## Supplementary Information

# A $d^{10}$-Cd Cluster Containing Sandwich-Type Arsenotungstate Exhibiting Fluorescent Recognition of Carcinogenic Dye in Methanol

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**Table S1** Crystallographic data and structural refinements for compound I

| | |
|---|---|
| Empirical formula | $C_{18}H_{86}As_2Cd_4N_{12}Cl_2O_{75}W_{18}$ |
| Formula weight | 5650.62 |
| Crystal system | Triclinic |
| Space group | *P–1* |
| *a* / Å | 12.5169(15) |
| *b* / Å | 12.5282(16) |
| *c* / Å | 15.952(3) |
| *α* / deg | 99.623(3) |
| *β* / deg | 98.647(3) |
| *γ* / deg | 112.828(2) |
| *V* / Å$^3$ | 2208.5(6) |
| *Z* | 1 |
| $D_c$ / g cm$^{-3}$ | 4.249 |
| *μ* / mm$^{-1}$ | 25.187 |
| *T* / K | 293(2) |
| Limiting indices | $-14 \le h \le 14$ |
| | $-14 \le k \le 14$ |
| | $-12 \le l \le 18$ |
| Measured reflections | 10995 |
| Independent reflections | 7649 |
| $R_{int}$ | 0.0939 |

| | |
|---|---|
| Data / restrains / parameters | 7649/ 262 /634 |
| GOF on $F^2$ | 0.996 |
| Final $R$ indices [$I > 2\sigma(I)$] | $R_1$ = 0.0785, $wR_2$ = 0.1726 |
| $R$ indices (all data) | $R_1$ = 0.0933 $wR_2$ = 0.1844 |

**Table S2** Selected bond length (Å) for compound I

| | | | |
|---|---|---|---|
| W(1)-O(1) | 1.747 | W(2)-O(2) | 1.754 |
| W(1)-O(10) | 1.774 | W(2)-O(11) | 1.773 |
| W(1)-O(12) | 1.924 | W(2)-O(13) | 1.943 |
| W(1)-O(30) | 1.963 | W(2)-O(12) | 1.941 |
| W(1)-O(25) | 2.020 | W(2)-O(14) | 1.999 |
| W(1)-O(31) | 2.322 | W(2)-O(31) | 2.360 |
| W(3)-O(3) | 1.715 | W(4)-O(4) | 1.711 |
| W(3)-O(25) | 1.859 | W(4)-O(20) | 1.767 |
| W(3)-O(14) | 1.884 | W(4)-O(13) | 1.887 |
| W(3)-O(19) | 1.935 | W(4)-O(17) | 1.997 |
| W(3)-O(15) | 1.937 | W(4)-O(18) | 2.002 |
| W(3)-O(31) | 2.483 | W(4)-O(32) | 2.355 |
| W(5)-O(5) | 1.710 | W(6)-O(6) | 1.728 |
| W(5)-O(18) | 1.881 | W(6)-O(22) | 1.786 |
| W(5)-O(21) | 1.888 | W(6)-O(17) | 1.873 |
| W(5)-O(15) | 1.895 | W(6)-O(28) | 1.989 |
| W(5)-O(16) | 1.959 | W(6)-O(21) | 1.995 |
| W(8)-O(8) | 1.718 | W(6)-O(32) | 2.369 |
| W(8)-O(26) | 1.805 | W(7)-O(7) | 1.711 |
| W(8)-O(29) | 1.883 | W(7)-O(27) | 1.849 |
| W(8)-O(28) | 1.900 | W(7)-O(19) | 1.898 |
| W(8)-O(23) | 1.981 | W(7)-O(16) | 1.906 |
| W(8)-O(33) | 2.332 | W(7)-O(23) | 1.908 |
| W(9)-O(9) | 1.715 | Cd(1)-O(11) | 2.221 |
| W(9)-O(24) | 1.780 | Cd(1)-O(10) | 2.243 |
| W(9)-O(30) | 1.889 | Cd(1)-O(26)#1 | 2.286 |
| W(9)-O(29) | 1.969 | Cd(1)-O(22)#1 | 2.315 |
| W(9)-O(27) | 2.051 | Cd(1)-Cl(1) | 2.512 |
| W(9)-O(33) | 2.378 | Cd(1)-O(34) | 2.510 |
| Cd(2)-O(24) | 2.165 | Cd(2)-O(34) | 2.340 |
| Cd(2)-O(20)#1 | 2.175 | As(1)-O(34) | 1.660 |
| Cd(2)-O(22)#1 | 2.254 | As(1)-O(32) | 1.673 |
| Cd(2)-O(26) | 2.290 | As(1)-O(33) | 1.690 |

| | | | |
|---|---|---|---|
| Cd(2)-O(34)#1 | 2.339 | As(1)-O(31) | 1.708 |