crystals

MDPI

Supplementary Material

Synthesis and Experimental-Computational Characterization of a Copper/Vanadium Compound with Potential Anticancer Activity

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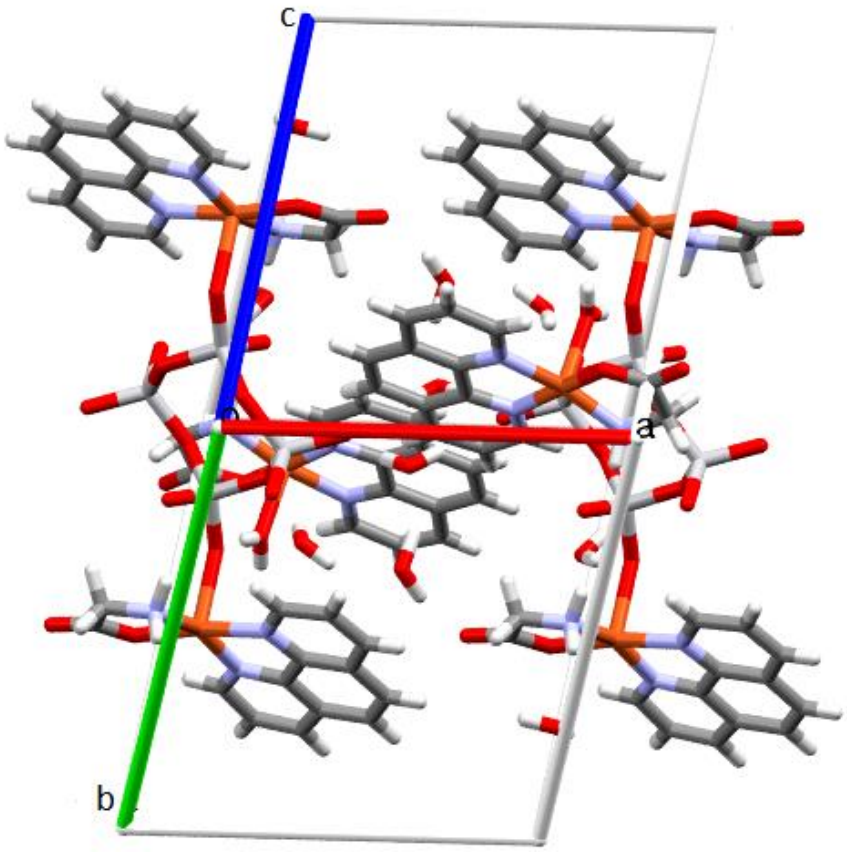

Figure 1. Packing of the unit cell of **Compound 1.**

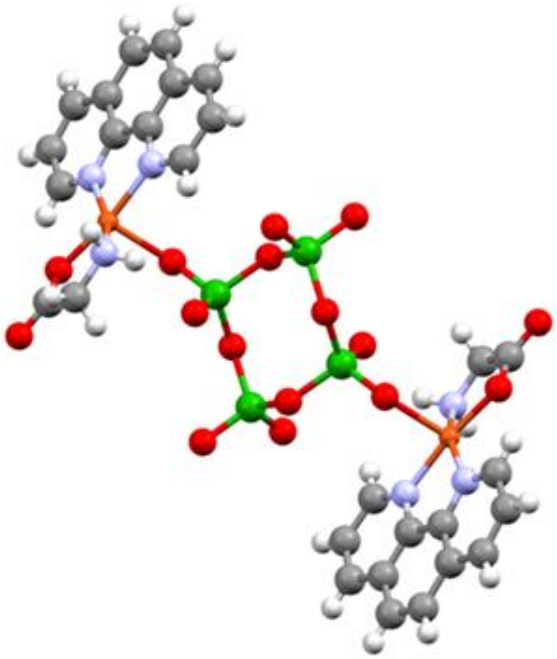

Figure 2. Ball and stick representation of the Cyclo-tetravanadate dicopper moiety of **Compound 1.**

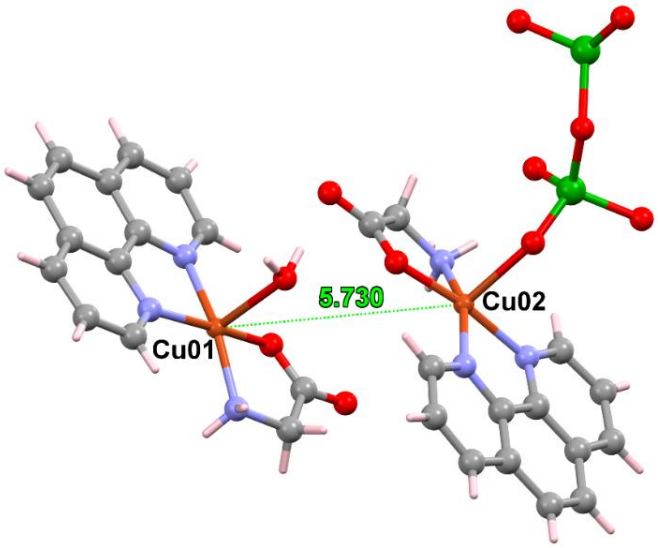

Figure S3. Copper-Copper distance Cu1---Cu2.

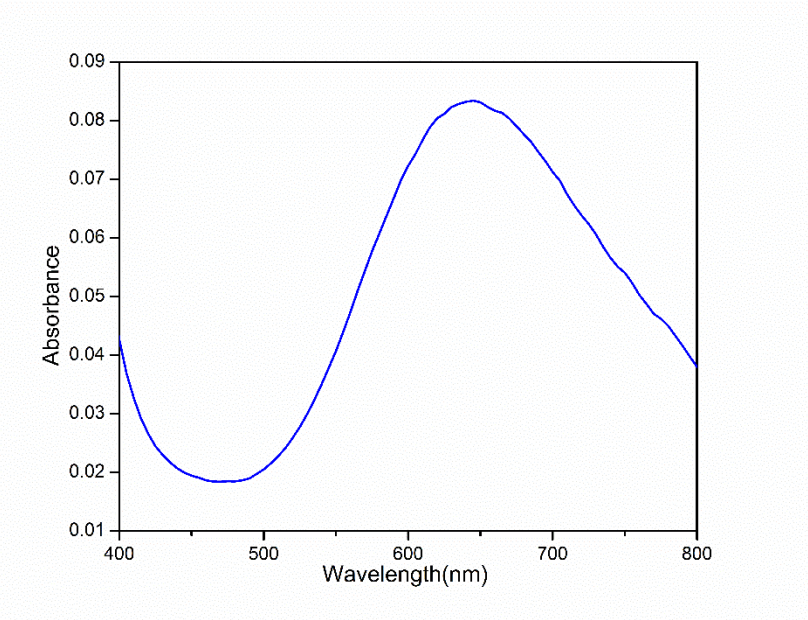

Figure 4. The visible spectrum of **Compound 1** in PBS.

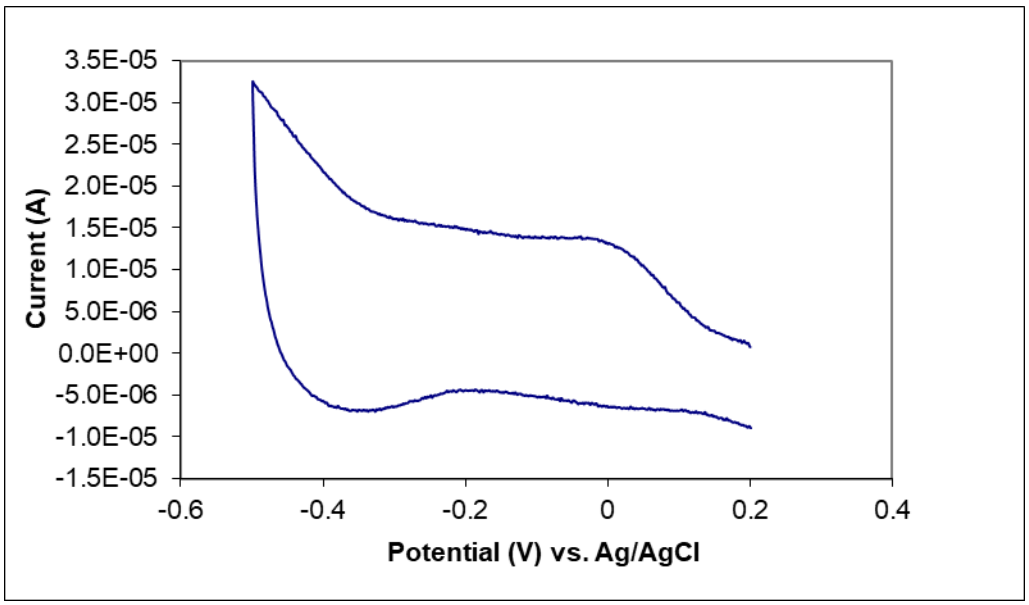

Figure 5. Cyclic voltammetry of NH_4VO_3 in phosphate buffer solution at pH 7.4, scan rate 0.5 V/s.

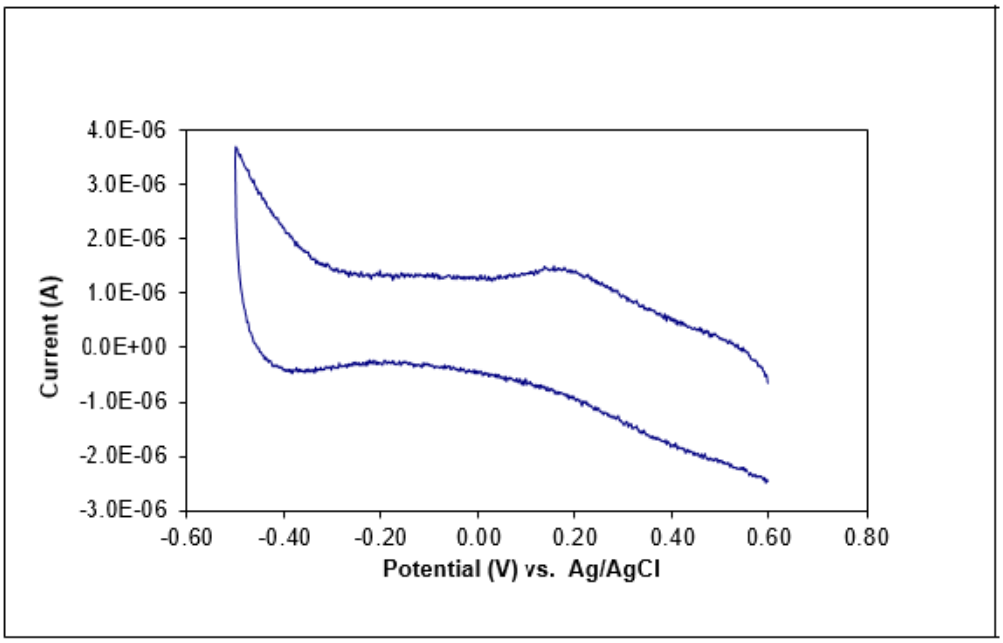

Figure 6. Cyclic voltammetry of $CuCl_2$ in phosphate buffer solution at pH 7.4, scan rate 0.1 V/s.

Table 1. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$) for Compound 1.

	x	y	z	U_{iso}*/U_{eq}
Cu2	0.19892 (3)	−0.04258 (3)	0.84002 (3)	0.03430 (9)
Cu1	0.92577 (3)	0.16576 (3)	0.67622 (3)	0.03308 (9)
V1	0.97277 (3)	0.35119 (3)	0.53147 (3)	0.02770 (9)
V2	1.17744 (3)	0.48690 (3)	0.42003 (3)	0.02986 (9)
O4	1.04723 (15)	0.35750 (14)	0.42210 (14)	0.0373 (3)
O15	1.07515 (17)	0.13990 (16)	0.67295 (17)	0.0442 (4)
N5	0.30241 (17)	−0.13297 (17)	0.80954 (15)	0.0333 (4)
O2	0.83818 (15)	0.37933 (15)	0.51131 (15)	0.0388 (3)
N2	0.80657 (19)	−0.01016 (17)	0.60011 (16)	0.0353 (4)
O1	0.92657 (16)	0.21601 (14)	0.53355 (14)	0.0375 (3)
N1	0.76305 (19)	0.17679 (18)	0.68907 (17)	0.0363 (4)
O5	1.1682 (2)	0.46206 (19)	0.29214 (18)	0.0544 (5)
N4	0.36962 (17)	0.09868 (17)	0.90687 (15)	0.0340 (4)
O7	0.11542 (18)	0.05541 (18)	0.8915 (2)	0.0565 (5)
C23	0.4642 (2)	0.0673 (2)	0.89997 (17)	0.0323 (4)
N6	0.03091 (19)	−0.18064 (19)	0.80635 (19)	0.0425 (4)
H6A	0.0129	−0.2356	0.7400	0.051*
H6B	0.0314	−0.2141	0.8536	0.051*
O3	1.07163 (18)	0.45263 (16)	0.64682 (16)	0.0472 (4)
C12	0.6855 (2)	−0.0332 (2)	0.60029 (18)	0.0351 (4)
C24	0.4281 (2)	−0.0578 (2)	0.84822 (17)	0.0324 (4)
N3	1.0438 (2)	0.3238 (2)	0.7942 (2)	0.0454 (5)

H3A	1.0353	0.3819	0.7803	0.054*
H3B	1.0254	0.3266	0.8569	0.054*
C11	0.6614 (2)	0.0672 (2)	0.64666 (18)	0.0350 (4)
C27	1.1791 (2)	0.2287 (2)	0.7333 (2)	0.0396 (5)
C7	0.5373 (2)	0.0503 (3)	0.6453 (2)	0.0416 (5)
C16	0.5203 (2)	−0.0985 (2)	0.83718 (19)	0.0379 (5)
C14	0.3514 (3)	−0.2971 (2)	0.7434 (2)	0.0456 (5)
H14	0.3224	−0.3790	0.7066	0.055*
O6	1.31462 (17)	0.50228 (19)	0.4777 (2)	0.0537 (5)
C19	0.5924 (2)	0.1509 (2)	0.93982 (19)	0.0386 (5)
O12	0.5150 (3)	0.5476 (2)	0.6438 (2)	0.0619 (5)
H12A	0.5753	0.5395	0.6195	0.093*
H12B	0.4551	0.5295	0.5916	0.093*
O16	1.28240 (19)	0.2275 (2)	0.7374 (2)	0.0554 (5)
O9	0.1777 (2)	−0.03556 (18)	0.67404 (17)	0.0559 (5)
H9A	0.1947	0.0356	0.6809	0.084*
H9B	0.1446	−0.0918	0.6126	0.084*
C22	0.3977 (2)	0.2136 (2)	0.9539 (2)	0.0427 (5)
H22	0.3327	0.2354	0.9598	0.051*
C18	0.6853 (2)	0.1074 (3)	0.9272 (2)	0.0464 (6)
H18	0.7707	0.1618	0.9530	0.056*
C13	0.2658 (2)	−0.2492 (2)	0.7582 (2)	0.0399 (5)
H13	0.1797	−0.3009	0.7309	0.048*
C26	−0.0647 (2)	−0.1354 (3)	0.8133 (3)	0.0555 (7)
H26A	−0.1192	−0.1674	0.8553	0.067*
H26B	−0.1167	−0.1632	0.7409	0.067*
C4	0.5855 (3)	−0.1503 (2)	0.5567 (2)	0.0433 (5)
C1	0.8327 (3)	−0.1010 (2)	0.5574 (2)	0.0460 (5)
H1	0.9156	−0.0852	0.5561	0.055*
C21	0.5240 (3)	0.3031 (2)	0.9952 (2)	0.0506 (6)
H21	0.5417	0.3832	1.0268	0.061*
C17	0.6511 (2)	−0.0114 (3)	0.8783 (2)	0.0455 (5)
H17	0.7134	−0.0369	0.8713	0.055*
O11	0.4805 (2)	0.4602 (3)	0.8073 (2)	0.0708 (7)
H11A	0.4698	0.4772	0.7437	0.106*
H11B	0.4219	0.3810	0.7917	0.106*
C9	0.6223 (3)	0.2630 (3)	0.7282 (3)	0.0525 (6)
H9	0.6117	0.3319	0.7553	0.063*
C28	1.1732 (3)	0.3416 (3)	0.8021 (3)	0.0539 (7)
H28A	1.2155	0.3668	0.8772	0.065*
H28B	1.2178	0.4049	0.7788	0.065*
C10	0.7435 (3)	0.2720 (2)	0.7279 (2)	0.0463 (5)
H10	0.8124	0.3475	0.7559	0.056*

O14	1.0233 (3)	0.2764 (3)	0.9999 (3)	0.0762 (7)
H14A	1.1035	0.3091	1.0147	0.114*
H14B	0.9933	0.2088	0.9467	0.114*
C3	0.6163 (3)	−0.2441 (2)	0.5136 (3)	0.0547 (7)
H3	0.5534	−0.3229	0.4846	0.066*
C8	0.5205 (3)	0.1533 (3)	0.6886 (2)	0.0507 (6)
H8	0.4402	0.1467	0.6904	0.061*
C6	0.4364 (2)	−0.0704 (3)	0.5988 (2)	0.0509 (7)
H6	0.3537	−0.0830	0.5971	0.061*
C15	0.4784 (3)	−0.2220 (3)	0.7835 (2)	0.0460 (5)
H15	0.5364	−0.2528	0.7753	0.055*
O10	0.7357 (3)	0.5978 (5)	0.8839 (3)	0.141 (2)
H10A	0.7486	0.5678	0.8227	0.211*
H10B	0.6621	0.5526	0.8849	0.211*
C20	0.6207 (2)	0.2724 (2)	0.9888 (2)	0.0471 (6)
H20	0.7043	0.3312	1.0166	0.057*
C25	−0.0041 (3)	−0.0003 (3)	0.8652 (3)	0.0610 (8)
O8	−0.0733 (2)	0.0477 (3)	0.8785 (4)	0.1127 (17)
O13	0.9412 (4)	0.4271 (4)	1.1286 (3)	0.0829 (14)
				0.789
H13A	0.9810	0.4405	1.1908	0.124*
H13B	0.9748	0.3938	1.0848	0.124*
C5	0.4595 (3)	−0.1650 (3)	0.5580 (2)	0.0516 (7)
H5	0.3926	−0.2418	0.5300	0.062*
C2	0.7388 (3)	−0.2201 (3)	0.5141 (3)	0.0561 (7)
H2	0.7598	−0.2824	0.4858	0.067*
O13A	0.945 (3)	0.4626 (19)	1.032 (2)	0.134 (11)
				0.211

Table 2. Geometric parameters (Å, º) for Compound 1.

Cu2—N5	2.0178 (19)	C23—C19	1.403 (3)
Cu2—N4	1.9990 (18)	N6—C26	1.480 (4)
Cu2—O7	1.931 (2)	C12—C11	1.427 (4)
Cu2—N6	1.990 (2)	C12—C4	1.409 (3)
Cu2—O9	2.270 (2)	C24—C16	1.403 (3)

Cu1—O15	1.9441 (18)	N3—C28	1.453 (4)
Cu1—N2	2.0127 (19)	C11—C7	1.405 (3)
Cu1—O1	2.2371 (17)	C27—O16	1.235 (3)
Cu1—N1	2.022 (2)	C27—C28	1.515 (4)
Cu1—N3	1.991 (2)	C7—C8	1.402 (4)
V1—O4	1.8067 (16)	C7—C6	1.442 (4)
V1—O2	1.8002 (17)	C16—C17	1.437 (4)
V1—O1	1.6665 (15)	C16—C15	1.403 (4)
V1—O3	1.6266 (19)	C14—C13	1.397 (4)
V2—O4	1.8166 (15)	C14—C15	1.370 (4)

V2—O2^{i}	1.8055 (17)	C19—C18	1.437 (4)
V2—O5	1.634 (2)	C19—C20	1.406 (4)
V2—O6	1.6448 (19)	C22—C21	1.407 (4)
O15—C27	1.269 (3)	C18—C17	1.359 (4)
N5—C24	1.357 (3)	C26—C25	1.510 (4)
N5—C13	1.326 (3)	C4—C3	1.396 (5)
O2—V2^{i}	1.8055 (17)	C4—C5	1.440 (4)
N2—C12	1.353 (3)	C1—C2	1.402 (4)
N2—C1	1.325 (4)	C21—C20	1.368 (5)
N1—C11	1.357 (3)	C9—C10	1.403 (4)
N1—C10	1.321 (4)	C9—C8	1.360 (5)
N4—C23	1.349 (3)	C3—C2	1.367 (5)
N4—C22	1.327 (3)	C6—C5	1.343 (5)
O7—C25	1.266 (4)	C25—O8	1.219 (5)
C23—C24	1.430 (3)	O13A—O13A^{ii}	1.80 (5)
N5—Cu2—O9	93.35 (8)	N4—C23—C19	123.0 (2)
N4—Cu2—N5	82.53 (8)	C19—C23—C24	120.3 (2)
N4—Cu2—O9	95.47 (8)	C26—N6—Cu2	107.92 (17)
O7—Cu2—N5	171.33 (9)	N2—C12—C11	117.2 (2)
O7—Cu2—N4	91.96 (8)	N2—C12—C4	122.6 (2)

O7—Cu2—N6	85.38 (9)	C4—C12—C11	120.2 (2)
O7—Cu2—O9	93.85 (10)	N5—C24—C23	116.9 (2)
N6—Cu2—N5	98.56 (9)	N5—C24—C16	122.6 (2)
N6—Cu2—N4	167.53 (9)	C16—C24—C23	120.5 (2)
N6—Cu2—O9	96.86 (9)	C28—N3—Cu1	109.80 (17)
O15—Cu1—N2	93.18 (8)	N1—C11—C12	116.7 (2)
O15—Cu1—O1	96.05 (8)	N1—C11—C7	123.0 (2)
O15—Cu1—N1	172.31 (8)	C7—C11—C12	120.3 (2)
O15—Cu1—N3	84.45 (9)	O15—C27—C28	116.9 (2)
N2—Cu1—O1	99.22 (7)	O16—C27—O15	123.5 (3)
N2—Cu1—N1	82.28 (9)	O16—C27—C28	119.5 (2)
N1—Cu1—O1	90.82 (7)	C11—C7—C6	118.3 (3)
N3—Cu1—N2	160.42 (10)	C8—C7—C11	117.0 (3)
N3—Cu1—O1	100.36 (9)	C8—C7—C6	124.6 (3)
N3—Cu1—N1	97.75 (9)	C24—C16—C17	118.3 (2)
O2—V1—O4	109.61 (8)	C15—C16—C24	117.5 (2)
O1—V1—O4	109.15 (8)	C15—C16—C17	124.1 (2)
O1—V1—O2	109.83 (8)	C15—C14—C13	119.3 (2)
O3—V1—O4	110.13 (9)	C23—C19—C18	118.3 (2)
O3—V1—O2	108.50 (10)	C23—C19—C20	117.1 (2)
O3—V1—O1	109.61 (9)	C20—C19—C18	124.6 (2)
$O2^{i}$—V2—O4	110.02 (8)	N4—C22—C21	121.3 (2)
O5—V2—O4	106.07 (10)	C17—C18—C19	121.4 (2)
O5—V2—$O2^{i}$	110.51 (10)	N5—C13—C14	122.6 (2)
O5—V2—O6	109.22 (13)	N6—C26—C25	111.8 (2)
O6—V2—O4	111.35 (10)	C12—C4—C5	118.3 (3)
O6—V2—$O2^{i}$	109.62 (10)	C3—C4—C12	117.1 (3)
V1—O4—V2	126.98 (10)	C3—C4—C5	124.6 (3)
C27—O15—Cu1	115.93 (17)	N2—C1—C2	121.9 (3)
C24—N5—Cu2	111.39 (15)	C20—C21—C22	120.1 (3)

C13—N5—Cu2	130.11 (16)	C18—C17—C16	121.2 (2)
C13—N5—C24	118.5 (2)	C8—C9—C10	119.7 (3)
V1—O2—$V2^{i}$	128.95 (10)	N3—C28—C27	111.9 (2)
C12—N2—Cu1	111.94 (16)	N1—C10—C9	122.3 (3)
C1—N2—Cu1	128.97 (18)	C2—C3—C4	120.0 (2)
C1—N2—C12	119.0 (2)	C9—C8—C7	119.6 (3)
V1—O1—Cu1	129.01 (9)	C5—C6—C7	121.4 (3)
C11—N1—Cu1	111.80 (16)	C14—C15—C16	119.5 (2)
C10—N1—Cu1	129.90 (18)	C21—C20—C19	119.3 (2)
C10—N1—C11	118.3 (2)	O7—C25—C26	117.6 (3)
C23—N4—Cu2	112.49 (15)	O8—C25—O7	124.4 (3)

C22—N4—Cu2	128.34 (17)	O8—C25—C26	118.0 (3)
C22—N4—C23	119.2 (2)	C6—C5—C4	121.4 (2)
C25—O7—Cu2	115.0 (2)	C3—C2—C1	119.5 (3)
N4—C23—C24	116.63 (19)		

Symmetry codes: (i) −x+2, −y+1, −z+1; (ii) −x+2, −y+1, −z+2