sub> (7).****Table 13.** Atomic coordinates and  $B_{\text{iso}}/B_{\text{eq}}$  for [DADMB]YEt(THF)<sub>2</sub> (7).

| atom  | x         | y          | z         | $B_{\text{eq}}$ |
|-------|-----------|------------|-----------|-----------------|
| Y(1)  | 0.500     | 0.19060(8) | 0.250     | 2.96(3)         |
| Si(1) | 0.3049(1) | 0.2211(1)  | 0.2772(1) | 2.93(5)         |
| O(1)  | 0.5296(3) | 0.1743(4)  | 0.3999(3) | 4.5(1)          |
| N(1)  | 0.3902(3) | 0.2725(4)  | 0.2579(4) | 2.9(1)          |
| C(1)  | 0.500     | 0.0117(6)  | 0.250     | 1.1(2)          |
| C(2)  | 0.498(2)  | -0.058(2)  | 0.288(1)  | 10.3(8)         |
| C(3)  | 0.4004(4) | 0.3471(5)  | 0.1996(5) | 2.7(2)          |
| C(4)  | 0.4705(3) | 0.4012(5)  | 0.2104(4) | 2.6(2)          |
| C(5)  | 0.4817(4) | 0.4701(5)  | 0.1485(5) | 2.7(2)          |
| C(6)  | 0.4251(4) | 0.4891(5)  | 0.0800(4) | 3.3(2)          |
| C(7)  | 0.3558(4) | 0.4385(5)  | 0.0706(5) | 4.3(2)          |
| C(8)  | 0.3441(4) | 0.3695(5)  | 0.1286(5) | 3.1(2)          |
| C(9)  | 0.5553(4) | 0.5301(5)  | 0.1603(5) | 3.6(2)          |
| C(10) | 0.2428(4) | 0.3062(6)  | 0.3313(5) | 3.5(2)          |
| C(11) | 0.2201(4) | 0.3964(6)  | 0.2769(5) | 4.5(2)          |
| C(12) | 0.2878(5) | 0.3389(6)  | 0.4170(5) | 5.2(2)          |
| C(13) | 0.1689(5) | 0.2532(6)  | 0.3472(6) | 4.4(2)          |
| C(14) | 0.2417(4) | 0.1680(5)  | 0.1818(5) | 3.8(2)          |
| C(15) | 0.3334(4) | 0.1155(5)  | 0.3499(5) | 4.3(2)          |
| C(16) | 0.5089(5) | 0.2414(6)  | 0.4625(6) | 4.9(2)          |
| C(17) | 0.5370(9) | 0.1981(8)  | 0.5468(7) | 8.9(4)          |
| C(18) | 0.6023(8) | 0.1337(9)  | 0.5284(8) | 10.3(4)         |
| C(19) | 0.5809(6) | 0.1014(8)  | 0.4440(8) | 8.1(3)          |
| H(1)  | 0.546     | 0.001      | 0.227     | 1.372           |
| H(2)  | 0.457     | 0.001      | 0.207     | 1.372           |
| H(3)  | 0.452     | -0.060     | 0.311     | 12.320          |
| H(4)  | 0.541     | -0.060     | 0.332     | 12.320          |
| H(5)  | 0.501     | -0.112     | 0.251     | 12.320          |
| H(6)  | 0.433     | 0.537      | 0.039     | 4.002           |
| H(7)  | 0.317     | 0.452      | 0.024     | 5.176           |
| H(8)  | 0.296     | 0.335      | 0.121     | 3.776           |
| H(9)  | 0.554     | 0.574      | 0.114     | 4.302           |

**Table 13.** Atomic coordinates and  $B_{\text{iso}}/B_{\text{eq}}$  for [DADMB]YEt(THF)<sub>2</sub> (7).

| atom  | x     | y     | z     | $B_{\text{eq}}$ |
|-------|-------|-------|-------|-----------------|
| H(10) | 0.599 | 0.488 | 0.162 | 4.302           |
| H(11) | 0.560 | 0.565 | 0.212 | 4.302           |
| H(12) | 0.265 | 0.432 | 0.270 | 5.460           |
| H(13) | 0.187 | 0.436 | 0.304 | 5.460           |
| H(14) | 0.194 | 0.377 | 0.223 | 5.460           |
| H(15) | 0.261 | 0.390 | 0.439 | 6.239           |
| H(16) | 0.338 | 0.361 | 0.409 | 6.239           |
| H(17) | 0.293 | 0.286 | 0.456 | 6.239           |
| H(18) | 0.183 | 0.198 | 0.382 | 5.300           |
| H(19) | 0.140 | 0.233 | 0.294 | 5.300           |
| H(20) | 0.138 | 0.296 | 0.375 | 5.300           |
| H(21) | 0.219 | 0.219 | 0.146 | 4.617           |
| H(22) | 0.202 | 0.130 | 0.200 | 4.617           |
| H(23) | 0.272 | 0.128 | 0.151 | 4.617           |
| H(24) | 0.364 | 0.138 | 0.401 | 5.188           |
| H(25) | 0.362 | 0.071 | 0.323 | 5.188           |
| H(26) | 0.288 | 0.085 | 0.363 | 5.188           |
| H(27) | 0.533 | 0.303 | 0.457 | 5.888           |
| H(28) | 0.454 | 0.250 | 0.455 | 5.888           |
| H(29) | 0.555 | 0.247 | 0.588 | 10.713          |
| H(30) | 0.498 | 0.161 | 0.567 | 10.713          |
| H(31) | 0.649 | 0.169 | 0.534 | 12.325          |
| H(32) | 0.609 | 0.080 | 0.566 | 12.325          |
| H(33) | 0.555 | 0.041 | 0.443 | 9.705           |
| H(34) | 0.625 | 0.094 | 0.417 | 9.705           |

$$B_{\text{eq}} = 8/3 \pi^2 (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos \gamma + 2U_{13}(aa^*cc^*)\cos \beta + 2U_{23}(bb^*cc^*)\cos \alpha)$$

**Table 14.** Anisotropic Displacement Parameters for [DADMB]YEt(THF)<sub>2</sub> (7).

| atom  | U <sub>11</sub> | U <sub>22</sub> | U <sub>33</sub> | U <sub>12</sub> | U <sub>13</sub> | U <sub>23</sub> |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Y(1)  | 0.0207(6)       | 0.0329(7)       | 0.0572(9)       | 0.000           | -0.0012(5)      | 0.000           |
| Si(1) | 0.026(1)        | 0.026(1)        | 0.051(2)        | -0.0024(9)      | 0.002(1)        | 0.005(1)        |
| O(1)  | 0.043(3)        | 0.053(4)        | 0.051(4)        | 0.012(3)        | -0.007(3)       | 0.008(3)        |
| N(1)  | 0.018(3)        | 0.024(4)        | 0.049(4)        | -0.002(3)       | 0.001(3)        | 0.008(3)        |
| C(3)  | 0.019(4)        | 0.025(4)        | 0.046(5)        | 0.006(3)        | 0.000(4)        | 0.002(4)        |
| C(4)  | 0.021(4)        | 0.023(4)        | 0.045(5)        | 0.000(3)        | 0.002(3)        | -0.001(4)       |
| C(5)  | 0.029(4)        | 0.023(4)        | 0.041(5)        | -0.001(3)       | 0.004(4)        | -0.003(4)       |
| C(6)  | 0.032(4)        | 0.038(5)        | 0.038(5)        | 0.007(4)        | 0.005(4)        | 0.010(4)        |
| C(7)  | 0.030(4)        | 0.036(5)        | 0.055(6)        | 0.004(4)        | -0.006(4)       | 0.013(4)        |
| C(8)  | 0.019(4)        | 0.036(5)        | 0.056(5)        | -0.005(3)       | -0.003(4)       | 0.006(4)        |
| C(9)  | 0.030(4)        | 0.034(5)        | 0.055(5)        | -0.005(4)       | 0.009(4)        | 0.002(4)        |
| C(10) | 0.034(4)        | 0.032(4)        | 0.053(5)        | 0.003(4)        | 0.008(4)        | 0.005(4)        |
| C(11) | 0.043(5)        | 0.043(6)        | 0.077(7)        | 0.008(4)        | 0.008(5)        | 0.004(5)        |
| C(12) | 0.056(6)        | 0.048(6)        | 0.062(6)        | -0.001(4)       | 0.014(5)        | -0.011(5)       |
| C(13) | 0.046(5)        | 0.047(6)        | 0.075(7)        | -0.003(4)       | 0.017(5)        | 0.003(5)        |
| C(14) | 0.040(5)        | 0.033(5)        | 0.064(6)        | -0.005(4)       | 0.000(4)        | 0.001(4)        |
| C(15) | 0.034(5)        | 0.037(5)        | 0.054(6)        | -0.002(4)       | 0.003(4)        | 0.012(4)        |
| C(16) | 0.049(6)        | 0.055(6)        | 0.053(6)        | -0.008(5)       | -0.006(5)       | -0.001(5)       |
| C(17) | 0.20(1)         | 0.068(8)        | 0.063(8)        | 0.039(9)        | -0.014(8)       | 0.003(7)        |
| C(18) | 0.15(1)         | 0.10(1)         | 0.11(1)         | 0.039(9)        | -0.080(10)      | 0.008(9)        |
| C(19) | 0.083(8)        | 0.108(9)        | 0.098(9)        | 0.062(7)        | 0.009(7)        | 0.039(8)        |

The general temperature factor expression:

$$\exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2a*b*U_{12}hk + 2a*c*U_{13}hl + 2b*c*U_{23}kl))$$

**Table 15.** Bond Lengths (Å) for [DADMB]YEt(THF)<sub>2</sub> (7).

| atom  | atom  | distance  | atom  | atom  | distance  |
|-------|-------|-----------|-------|-------|-----------|
| Y(1)  | O(1)  | 2.371(5)  | Y(1)  | O(1)  | 2.371(5)  |
| Y(1)  | N(1)  | 2.251(5)  | Y(1)  | N(1)  | 2.251(5)  |
| Y(1)  | C(1)  | 2.464(9)  | Y(1)  | C(3)  | 2.809(7)  |
| Y(1)  | C(3)  | 2.809(7)  | Si(1) | N(1)  | 1.726(5)  |
| Si(1) | C(10) | 1.898(7)  | Si(1) | C(14) | 1.879(7)  |
| Si(1) | C(15) | 1.877(7)  | O(1)  | C(16) | 1.448(9)  |
| O(1)  | C(19) | 1.452(9)  | N(1)  | C(3)  | 1.415(8)  |
| C(1)  | C(2)  | 1.13(2)   | C(1)  | C(2)  | 1.13(2)   |
| C(2)  | C(2)  | 1.21(5)   | C(3)  | C(4)  | 1.422(9)  |
| C(3)  | C(8)  | 1.411(9)  | C(4)  | C(4)  | 1.50(1)   |
| C(4)  | C(5)  | 1.405(9)  | C(5)  | C(6)  | 1.377(9)  |
| C(5)  | C(9)  | 1.517(9)  | C(6)  | C(7)  | 1.386(10) |
| C(7)  | C(8)  | 1.364(10) | C(10) | C(11) | 1.53(1)   |
| C(10) | C(12) | 1.531(10) | C(10) | C(13) | 1.54(1)   |
| C(16) | C(17) | 1.48(1)   | C(17) | C(18) | 1.51(2)   |
| C(18) | C(19) | 1.41(1)   |       |       |           |

**Table 16.** Bond Angles (°) for [DADMB]YEt(THF)<sub>2</sub> (7).

| atom  | atom  | atom  | angle    | atom  | atom  | atom  | angle    |
|-------|-------|-------|----------|-------|-------|-------|----------|
| O(1)  | Y(1)  | O(1)  | 169.1(3) | O(1)  | Y(1)  | N(1)  | 92.5(2)  |
| O(1)  | Y(1)  | N(1)  | 93.0(2)  | O(1)  | Y(1)  | C(1)  | 84.6(1)  |
| O(1)  | Y(1)  | C(3)  | 112.7(2) | O(1)  | Y(1)  | C(3)  | 76.1(2)  |
| O(1)  | Y(1)  | N(1)  | 93.0(2)  | O(1)  | Y(1)  | N(1)  | 92.5(2)  |
| O(1)  | Y(1)  | C(1)  | 84.6(1)  | O(1)  | Y(1)  | C(3)  | 76.1(2)  |
| O(1)  | Y(1)  | C(3)  | 112.7(2) | N(1)  | Y(1)  | N(1)  | 119.8(3) |
| N(1)  | Y(1)  | C(1)  | 120.1(1) | N(1)  | Y(1)  | C(3)  | 30.0(2)  |
| N(1)  | Y(1)  | C(3)  | 95.5(2)  | N(1)  | Y(1)  | C(1)  | 120.1(1) |
| N(1)  | Y(1)  | C(3)  | 95.5(2)  | N(1)  | Y(1)  | C(3)  | 30.0(2)  |
| C(1)  | Y(1)  | C(3)  | 140.2(1) | C(1)  | Y(1)  | C(3)  | 140.2(1) |
| C(3)  | Y(1)  | C(3)  | 79.7(3)  | N(1)  | Si(1) | C(10) | 113.7(3) |
| N(1)  | Si(1) | C(14) | 115.6(3) | N(1)  | Si(1) | C(15) | 106.0(3) |
| C(10) | Si(1) | C(14) | 107.6(3) | C(10) | Si(1) | C(15) | 108.3(3) |
| C(14) | Si(1) | C(15) | 105.2(3) | Y(1)  | O(1)  | C(16) | 126.4(4) |
| Y(1)  | O(1)  | C(19) | 124.9(6) | C(16) | O(1)  | C(19) | 108.2(7) |
| Y(1)  | N(1)  | Si(1) | 125.2(3) | Y(1)  | N(1)  | C(3)  | 97.4(4)  |
| Si(1) | N(1)  | C(3)  | 128.2(4) | Y(1)  | C(1)  | C(2)  | 147(1)   |
| Y(1)  | C(1)  | C(2)  | 147(1)   | C(2)  | C(1)  | C(2)  | 64(2)    |
| C(1)  | C(2)  | C(2)  | 57(1)    | Y(1)  | C(3)  | N(1)  | 52.6(3)  |
| Y(1)  | C(3)  | C(4)  | 83.3(4)  | Y(1)  | C(3)  | C(8)  | 136.0(5) |
| N(1)  | C(3)  | C(4)  | 119.9(6) | N(1)  | C(3)  | C(8)  | 122.6(6) |
| C(4)  | C(3)  | C(8)  | 117.5(7) | C(3)  | C(4)  | C(4)  | 124.5(7) |
| C(3)  | C(4)  | C(5)  | 118.9(6) | C(4)  | C(4)  | C(5)  | 115.9(5) |
| C(4)  | C(5)  | C(6)  | 121.4(6) | C(4)  | C(5)  | C(9)  | 119.5(6) |
| C(6)  | C(5)  | C(9)  | 119.0(7) | C(5)  | C(6)  | C(7)  | 119.9(7) |
| C(6)  | C(7)  | C(8)  | 120.1(6) | C(3)  | C(8)  | C(7)  | 122.2(6) |
| Si(1) | C(10) | C(11) | 111.1(5) | Si(1) | C(10) | C(12) | 109.6(5) |
| Si(1) | C(10) | C(13) | 109.8(5) | C(11) | C(10) | C(12) | 108.4(7) |
| C(11) | C(10) | C(13) | 109.1(6) | C(12) | C(10) | C(13) | 108.7(6) |
| O(1)  | C(16) | C(17) | 106.5(7) | C(16) | C(17) | C(18) | 102.3(9) |
| C(17) | C(18) | C(19) | 106.0(9) | O(1)  | C(19) | C(18) | 107.1(9) |

**Structural data for [DADMB]Y(NC<sub>5</sub>H<sub>6</sub>)(NC<sub>5</sub>H<sub>5</sub>)<sub>2</sub>·C<sub>5</sub>H<sub>12</sub> (9).****Table 17.** Atomic coordinates and B<sub>iso</sub>/B<sub>eq</sub> for [DADMB]Y(NC<sub>5</sub>H<sub>6</sub>)(NC<sub>5</sub>H<sub>5</sub>)<sub>2</sub>·C<sub>5</sub>H<sub>12</sub> (9).

| atom  | x          | y          | z          | B <sub>eq</sub> |
|-------|------------|------------|------------|-----------------|
| Y(1)  | 0.17019(2) | 0.07021(5) | 0.12763(1) | 2.52(1)         |
| Si(1) | 0.31982(6) | 0.0224(1)  | 0.14288(5) | 3.32(4)         |
| Si(2) | 0.02718(6) | 0.0277(1)  | 0.09807(5) | 3.00(4)         |
| N(1)  | 0.1680(2)  | 0.2596(4)  | 0.1382(1)  | 3.6(1)          |
| N(2)  | 0.2516(2)  | -0.0241(4) | 0.1365(1)  | 3.0(1)          |
| N(3)  | 0.0943(2)  | -0.0233(4) | 0.1040(1)  | 2.56(10)        |
| N(4)  | 0.1439(2)  | 0.0586(4)  | 0.1994(1)  | 2.5(1)          |
| N(5)  | 0.1928(2)  | 0.1144(4)  | 0.0566(1)  | 3.1(1)          |
| C(1)  | 0.2085(3)  | 0.3334(6)  | 0.1215(2)  | 5.0(2)          |
| C(2)  | 0.2423(3)  | 0.3964(7)  | 0.1508(3)  | 6.2(2)          |
| C(3)  | 0.2144(3)  | 0.4358(6)  | 0.1834(2)  | 5.9(2)          |
| C(4)  | 0.1601(3)  | 0.4027(5)  | 0.1897(2)  | 5.1(2)          |
| C(5)  | 0.1375(2)  | 0.3166(5)  | 0.1674(2)  | 4.2(2)          |
| C(6)  | 0.2258(2)  | -0.1119(4) | 0.1574(2)  | 2.6(1)          |
| C(7)  | 0.2385(2)  | -0.1358(5) | 0.1985(2)  | 3.2(1)          |
| C(8)  | 0.2087(2)  | -0.2139(5) | 0.2199(2)  | 3.4(1)          |
| C(9)  | 0.1661(2)  | -0.2739(5) | 0.2016(2)  | 3.6(2)          |
| C(10) | 0.1520(2)  | -0.2553(5) | 0.1613(2)  | 3.4(1)          |
| C(11) | 0.1804(2)  | -0.1727(4) | 0.1390(2)  | 2.7(1)          |
| C(12) | 0.1672(2)  | -0.1649(5) | 0.0944(2)  | 2.7(1)          |
| C(13) | 0.1220(2)  | -0.1004(4) | 0.0792(2)  | 2.7(1)          |
| C(14) | 0.1088(2)  | -0.1093(5) | 0.0378(2)  | 3.4(1)          |
| C(15) | 0.1386(3)  | -0.1798(6) | 0.0132(2)  | 3.7(2)          |
| C(16) | 0.1827(2)  | -0.2443(5) | 0.0284(2)  | 3.6(2)          |
| C(17) | 0.1969(2)  | -0.2378(5) | 0.0690(2)  | 3.4(1)          |
| C(18) | 0.2410(2)  | -0.3153(5) | 0.0855(2)  | 4.1(2)          |
| C(19) | 0.1072(2)  | -0.3277(5) | 0.1415(2)  | 4.3(2)          |
| C(20) | 0.3280(3)  | 0.1464(6)  | 0.1089(2)  | 5.2(2)          |
| C(21) | 0.3379(2)  | 0.0784(6)  | 0.1939(2)  | 5.0(2)          |
| C(22) | 0.3744(2)  | -0.0864(6) | 0.1282(2)  | 4.5(2)          |
| C(23) | 0.3673(3)  | -0.1184(7) | 0.0843(2)  | 5.4(2)          |
| C(24) | 0.3692(3)  | -0.1911(6) | 0.1556(2)  | 5.6(2)          |

**Table 17.** Atomic coordinates and  $B_{\text{iso}}/B_{\text{eq}}$  for [DADMB]Y(NC<sub>5</sub>H<sub>6</sub>)(NC<sub>5</sub>H<sub>5</sub>)<sub>2</sub>·C<sub>5</sub>H<sub>12</sub> (**9**).

| atom  | x          | y          | z          | $B_{\text{eq}}$ |
|-------|------------|------------|------------|-----------------|
| C(25) | 0.4340(3)  | -0.0356(6) | 0.1345(2)  | 5.6(2)          |
| C(26) | 0.0110(2)  | 0.1036(5)  | 0.0500(2)  | 4.4(2)          |
| C(27) | 0.0201(2)  | 0.1378(6)  | 0.1376(2)  | 4.6(2)          |
| C(28) | -0.0303(2) | -0.0820(5) | 0.1045(2)  | 3.6(1)          |
| C(29) | -0.0878(2) | -0.0299(6) | 0.0984(2)  | 4.4(2)          |
| C(30) | -0.0255(2) | -0.1320(6) | 0.1474(2)  | 4.0(2)          |
| C(31) | -0.0239(2) | -0.1788(6) | 0.0745(2)  | 4.3(2)          |
| C(32) | 0.2255(2)  | 0.0493(5)  | 0.0350(2)  | 3.5(1)          |
| C(33) | 0.2311(3)  | 0.0587(6)  | -0.0062(2) | 4.2(2)          |
| C(34) | 0.2001(3)  | 0.1372(7)  | -0.0261(2) | 4.6(2)          |
| C(35) | 0.1651(3)  | 0.2075(6)  | -0.0046(2) | 5.1(2)          |
| C(36) | 0.1631(2)  | 0.1939(5)  | 0.0372(2)  | 3.6(1)          |
| C(37) | 0.1070(2)  | -0.0179(5) | 0.2132(2)  | 3.4(1)          |
| C(38) | 0.0986(3)  | -0.0348(5) | 0.2536(2)  | 4.5(2)          |
| C(39) | 0.1302(3)  | 0.0246(6)  | 0.2814(2)  | 4.2(2)          |
| C(40) | 0.1682(2)  | 0.1032(5)  | 0.2678(2)  | 3.6(1)          |
| C(41) | 0.1731(2)  | 0.1173(5)  | 0.2272(2)  | 3.1(1)          |
| C(42) | 0.0000     | 0.243(1)   | 0.2500     | 11.2(5)         |
| C(43) | 0.0154(7)  | 0.343(1)   | 0.2362(5)  | 6.6(4)          |
| C(44) | 0.0000     | 0.455(1)   | 0.2500     | 7.8(4)          |
| C(45) | 0.0184(7)  | 0.563(1)   | 0.2354(5)  | 6.5(4)          |
| C(46) | 0.0000     | 0.677(1)   | 0.2500     | 8.2(4)          |
| C(47) | 0.0948(8)  | 0.493(2)   | 0.0369(6)  | 8.1(5)          |
| C(48) | -0.068(1)  | 0.530(2)   | -0.0533(8) | 11.7(7)         |
| C(49) | 0.0000     | 0.5000     | 0.0000     | 14.0(8)         |
| C(50) | 0.041(2)   | 0.457(3)   | 0.016(1)   | 15(1)           |
| C(51) | 0.043(1)   | 0.533(3)   | 0.031(1)   | 13.0(9)         |
| H(1)  | 0.2332     | 0.2897     | 0.1057     | 5.9442          |
| H(2)  | 0.1892     | 0.3859     | 0.1048     | 5.9442          |
| H(3)  | 0.2812     | 0.4092     | 0.1474     | 7.3805          |
| H(4)  | 0.2325     | 0.4859     | 0.2017     | 7.1093          |
| H(5)  | 0.1382     | 0.4394     | 0.2094     | 6.1072          |
| H(6)  | 0.0998     | 0.2949     | 0.1718     | 5.0948          |

**Table 17.** Atomic coordinates and  $B_{\text{iso}}/B_{\text{eq}}$  for [DADMB]Y(NC<sub>5</sub>H<sub>6</sub>)(NC<sub>5</sub>H<sub>5</sub>)<sub>2</sub>·C<sub>5</sub>H<sub>12</sub> (9).

| atom  | x       | y       | z       | $B_{\text{eq}}$ |
|-------|---------|---------|---------|-----------------|
| H(7)  | 0.2684  | -0.0967 | 0.2116  | 3.8210          |
| H(8)  | 0.2176  | -0.2263 | 0.2475  | 4.0703          |
| H(9)  | 0.1461  | -0.3284 | 0.2165  | 4.3722          |
| H(10) | 0.0788  | -0.0660 | 0.0267  | 4.0367          |
| H(11) | 0.1288  | -0.1844 | -0.0146 | 4.4683          |
| H(12) | 0.2030  | -0.2925 | 0.0111  | 4.2846          |
| H(13) | 0.2293  | -0.3910 | 0.0817  | 4.9480          |
| H(14) | 0.2751  | -0.3031 | 0.0718  | 4.9480          |
| H(15) | 0.2466  | -0.3009 | 0.1134  | 4.9480          |
| H(16) | 0.0730  | -0.3194 | 0.1555  | 5.1004          |
| H(17) | 0.1018  | -0.3049 | 0.1143  | 5.1004          |
| H(18) | 0.1186  | -0.4042 | 0.1423  | 5.1004          |
| H(19) | 0.3652  | 0.1745  | 0.1113  | 6.2828          |
| H(20) | 0.3206  | 0.1243  | 0.0818  | 6.2828          |
| H(21) | 0.3023  | 0.2036  | 0.1163  | 6.2828          |
| H(22) | 0.3344  | 0.0202  | 0.2133  | 5.9922          |
| H(23) | 0.3754  | 0.1055  | 0.1943  | 5.9922          |
| H(24) | 0.3131  | 0.1382  | 0.2002  | 5.9922          |
| H(25) | 0.3309  | -0.1490 | 0.0799  | 6.4523          |
| H(26) | 0.3718  | -0.0535 | 0.0680  | 6.4523          |
| H(27) | 0.3948  | -0.1728 | 0.0776  | 6.4523          |
| H(28) | 0.3333  | -0.2244 | 0.1516  | 6.7538          |
| H(29) | 0.3975  | -0.2440 | 0.1491  | 6.7538          |
| H(30) | 0.3736  | -0.1692 | 0.1830  | 6.7538          |
| H(31) | 0.4614  | -0.0900 | 0.1278  | 6.7691          |
| H(32) | 0.4379  | 0.0286  | 0.1178  | 6.7691          |
| H(33) | 0.4390  | -0.0142 | 0.1619  | 6.7691          |
| H(34) | 0.0373  | 0.1627  | 0.0466  | 5.2968          |
| H(35) | 0.0134  | 0.0526  | 0.0281  | 5.2968          |
| H(36) | -0.0258 | 0.1340  | 0.0508  | 5.2968          |
| H(37) | 0.0255  | 0.1047  | 0.1634  | 5.4821          |
| H(38) | 0.0475  | 0.1946  | 0.1338  | 5.4821          |
| H(39) | -0.0164 | 0.1700  | 0.1358  | 5.4821          |

**Table 17.** Atomic coordinates and  $B_{\text{iso}}/B_{\text{eq}}$  for [DADMB]Y(NC<sub>5</sub>H<sub>6</sub>)(NC<sub>5</sub>H<sub>5</sub>)<sub>2</sub>·C<sub>5</sub>H<sub>12</sub> (9).

| atom  | x       | y       | z       | $B_{\text{eq}}$ |
|-------|---------|---------|---------|-----------------|
| H(40) | -0.0930 | 0.0280  | 0.1177  | 5.3312          |
| H(41) | -0.0908 | 0.0011  | 0.0721  | 5.3312          |
| H(42) | -0.1158 | -0.0859 | 0.1015  | 5.3312          |
| H(43) | -0.0540 | -0.1868 | 0.1508  | 4.8430          |
| H(44) | 0.0103  | -0.1663 | 0.1510  | 4.8430          |
| H(45) | -0.0297 | -0.0738 | 0.1667  | 4.8430          |
| H(46) | -0.0524 | -0.2330 | 0.0787  | 5.1152          |
| H(47) | -0.0271 | -0.1505 | 0.0478  | 5.1152          |
| H(48) | 0.0119  | -0.2130 | 0.0783  | 5.1152          |
| H(49) | 0.2464  | -0.0076 | 0.0486  | 4.1948          |
| H(50) | 0.2561  | 0.0112  | -0.0202 | 5.0928          |
| H(51) | 0.2022  | 0.1440  | -0.0545 | 5.5552          |
| H(52) | 0.1431  | 0.2633  | -0.0179 | 6.1013          |
| H(53) | 0.1399  | 0.2426  | 0.0523  | 4.3642          |
| H(54) | 0.0860  | -0.0616 | 0.1943  | 4.0778          |
| H(55) | 0.0712  | -0.0871 | 0.2623  | 5.4294          |
| H(56) | 0.1260  | 0.0119  | 0.3094  | 5.0574          |
| H(57) | 0.1903  | 0.1463  | 0.2862  | 4.2679          |
| H(58) | 0.1989  | 0.1722  | 0.2181  | 3.7139          |

$$B_{\text{eq}} = 8/3 \pi^2 (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$$

**Table 18.** Anisotropic Displacement Parameters for [DADMB]Y(NC<sub>5</sub>H<sub>6</sub>)(NC<sub>5</sub>H<sub>5</sub>)<sub>2</sub>-C<sub>5</sub>H<sub>12</sub> (9).

| atom  | U <sub>11</sub> | U <sub>22</sub> | U <sub>33</sub> | U <sub>12</sub> | U <sub>13</sub> | U <sub>23</sub> |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Y(1)  | 0.0337(3)       | 0.0371(3)       | 0.0269(3)       | -0.0036(3)      | 0.0007(2)       | -0.0004(3)      |
| Si(1) | 0.0341(9)       | 0.047(1)        | 0.0431(9)       | -0.0013(8)      | -0.0015(7)      | -0.0003(8)      |
| Si(2) | 0.0340(9)       | 0.048(1)        | 0.0352(8)       | -0.0011(8)      | -0.0031(6)      | -0.0051(7)      |
| N(1)  | 0.055(3)        | 0.040(3)        | 0.040(3)        | -0.010(3)       | 0.007(2)        | -0.002(2)       |
| N(2)  | 0.032(3)        | 0.040(3)        | 0.035(2)        | -0.006(2)       | -0.001(2)       | 0.000(2)        |
| N(3)  | 0.039(3)        | 0.038(3)        | 0.025(2)        | -0.001(2)       | 0.001(2)        | -0.007(2)       |
| N(4)  | 0.035(3)        | 0.037(3)        | 0.031(2)        | -0.003(2)       | 0.001(2)        | -0.003(2)       |
| N(5)  | 0.040(3)        | 0.046(3)        | 0.031(3)        | -0.005(2)       | -0.003(2)       | 0.004(2)        |
| C(1)  | 0.068(5)        | 0.064(5)        | 0.063(4)        | -0.009(4)       | 0.002(3)        | 0.000(4)        |
| C(2)  | 0.076(6)        | 0.079(6)        | 0.108(7)        | -0.037(4)       | 0.023(5)        | -0.037(5)       |
| C(3)  | 0.074(5)        | 0.057(5)        | 0.095(6)        | -0.004(4)       | -0.014(4)       | -0.029(5)       |
| C(4)  | 0.067(5)        | 0.046(4)        | 0.082(5)        | -0.005(4)       | 0.007(4)        | -0.020(4)       |
| C(5)  | 0.053(4)        | 0.048(4)        | 0.055(4)        | -0.007(3)       | 0.000(3)        | -0.009(3)       |
| C(6)  | 0.035(3)        | 0.036(3)        | 0.032(3)        | 0.007(3)        | 0.011(2)        | -0.003(3)       |
| C(7)  | 0.039(3)        | 0.043(4)        | 0.039(3)        | 0.003(3)        | -0.002(2)       | -0.001(3)       |
| C(8)  | 0.053(4)        | 0.049(4)        | 0.037(3)        | 0.011(3)        | 0.005(3)        | 0.010(3)        |
| C(9)  | 0.053(4)        | 0.040(4)        | 0.052(4)        | 0.008(3)        | 0.014(3)        | 0.021(3)        |
| C(10) | 0.040(3)        | 0.036(3)        | 0.048(4)        | 0.002(3)        | 0.004(3)        | -0.003(3)       |
| C(11) | 0.043(3)        | 0.024(3)        | 0.038(3)        | 0.008(3)        | 0.007(2)        | -0.001(2)       |
| C(12) | 0.034(3)        | 0.039(3)        | 0.033(3)        | -0.009(3)       | 0.008(2)        | -0.008(3)       |
| C(13) | 0.037(3)        | 0.041(4)        | 0.029(3)        | -0.008(3)       | 0.004(2)        | -0.006(3)       |
| C(14) | 0.038(3)        | 0.047(4)        | 0.042(3)        | -0.006(3)       | 0.001(3)        | -0.006(3)       |
| C(15) | 0.056(4)        | 0.076(5)        | 0.038(4)        | -0.015(4)       | 0.008(3)        | -0.019(3)       |
| C(16) | 0.050(4)        | 0.050(4)        | 0.044(4)        | -0.004(3)       | 0.018(3)        | -0.018(3)       |
| C(17) | 0.040(3)        | 0.045(4)        | 0.045(4)        | -0.003(3)       | 0.005(3)        | -0.006(3)       |
| C(18) | 0.056(4)        | 0.056(4)        | 0.053(4)        | 0.002(3)        | 0.011(3)        | -0.017(3)       |
| C(19) | 0.053(4)        | 0.048(4)        | 0.058(4)        | -0.010(3)       | 0.013(3)        | 0.008(3)        |
| C(20) | 0.052(4)        | 0.062(5)        | 0.092(5)        | -0.016(4)       | -0.013(3)       | 0.022(4)        |
| C(21) | 0.044(4)        | 0.078(5)        | 0.069(4)        | 0.000(4)        | -0.001(3)       | -0.019(4)       |
| C(22) | 0.037(3)        | 0.065(5)        | 0.065(4)        | 0.007(3)        | 0.009(3)        | -0.008(4)       |
| C(23) | 0.081(5)        | 0.092(6)        | 0.061(5)        | -0.007(5)       | 0.029(4)        | -0.019(4)       |
| C(24) | 0.061(5)        | 0.052(5)        | 0.114(6)        | 0.017(4)        | 0.013(4)        | 0.021(4)        |
| C(25) | 0.034(4)        | 0.092(6)        | 0.104(6)        | 0.013(4)        | 0.011(3)        | -0.001(5)       |

**Table 18.** Anisotropic Displacement Parameters for [DADMB]Y(NC<sub>5</sub>H<sub>6</sub>)(NC<sub>5</sub>H<sub>5</sub>)<sub>2</sub>-C<sub>5</sub>H<sub>12</sub> (9).

| atom  | U <sub>11</sub> | U <sub>22</sub> | U <sub>33</sub> | U <sub>12</sub> | U <sub>13</sub> | U <sub>23</sub> |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| C(26) | 0.049(4)        | 0.058(4)        | 0.050(4)        | -0.003(3)       | -0.008(3)       | 0.005(3)        |
| C(27) | 0.042(4)        | 0.066(5)        | 0.060(4)        | 0.014(4)        | -0.013(3)       | -0.019(4)       |
| C(28) | 0.038(3)        | 0.061(4)        | 0.037(3)        | -0.002(3)       | -0.003(2)       | 0.000(3)        |
| C(29) | 0.034(3)        | 0.093(6)        | 0.056(4)        | -0.007(4)       | 0.003(3)        | -0.001(4)       |
| C(30) | 0.051(4)        | 0.075(5)        | 0.045(4)        | -0.014(4)       | 0.007(3)        | 0.004(4)        |
| C(31) | 0.050(4)        | 0.070(5)        | 0.050(4)        | -0.020(3)       | 0.000(3)        | -0.005(4)       |
| C(32) | 0.052(4)        | 0.050(4)        | 0.038(3)        | -0.010(3)       | 0.005(3)        | -0.001(3)       |
| C(33) | 0.073(5)        | 0.067(5)        | 0.040(4)        | -0.023(4)       | 0.013(3)        | -0.013(4)       |
| C(34) | 0.066(5)        | 0.089(6)        | 0.035(4)        | -0.030(4)       | -0.001(3)       | -0.002(4)       |
| C(35) | 0.058(4)        | 0.072(5)        | 0.056(4)        | -0.020(4)       | -0.010(3)       | 0.029(4)        |
| C(36) | 0.046(4)        | 0.056(4)        | 0.039(3)        | -0.009(3)       | 0.001(3)        | 0.011(3)        |
| C(37) | 0.041(3)        | 0.045(4)        | 0.039(3)        | 0.000(3)        | -0.001(2)       | -0.003(3)       |
| C(38) | 0.060(4)        | 0.061(4)        | 0.042(4)        | -0.004(3)       | 0.015(3)        | 0.004(3)        |
| C(39) | 0.070(4)        | 0.077(5)        | 0.026(3)        | 0.003(4)        | 0.004(3)        | -0.003(3)       |
| C(40) | 0.046(4)        | 0.066(5)        | 0.029(3)        | -0.001(3)       | -0.001(2)       | -0.006(3)       |
| C(41) | 0.039(3)        | 0.044(4)        | 0.043(4)        | -0.008(3)       | 0.001(3)        | -0.001(3)       |
| C(42) | 0.28(2)         | 0.08(1)         | 0.09(1)         | 0.0000          | 0.00(1)         | 0.0000          |
| C(44) | 0.16(1)         | 0.11(1)         | 0.039(6)        | 0.0000          | -0.017(7)       | 0.0000          |
| C(46) | 0.12(1)         | 0.076(9)        | 0.11(1)         | 0.0000          | -0.002(8)       | 0.0000          |
| C(49) | 0.13(2)         | 0.25(2)         | 0.18(2)         | 0.02(2)         | -0.06(1)        | 0.04(2)         |

The general temperature factor expression:

$$\exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2a*b*U_{12}hk + 2a*c*U_{13}hl + 2b*c*U_{23}kl))$$

**Table 19.** Bond Lengths (Å) for [DADMB]Y(NC<sub>5</sub>H<sub>6</sub>)(NC<sub>5</sub>H<sub>5</sub>)<sub>2</sub>·C<sub>5</sub>H<sub>12</sub> (**9**).

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| Y(1)  | N(1)  | 2.280(5) | Y(1)  | N(2)  | 2.254(4) |
| Y(1)  | N(3)  | 2.253(4) | Y(1)  | N(4)  | 2.481(4) |
| Y(1)  | N(5)  | 2.486(4) | Y(1)  | C(6)  | 2.717(5) |
| Y(1)  | C(13) | 2.822(5) | Si(1) | N(2)  | 1.728(4) |
| Si(1) | C(20) | 1.870(7) | Si(1) | C(21) | 1.866(6) |
| Si(1) | C(22) | 1.905(6) | Si(2) | N(3)  | 1.718(4) |
| Si(2) | C(26) | 1.869(6) | Si(2) | C(27) | 1.865(6) |
| Si(2) | C(28) | 1.906(6) | N(1)  | C(1)  | 1.424(7) |
| N(1)  | C(5)  | 1.397(7) | N(2)  | C(6)  | 1.403(6) |
| N(3)  | C(13) | 1.408(6) | N(4)  | C(37) | 1.352(7) |
| N(4)  | C(41) | 1.343(7) | N(5)  | C(32) | 1.320(7) |
| N(5)  | C(36) | 1.340(7) | C(1)  | C(2)  | 1.459(9) |
| C(2)  | C(3)  | 1.365(9) | C(3)  | C(4)  | 1.372(9) |
| C(4)  | C(5)  | 1.369(8) | C(6)  | C(7)  | 1.422(7) |
| C(6)  | C(11) | 1.429(7) | C(7)  | C(8)  | 1.375(7) |
| C(8)  | C(9)  | 1.375(8) | C(9)  | C(10) | 1.393(7) |
| C(10) | C(11) | 1.410(7) | C(10) | C(19) | 1.514(8) |
| C(11) | C(12) | 1.513(7) | C(12) | C(13) | 1.408(7) |
| C(12) | C(17) | 1.411(7) | C(13) | C(14) | 1.407(7) |
| C(14) | C(15) | 1.378(8) | C(15) | C(16) | 1.388(8) |
| C(16) | C(17) | 1.387(8) | C(17) | C(18) | 1.493(8) |
| C(22) | C(23) | 1.514(9) | C(22) | C(24) | 1.550(9) |
| C(22) | C(25) | 1.553(8) | C(28) | C(29) | 1.516(8) |
| C(28) | C(30) | 1.546(8) | C(28) | C(31) | 1.533(8) |
| C(32) | C(33) | 1.383(8) | C(33) | C(34) | 1.356(9) |
| C(34) | C(35) | 1.387(9) | C(35) | C(36) | 1.400(8) |
| C(37) | C(38) | 1.377(7) | C(38) | C(39) | 1.375(8) |
| C(39) | C(40) | 1.382(8) | C(40) | C(41) | 1.367(7) |
| C(42) | C(43) | 1.33(2)  | C(42) | C(43) | 1.33(2)  |
| C(43) | C(43) | 1.19(3)  | C(43) | C(44) | 1.46(2)  |
| C(44) | C(45) | 1.44(2)  | C(44) | C(45) | 1.44(2)  |
| C(45) | C(45) | 1.32(3)  | C(45) | C(46) | 1.50(2)  |
| C(47) | C(48) | 0.89(3)  | C(47) | C(50) | 1.52(5)  |

**Table 19.** Bond Lengths (Å) for [DADMB]Y(NC<sub>5</sub>H<sub>6</sub>)(NC<sub>5</sub>H<sub>5</sub>)<sub>2</sub>·C<sub>5</sub>H<sub>12</sub> (**9**).

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| C(47) | C(51) | 1.34(4)  | C(48) | C(50) | 1.40(5)  |
| C(48) | C(51) | 1.22(4)  | C(49) | C(50) | 1.21(4)  |
| C(49) | C(50) | 1.21(4)  | C(49) | C(51) | 1.47(4)  |
| C(49) | C(51) | 1.47(4)  | C(50) | C(51) | 1.03(4)  |

**Table 20.** Bond Angles (°) for [DADMB]Y(NC<sub>5</sub>H<sub>6</sub>)(NC<sub>5</sub>H<sub>5</sub>)<sub>2</sub>·C<sub>5</sub>H<sub>12</sub> (**9**).

| atom  | atom  | atom  | angle    | atom  | atom  | atom  | angle    |
|-------|-------|-------|----------|-------|-------|-------|----------|
| N(1)  | Y(1)  | N(2)  | 119.5(2) | N(1)  | Y(1)  | N(3)  | 121.4(2) |
| N(1)  | Y(1)  | N(4)  | 84.2(1)  | N(1)  | Y(1)  | N(5)  | 86.8(2)  |
| N(1)  | Y(1)  | C(6)  | 138.0(2) | N(1)  | Y(1)  | C(13) | 142.0(2) |
| N(2)  | Y(1)  | N(3)  | 118.9(1) | N(2)  | Y(1)  | N(4)  | 94.5(1)  |
| N(2)  | Y(1)  | N(5)  | 91.6(1)  | N(2)  | Y(1)  | C(6)  | 31.0(1)  |
| N(2)  | Y(1)  | C(13) | 93.3(2)  | N(3)  | Y(1)  | N(4)  | 95.3(1)  |
| N(3)  | Y(1)  | N(5)  | 87.7(1)  | N(3)  | Y(1)  | C(6)  | 96.7(2)  |
| N(3)  | Y(1)  | C(13) | 29.6(1)  | N(4)  | Y(1)  | N(5)  | 170.8(2) |
| N(4)  | Y(1)  | C(6)  | 74.7(1)  | N(4)  | Y(1)  | C(13) | 113.7(1) |
| N(5)  | Y(1)  | C(6)  | 113.6(1) | N(5)  | Y(1)  | C(13) | 72.7(1)  |
| C(6)  | Y(1)  | C(13) | 79.9(2)  | N(2)  | Si(1) | C(20) | 106.6(3) |
| N(2)  | Si(1) | C(21) | 115.3(2) | N(2)  | Si(1) | C(22) | 113.4(3) |
| C(20) | Si(1) | C(21) | 104.1(3) | C(20) | Si(1) | C(22) | 107.6(3) |
| C(21) | Si(1) | C(22) | 109.1(3) | N(3)  | Si(2) | C(26) | 116.4(2) |
| N(3)  | Si(2) | C(27) | 105.2(2) | N(3)  | Si(2) | C(28) | 114.4(2) |
| C(26) | Si(2) | C(27) | 104.2(3) | C(26) | Si(2) | C(28) | 106.9(3) |
| C(27) | Si(2) | C(28) | 109.0(3) | Y(1)  | N(1)  | C(1)  | 122.1(4) |
| Y(1)  | N(1)  | C(5)  | 126.9(4) | C(1)  | N(1)  | C(5)  | 109.6(5) |
| Y(1)  | N(2)  | Si(1) | 131.5(2) | Y(1)  | N(2)  | C(6)  | 93.0(3)  |
| Si(1) | N(2)  | C(6)  | 126.6(4) | Y(1)  | N(3)  | Si(2) | 127.3(2) |
| Y(1)  | N(3)  | C(13) | 98.2(3)  | Si(2) | N(3)  | C(13) | 127.5(3) |
| Y(1)  | N(4)  | C(37) | 122.8(3) | Y(1)  | N(4)  | C(41) | 119.7(3) |
| C(37) | N(4)  | C(41) | 116.6(4) | Y(1)  | N(5)  | C(32) | 122.2(4) |
| Y(1)  | N(5)  | C(36) | 119.0(4) | C(32) | N(5)  | C(36) | 117.5(5) |
| N(1)  | C(1)  | C(2)  | 115.2(6) | C(1)  | C(2)  | C(3)  | 115.8(6) |
| C(2)  | C(3)  | C(4)  | 119.8(6) | C(3)  | C(4)  | C(5)  | 119.6(6) |
| N(1)  | C(5)  | C(4)  | 122.3(6) | Y(1)  | C(6)  | N(2)  | 56.0(2)  |
| Y(1)  | C(6)  | C(7)  | 127.0(4) | Y(1)  | C(6)  | C(11) | 83.5(3)  |
| N(2)  | C(6)  | C(7)  | 122.6(5) | N(2)  | C(6)  | C(11) | 119.9(5) |
| C(7)  | C(6)  | C(11) | 117.0(5) | C(6)  | C(7)  | C(8)  | 122.0(5) |
| C(7)  | C(8)  | C(9)  | 120.3(5) | C(8)  | C(9)  | C(10) | 120.4(5) |
| C(9)  | C(10) | C(11) | 120.4(5) | C(9)  | C(10) | C(19) | 118.9(5) |
| C(11) | C(10) | C(19) | 120.7(5) | C(6)  | C(11) | C(10) | 119.7(5) |