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Table 1. Anisotropic Temperature Factors for **11**

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

| | u11(U) | u22 | u33 | u12 | u13 | u23 |
|---|---|---|---|---|---|---|
| W1 | 2.77(3) | 1.975(22) | 1.579(22) | 0.021(17) | -0.104(15) | 0.051(16) |
| I1 | 3.43(4) | 3.41 (4) | 2.20 (3) | 0.99 (3) | 0.15 (3) | 0.12 (3) |
| C1 | 4.6 (7) | 2.9 (6) | 3.7 (6) | 0.9 (5) | -1.5 (5) | -1.4 (5) |
| O1 | 5.6 (5) | 5.4 (5) | 2.3 (4) | 0.7 (4) | 1.5 (4) | 1.1 (4) |
| C2 | 3.3 (6) | 1.1 (4) | 2.8 (5) | -0.5 (4) | -1.0 (4) | -0.5 (4) |
| C3 | 3.0 (6) | 2.9 (5) | 3.4 (6) | 0.7 (4) | -1.8 (5) | -0.4 (5) |
| C4 | 6.7 (8) | 3.6 (6) | 2.0 (5) | 0.1 (5) | -1.2 (5) | 0.3 (5) |
| C5 | 6.1 (8) | 5.1 (7) | 2.2 (5) | 0.0 (6) | -0.8 (5) | -1.4 (5) |
| C6 | 4.6 (7) | 4.6 (6) | 4.4 (7) | 1.3 (6) | -0.4 (5) | -0.8 (6) |
| C7 | 5.9 (8) | 4.3 (7) | 6.2 (8) | 0.1 (6) | -2.3 (7) | -1.2 (6) |
| C8 | 4.7 (8) | 3.6 (6) | 9.2 (10) | -0.4 (6) | 0.0 (7) | -1.8 (7) |
| C9 | 4.9 (8) | 3.2 (6) | 6.5 (8) | -0.7 (5) | 0.6 (6) | 0.1 (6) |
| C10 | 2.5 (6) | 4.9 (7) | 8.9 (10) | -1.6 (5) | -0.8 (6) | -0.7 (7) |
| C11 | 2.5 (6) | 3.7 (6) | 5.1 (7) | 0.2 (5) | -0.2 (5) | -1.3 (5) |
| B1 | 4.2 (7) | 2.0 (5) | 1.6 (5) | 0.8 (5) | -0.2 (5) | -1.3 (4) |
| N11 | 3.0 (5) | 2.0 (4) | 2.7 (4) | 0.5 (3) | 0.2 (3) | 0.0 (3) |
| N12 | 2.8 (5) | 2.3 (4) | 1.6 (4) | 0.1 (3) | 0.1 (3) | -0.8 (3) |
| C13 | 2.4 (6) | 3.2 (5) | 2.4 (5) | -0.4 (4) | 0.1 (4) | -0.3 (4) |
| C14 | 4.5 (7) | 2.8 (5) | 1.9 (5) | -0.3 (5) | 0.6 (4) | 0.2 (4) |
| C15 | 2.9 (6) | 2.4 (5) | 2.5 (5) | -0.5 (4) | -0.2 (4) | 0.1 (4) |
| C16 | 4.8 (7) | 3.8 (6) | 3.1 (6) | -0.2 (5) | 0.5 (5) | -0.2 (5) |
| C17 | 3.9 (6) | 2.0 (5) | 3.4 (6) | -0.4 (4) | 0.7 (5) | 0.1 (4) |
| N21 | 2.2 (4) | 2.7 (4) | 3.0 (4) | -0.3 (4) | -0.2 (3) | 0.7 (4) |
| N22 | 3.1 (5) | 2.0 (4) | 1.6 (4) | 0.5 (3) | -0.4 (3) | 0.5 (3) |
| C23 | 3.6 (6) | 2.1 (5) | 2.9 (5) | -1.5 (4) | -1.2 (5) | 0.9 (4) |
| C24 | 3.6 (7) | 3.6 (6) | 3.9 (6) | -1.1 (5) | -0.4 (5) | 1.5 (5) |
| C25 | 3.2 (6) | 3.1 (5) | 3.1 (5) | -0.8 (5) | -0.3 (4) | 0.2 (5) |
| C26 | 5.2 (7) | 3.0 (5) | 3.9 (6) | -1.8 (5) | -1.5 (5) | 0.0 (5) |
| C27 | 3.5 (7) | 5.0 (7) | 5.4 (7) | -0.9 (5) | 1.3 (5) | 0.2 (6) |
| N31 | 2.9 (5) | 2.0 (4) | 2.8 (4) | -0.2 (4) | -0.1 (4) | 1.0 (4) |
| N32 | 2.9 (5) | 2.4 (4) | 3.3 (5) | 0.1 (4) | 0.3 (4) | -0.2 (4) |
| C33 | 3.0 (6) | 2.8 (5) | 4.1 (6) | 0.3 (5) | 0.5 (5) | 0.8 (5) |
| C34 | 3.0 (6) | 3.1 (5) | 3.8 (6) | -0.3 (5) | 0.1 (5) | 1.6 (5) |
| C35 | 2.1 (5) | 2.6 (5) | 3.2 (5) | -0.6 (4) | -0.2 (4) | 0.8 (4) |
| C36 | 5.4 (8) | 4.6 (7) | 4.9 (7) | 2.0 (6) | 0.8 (6) | 1.1 (6) |
| C37 | 3.6 (6) | 4.4 (6) | 3.3 (6) | 0.4 (5) | -1.2 (5) | 1.3 (5) |
| H4a | 5.1 | | | | | |
| H4b | 5.1 | | | | | |
| H5a | 5.5 | | | | | |
| H5b | 5.5 | | | | | |
| H6a | 5.6 | | | | | |
| H6b | 5.6 | | | | | |
| H7a | 6.5 | | | | | |
| H7b | 6.5 | | | | | |
| H8a | 6.8 | | | | | |
| H8b | 6.8 | | | | | |
| H9a | 5.9 | | | | | |

| | |
|---|---|
| H9b | 5.9 |
| H10a | 6.4 |
| H10b | 6.4 |
| H11a | 4.8 |
| H11b | 4.8 |
| H1 | 3.6 |
| H14 | 4.1 |
| H16a | 4.9 |
| H16b | 4.9 |
| H16c | 4.9 |
| H17a | 4.1 |
| H17b | 4.1 |
| H17c | 4.1 |
| H24 | 4.7 |
| H26a | 5.0 |
| H26b | 5.0 |
| H26c | 5.0 |
| H27a | 5.6 |
| H27b | 5.6 |
| H27c | 5.6 |
| H34 | 4.3 |
| H36a | 6.0 |
| H36b | 6.0 |
| H36c | 6.0 |
| H37a | 4.8 |
| H37b | 4.8 |
| H37c | 4.8 |

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)

Table 2. Complete Bond Distances for **11**

| | | | |
|---|---|---|---|
| W(1)-I(1) | 2.7905(7) | N(11)-N(12) | 1.387(10) |
| W(1)-C(1) | 1.913(12) | N(11)-C(15) | 1.352(11) |
| W(1)-C(2) | 2.023(9) | N(12)-C(13) | 1.351(12) |
| W(1)-C(3) | 2.060(9) | C(13)-C(14) | 1.391(13) |
| W(1)-N(11) | 2.253(7) | C(13)-C(16) | 1.479(13) |
| W(1)-N(21) | 2.255(7) | C(14)-C(15) | 1.404(13) |
| W(1)-N(31) | 2.196(7) | C(15)-C(17) | 1.475(12) |
| C(1)-O(1) | 1.190(13) | N(21)-N(22) | 1.390(10) |
| C(2)-C(3) | 1.302(14) | N(21)-C(25) | 1.341(12) |
| C(2)-C(11) | 1.494(14) | N(22)-C(23) | 1.351(11) |
| C(3)-C(4) | 1.509(13) | C(23)-C(24) | 1.361(16) |
| C(4)-C(5) | 1.538(16) | C(23)-C(26) | 1.474(14) |
| C(5)-C(6) | 1.518(16) | C(24)-C(25) | 1.389(14) |
| C(6)-C(7) | 1.536(17) | C(25)-C(27) | 1.505(15) |
| C(7)-C(8) | 1.518(20) | N(31)-N(32) | 1.381(11) |
| C(8)-C(9) | 1.530(17) | N(31)-C(35) | 1.337(11) |
| C(9)-C(10) | 1.516(16) | N(32)-C(33) | 1.335(12) |
| C(10)-C(11) | 1.535(14) | C(33)-C(34) | 1.361(14) |
| B(1)-N(12) | 1.520(13) | C(33)-C(36) | 1.495(15) |
| B(1)-N(22) | 1.522(14) | C(34)-C(35) | 1.391(14) |
| B(1)-N(32) | 1.540(13) | C(35)-C(37) | 1.505(14) |

Table 3. Complete Bond Angles for **11**

| | | | |
|---|---|---|---|
| I(1)-W(1)-C(1) | 89.3(3) | W(1)-N(11)-N(12) | 119.1(5) |
| I(1)-W(1)-C(2) | 105.57(24) | W(1)-N(11)-C(15) | 134.0(6) |
| I(1)-W(1)-C(3) | 100.65(25) | N(12)-N(11)-C(15) | 106.5(7) |
| I(1)-W(1)-N(11) | 84.97(18) | B(1)-N(12)-N(11) | 120.1(7) |
| I(1)-W(1)-N(21) | 87.68(19) | B(1)-N(12)-C(13) | 129.6(7) |
| I(1)-W(1)-N(31) | 164.55(19) | N(11)-N(12)-C(13) | 110.4(7) |
| C(1)-W(1)-C(2) | 106.1(4) | N(12)-C(13)-C(14) | 107.3(8) |
| C(1)-W(1)-C(3) | 69.1(4) | N(12)-C(13)-C(16) | 124.0(8) |
| C(1)-W(1)-N(11) | 168.6(4) | C(14)-C(13)-C(16) | 128.7(9) |
| C(1)-W(1)-N(21) | 88.0(3) | C(13)-C(14)-C(15) | 106.6(8) |
| C(1)-W(1)-N(31) | 96.2(3) | N(11)-C(15)-C(14) | 109.3(8) |
| C(2)-W(1)-C(3) | 37.2(4) | N(11)-C(15)-C(17) | 125.3(8) |
| C(2)-W(1)-N(11) | 85.0(3) | C(14)-C(15)-C(17) | 125.4(8) |
| C(2)-W(1)-N(21) | 160.5(3) | W(1)-N(21)-N(22) | 118.3(5) |
| C(2)-W(1)-N(31) | 86.8(3) | W(1)-N(21)-C(25) | 134.8(6) |
| C(3)-W(1)-N(11) | 121.6(4) | N(22)-N(21)-C(25) | 106.6(7) |
| C(3)-W(1)-N(21) | 155.3(3) | B(1)-N(22)-N(21) | 120.9(7) |
| C(3)-W(1)-N(31) | 94.8(3) | B(1)-N(22)-C(23) | 129.7(8) |
| N(11)-W(1)-N(21) | 82.0(3) | N(21)-N(22)-C(23) | 109.1(8) |
| N(11)-W(1)-N(31) | 87.0(3) | N(22)-C(23)-C(24) | 108.0(8) |
| N(21)-W(1)-N(31) | 78.1(3) | N(22)-C(23)-C(26) | 123.2(9) |
| W(1)-C(1)-O(1) | 178.3(8) | C(24)-C(23)-C(26) | 128.8(9) |
| W(1)-C(2)-C(3) | 73.0(6) | C(23)-C(24)-C(25) | 107.3(9) |
| W(1)-C(2)-C(11) | 144.4(7) | N(21)-C(25)-C(24) | 109.1(9) |
| C(3)-C(2)-C(11) | 141.5(8) | N(21)-C(25)-C(27) | 124.4(8) |
| W(1)-C(3)-C(2) | 69.9(5) | C(24)-C(25)-C(27) | 126.5(9) |
| W(1)-C(3)-C(4) | 148.9(8) | W(1)-N(31)-N(32) | 120.2(5) |
| C(2)-C(3)-C(4) | 141.2(9) | W(1)-N(31)-C(35) | 133.8(6) |
| C(3)-C(4)-C(5) | 114.6(8) | N(32)-N(31)-C(35) | 105.7(7) |
| C(4)-C(5)-C(6) | 114.7(9) | B(1)-N(32)-N(31) | 119.2(7) |
| C(5)-C(6)-C(7) | 115.4(9) | B(1)-N(32)-C(33) | 129.8(8) |
| C(6)-C(7)-C(8) | 114.0(9) | N(31)-N(32)-C(33) | 110.1(7) |
| C(7)-C(8)-C(9) | 114.2(9) | N(32)-C(33)-C(34) | 108.0(9) |
| C(8)-C(9)-C(10) | 115.9(10) | N(32)-C(33)-C(36) | 121.9(9) |
| C(9)-C(10)-C(11) | 112.2(9) | C(34)-C(33)-C(36) | 130.1(9) |
| C(2)-C(11)-C(10) | 112.4(8) | C(33)-C(34)-C(35) | 106.4(8) |
| N(12)-B(1)-N(22) | 110.5(7) | N(31)-C(35)-C(34) | 109.8(8) |
| N(12)-B(1)-N(32) | 110.3(8) | N(31)-C(35)-C(37) | 123.1(8) |
| N(22)-B(1)-N(32) | 107.8(7) | C(34)-C(35)-C(37) | 127.0(8) |

Table 4. Atomic Parameters x, y, z and Biso for **11**

Table .Atomic Parameters x,y,z and Biso.
E.S.Ds. refer to the last digit printed.

| | x | y | z | Biso |
|---|---|---|---|---|
| W1 | 0.13299(4) | 0.826262(16) | 0.108246(24) | 1.665(18) |
| I1 | 0.34892(7) | 0.74250 (3) | 0.15417 (4) | 2.38 (3) |
| C1 | 0.2114 (11) | 0.8382 (5) | -0.0133 (7) | 3.0 (4) |
| O1 | 0.2603 (8) | 0.8440 (3) | -0.0892 (5) | 3.5 (3) |
| C2 | -0.0358 (10) | 0.7702 (4) | 0.0881 (6) | 1.9 (4) |
| C3 | 0.0276 (10) | 0.7732 (4) | 0.0080 (7) | 2.5 (4) |
| C4 | 0.0143 (12) | 0.7507 (5) | -0.0926 (7) | 3.2 (5) |
| C5 | 0.1093 (12) | 0.6943 (5) | -0.1178 (7) | 3.5 (5) |
| C6 | 0.0854 (12) | 0.6337 (5) | -0.0611 (8) | 3.6 (5) |
| C7 | -0.0613 (13) | 0.6055 (5) | -0.0686 (9) | 4.3 (5) |
| C8 | -0.1164 (13) | 0.5806 (5) | 0.0240 (10) | 4.6 (6) |
| C9 | -0.1210 (12) | 0.6308 (5) | 0.1023 (8) | 3.8 (5) |
| C10 | -0.2217 (11) | 0.6856 (5) | 0.0868 (10) | 4.3 (6) |
| C11 | -0.1688 (10) | 0.7485 (5) | 0.1301 (7) | 3.0 (5) |
| B1 | 0.0701 (12) | 0.9404 (5) | 0.2638 (7) | 2.1 (4) |
| N11 | 0.0811 (8) | 0.8198 (3) | 0.2620 (5) | 2.0 (3) |
| N12 | 0.0544 (8) | 0.8757 (3) | 0.3114 (5) | 1.8 (3) |
| C13 | 0.0123 (10) | 0.8617 (4) | 0.3993 (6) | 2.1 (4) |
| C14 | 0.0129 (11) | 0.7953 (4) | 0.4081 (6) | 2.4 (4) |
| C15 | 0.0544 (10) | 0.7707 (4) | 0.3210 (6) | 2.0 (4) |
| C16 | -0.0248 (11) | 0.9105 (5) | 0.4701 (7) | 3.1 (5) |
| C17 | 0.0715 (11) | 0.7022 (4) | 0.2986 (7) | 2.4 (4) |
| N21 | 0.2692 (8) | 0.9068 (3) | 0.1607 (5) | 2.1 (3) |
| N22 | 0.2165 (8) | 0.9485 (3) | 0.2275 (5) | 1.8 (3) |
| C23 | 0.3084 (11) | 0.9963 (4) | 0.2430 (7) | 2.3 (4) |
| C24 | 0.4198 (11) | 0.9856 (5) | 0.1876 (7) | 2.9 (4) |
| C25 | 0.3934 (10) | 0.9300 (4) | 0.1368 (7) | 2.5 (4) |
| C26 | 0.2850 (12) | 1.0488 (5) | 0.3103 (7) | 3.2 (5) |
| C27 | 0.4878 (11) | 0.8990 (5) | 0.0669 (8) | 3.7 (5) |
| N31 | -0.0088 (8) | 0.9084 (3) | 0.1005 (5) | 2.0 (3) |
| N32 | -0.0306 (8) | 0.9459 (3) | 0.1791 (5) | 2.3 (3) |
| C33 | -0.1291 (10) | 0.9892 (4) | 0.1610 (7) | 2.6 (4) |
| C34 | -0.1737 (10) | 0.9808 (4) | 0.0705 (7) | 2.6 (4) |
| C35 | -0.0961 (9) | 0.9307 (4) | 0.0343 (6) | 2.1 (4) |
| C36 | -0.1735 (13) | 1.0368 (5) | 0.2332 (8) | 3.9 (5) |
| C37 | -0.1095 (11) | 0.9016 (5) | -0.0623 (7) | 3.0 (4) |
| H4a | -0.079 | 0.737 | -0.103 | 4.0 |
| H4b | 0.034 | 0.786 | -0.133 | 4.0 |
| H5a | 0.203 | 0.708 | -0.108 | 4.3 |
| H5b | 0.094 | 0.684 | -0.183 | 4.3 |
| H6a | 0.102 | 0.644 | 0.004 | 4.4 |
| H6b | 0.149 | 0.601 | -0.081 | 4.4 |
| H7a | -0.120 | 0.639 | -0.091 | 5.1 |
| H7b | -0.061 | 0.571 | -0.114 | 5.1 |
| H8a | -0.209 | 0.566 | 0.013 | 5.4 |
| H8b | -0.060 | 0.545 | 0.045 | 5.4 |

| | | | | |
|---|---|---|---|---|
| H9a | -0.030 | 0.650 | 0.108 | 4.6 |
| H9b | -0.143 | 0.610 | 0.160 | 4.6 |
| H10a | -0.236 | 0.691 | 0.020 | 5.1 |
| H10b | -0.308 | 0.674 | 0.115 | 5.1 |
| H11a | -0.155 | 0.743 | 0.197 | 3.8 |
| H11b | -0.237 | 0.781 | 0.119 | 3.8 |
| H1 | 0.050 | 0.974 | 0.308 | 2.9 |
| H14 | -0.012 | 0.771 | 0.463 | 3.2 |
| H16a | -0.049 | 0.889 | 0.527 | 3.9 |
| H16b | 0.052 | 0.939 | 0.482 | 3.9 |
| H16c | -0.102 | 0.935 | 0.447 | 3.9 |
| H17a | 0.043 | 0.677 | 0.352 | 3.2 |
| H17b | 0.016 | 0.691 | 0.244 | 3.2 |
| H17c | 0.167 | 0.694 | 0.286 | 3.2 |
| H24 | 0.501 | 1.012 | 0.184 | 3.7 |
| H26a | 0.361 | 1.078 | 0.311 | 4.0 |
| H26b | 0.202 | 1.071 | 0.291 | 4.0 |
| H26c | 0.274 | 1.031 | 0.372 | 4.0 |
| H27a | 0.569 | 0.925 | 0.061 | 4.5 |
| H27b | 0.514 | 0.857 | 0.089 | 4.5 |
| H27c | 0.441 | 0.896 | 0.007 | 4.5 |
| H34 | -0.246 | 1.004 | 0.038 | 3.4 |
| H36a | -0.245 | 1.064 | 0.206 | 4.7 |
| H36b | -0.209 | 1.014 | 0.286 | 4.7 |
| H36c | -0.097 | 1.063 | 0.253 | 4.7 |
| H37a | -0.178 | 0.925 | -0.098 | 3.8 |
| H37b | -0.022 | 0.904 | -0.093 | 3.8 |
| H37c | -0.137 | 0.857 | -0.058 | 3.8 |

Biso is the Mean of the Principal Axes of the Thermal Ellipsoid