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2-Aminopyrimidinium Decavanadate: Experimental and Theoretical Characterization, Molecular Docking, and Potential Antineoplastic Activity

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Table S1. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **Compound 1**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1A	5297(3)	-2(3)	6515(2)	24.7(6)
C2A	7590(3)	330(3)	6297(3)	34.4(7)
C3A	7392(4)	-759(3)	5332(3)	37.5(8)
C4A	6077(3)	-1456(3)	4991(3)	32.4(7)
N1A	4280(3)	371(3)	7077(2)	33.2(6)
N2A	6592(3)	709(2)	6893(2)	30.2(6)
N3A	5037(3)	-1061(2)	5575(2)	26.3(5)
C1B	13668(3)	6805(3)	10280(2)	29.1(6)
C2B	16004(3)	6887(3)	10264(3)	36.2(7)
C3B	15809(4)	5965(3)	9193(3)	35.9(7)
C4B	14464(4)	5506(3)	8677(3)	32.4(7)
N1B	12627(3)	7177(3)	10803(3)	46.5(8)
N2B	14992(3)	7312(3)	10807(2)	32.4(6)
N3B	13409(3)	5936(2)	9219(2)	30.3(6)
C1C	5475(3)	1560(3)	1611(2)	23.2(6)
C2C	3141(3)	1372(3)	1693(3)	33.9(7)
C3C	3360(3)	2370(3)	2714(3)	31.1(7)
C4C	4716(3)	2954(3)	3144(3)	27.6(6)
N1C	6513(3)	1155(3)	1076(2)	36.1(7)
N2C	4159(3)	956(3)	1130(2)	30.5(6)
N3C	5777(2)	2550(2)	2605.5(19)	22.6(5)
O1	8477.6(19)	5610.9(18)	7484.3(15)	22.2(4)
O2	6244(2)	3651(2)	6907.2(18)	32.0(5)
O3	7469.6(19)	2519.9(18)	5129.4(16)	22.0(4)
O4	8566(2)	1083.4(19)	3394.4(18)	29.6(5)
O5	10083(2)	2093.7(18)	5453.5(17)	24.3(4)
O6	11573(3)	2834(2)	7553(2)	39.7(6)
O7	12230.6(19)	3987.7(19)	6017.7(16)	22.2(4)
O8	7077.4(18)	4875.6(18)	5442.9(15)	20.3(4)
O9	11092(2)	5191.2(19)	7773.4(15)	23.9(4)
O10	8275.1(18)	3598.6(17)	3654.2(14)	17.6(4)
O11	10593(2)	7588(2)	8265.4(16)	30.4(5)
O12	8926(2)	3283(2)	7194.9(16)	26.0(4)
O13	9311.7(18)	6808.4(17)	6067.0(15)	17.7(4)
O14	9655.0(18)	4442.2(17)	5716.0(14)	16.7(4)
V1	9055.4(5)	2430.0(4)	4428.6(4)	18.89(11)
V2	7681.5(5)	3917.4(5)	6468.4(4)	21.63(11)
V3	10689.7(5)	3476.0(5)	6853.7(4)	24.46(12)
V4	8412.2(4)	5313.1(4)	4843.2(3)	16.14(10)
V5	10113.1(5)	6232.1(4)	7245.6(4)	19.20(11)

Atom	*x*	*y*	*z*	U(eq)
O1W	9553(5)	6138(7)	9966(4)	180(3)
O2W	9810(20)	177(19)	10187(16)	180(6)
O3W	10485(10)	958(9)	8635(8)	257(4)

Table S2. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **Compound 1**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1A	23.4(14)	23.4(14)	25.5(14)	10.4(11)	-1.6(11)	-1.9(11)
C2A	20.2(15)	30.9(16)	46.8(19)	11.0(14)	3.5(13)	-3.5(12)
C3A	29.2(17)	36.0(18)	44.9(19)	9.4(15)	12.9(14)	7.8(14)
C4A	34.9(17)	23.4(15)	34.0(16)	4.5(13)	4.0(13)	5.8(13)
N1A	23.2(13)	36.5(15)	30.1(13)	2.9(11)	4.0(10)	-2.8(11)
N2A	22.5(13)	27.3(13)	33.2(14)	4.9(11)	1.5(10)	-2.6(10)
N3A	22.4(12)	21.8(12)	30.3(13)	7.4(10)	-1.5(10)	-1.9(9)
C1B	26.3(15)	31.8(16)	25.1(14)	7.9(12)	-0.3(12)	0.3(12)
C2B	22.6(15)	47(2)	34.9(17)	12.7(15)	-1.7(13)	3.1(14)
C3B	32.1(17)	43.4(19)	32.2(17)	11.3(15)	6.0(13)	12.4(14)
C4B	39.8(18)	30.9(16)	23.0(14)	6.3(12)	0.9(13)	7.0(14)
N1B	25.9(15)	61(2)	36.2(16)	0.3(14)	2.7(12)	1.9(14)
N2B	24.5(13)	39.2(15)	24.1(12)	4.0(11)	-4.2(10)	-0.1(11)
N3B	25.8(13)	31.7(14)	25.5(12)	5.4(11)	-6.9(10)	-0.1(11)
C1C	19.4(13)	23.8(14)	21.5(13)	4.0(11)	-0.2(10)	1.5(11)
C2C	18.0(14)	41.8(18)	37.1(17)	9.3(14)	0.9(12)	5.6(13)
C3C	22.0(15)	37.5(17)	34.0(16)	9.8(14)	8.1(12)	12.1(13)
C4C	27.9(15)	26.4(15)	25.9(14)	5.7(12)	1.8(12)	7.7(12)
N1C	17.2(12)	41.9(16)	30.6(14)	-7.4(12)	2.1(10)	-1.3(11)
N2C	17.3(12)	36.6(14)	26.3(12)	0.7(11)	-2.3(10)	-0.2(10)
N3C	17.5(11)	22.5(11)	21.7(11)	2.8(9)	-2.2(9)	1.0(9)
O1	17.2(9)	25.1(10)	18.2(9)	1.3(8)	4.3(7)	0.3(8)
O2	23.1(11)	36.2(12)	31.7(11)	6.7(9)	11.1(9)	-1.9(9)
O3	16.4(9)	20.4(9)	23.3(9)	2.0(8)	4.2(7)	-2.1(7)
O4	27.1(11)	20.6(10)	30.1(11)	-2.5(8)	5.4(9)	-2.0(8)
O5	20.8(10)	22.1(10)	29.2(10)	7.8(8)	3.7(8)	5.3(8)
O6	37.8(13)	48.8(15)	38.6(13)	23.6(11)	-1.0(10)	12.3(11)
O7	14.8(9)	26.6(10)	23.3(9)	7.1(8)	-0.5(7)	4.9(8)
O8	12.8(9)	21.8(9)	20.1(9)	0.5(7)	3.0(7)	0.4(7)
O9	16.3(9)	32.7(11)	18.0(9)	5.6(8)	-1.7(7)	1.2(8)
O10	12.5(8)	19.0(9)	14.9(8)	-0.3(7)	0.7(7)	-0.2(7)
O11	25.7(11)	32.1(11)	19.3(9)	-4.7(8)	3.1(8)	-3.9(9)
O12	24.3(10)	29.4(11)	22.5(10)	9.0(8)	4.0(8)	-0.1(8)
O13	12.1(8)	18.7(9)	17.2(8)	0.2(7)	2.0(7)	2.4(7)
O14	13.1(8)	18.4(9)	15.1(8)	1.8(7)	2.1(7)	1.9(7)
V1	14.9(2)	16.5(2)	20.1(2)	1.27(17)	2.51(17)	0.07(16)
V2	16.9(2)	23.5(2)	20.0(2)	3.17(18)	5.31(17)	-0.75(18)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
V3	20.8(2)	29.8(3)	22.1(2)	9.9(2)	0.31(18)	3.06(19)
V4	9.27(19)	18.8(2)	15.7(2)	1.16(16)	0.67(15)	1.43(16)
V5	14.4(2)	22.6(2)	13.3(2)	-0.92(17)	1.38(16)	-0.47(17)
O1W	73(3)	401(10)	60(3)	99(4)	7(2)	-20(4)
O2W	125(11)	143(13)	150(13)	-99(9)	-23(9)	58(8)
O3W	240(10)	277(11)	276(11)	139(10)	64(8)	-1(8)

Table S3. Bond Lengths for **Compound 1**.[a]

Atoms	Length/Å	Atoms	Length/Å
C1A-N1A	1.316(4)	O6-V3	1.595(2)
C1A-N2A	1.353(4)	O7-V3	2.069(2)
C1A-N3A	1.350(4)	O7-V4[a]	1.686(2)
C2A-C3A	1.390(5)	O8-V2	2.064(2)
C2A-N2A	1.324(4)	O8-V4	1.6838(19)
C3A-C4A	1.361(5)	O9-V3	1.855(2)
C4A-N3A	1.356(4)	O9-V5	1.866(2)
C1B-N1B	1.311(4)	O10-V1	2.084(2)
C1B-N2B	1.353(4)	O10-V4	1.9903(19)
C1B-N3B	1.353(4)	O10-V5(i)	2.0719(19)
C2B-C3B	1.387(5)	O11-V5	1.611(2)
C2B-N2B	1.315(4)	O12-V2	1.827(2)
C3B-C4B	1.361(5)	O12-V3	1.826(2)
C4B-N3B	1.351(4)	O13-V1(i)	1.979(2)
C1C-N1C	1.325(4)	O13-V4	1.9002(18)
C1C-N2C	1.351(4)	O13-V5	1.979(2)
C1C-N3C	1.352(3)	O14-V1	2.2633(19)
C2C-C3C	1.380(4)	O14-V2	2.3403(19)
C2C-N2C	1.329(4)	O14-V3	2.336(2)
C3C-C4C	1.369(4)	O14-V4(i)	2.106(2)
C4C-N3C	1.347(4)	O14-V4	2.1248(19)
O1-V2	1.914(2)	O14-V5	2.2378(18)
O1-V5	1.760(2)	V1-V3	3.1067(12)
O2-V2	1.596(2)	V2-V3	3.0701(16)
O3-V1	1.866(2)	V2-V4	3.1042(11)
O3-V2	1.8631(19)	V2-V5	3.0988(12)
O4-V1	1.613(2)	V3-V4(i)	3.0862(11)
O5-V1	1.754(2)	V3-V5	3.1182(15)
O5-V3	1.908(2)	V4-V5	3.1154(12)

[a] Symmetry operation: (i) = 2-*x*, 1-*y*, 1-*z*.

Table S4. Bond Angles for **Compound 1**.[a]

Atoms	Angle/°	Atoms	Angle/°
N1A-C1A-N2A	118.5(3)	O5-V3-V4(i)	77.72(7)

Atoms	Angle/°	Atoms	Angle/°
N1A-C1A-N3A	120.2(3)	O5-V3-V5	122.33(7)
N3A-C1A-N2A	121.3(3)	O6-V3-O5	102.04(12)
N2A-C2A-C3A	124.1(3)	O6-V3-O7	98.64(11)
C4A-C3A-C2A	116.6(3)	O6-V3-O9	102.27(12)
N3A-C4A-C3A	120.0(3)	O6-V3-O12	105.64(12)
C2A-N2A-C1A	117.3(3)	O6-V3-O14	172.46(10)
C1A-N3A-C4A	120.7(3)	O6-V3-V1	132.53(10)
N1B-C1B-N2B	119.2(3)	O6-V3-V2	138.45(10)
N1B-C1B-N3B	119.9(3)	O6-V3-V4(i)	129.49(10)
N2B-C1B-N3B	120.9(3)	O6-V3-V5	135.36(10)
N2B-C2B-C3B	124.7(3)	O7-V3-O14	73.85(8)
C4B-C3B-C2B	116.3(3)	O7-V3-V1	80.26(6)
N3B-C4B-C3B	119.9(3)	O7-V3-V2	122.84(6)
C2B-N2B-C1B	117.2(3)	O7-V3-V4(i)	30.85(5)
C4B-N3B-C1B	120.9(3)	O7-V3-V5	83.26(6)
N1C-C1C-N2C	118.0(3)	O9-V3-O5	154.01(9)
N1C-C1C-N3C	118.8(3)	O9-V3-O7	84.30(9)
N2C-C1C-N3C	123.1(3)	O9-V3-O14	78.01(8)
N2C-C2C-C3C	123.8(3)	O9-V3-V1	124.53(7)
C4C-C3C-C2C	116.5(3)	O9-V3-V2	85.60(6)
N3C-C4C-C3C	121.4(3)	O9-V3-V4(i)	79.82(7)
C2C-N2C-C1C	116.7(3)	O9-V3-V5	33.20(6)
C4C-N3C-C1C	118.5(2)	O12-V3-O5	89.57(9)
V5-O1-V2	114.95(10)	O12-V3-O7	155.61(9)
V2-O3-V1	113.78(10)	O12-V3-O9	92.62(9)
V1-O5-V3	116.00(11)	O12-V3-O14	81.84(8)
V4(i)-O7-V3	110.14(10)	O12-V3-V1	81.69(7)
V4-O8-V2	111.43(10)	O12-V3-V2	32.82(7)
V3-O9-V5	113.83(10)	O12-V3-V4(i)	124.80(7)
V4-O10-V1	106.92(9)	O12-V3-V5	81.11(7)
V4-O10-V5(i)	106.04(8)	O14-V3-V1	46.53(5)
V5[a]-O10-V1	98.07(8)	O14-V3-V2	49.02(4)
V3-O12-V2	114.39(11)	O14-V3-V4(i)	43.00(5)
V4-O13-V1(i)	107.29(9)	O14-V3-V5	45.71(5)
V4-O13-V5	106.85(9)	V1-V3-V5	91.93(2)
V5-O13-V1(i)	104.91(9)	V2-V3-V1	60.75(2)
V1-O14-V2	85.44(6)	V2-V3-V4(i)	91.99(3)
V1-O14-V3	84.96(7)	V2-V3-V5	60.093(16)
V3-O14-V2	82.07(7)	V4(i)-V3-V1	60.60(3)
V4-O14-V1	96.45(7)	V4(i)-V3-V5	63.08(2)
V4(i)-O14-V1	91.23(7)	O7(i)-V4-O10	95.75(9)
V4(i)-O14-V2	169.61(10)	O7(i)-V4-O13	98.96(10)
V4-O14-V2	87.95(7)	O7(i)-V4-O14(i)	88.16(9)
V4(i)-O14-V3	87.85(7)	O7(i)-V4-O14	165.77(8)

Atoms	Angle/°	Atoms	Angle/°
V4-O14-V3	169.78(9)	O7(i)-V4-V2	144.98(7)
V4(i)-O14-V4	102.21(8)	O7(i)-V4-V3(i)	39.00(7)
V4(i)-O14-V5	96.64(7)	O7(i)-V4-V5	136.37(7)
V4-O14-V5	91.10(7)	O8-V4-O7(i)	106.82(10)
V5-O14-V1	167.72(9)	O8-V4-O10	95.42(8)
V5-O14-V2	85.17(6)	O8-V4-O13	98.48(9)
V5-O14-V3	85.92(7)	O8-V4-O14(i)	164.76(9)
O3-V1-O10	86.43(8)	O8-V4-O14	87.13(9)
O3-V1-O13(i)	153.14(8)	O8-V4-V2	38.24(7)
O3-V1-O14	80.41(7)	O8-V4-V3(i)	145.77(7)
O3-V1-V3	84.81(7)	O8-V4-V5	84.53(7)
O4-V1-O3	100.61(10)	O10-V4-O14	79.74(8)
O4-V1-O5	105.69(11)	O10-V4-O14(i)	79.90(7)
O4-V1-O10	97.82(10)	O10-V4-V2	87.79(7)
O4-V1-O13(i)	101.14(9)	O10-V4-V3(i)	88.37(6)
O4-V1-O14	172.38(10)	O10-V4-V5	125.64(6)
O4-V1-V3	138.98(9)	O13-V4-O10	155.87(8)
O5-V1-O3	95.59(10)	O13-V4-O14(i)	81.56(7)
O5-V1-O10	155.56(8)	O13-V4-O14	81.35(8)
O5-V1-O13(i)	93.52(9)	O13-V4-V2	91.00(7)
O5-V1-O14	81.65(8)	O13-V4-V3(i)	91.11(7)
O5-V1-V3	33.51(7)	O13-V4-V5	37.44(6)
O10-V1-O14	74.66(7)	O14(i)-V4-O14	77.79(8)
O10-V1-V3	123.17(5)	O14(i)-V4-V2	126.64(5)
O13(i)-V1-O10	75.16(8)	O14-V4-V2	48.89(5)
O13(i)-V1-O14	75.99(7)	O14(i)-V4-V3(i)	49.15(5)
O13(i)-V1-V3	89.04(6)	O14-V4-V3(i)	126.92(6)
O14-V1-V3	48.51(5)	O14-V4-V5	45.90(5)
O1-V2-O8	82.86(9)	O14(i)-V4-V5	86.49(6)
O1-V2-O14	76.73(7)	V2-V4-V5	59.77(3)
O1-V2-V3	82.42(6)	V3(i)-V4-V2	174.85(2)
O1-V2-V4	77.88(7)	V3(i)-V4-V5	120.33(3)
O1-V2-V5	31.00(6)	O1-V5-O9	95.07(10)
O2-V2-O1	102.30(10)	O1-V5-O10[a]	156.99(8)
O2-V2-O3	101.66(10)	O1-V5-O13	94.18(9)
O2-V2-O8	99.78(10)	O1-V5-O14	82.54(8)
O2-V2-O12	105.00(11)	O1-V5-V2	34.06(6)
O2-V2-O14	173.26(10)	O1-V5-V3	83.30(7)
O2-V2-V3	137.79(9)	O1-V5-V4	79.50(7)
O2-V2-V4	130.11(9)	O9-V5-O10(i)	86.88(9)
O2-V2-V5	133.30(8)	O9-V5-O13	154.08(8)
O3-V2-O1	154.39(8)	O9-V5-O14	80.41(8)
O3-V2-O8	84.28(9)	O9-V5-V2	84.58(7)
O3-V2-O14	78.42(7)	O9-V5-V3	32.97(6)

Atoms	Angle/°	Atoms	Angle/°
O3-V2-V3	85.93(6)	O9-V5-V4	123.39(6)
O3-V2-V4	79.84(7)	O10(i)-V5-O14	75.17(7)
O3-V2-V5	124.42(6)	O10(i)-V5-V2	123.98(5)
O8-V2-O14	73.49(7)	O10(i)-V5-V3	86.10(6)
O8-V2-V3	122.36(5)	O10(i)-V5-V4	80.33(6)
O8-V2-V4	30.33(5)	O11-V5-O1	104.59(10)
O8-V2-V5	79.54(6)	O11-V5-O9	100.90(11)
O12-V2-O1	89.37(9)	O11-V5-O10(i)	97.51(9)
O12-V2-O3	93.09(9)	O11-V5-O13	100.10(11)
O12-V2-O8	155.08(8)	O11-V5-O14	172.53(9)
O12-V2-O14	81.70(8)	O11-V5-V2	138.48(8)
O12-V2-V3	32.79(6)	O11-V5-V3	133.73(9)
O12-V2-V4	124.82(7)	O11-V5-V4	135.26(9)
O12-V2-V5	81.65(7)	O13-V5-O10(i)	75.44(8)
O14-V2-V3	48.91(5)	O13-V5-O14	76.86(8)
O14-V2-V4	43.16(5)	O13-V5-V2	89.70(6)
O14-V2-V5	46.02(5)	O13-V5-V3	125.12(6)
V3-V2-V4	92.05(2)	O13-V5-V4	35.72(5)
V3-V2-V5	60.72(3)	O14-V5-V2	48.81(5)
V5-V2-V4	60.30(3)	O14-V5-V3	48.36(5)
O5-V3-O7	83.12(8)	O14-V5-V4	42.99(5)
O5-V3-O14	76.68(8)	V2-V5-V3	59.19(3)
O5-V3-V1	30.49(6)	V2-V5-V4	59.937(19)
O5-V3-V2	82.30(6)	V4-V5-V3	90.93(2)

[a] Symmetry operation: (i) = 2-*x*, 1-*y*, 1-*z*.

Table S5. Torsion Angles for **Compound 1**.[a]

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C2A	C3A	C4A	N3A	1.3(5)	V2	O3	V1	V3	36.22(10)
C3A	C2A	N2A	C1A	-1.5(5)	V2	O8	V4	O7(i)	177.14(9)
C3A	C4A	N3A	C1A	-2.2(5)	V2	O8	V4	O10	79.45(10)
N1A	C1A	N2A	C2A	-178.4(3)	V2	O8	V4	O13	-80.76(10)
N1A	C1A	N3A	C4A	-179.8(3)	V2	O8	V4	O14	0.04(9)
N2A	C1A	N3A	C4A	1.3(4)	V2	O8	V4	O14(i)	8.2(4)
N2A	C2A	C3A	C4A	0.5(6)	V2	O8	V4	V3(i)	174.53(4)
N3A	C1A	N2A	C2A	0.6(4)	V2	O8	V4	V5	-45.92(8)
C2B	C3B	C4B	N3B	-1.3(5)	V2	O12	V3	O5	-76.37(12)
C3B	C2B	N2B	C1B	0.3(5)	V2	O12	V3	O6	-178.76(13)
C3B	C4B	N3B	C1B	-1.1(5)	V2	O12	V3	O7	-4.2(3)
N1B	C1B	N2B	C2B	178.2(3)	V2	O12	V3	O9	77.72(12)
N1B	C1B	N3B	C4B	-177.8(3)	V2	O12	V3	O14	0.24(10)
N2B	C1B	N3B	C4B	3.3(5)	V2	O12	V3	V1	-46.80(10)
N2B	C2B	C3B	C4B	1.7(6)	V2	O12	V3	V4(i)	-1.69(14)
N3B	C1B	N2B	C2B	-2.8(5)	V2	O12	V3	V5	46.49(9)

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C2C	C3C	C4C	N3C	-1.5(5)	V3	O5	V1	O3	-71.79(12)
C3C	C2C	N2C	C1C	0.3(5)	V3	O5	V1	O4	-174.48(11)
C3C	C4C	N3C	C1C	1.1(4)	V3	O5	V1	O10	21.9(3)
N1C	C1C	N2C	C2C	179.2(3)	V3	O5	V1	O13(i)	82.91(11)
N1C	C1C	N3C	C4C	-179.9(3)	V3	O5	V1	O14	7.63(10)
N2C	C1C	N3C	C4C	0.0(4)	V3	O9	V5	O1	69.38(11)
N2C	C2C	C3C	C4C	0.8(5)	V3	O9	V5	O10(i)	-87.63(11)
N3C	C1C	N2C	C2C	-0.8(5)	V3	O9	V5	O11	175.32(11)
V1	O3	V2	O1	26.3(3)	V3	O9	V5	O13	-41.1(2)
V1	O3	V2	O2	-174.69(12)	V3	O9	V5	O14	-12.15(10)
V1	O3	V2	O8	86.47(11)	V3	O9	V5	V2	36.94(9)
V1	O3	V2	O12	-68.67(12)	V3	O9	V5	V4	-11.37(13)
V1	O3	V2	O14	12.20(10)	V3	O12	V2	O1	-76.92(12)
V1	O3	V2	V3	-36.65(10)	V3	O12	V2	O2	-179.49(11)
V1	O3	V2	V4	56.17(9)	V3	O12	V2	O3	77.57(12)
V1	O3	V2	V5	13.32(14)	V3	O12	V2	O8	-5.5(3)
V2	O1	V5	O9	-72.51(12)	V3	O12	V2	O14	-0.24(10)
V2	O1	V5	O10(i)	21.5(3)	V3	O12	V2	V4	-2.19(14)
V2	O1	V5	O11	-175.17(12)	V3	O12	V2	V5	-46.78(9)
V2	O1	V5	O13	83.24(12)	V5	O9	V3	O5	25.0(3)
V2	O1	V5	O14	7.10(10)	V5	O9	V3	O6	-175.98(12)
V2	O1	V5	V3	-41.65(10)	V5	O9	V3	O7	86.39(11)
V2	O1	V5	V4	50.55(9)	V5	O9	V3	O12	-69.36(12)
V2	O3	V1	O4	175.14(12)	V5	O9	V3	O14	11.73(9)
V2	O3	V1	O5	67.99(12)	V5	O9	V3	V1	12.35(14)
V2	O3	V1	O10	-87.57(11)	V5	O9	V3	V2	-37.27(9)
V2	O3	V1	O13(i)	-41.3(2)	V5	O9	V3	V4(i)	55.55(9)
V2	O3	V1	O14	-12.54(10)					

[a] Symmetry operation: (i) = 2-*x*, 1-*y*, 1-*z*.

Table S6. Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for **Compound 1**.

Atom	*x*	*y*	*z*	U(eq)
H2A	8478.95	824.51	6540.71	41
H3A	8120.66	-999.06	4937.93	45
H4A	5893.17	-2203.74	4359.09	39
H1AA	4409.49	1037.89	7638.62	40
H1AB	3494.19	6.49	6893.82	40
H3AA	4209.92	-1484.59	5343.4	32
H2B	16916.53	7230.11	10623.18	43
H3B	16555.89	5675.16	8847.5	43
H4B	14270.93	4898.56	7953.1	39
H1BA	12784.5	7718.57	11550.57	56
H1BB	11946.2	6917.07	10524.57	56
H3BA	12650.98	5730.9	8900.87	36

Atom	*x*	*y*	*z*	U(eq)
H2C	2227.96	967.03	1379.4	41
H3C	2625.44	2632.78	3091.38	37
H4C	4908.73	3644.46	3822.87	33
H1CA	6329.07	577.81	468.38	43
H1CB	7329.57	1451.31	1319.88	43
H3CA	6825.79	3037.48	3039.98	27
H1WA	9746.49	6890.5	10457.75	270
H1WB	9378.19	6247.7	9348.35	270
H2WA	9847.38	-94.13	9487.59	270
H2WB	9956.58	987.37	10383.59	270
H3WA	10546.19	1637.16	8485.98	385
H3WB	10722.19	368.06	8103.98	385

Table S7. Atomic Occupancy for **Compound 1**.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
O2W	0.5	H2WA	0.5	H2WB	0.5

Thermogravimetric analysis

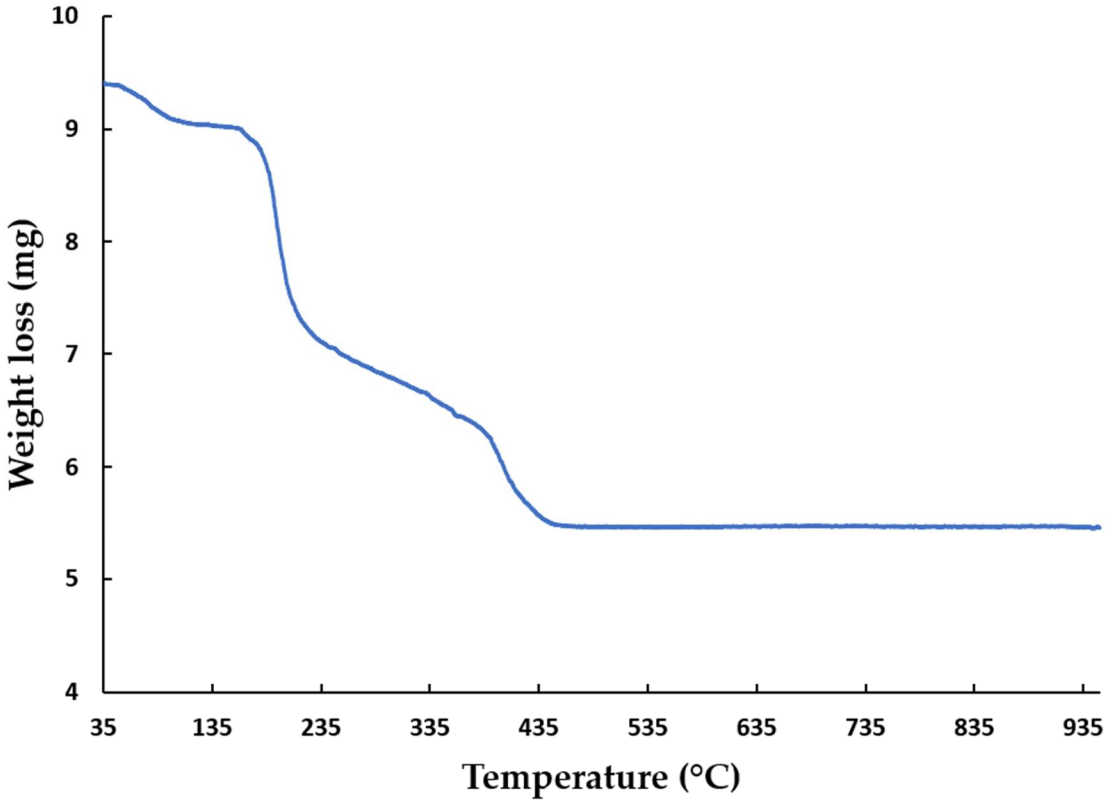

Figure S1. TG spectrum of **Compound 1** in the range of 35-950°C.