# APPENDIX

**TABLE 1. CRYSTAL DATA AND STRUCTURE REFINEMENT FOR 2M_JN1_S.**

| | | |
|---|---|---|
| Identification code | 2m_jn1_s | |
| Empirical formula | C18 H15 N | |
| Formula weight | 245.31 | |
| Temperature | 293(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Orthorhombic | |
| Space group | Pbca | |
| Unit cell dimensions | a = 11.4419(14) Å | α= 90°. |
| | b = 14.1679(17) Å | β= 90°. |
| | c = 16.1234(19) Å | γ = 90°. |
| Volume | 2613.7(5) $Å^3$ | |
| Z | 8 | |
| Density (calculated) | 1.247 $Mg/m^3$ | |
| Absorption coefficient | 0.072 $mm^{-1}$ | |
| F(000) | 1040 | |
| Crystal size | 0.40 x 0.36 x 0.20 $mm^3$ | |
| Theta range for data collection | 2.53 to 26.00°. | |
| Index ranges | -10<=h<=14, -15<=k<=17, -19<=l<=19 | |
| Reflections collected | 14591 | |
| Independent reflections | 2566 [R(int) = 0.0481] | |
| Completeness to theta = 26.00° | 100.0 % | |
| Absorption correction | None | |
| Max. and min. transmission | 0.9857 and 0.9717 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 2566 / 0 / 174 | |
| Goodness-of-fit on $F^2$ | 1.073 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0758, wR2 = 0.2184 | |
| R indices (all data) | R1 = 0.1143, wR2 = 0.2517 | |
| Largest diff. peak and hole | 0.741 and -0.286 $e.Å^{-3}$ | |

**TABLE 2: ATOMIC COORDINATES (X104) AND EQUIVALENT ISOTROPIC DISPLACEMENT PARAMETERS (Å2X 103) FOR 2M_JN1_S. U(EQ) IS DEFINED AS ONE THIRD OF THE TRACE OF THE ORTHOGONALIZED UIJ TENSOR.**

| | x | y | z | U(eq) |
|---|---|---|---|---|
| C(1) | -2212(4) | 10328(3) | 3428(2) | 76(1) |
| C(2) | -3297(4) | 9936(3) | 3451(2) | 86(1) |
| C(3) | -3451(4) | 9026(3) | 3768(2) | 83(1) |
| C(4) | -2523(4) | 8534(3) | 4062(2) | 72(1) |
| C(5) | -399(3) | 8415(3) | 4339(2) | 66(1) |
| C(6) | 734(4) | 8759(3) | 4336(2) | 89(1) |
| C(8) | 2459(3) | 11731(3) | 3410(2) | 71(1) |
| C(9) | 2009(4) | 12518(3) | 3024(2) | 77(1) |
| C(10) | 832(4) | 12584(3) | 2844(2) | 78(1) |
| C(11) | 70(3) | 11872(2) | 3051(2) | 68(1) |
| C(12) | -500(4) | 7427(3) | 4683(3) | 93(1) |
| C(13) | 3160(4) | 9844(3) | 4175(3) | 98(1) |
| C(4A) | -1382(3) | 8912(2) | 4049(2) | 61(1) |
| C(6A) | 893(4) | 9635(3) | 4031(2) | 79(1) |
| C(7A) | 1709(3) | 10992(2) | 3610(2) | 58(1) |
| C(11A) | 488(3) | 11049(2) | 3440(2) | 57(1) |
| C(11B) | -58(3) | 10192(2) | 3713(2) | 55(1) |
| C(11C) | -1219(3) | 9846(2) | 3719(2) | 60(1) |
| N(7) | 1989(3) | 10141(2) | 3963(2) | 69(1) |

**TABLE 3: BOND LENGTHS [Å] AND ANGLES [°] FOR 2M_JN1_S.**

| | | | |
|---|---|---|---|
| C(1)-C(2) | 1.361(5) | C(4)-H(4) | 0.9300 |
| C(1)-C(11C) | 1.406(5) | C(5)-C(6) | 1.386(6) |
| C(1)-H(1) | 0.9300 | C(5)-C(4A) | 1.407(5) |
| C(2)-C(3) | 1.398(6) | C(5)-C(12) | 1.510(5) |
| C(2)-H(2) | 0.9300 | C(6)-C(6A) | 1.347(5) |
| C(3)-C(4) | 1.356(6) | C(6)-H(6) | 0.9300 |
| C(3)-H(3) | 0.9300 | C(8)-C(9) | 1.377(5) |
| C(4)-C(4A) | 1.411(5) | C(8)-C(7A) | 1.392(5) |

| | | | |
|---|---|---|---|
| C(8)-H(8) | 0.9300 | C(6A)-C(6)-H(6) | 121.6 |
| C(9)-C(10) | 1.381(5) | C(5)-C(6)-H(6) | 121.6 |
| C(9)-H(9) | 0.9300 | C(9)-C(8)-C(7A) | 118.8(4) |
| C(10)-C(11) | 1.375(5) | C(9)-C(8)-H(8) | 120.6 |
| C(10)-H(10) | 0.9300 | C(7A)-C(8)-H(8) | 120.6 |
| C(11)-C(11A) | 1.407(4) | C(8)-C(9)-C(10) | 121.0(4) |
| C(11)-H(11) | 0.9300 | C(8)-C(9)-H(9) | 119.5 |
| C(12)-H(12A) | 0.9600 | C(10)-C(9)-H(9) | 119.5 |
| C(12)-H(12B) | 0.9600 | C(11)-C(10)-C(9) | 121.2(4) |
| C(12)-H(12C) | 0.9600 | C(11)-C(10)-H(10) | 119.4 |
| C(13)-N(7) | 1.446(5) | C(9)-C(10)-H(10) | 119.4 |
| C(13)-H(13A) | 0.9600 | C(10)-C(11)-C(11A) | 120.0(4) |
| C(13)-H(13B) | 0.9600 | C(10)-C(11)-H(11) | 120.0 |
| C(13)-H(13C) | 0.9600 | C(11A)-C(11)-H(11) | 120.0 |
| C(4A)-C(11C) | 1.437(4) | C(5)-C(12)-H(12A) | 109.5 |
| C(6A)-C(11B) | 1.439(5) | C(5)-C(12)-H(12B) | 109.5 |
| C(6A)-N(7) | 1.449(5) | H(12A)-C(12)-H(12B) | 109.5 |
| C(7A)-N(7) | 1.371(4) | C(5)-C(12)-H(12C) | 109.5 |
| C(7A)-C(11A) | 1.426(5) | H(12A)-C(12)-H(12C) | 109.5 |
| C(11A)-C(11B) | 1.435(4) | H(12B)-C(12)-H(12C) | 109.5 |
| C(11B)-C(11C) | 1.415(5) | N(7)-C(13)-H(13A) | 109.5 |
| C(2)-C(1)-C(11C) | 122.0(4) | N(7)-C(13)-H(13B) | 109.5 |
| C(2)-C(1)-H(1) | 119.0 | H(13A)-C(13)-H(13B) | 109.5 |
| C(11C)-C(1)-H(1) | 119.0 | N(7)-C(13)-H(13C) | 109.5 |
| C(1)-C(2)-C(3) | 120.1(4) | H(13A)-C(13)-H(13C) | 109.5 |
| C(1)-C(2)-H(2) | 120.0 | H(13B)-C(13)-H(13C) | 109.5 |
| C(3)-C(2)-H(2) | 120.0 | C(5)-C(4A)-C(4) | 122.9(3) |
| C(4)-C(3)-C(2) | 120.2(4) | C(5)-C(4A)-C(11C) | 118.6(3) |
| C(4)-C(3)-H(3) | 119.9 | C(4)-C(4A)-C(11C) | 118.4(3) |
| C(2)-C(3)-H(3) | 119.9 | C(6)-C(6A)-C(11B) | 122.2(4) |
| C(3)-C(4)-C(4A) | 121.6(3) | C(6)-C(6A)-N(7) | 126.9(4) |
| C(3)-C(4)-H(4) | 119.2 | C(11B)-C(6A)-N(7) | 110.8(3) |
| C(4A)-C(4)-H(4) | 119.2 | N(7)-C(7A)-C(8) | 127.8(3) |
| C(6)-C(5)-C(4A) | 124.8(3) | N(7)-C(7A)-C(11A) | 111.0(3) |
| C(6)-C(5)-C(12) | 113.5(4) | C(8)-C(7A)-C(11A) | 121.2(3) |
| C(4A)-C(5)-C(12) | 121.7(3) | C(11)-C(11A)-C(7A) | 117.7(3) |
| C(6A)-C(6)-C(5) | 116.8(4) | C(11)-C(11A)-C(11B) | 133.6(3) |

| | | | |
|---|---|---|---|
| C(7A)-C(11A)-C(11B) | 108.7(3) | C(1)-C(11C)-C(4A) | 117.7(3) |
| C(11C)-C(11B)-C(11A) | 134.7(3) | C(11B)-C(11C)-C(4A) | 116.3(3) |
| C(11C)-C(11B)-C(6A) | 121.2(3) | C(7A)-N(7)-C(13) | 124.9(3) |
| C(11A)-C(11B)-C(6A) | 104.1(3) | C(7A)-N(7)-C(6A) | 105.3(3) |
| C(1)-C(11C)-C(11B) | 126.0(3) | C(13)-N(7)-C(6A) | 129.7(3) |

Symmetry transformations used to generate equivalent atoms:

**TABLE 4: ANISOTROPIC DISPLACEMENT PARAMETERS (Å2X 103) FOR 2M_JN1_S. THE ANISOTROPIC DISPLACEMENT FACTOR EXPONENT TAKES THE FORM: -2□2[ H2 A*2U11 + ... + 2 H K A* B* U12 ]**

| | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| C(1) | 90(3) | 73(2) | 64(2) | 16(2) | 0(2) | -1(2) |
| C(2) | 83(3) | 100(3) | 74(2) | 16(2) | -10(2) | 5(2) |
| C(3) | 81(3) | 91(3) | 76(2) | -1(2) | -3(2) | -15(2) |
| C(4) | 91(3) | 62(2) | 62(2) | -3(2) | 6(2) | -14(2) |
| C(5) | 72(2) | 76(2) | 51(2) | -10(2) | 10(2) | -14(2) |
| C(6) | 129(4) | 75(3) | 62(2) | -7(2) | -1(2) | 29(3) |
| C(8) | 76(2) | 76(2) | 60(2) | -12(2) | 15(2) | -10(2) |
| C(9) | 101(3) | 69(2) | 60(2) | -5(2) | 22(2) | -15(2) |
| C(10) | 105(3) | 68(2) | 60(2) | 8(2) | 13(2) | 0(2) |
| C(11) | 78(2) | 71(2) | 55(2) | 3(2) | 1(2) | 8(2) |
| C(12) | 118(3) | 82(3) | 79(3) | 3(2) | 8(2) | 20(2) |
| C(13) | 100(3) | 95(3) | 98(3) | -17(2) | -23(2) | 26(2) |
| C(4A) | 88(2) | 54(2) | 42(2) | -4(1) | 8(2) | -9(2) |
| C(6A) | 118(3) | 71(2) | 50(2) | -13(2) | 6(2) | 13(2) |
| C(7A) | 64(2) | 62(2) | 47(2) | -7(1) | 7(1) | 1(2) |
| C(11A) | 66(2) | 63(2) | 44(2) | -5(1) | 4(1) | 3(2) |
| C(11B) | 73(2) | 53(2) | 41(1) | -1(1) | -1(1) | 10(2) |
| C(11C) | 83(2) | 56(2) | 41(2) | 1(1) | 4(2) | -3(2) |
| N(7) | 72(2) | 72(2) | 64(2) | -6(1) | 2(1) | -8(2) |

**TABLE 5: HYDROGEN COORDINATES ( X $10^4$) AND ISOTROPIC DISPLACEMENT PARAMETERS (Å2X $10^3$) FOR 2M_JN1_S.**

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1) | -2124 | 10933 | 3214 | 91 |
| H(2) | -3937 | 10273 | 3255 | 103 |
| H(3) | -4192 | 8757 | 3776 | 99 |
| H(4) | -2641 | 7932 | 4278 | 86 |
| H(6) | 1356 | 8402 | 4536 | 106 |
| H(8) | 3251 | 11694 | 3536 | 85 |
| H(9) | 2505 | 13012 | 2882 | 92 |
| H(10) | 550 | 13119 | 2577 | 93 |
| H(11) | -723 | 11934 | 2935 | 82 |
| H(12A) | 250 | 7223 | 4880 | 140 |
| H(12B) | -765 | 7008 | 4254 | 140 |
| H(12C) | -1050 | 7423 | 5133 | 140 |
| H(13A) | 3540 | 9596 | 3691 | 147 |
| H(13B) | 3123 | 9364 | 4595 | 147 |
| H(13C) | 3594 | 10374 | 4381 | 147 |

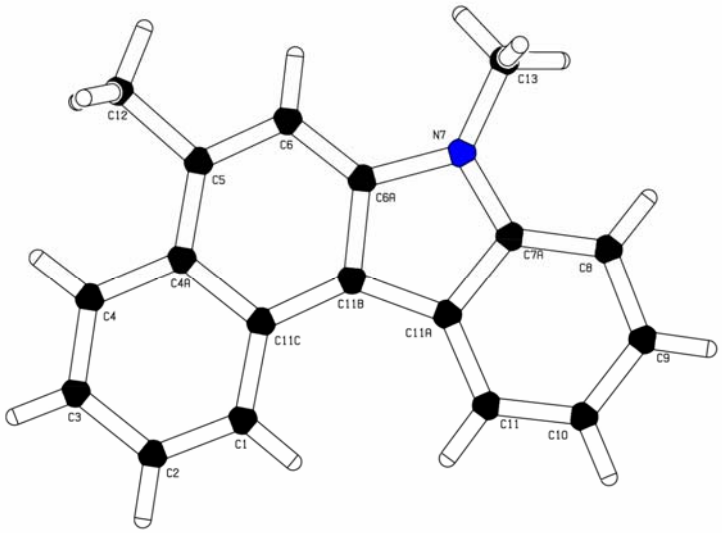
**TABLE 6. TORSION ANGLES [°] FOR 2M_JN1_S.**

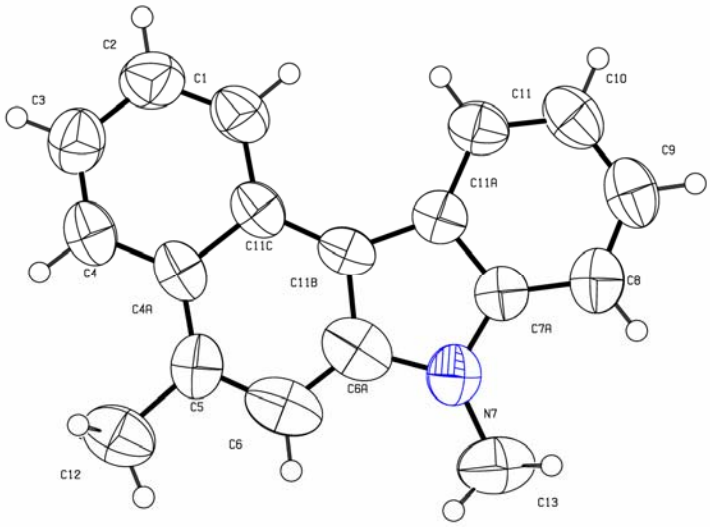
| | | | |
|---|---|---|---|
| C(11C)-C(1)-C(2)-C(3) | -0.2(6) | C(3)-C(4)-C(4A)-C(5) | -179.1(3) |
| C(1)-C(2)-C(3)-C(4) | 0.7(6) | C(3)-C(4)-C(4A)-C(11C) | 0.5(5) |
| C(2)-C(3)-C(4)-C(4A) | -0.9(6) | C(5)-C(6)-C(6A)-C(11B) | -0.7(5) |
| C(4A)-C(5)-C(6)-C(6A) | 0.0(5) | C(5)-C(6)-C(6A)-N(7) | -179.8(3) |
| C(12)-C(5)-C(6)-C(6A) | 179.5(3) | C(9)-C(8)-C(7A)-N(7) | 177.3(3) |
| C(7A)-C(8)-C(9)-C(10) | 0.8(5) | C(9)-C(8)-C(7A)-C(11A) | -1.6(5) |
| C(8)-C(9)-C(10)-C(11) | 0.7(5) | C(10)-C(11)-C(11A)-C(7A) | 0.4(4) |
| C(9)-C(10)-C(11)-C(11A) | -1.3(5) | C(10)-C(11)-C(11A)-C(11B) | -178.4(3) |
| C(6)-C(5)-C(4A)-C(4) | 179.9(3) | N(7)-C(7A)-C(11A)-C(11) | -178.0(3) |
| C(12)-C(5)-C(4A)-C(4) | 0.5(5) | C(8)-C(7A)-C(11A)-C(11) | 1.0(4) |
| C(6)-C(5)-C(4A)-C(11C) | 0.3(5) | N(7)-C(7A)-C(11A)-C(11B) | 1.1(3) |
| C(12)-C(5)-C(4A)-C(11C) | -179.2(3) | C(8)-C(7A)-C(11A)-C(11B) | -179.9(3) |

| | | | |
|---|---|---|---|
| C(11)-C(11A)-C(11B)-C(11C) | -1.8(6) | C(6A)-C(11B)-C(11C)-C(4A) | -0.7(4) |
| C(7A)-C(11A)-C(11B)-C(11C) | 179.3(3) | C(5)-C(4A)-C(11C)-C(1) | 179.7(3) |
| C(11)-C(11A)-C(11B)-C(6A) | 178.0(3) | C(4)-C(4A)-C(11C)-C(1) | 0.0(4) |
| C(7A)-C(11A)-C(11B)-C(6A) | -1.0(3) | C(5)-C(4A)-C(11C)-C(11B) | 0.1(4) |
| C(6)-C(6A)-C(11B)-C(11C) | 1.1(5) | C(4)-C(4A)-C(11C)-C(11B) | -179.6(3) |
| N(7)-C(6A)-C(11B)-C(11C) | -179.6(3) | C(8)-C(7A)-N(7)-C(13) | -1.9(5) |
| C(6)-C(6A)-C(11B)-C(11A) | -178.7(3) | C(11A)-C(7A)-N(7)-C(13) | 177.1(3) |
| N(7)-C(6A)-C(11B)-C(11A) | 0.6(3) | C(8)-C(7A)-N(7)-C(6A) | -179.7(3) |
| C(2)-C(1)-C(11C)-C(11B) | 179.3(3) | C(11A)-C(7A)-N(7)-C(6A) | -0.7(3) |
| C(2)-C(1)-C(11C)-C(4A) | -0.2(5) | C(6)-C(6A)-N(7)-C(7A) | 179.3(3) |
| C(11A)-C(11B)-C(11C)-C(1) | -0.5(6) | C(11B)-C(6A)-N(7)-C(7A) | 0.1(4) |
| C(6A)-C(11B)-C(11C)-C(1) | 179.7(3) | C(6)-C(6A)-N(7)-C(13) | 1.7(6) |
| C(11A)-C(11B)-C(11C)-C(4A) | 179.0(3) | C(11B)-C(6A)-N(7)-C(13) | -177.6(3) |

Symmetry transformations used to generate equivalent atoms:

**DIAGRAMS:**


C13
C12
C6
N7
C5
C6A
C7A
C8
C4A
C4
C11B
C11C
C11A
C9
C3
C11
C10
C1
C2


C2
C1
C3
C11
C10
C9
C11A
C11C
C4
C11B
C8
C4A
C7A
C6A
C5
N7
C6
C12
C13