# Supporting Information for

# Comparisons of Zinc with Cadmium in $N_2S_2$ Coordination and as S-Bonded Adducts to Tungsten Carbonyls

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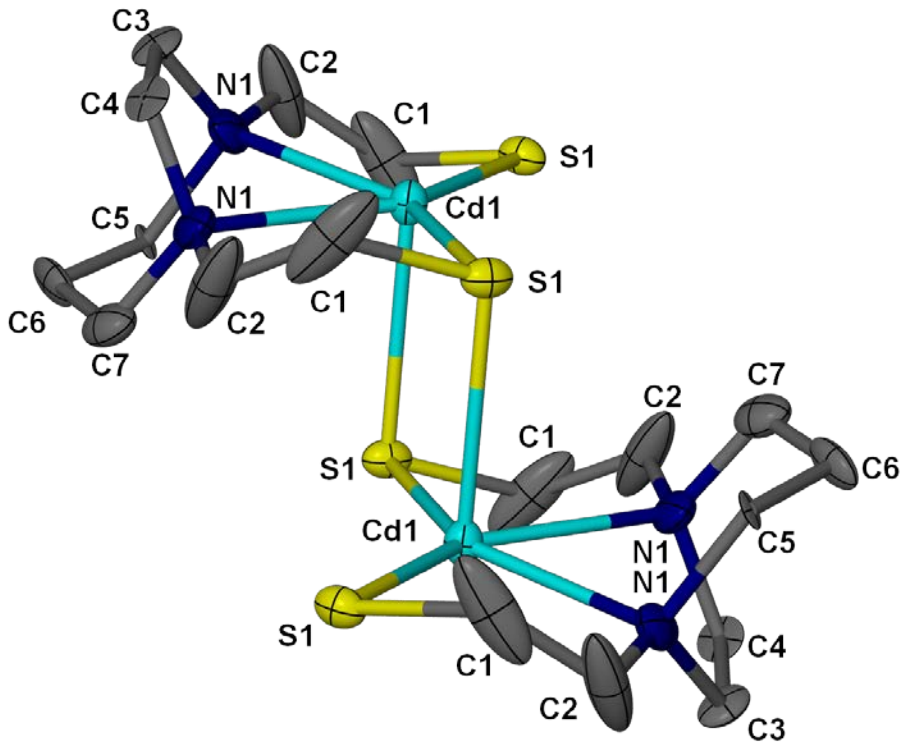


**Figure S1.** Thermal ellipsoid plot at 50% probability for **[Cd-1']x**.

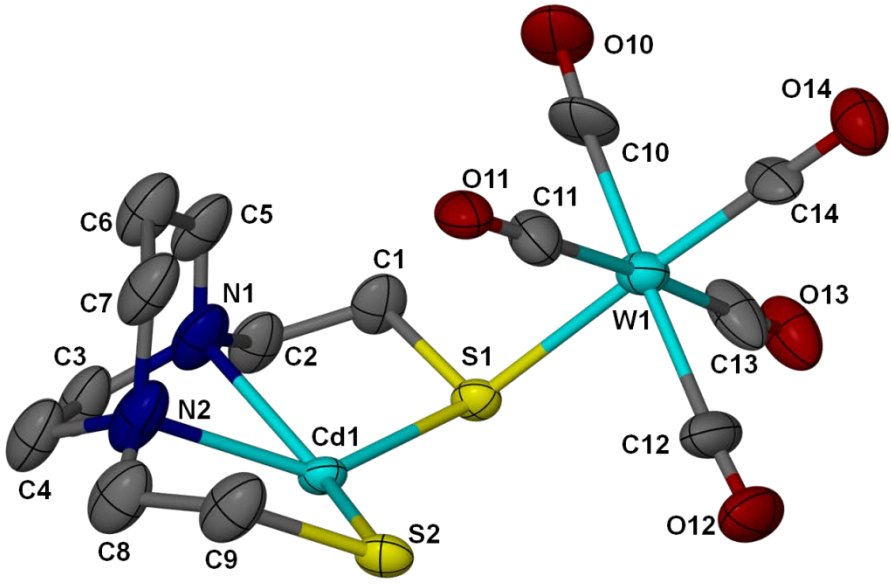


**Figure S2.** Thermal ellipsoid plot at 50% probability for monomeric unit of **[Cd-1'-W(CO)$_5$]$_2$**.

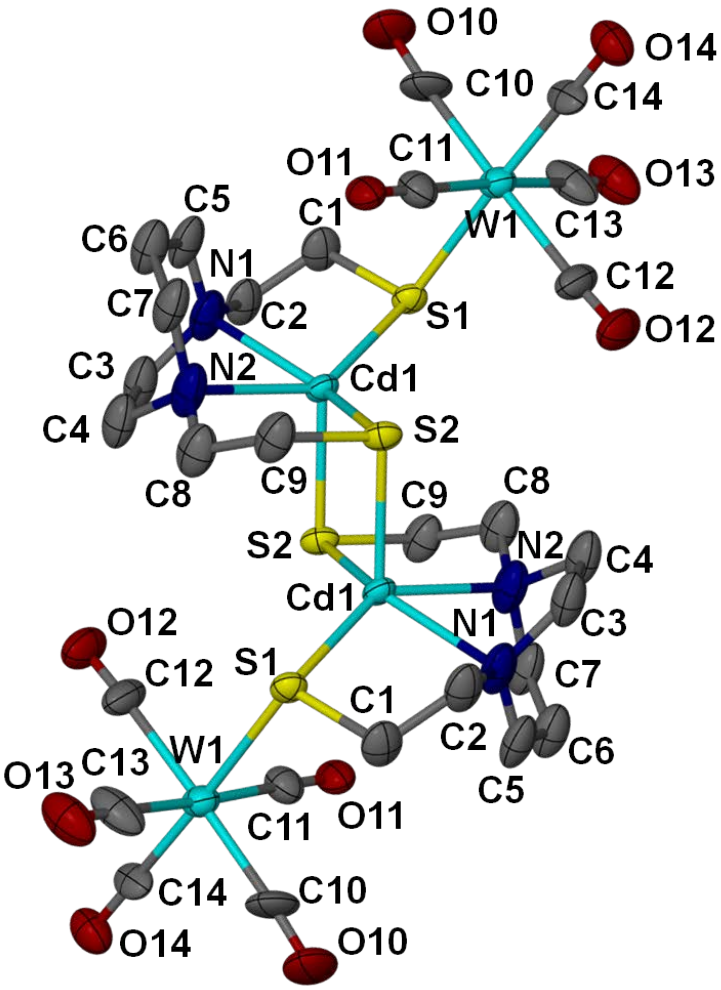


**Figure S3.** Thermal ellipsoid plot at 50% probability for dimeric **[Cd-1'-W(CO)$_5$]$_2$**.

**Table S1**. Crystal data and structure refinement for **[Cd-1']$_x$**.

| | | |
|---|---|---|
| Identification code | **[Cd-1']$_x$** | |
| Empirical formula | C9 H18 Cd N2 S2 | |
| Formula weight | 330.77 | |
| Temperature | 110(2) K | |
| Wavelength | 1.54184 Å | |
| Crystal system | Monoclinic | |
| Space group | C2/c | |
| Unit cell dimensions | a = 14.690(5) Å | α = 90°. |
| | b = 11.059(3) Å | β = 110.033(15)°. |
| | c = 7.516(2) Å | γ = 90°. |
| Volume | 1147.1(6) Å$^3$ | |
| Z | 4 | |
| Density (calculated) | 1.915 Mg/m$^3$ | |
| Absorption coefficient | 18.344 mm$^{-1}$ | |
| F(000) | 664 | |
| Crystal size | 0.20 x 0.01 x 0.01 mm$^3$ | |
| Theta range for data collection | 7.20 to 59.83°. | |
| Index ranges | -16<=h<=15, -12<=k<=12, -7<=l<=8 | |
| Reflections collected | 3023 | |
| Independent reflections | 656 [R(int) = 0.0498] | |
| Completeness to theta = 59.83° | 76.9 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.8378 and 0.1205 | |
| Refinement method | Full-matrix least-squares on F$^2$ | |
| Data / restraints / parameters | 656 / 16 / 87 | |
| Goodness-of-fit on F$^2$ | 1.012 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0253, wR2 = 0.0491 | |
| R indices (all data) | R1 = 0.0346, wR2 = 0.0505 | |
| Largest diff. peak and hole | 0.529 and -0.420 e.Å$^{-3}$ | |

**Table S2**. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for **[Cd-1']$_x$**. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Cd(1) | 0 | 496(1) | 2500 | 19(1) |
| S(1) | -1284(1) | -437(1) | 3685(2) | 23(1) |
| N(1) | -653(3) | 2400(3) | 3382(6) | 29(1) |
| C(1) | -1957(5) | 963(6) | 3470(12) | 70(3) |
| C(2) | -1366(6) | 2038(5) | 4264(12) | 69(3) |
| C(3) | 306(8) | 3099(10) | 4388(18) | 23(3) |
| C(4) | 1052(10) | 2990(20) | 3400(30) | 24(5) |
| C(5) | -1238(9) | 3110(16) | 1570(20) | 10(4) |
| C(6) | -616(7) | 3827(10) | 695(16) | 28(3) |
| C(7) | 102(10) | 3119(9) | 55(18) | 33(3) |

**Table S3**. Bond lengths [Å] and angles [°] for **[Cd-1']$_x$**.

| | |
|---|---|
| Cd(1)-N(1)#1 | 2.496(4) |
| Cd(1)-N(1) | 2.496(4) |
| Cd(1)-S(1) | 2.5620(12) |
| Cd(1)-S(1)#1 | 2.5620(12) |
| Cd(1)-S(1)#2 | 2.8417(14) |
| Cd(1)-S(1)#3 | 2.8417(14) |
| S(1)-C(1) | 1.815(6) |
| S(1)-Cd(1)#3 | 2.8417(14) |
| N(1)-C(7)#1 | 1.420(13) |
| N(1)-C(4)#1 | 1.425(18) |
| N(1)-C(2) | 1.474(8) |
| N(1)-C(5) | 1.551(11) |
| N(1)-C(3) | 1.557(11) |
| C(1)-C(2) | 1.472(10) |
| C(1)-H(1A) | 0.9900 |
| C(1)-H(1B) | 0.9900 |
| C(2)-H(2A) | 0.9900 |
| C(2)-H(2B) | 0.9900 |
| C(3)-C(4) | 1.522(10) |
| C(3)-H(3A) | 0.9900 |
| C(3)-H(3B) | 0.9900 |
| C(4)-N(1)#1 | 1.425(18) |
| C(4)-H(4A) | 0.9900 |
| C(4)-H(4B) | 0.9900 |
| C(5)-C(6) | 1.520(10) |
| C(5)-H(5A) | 0.9900 |
| C(5)-H(5B) | 0.9900 |
| C(6)-C(7) | 1.517(10) |
| C(6)-H(6A) | 0.9900 |
| C(6)-H(6B) | 0.9900 |
| C(7)-N(1)#1 | 1.420(13) |
| C(7)-H(7A) | 0.9900 |
| C(7)-H(7B) | 0.9900 |

| | |
|---|---|
| N(1)#1-Cd(1)-N(1) | 64.9(2) |
| N(1)#1-Cd(1)-S(1) | 145.87(11) |
| N(1)-Cd(1)-S(1) | 81.48(11) |
| N(1)#1-Cd(1)-S(1)#1 | 81.48(11) |
| N(1)-Cd(1)-S(1)#1 | 145.87(11) |
| S(1)-Cd(1)-S(1)#1 | 132.50(5) |
| N(1)#1-Cd(1)-S(1)#2 | 86.21(10) |
| N(1)-Cd(1)-S(1)#2 | 96.02(10) |
| S(1)-Cd(1)-S(1)#2 | 91.64(4) |
| S(1)#1-Cd(1)-S(1)#2 | 87.30(4) |
| N(1)#1-Cd(1)-S(1)#3 | 96.02(10) |
| N(1)-Cd(1)-S(1)#3 | 86.21(10) |
| S(1)-Cd(1)-S(1)#3 | 87.30(4) |
| S(1)#1-Cd(1)-S(1)#3 | 91.64(4) |
| S(1)#2-Cd(1)-S(1)#3 | 177.37(5) |
| C(1)-S(1)-Cd(1) | 93.97(19) |
| C(1)-S(1)-Cd(1)#3 | 105.2(3) |
| Cd(1)-S(1)-Cd(1)#3 | 92.70(4) |
| C(7)#1-N(1)-C(4)#1 | 117.2(11) |
| C(7)#1-N(1)-C(2) | 94.2(7) |
| C(4)#1-N(1)-C(2) | 114.9(6) |
| C(7)#1-N(1)-C(5) | 115.4(9) |
| C(4)#1-N(1)-C(5) | 10.5(9) |
| C(2)-N(1)-C(5) | 105.4(6) |
| C(7)#1-N(1)-C(3) | 32.4(5) |
| C(4)#1-N(1)-C(3) | 104.0(9) |
| C(2)-N(1)-C(3) | 125.5(7) |
| C(5)-N(1)-C(3) | 108.2(8) |
| C(7)#1-N(1)-Cd(1) | 122.0(5) |
| C(4)#1-N(1)-Cd(1) | 101.9(9) |
| C(2)-N(1)-Cd(1) | 106.7(3) |
| C(5)-N(1)-Cd(1) | 110.0(8) |
| C(3)-N(1)-Cd(1) | 100.5(5) |
| C(2)-C(1)-S(1) | 115.1(5) |
| C(2)-C(1)-H(1A) | 108.5 |
| S(1)-C(1)-H(1A) | 108.5 |

| | |
|---|---|
| C(2)-C(1)-H(1B) | 108.5 |
| S(1)-C(1)-H(1B) | 108.5 |
| H(1A)-C(1)-H(1B) | 107.5 |
| C(1)-C(2)-N(1) | 116.6(6) |
| C(1)-C(2)-H(2A) | 108.1 |
| N(1)-C(2)-H(2A) | 108.1 |
| C(1)-C(2)-H(2B) | 108.1 |
| N(1)-C(2)-H(2B) | 108.1 |
| H(2A)-C(2)-H(2B) | 107.3 |
| C(4)-C(3)-N(1) | 114.0(11) |
| C(4)-C(3)-H(3A) | 108.8 |
| N(1)-C(3)-H(3A) | 108.8 |
| C(4)-C(3)-H(3B) | 108.8 |
| N(1)-C(3)-H(3B) | 108.8 |
| H(3A)-C(3)-H(3B) | 107.6 |
| N(1)#1-C(4)-C(3) | 111.2(12) |
| N(1)#1-C(4)-H(4A) | 109.4 |
| C(3)-C(4)-H(4A) | 109.4 |
| N(1)#1-C(4)-H(4B) | 109.4 |
| C(3)-C(4)-H(4B) | 109.4 |
| H(4A)-C(4)-H(4B) | 108.0 |
| C(6)-C(5)-N(1) | 114.2(9) |
| C(6)-C(5)-H(5A) | 108.7 |
| N(1)-C(5)-H(5A) | 108.7 |
| C(6)-C(5)-H(5B) | 108.7 |
| N(1)-C(5)-H(5B) | 108.7 |
| H(5A)-C(5)-H(5B) | 107.6 |
| C(7)-C(6)-C(5) | 117.0(11) |
| C(7)-C(6)-H(6A) | 108.0 |
| C(5)-C(6)-H(6A) | 108.0 |
| C(7)-C(6)-H(6B) | 108.0 |
| C(5)-C(6)-H(6B) | 108.0 |
| H(6A)-C(6)-H(6B) | 107.3 |
| N(1)#1-C(7)-C(6) | 106.8(10) |
| N(1)#1-C(7)-H(7A) | 110.4 |
| C(6)-C(7)-H(7A) | 110.4 |

| | |
|---|---|
| N(1)#1-C(7)-H(7B) | 110.4 |
| C(6)-C(7)-H(7B) | 110.4 |
| H(7A)-C(7)-H(7B) | 108.6 |

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Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2 #2 x,-y,z-1/2 #3 -x,-y,-z+1

**Table S4**. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **[Cd-1']$_x$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Cd(1) | 18(1) | 18(1) | 25(1) | 0 | 12(1) | 0 |
| S(1) | 18(1) | 30(1) | 20(1) | 3(1) | 7(1) | -4(1) |
| N(1) | 39(3) | 22(2) | 24(3) | 6(2) | 7(2) | 14(2) |
| C(1) | 50(4) | 79(5) | 107(7) | 65(4) | 62(5) | 38(4) |
| C(2) | 122(7) | 34(3) | 94(6) | 33(4) | 93(5) | 35(4) |
| C(3) | 11(7) | 29(6) | 24(8) | -11(5) | 0(5) | -9(6) |
| C(4) | 15(6) | 25(6) | 28(7) | -6(4) | 3(4) | -18(4) |
| C(5) | 7(5) | 7(5) | 15(5) | 8(3) | 4(4) | 6(4) |
| C(6) | 23(6) | 30(6) | 28(7) | 17(5) | 3(5) | -11(5) |
| C(7) | 35(8) | 37(6) | 25(8) | -8(5) | 8(6) | -18(6) |

**Table S5**. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters (Å$^2$x $10^3$) for **[Cd-1']$_x$**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1A) | -2319 | 1112 | 2112 | 84 |
| H(1B) | -2439 | 859 | 4111 | 84 |
| H(2A) | -1015 | 1889 | 5627 | 83 |
| H(2B) | -1810 | 2727 | 4172 | 83 |
| H(3A) | 152 | 3964 | 4462 | 27 |
| H(3B) | 595 | 2792 | 5699 | 27 |
| H(4A) | 1280 | 3805 | 3217 | 28 |
| H(4B) | 1617 | 2523 | 4219 | 28 |
| H(5A) | -1639 | 2532 | 620 | 12 |
| H(5B) | -1683 | 3674 | 1891 | 12 |
| H(6A) | -1054 | 4270 | -414 | 34 |
| H(6B) | -251 | 4439 | 1628 | 34 |
| H(7A) | -245 | 2600 | -1041 | 39 |
| H(7B) | 530 | 3678 | -322 | 39 |

**Table S6**. Crystal data and structure refinement for **[Cd-1'-W(CO)$_5$]$_2$**.

| | | |
|---|---|---|
| Identification code | **[Cd-1'-W(CO)$_5$]$_2$** | |
| Empirical formula | C14 H16 Cd N2 O5 S2 W | |
| Formula weight | 652.66 | |
| Temperature | 110(2) K | |
| Wavelength | 1.54178 Å | |
| Crystal system | Monoclinic | |
| Space group | P2(1)/c | |
| Unit cell dimensions | a = 14.574(3) Å | α = 90°. |
| | b = 11.540(3) Å | β = 115.686(11)°. |
| | c = 12.711(3) Å | γ = 90°. |
| Volume | 1926.5(8) Å$^3$ | |
| Z | 4 | |
| Density (calculated) | 2.250 Mg/m$^3$ | |
| Absorption coefficient | 21.983 mm$^{-1}$ | |
| F(000) | 1232 | |
| Crystal size | 0.03 x 0.02 x 0.01 mm$^3$ | |
| Theta range for data collection | 3.36 to 60.84°. | |
| Index ranges | -15<=h<=16, -12<=k<=13, -14<=l<=14 | |
| Reflections collected | 14013 | |
| Independent reflections | 2868 [R(int) = 0.1997] | |
| Completeness to theta = 60.84° | 97.9 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.8101 and 0.5584 | |
| Refinement method | Full-matrix least-squares on F$^2$ | |
| Data / restraints / parameters | 2868 / 175 / 226 | |
| Goodness-of-fit on F$^2$ | 1.070 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0913, wR2 = 0.2265 | |
| R indices (all data) | R1 = 0.1401, wR2 = 0.2592 | |
| Largest diff. peak and hole | 1.939 and -2.371 e.Å$^{-3}$ | |

**Table S7**. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for **[Cd-1'-W(CO)$_5$]$_2$**. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Cd(1) | 6287(1) | 4988(2) | 259(2) | 28(1) |
| S(1) | 7688(4) | 6265(6) | 1673(5) | 30(1) |
| S(2) | 4680(4) | 5874(6) | -1375(5) | 30(1) |
| N(1) | 7684(18) | 3690(20) | 640(20) | 51(3) |
| N(2) | 5945(19) | 3510(20) | -1190(20) | 52(3) |
| C(1) | 8750(20) | 5220(20) | 2030(30) | 46(4) |
| C(2) | 8410(20) | 3980(30) | 1910(30) | 48(3) |
| C(3) | 7290(20) | 2500(30) | 760(30) | 54(3) |
| C(4) | 6270(20) | 2330(30) | -490(30) | 54(3) |
| C(5) | 8160(20) | 3840(30) | -10(30) | 53(3) |
| C(6) | 7580(20) | 3570(30) | -1160(30) | 56(3) |
| C(7) | 6460(20) | 3760(30) | -1920(30) | 53(3) |
| C(8) | 4850(20) | 3540(30) | -2000(30) | 53(3) |
| C(9) | 4430(20) | 4700(30) | -2490(30) | 49(4) |
| W(1) | 8017(1) | 8065(1) | 679(1) | 34(1) |
| C(10) | 9380(20) | 7500(30) | 830(30) | 62(5) |
| C(11) | 7330(20) | 7240(20) | -900(30) | 41(4) |
| C(12) | 6600(20) | 8700(30) | 520(30) | 51(4) |
| C(13) | 8670(30) | 8810(30) | 2310(30) | 58(5) |
| C(14) | 8240(20) | 9430(30) | -30(20) | 39(4) |
| O(10) | 10147(16) | 7240(20) | 870(20) | 71(5) |
| O(11) | 7010(15) | 6697(16) | -1734(16) | 41(4) |
| O(12) | 5867(16) | 9077(19) | 344(19) | 56(5) |
| O(13) | 9012(18) | 9270(20) | 3149(18) | 64(5) |
| O(14) | 8398(17) | 10280(18) | -431(17) | 51(4) |

**Table S8**. Bond lengths [Å] and angles [°] for **[Cd-1'-W(CO)$_5$]$_2$**.

| | |
|---|---|
| Cd(1)-N(2) | 2.40(2) |
| Cd(1)-N(1) | 2.40(2) |
| Cd(1)-S(1) | 2.527(6) |
| Cd(1)-S(2) | 2.574(6) |
| Cd(1)-S(2)#1 | 2.593(6) |
| S(1)-C(1) | 1.86(3) |
| S(1)-W(1) | 2.583(7) |
| S(2)-C(9) | 1.88(3) |
| S(2)-Cd(1)#1 | 2.593(6) |
| N(1)-C(5) | 1.30(4) |
| N(1)-C(3) | 1.52(4) |
| N(1)-C(2) | 1.54(3) |
| N(2)-C(7) | 1.46(4) |
| N(2)-C(8) | 1.48(4) |
| N(2)-C(4) | 1.58(4) |
| C(1)-C(2) | 1.50(4) |
| C(1)-H(1A) | 0.9900 |
| C(1)-H(1B) | 0.9900 |
| C(2)-H(2A) | 0.9900 |
| C(2)-H(2B) | 0.9900 |
| C(3)-C(4) | 1.65(4) |
| C(3)-H(3A) | 0.9900 |
| C(3)-H(3B) | 0.9900 |
| C(4)-H(4A) | 0.9900 |
| C(4)-H(4B) | 0.9900 |
| C(5)-C(6) | 1.37(4) |
| C(5)-H(5) | 0.9500 |
| C(6)-C(7) | 1.51(4) |
| C(6)-H(6) | 0.9500 |
| C(7)-H(7A) | 0.9900 |
| C(7)-H(7B) | 0.9900 |
| C(8)-C(9) | 1.49(4) |
| C(8)-H(8A) | 0.9900 |
| C(8)-H(8B) | 0.9900 |

| | |
|---|---|
| C(9)-H(9A) | 0.9900 |
| C(9)-H(9B) | 0.9900 |
| W(1)-C(14) | 1.91(3) |
| W(1)-C(10) | 2.02(3) |
| W(1)-C(11) | 2.05(3) |
| W(1)-C(13) | 2.06(3) |
| W(1)-C(12) | 2.11(3) |
| C(10)-O(10) | 1.13(3) |
| C(11)-O(11) | 1.14(3) |
| C(12)-O(12) | 1.09(3) |
| C(13)-O(13) | 1.10(3) |
| C(14)-O(14) | 1.18(3) |

| | |
|---|---|
| N(2)-Cd(1)-N(1) | 65.5(8) |
| N(2)-Cd(1)-S(1) | 142.7(7) |
| N(1)-Cd(1)-S(1) | 82.4(6) |
| N(2)-Cd(1)-S(2) | 81.3(6) |
| N(1)-Cd(1)-S(2) | 143.6(6) |
| S(1)-Cd(1)-S(2) | 121.0(2) |
| N(2)-Cd(1)-S(2)#1 | 99.5(7) |
| N(1)-Cd(1)-S(2)#1 | 105.4(7) |
| S(1)-Cd(1)-S(2)#1 | 107.3(2) |
| S(2)-Cd(1)-S(2)#1 | 94.2(2) |
| C(1)-S(1)-Cd(1) | 97.4(9) |
| C(1)-S(1)-W(1) | 109.2(10) |
| Cd(1)-S(1)-W(1) | 112.6(2) |
| C(9)-S(2)-Cd(1) | 97.6(9) |
| C(9)-S(2)-Cd(1)#1 | 99.5(11) |
| Cd(1)-S(2)-Cd(1)#1 | 85.8(2) |
| C(5)-N(1)-C(3) | 121(3) |
| C(5)-N(1)-C(2) | 109(2) |
| C(3)-N(1)-C(2) | 102(2) |
| C(5)-N(1)-Cd(1) | 115(2) |
| C(3)-N(1)-Cd(1) | 105.2(17) |
| C(2)-N(1)-Cd(1) | 102.1(16) |
| C(7)-N(2)-C(8) | 104(2) |

| | |
|---|---|
| C(7)-N(2)-C(4) | 115(2) |
| C(8)-N(2)-C(4) | 112(3) |
| C(7)-N(2)-Cd(1) | 110.9(19) |
| C(8)-N(2)-Cd(1) | 108.9(17) |
| C(4)-N(2)-Cd(1) | 105.6(16) |
| C(2)-C(1)-S(1) | 112.8(19) |
| C(2)-C(1)-H(1A) | 109.0 |
| S(1)-C(1)-H(1A) | 109.0 |
| C(2)-C(1)-H(1B) | 109.0 |
| S(1)-C(1)-H(1B) | 109.0 |
| H(1A)-C(1)-H(1B) | 107.8 |
| C(1)-C(2)-N(1) | 112(2) |
| C(1)-C(2)-H(2A) | 109.3 |
| N(1)-C(2)-H(2A) | 109.3 |
| C(1)-C(2)-H(2B) | 109.3 |
| N(1)-C(2)-H(2B) | 109.3 |
| H(2A)-C(2)-H(2B) | 108.0 |
| N(1)-C(3)-C(4) | 103(2) |
| N(1)-C(3)-H(3A) | 111.2 |
| C(4)-C(3)-H(3A) | 111.2 |
| N(1)-C(3)-H(3B) | 111.2 |
| C(4)-C(3)-H(3B) | 111.2 |
| H(3A)-C(3)-H(3B) | 109.1 |
| N(2)-C(4)-C(3) | 112(2) |
| N(2)-C(4)-H(4A) | 109.3 |
| C(3)-C(4)-H(4A) | 109.3 |
| N(2)-C(4)-H(4B) | 109.3 |
| C(3)-C(4)-H(4B) | 109.3 |
| H(4A)-C(4)-H(4B) | 108.0 |
| N(1)-C(5)-C(6) | 113(3) |
| N(1)-C(5)-H(5) | 123.4 |
| C(6)-C(5)-H(5) | 123.4 |
| C(5)-C(6)-C(7) | 130(3) |
| C(5)-C(6)-H(6) | 114.9 |
| C(7)-C(6)-H(6) | 114.9 |
| N(2)-C(7)-C(6) | 106(3) |

| | |
|---|---|
| N(2)-C(7)-H(7A) | 110.6 |
| C(6)-C(7)-H(7A) | 110.6 |
| N(2)-C(7)-H(7B) | 110.6 |
| C(6)-C(7)-H(7B) | 110.6 |
| H(7A)-C(7)-H(7B) | 108.7 |
| N(2)-C(8)-C(9) | 116(3) |
| N(2)-C(8)-H(8A) | 108.4 |
| C(9)-C(8)-H(8A) | 108.4 |
| N(2)-C(8)-H(8B) | 108.4 |
| C(9)-C(8)-H(8B) | 108.4 |
| H(8A)-C(8)-H(8B) | 107.4 |
| C(8)-C(9)-S(2) | 115(2) |
| C(8)-C(9)-H(9A) | 108.6 |
| S(2)-C(9)-H(9A) | 108.6 |
| C(8)-C(9)-H(9B) | 108.6 |
| S(2)-C(9)-H(9B) | 108.6 |
| H(9A)-C(9)-H(9B) | 107.5 |
| C(14)-W(1)-C(10) | 87.2(13) |
| C(14)-W(1)-C(11) | 91.5(11) |
| C(10)-W(1)-C(11) | 89.1(14) |
| C(14)-W(1)-C(13) | 92.0(12) |
| C(10)-W(1)-C(13) | 91.9(15) |
| C(11)-W(1)-C(13) | 176.3(11) |
| C(14)-W(1)-C(12) | 91.4(12) |
| C(10)-W(1)-C(12) | 178.5(13) |
| C(11)-W(1)-C(12) | 91.6(13) |
| C(13)-W(1)-C(12) | 87.5(15) |
| C(14)-W(1)-S(1) | 178.0(9) |
| C(10)-W(1)-S(1) | 94.4(10) |
| C(11)-W(1)-S(1) | 89.6(8) |
| C(13)-W(1)-S(1) | 86.8(9) |
| C(12)-W(1)-S(1) | 87.0(9) |
| O(10)-C(10)-W(1) | 175(3) |
| O(11)-C(11)-W(1) | 174(3) |
| O(12)-C(12)-W(1) | 174(3) |
| O(13)-C(13)-W(1) | 175(3) |

O(14)-C(14)-W(1) 178(2)

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Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z

**Table S9**. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **[Cd-1'-W(CO)$_5$]$_2$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Cd(1) | 19(1) | 33(1) | 33(1) | -3(1) | 13(1) | 1(1) |
| S(1) | 19(3) | 37(3) | 33(3) | -3(2) | 9(2) | -1(2) |
| S(2) | 19(3) | 42(4) | 29(3) | 0(3) | 9(2) | -2(2) |
| N(1) | 36(4) | 52(4) | 55(6) | -14(4) | 9(4) | 16(4) |
| N(2) | 45(5) | 55(5) | 45(5) | -21(4) | 8(4) | 12(4) |
| C(1) | 27(5) | 47(5) | 53(7) | -2(5) | 5(5) | 10(4) |
| C(2) | 31(5) | 48(4) | 54(6) | -8(5) | 7(4) | 13(4) |
| C(3) | 43(5) | 50(4) | 55(6) | -17(5) | 8(5) | 15(4) |
| C(4) | 46(6) | 52(4) | 50(6) | -20(4) | 9(5) | 12(4) |
| C(5) | 39(5) | 57(6) | 55(6) | -16(5) | 11(4) | 20(5) |
| C(6) | 45(5) | 58(6) | 54(6) | -16(5) | 10(5) | 15(5) |
| C(7) | 46(5) | 57(6) | 48(5) | -22(5) | 11(4) | 12(5) |
| C(8) | 45(5) | 58(5) | 43(6) | -18(5) | 7(4) | 8(5) |
| C(9) | 41(7) | 58(7) | 39(6) | -16(5) | 8(5) | 7(6) |
| W(1) | 29(1) | 40(1) | 36(1) | -2(1) | 17(1) | -2(1) |
| C(10) | 27(6) | 67(13) | 101(15) | 5(10) | 34(7) | -8(7) |
| C(11) | 48(9) | 38(10) | 41(5) | -2(5) | 22(7) | -8(8) |
| C(12) | 49(7) | 47(10) | 73(12) | 16(8) | 42(8) | 13(7) |
| C(13) | 84(12) | 55(10) | 34(6) | 0(7) | 23(8) | -31(10) |
| C(14) | 55(11) | 46(8) | 30(9) | -13(6) | 30(9) | -14(7) |
| O(10) | 29(7) | 73(13) | 112(15) | 1(11) | 31(8) | 0(8) |
| O(11) | 49(9) | 44(10) | 41(7) | -6(6) | 30(7) | -9(7) |
| O(12) | 49(7) | 52(10) | 78(12) | 17(9) | 38(9) | 19(8) |
| O(13) | 86(12) | 61(11) | 41(7) | -10(7) | 22(9) | -30(10) |
| O(14) | 67(11) | 42(9) | 45(10) | -6(7) | 25(9) | -14(8) |

**Table S10**. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters (Å$^2$x $10^3$) for **[Cd-1'-W(CO)$_5$]$_2$**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1A) | 9084 | 5366 | 1510 | 56 |
| H(1B) | 9265 | 5359 | 2844 | 56 |
| H(2A) | 8063 | 3843 | 2415 | 58 |
| H(2B) | 9014 | 3471 | 2176 | 58 |
| H(3A) | 7115 | 2474 | 1430 | 65 |
| H(3B) | 7805 | 1887 | 868 | 65 |
| H(4A) | 6413 | 1750 | -972 | 65 |
| H(4B) | 5702 | 2040 | -337 | 65 |
| H(5) | 8841 | 4106 | 282 | 64 |
| H(6) | 7939 | 3195 | -1534 | 67 |
| H(7A) | 6340 | 4576 | -2200 | 64 |
| H(7B) | 6218 | 3242 | -2608 | 64 |
| H(8A) | 4461 | 3239 | -1587 | 63 |
| H(8B) | 4733 | 3006 | -2656 | 63 |
| H(9A) | 3688 | 4625 | -2964 | 59 |
| H(9B) | 4731 | 4938 | -3027 | 59 |