Electronic Supplementary Information

**Crystal structure and X-ray powder diffraction data for two solid state forms of topiroxostat**

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TABLE SI X-ray crystal structural data for TOPI-II and TOPI-H2O.

|  |  |  |
| --- | --- | --- |
| System | TOPI-IIMonoclinic | TOPI-H2OTriclinic |
| Chemical Formula | C13H8N6 | C13H8N6‧H2O |
| Formula weight | 248.25 | 266.27 |
| Space group | *P*21/*c* | *P-1* |
| Temperature (K) | 293 | 293 |
| Unit-cell parameters (Å, °) | a = 7.346(2) | *a* = 7.418 (6) |
| b = 12.955(2) | *b* = 8.532(8) |
| *c* = 12.130(7) | *c* = 11.183(9) |
| α = 90 | α = 74.807(1) |
| β = 96.91(6) | β = 81.129(0) |
| *γ* = 90 | *γ* = 66.32(1) |
| Vol (Å3) | 1146.1(3) | 624.7(3) |
| *Z*  | 4 | 2 |
| *D*cal (g cm−3) | 1.439 | 1.415 |
| *μ* (mm−1) | 0.095 | 0.098 |
| F(000) | 512 | 276 |
| θ range for data collection (°) | 2.793-27.269 | 2.673-27.121 |
| Index ranges | −9 ≤ h ≤ 9, −13 ≤ k ≤ 16, −15 ≤ l ≤ 15 | −9 ≤ h ≤ 9, −10 ≤ k ≤ 10, −14 ≤ l ≤ 13 |
| Reflection collected/ Independent | 11200/2552（Rint = 0.0473） | 12882/2755（Rint = 0.0239） |
| Data/restraints/parameters | 2552/0/176 | 2755/0/184 |
| Goodness-of-fit (S)b on F2 | 1.192 | 1.060 |
| Final R indexes [I≥2σ(I)] | R1 = 0.0757wR2 = 0.2414 | R1 = 0.0379wR2 = 0.1121 |
| Residual density max / min / (e. Å-3) | 0.0331/-0.341 | 0.202/-0.202 |

TABLE SII Fractional atomic coordinates (×104) and equivalent isotropic displacement parameters (Å2×103) for TOPI-II. Ueq is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Atom | x | y | z | U(eq) |
| N5 | 7124(4) | 5967(2) | 4582(2) | 33.8(6) |
| N6 | 9846(4) | 3405(2) | 7540(2) | 40.5(7) |
| N4 | 8511(4) | 7023(2) | 5815(2) | 39.0(7) |
| N3 | 7735(4) | 7646(2) | 4984(2) | 39.7(7) |
| N2 | 3822(5) | 7898(2) | 1218(2) | 51.3(8) |
| C8 | 8112(4) | 6039(2) | 5568(2) | 32.8(7) |
| C4 | 5877(4) | 7289(2) | 3211(2) | 33.7(7) |
| C2 | 4233(5) | 6914(3) | 1445(3) | 38.8(8) |
| C9 | 8710(4) | 5149(2) | 6276(2) | 32.8(7) |
| C10 | 8290(4) | 4160(2) | 5890(3) | 36.7(7) |
| C3 | 5241(5) | 6576(3) | 2409(3) | 38.9(8) |
| C7 | 6921(4) | 6964(2) | 4260(2) | 35.4(7) |
| C11 | 8886(5) | 3320(3) | 6543(3) | 39.8(8) |
| C13 | 9709(5) | 5242(3) | 7320(3) | 42.9(8) |
| C5 | 5487(5) | 8331(3) | 2982(3) | 46.4(9) |
| C12 | 10242(5) | 4357(3) | 7912(3) | 46.6(9) |
| C1 | 3499(6) | 6198(3) | 601(3) | 52.6(10) |
| C6 | 4473(6) | 8575(3) | 1986(3) | 57.0(11) |

TABLE SIII Fractional atomic coordinates (×104) and equivalent isotropic displacement parameters (Å2×103) for TOPI-H2O. Ueq is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Atom | x | y | z | U(eq) |
| O1 | 2556.1(14) | 5598.2(12) | 1093.3(8) | 49.4(3) |
| N5 | 5475.7(15) | 2037.6(12) | 5034.1(9) | 37.6(2) |
| N3 | 2853.8(15) | 4450.9(13) | 4284.2(9) | 40.5(3) |
| N4 | 3866.5(15) | 3618.4(13) | 3368.7(9) | 39.1(2) |
| N2 | 2316.4(16) | 4647.8(14) | 8848.8(9) | 45.2(3) |
| N6 | 9638.5(17) | -1355.8(14) | 1763.5(11) | 49.4(3) |
| C4 | 3324.1(17) | 3856.5(15) | 6497.9(10) | 34.4(3) |
| C7 | 3878.2(17) | 3446.2(14) | 5264.5(10) | 34.3(3) |
| C8 | 5416.7(17) | 2192.0(14) | 3827.0(10) | 34.2(3) |
| C2 | 1258.0(18) | 5661.6(15) | 7863.6(11) | 37.6(3) |
| C3 | 1682.1(17) | 5334.3(15) | 6686.0(11) | 37.7(3) |
| C9 | 6849.7(17) | 990.0(14) | 3095.1(10) | 35.4(3) |
| C5 | 4419.5(19) | 2778.0(16) | 7505.4(11) | 41.3(3) |
| N1 | -1774(2) | 8375.6(17) | 8295.8(14) | 64.3(4) |
| C13 | 6713.6(19) | 1208.5(17) | 1834.3(11) | 44.5(3) |
| C10 | 8428(2) | -412.8(16) | 3667.4(12) | 46.1(3) |
| C12 | 8124(2) | 6.4(18) | 1217.0(12) | 49.2(3) |
| C1 | -439(2) | 7183.2(17) | 8106.8(12) | 45.4(3) |
| C6 | 3857(2) | 3230.5(18) | 8647.9(12) | 48.9(3) |
| C11 | 9768(2) | -1529.0(17) | 2967.6(13) | 52.0(3) |
| N6 | 9638.5(17) | -1355.8(14) | 1763.5(11) | 49.4(3) |
| C4 | 3324.1(17) | 3856.5(15) | 6497.9(10) | 34.4(3) |