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Letter to the Editor

The space group of vanadium(V) oxide-*o*-phenanthroline (2/2)

The crystal structure of the 2/2 adduct of vanadium(V) oxide with *o*-phenanthroline, $[(C_{12}H_8N_2)_2V_4O_{10}]$, was published in the triclinic *P*-1 space group ($a = 9.782$, $b = 6.512$, $c = 19.765$ Å; $\alpha = 89.94$, $\beta = 100.66$, $\gamma = 89.86°$) by Wang and co-workers [1]; Wang with a slightly different group of co-workers simultaneously published the identical structure elsewhere [2] but without anisotropic temperature factors and hydrogen positions. There are several typographical errors in both reports; among these, the U_{23}, U_{13} and U_{12} parameters should be smaller by a factor of 10. The α and γ angles are almost 90°, and the *y*-coordinate of the V, N, C atoms, along with six of the ten O atoms, is either nearly $\frac{1}{4}$ or almost $\frac{3}{4}$. The crystal system should be monoclinic. The 4526 reflections that are calculated [3] from the published crystallographic information clearly show the presence of the two-fold screw axis as the $0\,k\,0 = 2n + 1$ reflections are systematically absent. In the $P2_1/m$ space group, the structure could be refined on the 2484 simulated unique ($R_{int} = 0.013$) reflections to $R = 0.005$ (Table 1). In the higher-symmetry setting, all but two O atoms lie on the mirror plane (Fig. 1). The structure is better regarded as a helical ribbon motif that runs along the *b*-axis of the unit cell.

Table 1
Atomic coordinates for $[(C_{12}H_8N_2)_2V_4O_{10}]$ in $P2_1/m$ ($a = 9.782$, $b = 6.512$, $c = 19.765$ Å; $\beta = 100.66°$)

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
V1a	0.5487	3/4	0.3681	V1b	0.4341	1/4	0.1582
V2a	0.3729	3/4	0.1973	V2b	0.5999	1/4	0.3241
O1a	0.2167	3/4	0.2118	O1b	0.7481	1/4	0.3001
O2a	0.4926	3/4	0.2763	O2b	0.4632	1/4	0.2506
O3a	0.4116	3/4	0.4006	O3b	0.5834	1/4	0.1374
O4a	0.5825	0.4649	0.3734	O4b	0.4013	0.5351	0.1502
N1a	0.6806	3/4	0.4697	N1b	0.3368	1/4	0.0492
N2a	0.7752	3/4	0.3515	N2b	0.1975	1/4	0.1530
C1a	0.8210	3/4	0.4735	C1b	0.1962	1/4	0.0329
C2a	0.6319	3/4	0.5283	C2b	0.4086	1/4	−0.0016
C3a	0.7198	3/4	0.5922	C3b	0.3448	1/4	−0.0707
C4a	0.8591	3/4	0.5964	C4b	0.2030	1/4	−0.0871
C5a	0.9153	3/4	0.5360	C5b	0.1250	1/4	−0.0356
C6a	1.0606	3/4	0.5355	C6b	−0.0241	1/4	−0.0475
C7a	1.1089	3/4	0.4757	C7b	−0.0946	1/4	0.0045
C8a	1.0152	3/4	0.4110	C8b	−0.0245	1/4	0.0748
C9a	1.0582	3/4	0.3467	C9b	−0.0909	1/4	0.1313
C10a	0.9609	3/4	0.2882	C10b	−0.0145	1/4	0.1965
C11a	0.8197	3/4	0.2925	C11b	0.1305	1/4	0.2050
C12a	0.8716	3/4	0.4100	C12b	0.1218	1/4	0.0886

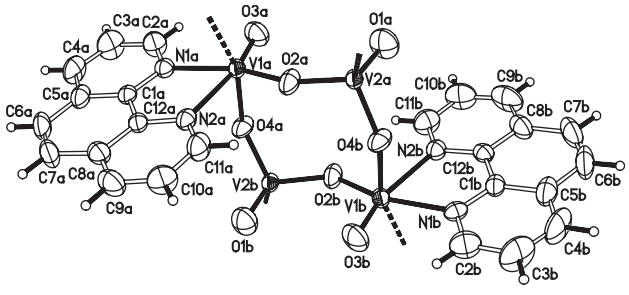

Fig. 1. ORTEP plot of $[(C_{12}H_8N_2)_2V_4O_{10}]$ at the 75% probability level.

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