

atoms) which was used for all calculations. Geometrical analysis performed using the program *PARST* (Nardelli, 1983).

Related literature. The formation of Zn(en)Ni(CN)₄ as an intermediate in the course of the thermal decomposition of Zn(en)₃Ni(CN)₄·H₂O via Zn(en)₃Ni(CN)₄ and Zn(en)₂Ni(CN)₄ was not observed (Černák, Potočňák & Chomič, 1991). On the other hand, in the course of the thermal decomposition of Cd(en)₃Ni(CN)₄, the complexes Cd(en)₂Ni(CN)₄ and Cd(en)Ni(CN)₄ are successively formed. The structure of Cd(en)Ni(CN)₄ consists of a three-dimensional network with CN ligands bridging Cd and Ni atoms (Jameson, Bachmann, Oswald & Dubler, 1981). Similarly, Ni(en)Ni(CN)₄ is formed in the course of the thermal decomposition of Ni(en)₃Ni(CN)₄·H₂O (Černák, Chomič & Potočňák, 1989). The crystal structures of the ionic complexes Zn(en)₃Ni(CN)₄·H₂O and Zn(en)₃Ni(CN)₄

were described by Černák, Chomič, Dunaj-Jurčo & Kappenstein (1984), while the chain structure of Zn(en)₂Ni(CN)₄ was described by Černák, Potočňák, Chomič & Dunaj-Jurčo (1990).

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Structure of (η⁵-C₅H₅)₂W_{1.2}Mo_{0.8}Fe(μ₃-Te)₂(CO)₇ Containing a Te···Te Bonding Interaction

BY BIXIAN ZHENG, JINSHUN HUANG,* QIANER ZHANG AND JIAXI LU

Fuzhou Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, People's Republic of China

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Abstracts. [FeMo_{0.8}Te₂W_{1.2}(C₅H₅)₂(CO)₇], *M_r* = 934.68, triclinic, *P*1̄, *a* = 13.195 (2), *b* = 15.892 (2), *c* = 21.632 (2) Å, α = 100.28 (1), β = 104.76 (1), γ = 94.07 (1)°, *V* = 4283.6 (9) Å³, *Z* = 8, *D_x* = 2.899 g cm⁻³, λ(Mo *K*α) = 0.71073 Å, μ = 107.41 cm⁻¹, *F*(000) = 3363.2, *T* = 295 K, *R* = 0.051 for 8302 observed reflections. The four molecules per asymmetric unit are quite similar. The title compound features Te···Te distances of 3.140–3.154 Å, which indicate strong Te···Te bonding interactions.

Experimental. The reaction of (η⁵-C₅H₅)₂Mo₂(CO)₆ and (η⁵-C₅H₅)W₂(CO)₆ with Fe₃Te₂(CO)₉ in toluene yielded dark-brown crystals of the title compound. Qualitative elemental analysis showed Mo, W and Fe were present. The crystal chosen for X-ray study had approximate dimensions 0.20 × 0.20 × 0.11 mm. The intensity data were collected on an Enraf–Nonius CAD-4 diffractometer with graphite-monochroma-

tized Mo *K*α radiation. The lattice parameters were refined from the angle values of 25 reflections with 28 ≤ 2θ ≤ 30°. 15 481 reflections with 2 ≤ 2θ ≤ 50° were collected using the ω-scan mode with a variable rate of 1 to 7° min⁻¹ and a scan range of (0.40 + 0.35tan2θ)°. The index range was -15 ≤ *h* ≤ 15, -18 ≤ *k* ≤ 18, 0 ≤ *l* ≤ 25. Three standard reflections measured at exposure intervals of 2 h exhibited no significant variation. Data were corrected for Lorentz–polarization effects and empirically for absorption using the program *DIFABS* (Walker & Stuart, 1983). Max. and min. transmission factors were 1.152 and 0.820, respectively. 8302 reflections with *I* > 3σ(*I*) were used in subsequent calculations.

The structure was solved using direct methods, which located the positions of all Te, W/Mo and Fe atoms in the four independent molecules. The remaining non-H atoms were located from difference Fourier syntheses. All non-H atoms except the C atoms were refined with anisotropic temperature factors. All H atoms were located according to their

* To whom all correspondence should be addressed.

Table 1. Positional parameters and equivalent isotropic thermal parameters for $(\eta^5\text{-C}_5\text{H}_5)_2\text{W}_{1.2}\text{Mo}_{0.8}\text{Fe}(\mu_3\text{-Te})_2(\text{CO})_7$ at 295 K

$$B_{\text{eq}} = (4/3)\sum_i\sum_j\beta_{ij}\mathbf{a}_i\cdot\mathbf{a}_j$$

| | <i>x</i> | <i>y</i> | <i>z</i> | <i>B</i> _{eq} (Å ²) |
|--------|--------------|-------------|-------------|------------------------------------------|
| WM(1) | 0.52817 (7) | 0.24134 (6) | 0.03599 (4) | 2.99 (2) |
| MW(1) | 0.5219 (1) | 0.22447 (8) | 0.22898 (6) | 2.82 (3) |
| WM(2) | 0.63136 (7) | 0.13653 (6) | 0.68799 (4) | 2.96 (2) |
| MW(2) | 0.5037 (1) | 0.28725 (8) | 0.54987 (6) | 2.81 (3) |
| WM(3) | 1.01127 (8) | 0.13637 (6) | 0.18015 (4) | 3.18 (2) |
| MW(3) | 1.0458 (1) | 0.28753 (8) | 0.04221 (6) | 2.83 (3) |
| WM(4) | -0.00518 (8) | 0.24383 (6) | 0.52754 (5) | 3.15 (2) |
| MW(4) | 0.1608 (1) | 0.18897 (9) | 0.71005 (6) | 3.20 (3) |
| Te(1) | 0.6602 (1) | 0.28298 (9) | 0.16171 (6) | 3.14 (3) |
| Te(2) | 0.4159 (1) | 0.29694 (8) | 0.12470 (6) | 2.55 (3) |
| Te(3) | 0.6979 (1) | 0.26600 (9) | 0.63206 (7) | 3.19 (3) |
| Te(4) | 0.4823 (1) | 0.25151 (9) | 0.66850 (6) | 2.88 (3) |
| Te(5) | 0.9137 (1) | 0.26186 (9) | 0.12243 (6) | 2.94 (3) |
| Te(6) | 1.1598 (1) | 0.25551 (9) | 0.16248 (6) | 2.84 (3) |
| Te(7) | 0.1923 (1) | 0.28545 (9) | 0.61725 (6) | 3.07 (3) |
| Te(8) | -0.0216 (1) | 0.25880 (9) | 0.65391 (6) | 2.96 (3) |
| Fe(1) | 0.5660 (2) | 0.4060 (2) | 0.1185 (1) | 3.00 (7) |
| Fe(2) | 0.6667 (3) | 0.3141 (2) | 0.7450 (2) | 3.57 (8) |
| Fe(3) | 1.0436 (2) | 0.3139 (2) | 0.2366 (1) | 3.01 (7) |
| Fe(4) | 0.0572 (2) | 0.3948 (2) | 0.6245 (1) | 3.15 (7) |
| O(1) | 0.714 (1) | 0.328 (1) | -0.0077 (7) | 5.4 (4) |
| O(2) | 0.381 (1) | 0.343 (1) | -0.0540 (8) | 5.7 (5) |
| O(3) | 0.626 (1) | 0.057 (1) | 0.201 (1) | 7.7 (6) |
| O(4) | 0.335 (1) | 0.0785 (9) | 0.1627 (8) | 5.7 (5) |
| O(5) | 0.588 (1) | 0.515 (1) | 0.2460 (8) | 6.5 (5) |
| O(6) | 0.417 (1) | 0.5077 (9) | 0.0479 (8) | 6.3 (5) |
| O(7) | 0.755 (1) | 0.493 (1) | 0.0956 (8) | 5.7 (4) |
| O(8) | 0.590 (1) | 0.138 (1) | 0.8231 (8) | 8.6 (5) |
| O(9) | 0.868 (1) | 0.147 (1) | 0.7673 (8) | 6.1 (4) |
| O(10) | 0.597 (1) | 0.154 (1) | 0.4639 (7) | 5.2 (4) |
| O(11) | 0.316 (1) | 0.140 (1) | 0.4945 (8) | 6.0 (5) |
| O(12) | 0.659 (2) | 0.492 (1) | 0.734 (1) | 8.7 (7) |
| O(13) | 0.884 (1) | 0.339 (1) | 0.820 (1) | 8.0 (6) |
| O(14) | 0.573 (2) | 0.332 (1) | 0.8561 (9) | 9.7 (6) |
| O(15) | 1.177 (2) | 0.139 (1) | 0.3119 (8) | 8.0 (6) |
| O(16) | 0.855 (1) | 0.146 (1) | 0.2652 (8) | 6.0 (5) |
| O(17) | 1.174 (1) | 0.149 (1) | -0.0072 (8) | 5.7 (5) |
| O(18) | 0.867 (1) | 0.154 (1) | -0.0529 (8) | 6.8 (6) |
| O(19) | 1.073 (1) | 0.491 (1) | 0.2209 (8) | 6.6 (5) |
| O(20) | 1.224 (1) | 0.342 (1) | 0.3544 (8) | 8.1 (6) |
| O(21) | 0.888 (1) | 0.345 (1) | 0.3124 (7) | 6.0 (5) |
| O(22) | -0.209 (1) | 0.334 (1) | 0.4960 (8) | 5.4 (5) |
| O(23) | 0.079 (2) | 0.371 (1) | 0.4525 (8) | 7.0 (5) |
| O(24) | -0.008 (1) | 0.027 (1) | 0.6666 (8) | 6.0 (5) |
| O(25) | 0.259 (1) | 0.055 (1) | 0.6278 (9) | 6.1 (5) |
| O(26) | 0.161 (1) | 0.478 (1) | 0.7602 (8) | 6.7 (5) |
| O(27) | -0.134 (1) | 0.479 (1) | 0.6177 (8) | 6.1 (5) |
| O(28) | 0.163 (2) | 0.518 (1) | 0.5705 (9) | 8.6 (6) |
| C(1) | 0.646 (1) | 0.299 (1) | 0.0114 (9) | 2.7 (4)* |
| C(2) | 0.440 (2) | 0.311 (1) | -0.018 (1) | 3.6 (5)* |
| C(3) | 0.590 (2) | 0.124 (1) | 0.211 (1) | 3.7 (5)* |
| C(4) | 0.407 (2) | 0.136 (1) | 0.187 (1) | 4.2 (5)* |
| C(5) | 0.577 (2) | 0.469 (1) | 0.195 (1) | 4.8 (5)* |
| C(6) | 0.477 (2) | 0.466 (1) | 0.073 (1) | 3.3 (4)* |
| C(7) | 0.679 (1) | 0.457 (1) | 0.1018 (9) | 3.0 (4)* |
| C(8) | 0.611 (2) | 0.143 (1) | 0.774 (1) | 4.0 (5)* |
| C(9) | 0.783 (2) | 0.150 (1) | 0.740 (1) | 3.9 (5)* |
| C(10) | 0.564 (2) | 0.208 (1) | 0.498 (1) | 3.9 (5)* |
| C(11) | 0.386 (2) | 0.199 (1) | 0.517 (1) | 4.8 (5)* |
| C(12) | 0.663 (2) | 0.420 (2) | 0.737 (1) | 5.3 (6)* |
| C(13) | 0.797 (2) | 0.330 (2) | 0.791 (1) | 6.3 (7)* |
| C(14) | 0.615 (2) | 0.325 (2) | 0.815 (1) | 5.5 (6)* |
| C(15) | 1.117 (2) | 0.139 (1) | 0.262 (1) | 4.8 (5)* |
| C(16) | 0.913 (2) | 0.148 (1) | 0.234 (1) | 4.2 (5)* |
| C(17) | 1.124 (2) | 0.202 (1) | 0.013 (1) | 3.8 (5)* |
| C(18) | 0.935 (2) | 0.201 (1) | -0.0163 (9) | 3.1 (4)* |
| C(19) | 1.064 (2) | 0.423 (1) | 0.229 (1) | 4.7 (5)* |
| C(20) | 1.150 (2) | 0.327 (1) | 0.307 (1) | 4.9 (6)* |
| C(21) | 0.946 (2) | 0.331 (1) | 0.280 (1) | 4.0 (5)* |
| C(22) | -0.132 (2) | 0.303 (2) | 0.509 (1) | 5.0 (6)* |
| C(23) | 0.049 (2) | 0.325 (2) | 0.484 (1) | 5.0 (6)* |
| C(24) | 0.052 (2) | 0.089 (1) | 0.683 (1) | 3.5 (4)* |
| C(25) | 0.221 (2) | 0.108 (1) | 0.659 (1) | 3.5 (4)* |
| C(26) | 0.123 (2) | 0.447 (1) | 0.707 (1) | 4.0 (5)* |
| C(27) | -0.063 (2) | 0.445 (1) | 0.618 (1) | 4.2 (5)* |
| C(28) | 0.119 (2) | 0.471 (1) | 0.592 (1) | 4.9 (6)* |
| CP(11) | 0.447 (2) | 0.101 (2) | 0.029 (1) | 6.2 (7)* |
| CP(12) | 0.409 (2) | 0.129 (2) | -0.029 (1) | 5.1 (6)* |
| CP(13) | 0.500 (2) | 0.139 (1) | -0.053 (1) | 4.8 (5)* |
| CP(14) | 0.585 (2) | 0.124 (2) | -0.013 (1) | 6.2 (7)* |

Table 1 (cont.)

| | <i>x</i> | <i>y</i> | <i>z</i> | <i>B</i> _{eq} (Å ²) |
|--------|------------|------------|------------|------------------------------------------|
| CP(15) | 0.553 (2) | 0.099 (2) | 0.040 (1) | 7.0 (8)* |
| CP(21) | 0.604 (2) | 0.342 (1) | 0.316 (1) | 4.6 (5)* |
| CP(22) | 0.626 (2) | 0.265 (2) | 0.337 (1) | 5.6 (6)* |
| CP(23) | 0.528 (2) | 0.225 (2) | 0.333 (1) | 5.7 (6)* |
| CP(24) | 0.448 (2) | 0.273 (2) | 0.311 (1) | 5.3 (6)* |
| CP(25) | 0.496 (2) | 0.349 (2) | 0.302 (1) | 4.9 (6)* |
| CP(31) | 0.628 (2) | -0.008 (1) | 0.682 (1) | 4.6 (5)* |
| CP(32) | 0.520 (2) | 0.010 (2) | 0.661 (1) | 5.9 (6)* |
| CP(33) | 0.506 (2) | 0.040 (2) | 0.603 (1) | 5.2 (6)* |
| CP(34) | 0.603 (2) | 0.042 (1) | 0.588 (1) | 4.7 (5)* |
| CP(35) | 0.677 (2) | 0.012 (2) | 0.635 (1) | 5.0 (6)* |
| CP(41) | 0.549 (2) | 0.399 (2) | 0.503 (1) | 5.0 (6)* |
| CP(42) | 0.566 (2) | 0.436 (1) | 0.568 (1) | 4.8 (5)* |
| CP(43) | 0.469 (2) | 0.430 (2) | 0.584 (1) | 4.9 (6)* |
| CP(44) | 0.392 (2) | 0.391 (1) | 0.525 (1) | 3.9 (5)* |
| CP(45) | 0.443 (2) | 0.370 (1) | 0.475 (1) | 4.3 (5)* |
| CP(51) | 1.043 (2) | 0.041 (2) | 0.094 (1) | 5.0 (6)* |
| CP(52) | 1.076 (2) | 0.008 (2) | 0.150 (1) | 5.4 (6)* |
| CP(53) | 0.981 (2) | -0.006 (2) | 0.167 (1) | 5.0 (6)* |
| CP(54) | 0.899 (2) | 0.015 (2) | 0.124 (1) | 5.6 (6)* |
| CP(55) | 0.939 (2) | 0.047 (2) | 0.077 (1) | 5.8 (6)* |
| CP(61) | 1.148 (2) | 0.398 (1) | 0.021 (1) | 4.8 (6)* |
| CP(62) | 1.125 (2) | 0.435 (1) | 0.076 (1) | 4.5 (5)* |
| CP(63) | 1.017 (2) | 0.435 (1) | 0.060 (1) | 4.6 (5)* |
| CP(64) | 0.975 (2) | 0.396 (1) | -0.005 (1) | 4.2 (5)* |
| CP(65) | 1.060 (2) | 0.372 (1) | -0.031 (1) | 4.6 (5)* |
| CP(71) | -0.074 (2) | 0.153 (2) | 0.428 (1) | 5.6 (6)* |
| CP(72) | 0.027 (2) | 0.146 (2) | 0.447 (1) | 5.2 (6)* |
| CP(73) | 0.050 (2) | 0.110 (2) | 0.500 (1) | 6.0 (6)* |
| CP(74) | -0.043 (2) | 0.093 (2) | 0.517 (1) | 5.5 (6)* |
| CP(75) | -0.122 (2) | 0.127 (2) | 0.472 (1) | 5.5 (6)* |
| CP(81) | 0.242 (2) | 0.165 (1) | 0.810 (1) | 4.3 (5)* |
| CP(82) | 0.316 (2) | 0.219 (2) | 0.792 (1) | 5.7 (6)* |
| CP(83) | 0.269 (2) | 0.297 (1) | 0.793 (1) | 4.5 (5)* |
| CP(84) | 0.178 (2) | 0.292 (1) | 0.809 (1) | 4.5 (5)* |
| CP(85) | 0.160 (2) | 0.208 (1) | 0.817 (1) | 4.7 (5)* |

* Atoms refined isotropically.

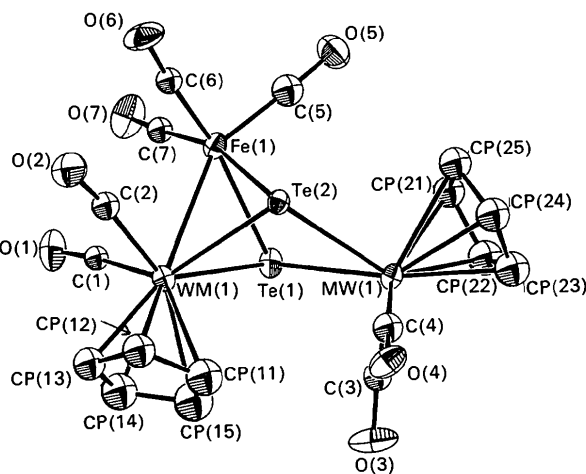


Fig. 1. Molecular structure of the title compound with numbering of the atoms.

ideal molecular geometries and added to the structure-factor calculations with their positions and isotropic temperature factors fixed. MW and WM stand for site-disordered atomic symbols which contain both W and Mo, MW means 0.65 Mo and 0.35 W; WM 0.15 Mo and 0.85 W. The Mo and W occupancies were determined by refining their multiplicity factors. The function minimized in the least-squares program was $\sum w(|F_o| - |F_c|)^2$ with $w =$

Table 2. Selected interatomic distances (Å) and bond angles (°)

| Molecule 1 | | Molecule 2 | | Molecule 3 | | Molecule 4 | |
|---------------|-----------|---------------|-----------|---------------|-----------|---------------|-----------|
| WM(1)···MW(1) | 4.252 (2) | WM(2)···MW(2) | 4.250 (2) | WM(3)···MW(3) | 4.240 (2) | WM(4)···MW(4) | 4.270 (2) |
| WM(1)—Te(1) | 2.765 (1) | WM(2)—Te(3) | 2.764 (2) | WM(3)—Te(5) | 2.762 (2) | WM(4)—Te(7) | 2.777 (1) |
| WM(1)—Te(2) | 2.772 (2) | WM(2)—Te(4) | 2.783 (2) | WM(3)—Te(6) | 2.772 (2) | WM(4)—Te(8) | 2.766 (2) |
| WM(1)—Fe(1) | 2.824 (3) | WM(2)—Fe(2) | 2.825 (4) | WM(3)—Fe(3) | 2.822 (3) | WM(4)—Fe(4) | 2.806 (3) |
| MW(1)—Te(1) | 2.812 (2) | MW(2)—Te(3) | 2.803 (2) | MW(3)—Te(5) | 2.812 (2) | MW(4)—Te(7) | 2.826 (2) |
| MW(1)—Te(2) | 2.814 (2) | MW(2)—Te(4) | 2.802 (3) | MW(2)—Te(6) | 2.807 (2) | MW(4)—Te(8) | 2.805 (2) |
| MW(1)···Fe(1) | 4.160 (4) | MW(2)···Fe(2) | 4.151 (3) | MW(3)···Fe(3) | 4.158 (3) | MW(4)···Fe(4) | 4.182 (3) |
| Te(1)—Te(2) | 3.151 (2) | Te(3)—Te(4) | 3.143 (2) | Te(5)—Te(6) | 3.154 (2) | Te(7)—Te(8) | 3.140 (2) |
| Te(1)—Fe(1) | 2.577 (3) | Te(3)—Fe(2) | 2.571 (4) | Te(5)—Fe(3) | 2.575 (3) | Te(7)—Fe(4) | 2.589 (3) |
| Te(2)—Fe(1) | 2.583 (3) | Te(4)—Fe(2) | 2.581 (4) | Te(6)—Fe(3) | 2.589 (4) | Te(8)—Fe(4) | 2.581 (3) |
| WM(1)—C(1) | 1.99 (3) | WM(2)—C(8) | 1.93 (2) | WM(3)—C(15) | 1.95 (2) | WM(4)—C(22) | 1.97 (2) |
| WM(1)—C(2) | 1.97 (2) | WM(2)—C(9) | 2.00 (2) | WM(3)—C(16) | 1.95 (3) | WM(4)—C(23) | 1.93 (3) |
| WM(1)—CP(11) | 2.37 (3) | WM(2)—CP(31) | 2.27 (2) | WM(3)—CP(51) | 2.33 (2) | WM(4)—CP(71) | 2.29 (2) |
| WM(1)—CP(12) | 2.29 (3) | WM(2)—CP(32) | 2.29 (2) | WM(3)—CP(52) | 2.32 (3) | WM(4)—CP(72) | 2.26 (2) |
| WM(1)—CP(13) | 2.21 (2) | WM(2)—CP(33) | 2.36 (3) | WM(3)—CP(53) | 2.23 (2) | WM(4)—CP(73) | 2.33 (3) |
| WM(1)—CP(14) | 2.25 (3) | WM(2)—CP(34) | 2.34 (2) | WM(3)—CP(54) | 2.29 (2) | WM(4)—CP(74) | 2.37 (3) |
| WM(1)—CP(15) | 2.32 (3) | WM(2)—CP(35) | 2.31 (2) | WM(3)—CP(55) | 2.34 (2) | WM(4)—CP(75) | 2.27 (2) |
| MW(1)—C(3) | 1.93 (2) | MW(2)—C(10) | 1.88 (2) | MW(3)—C(17) | 1.89 (2) | MW(4)—C(24) | 1.96 (2) |
| MW(1)—C(4) | 1.91 (2) | MW(2)—C(11) | 1.91 (2) | MW(3)—C(18) | 1.95 (2) | MW(4)—C(25) | 1.90 (2) |
| MW(1)—CP(21) | 2.37 (2) | MW(2)—CP(41) | 2.31 (3) | MW(3)—CP(61) | 2.32 (3) | MW(4)—CP(81) | 2.27 (2) |
| MW(1)—CP(22) | 2.33 (2) | MW(2)—CP(42) | 2.38 (2) | MW(3)—CP(62) | 2.40 (2) | MW(4)—CP(82) | 2.29 (2) |
| MW(1)—CP(23) | 2.23 (3) | MW(2)—CP(43) | 2.37 (2) | MW(3)—CP(63) | 2.37 (2) | MW(4)—CP(83) | 2.33 (2) |
| MW(1)—CP(24) | 2.28 (3) | MW(2)—CP(44) | 2.32 (2) | MW(3)—CP(64) | 2.29 (2) | MW(4)—CP(84) | 2.40 (2) |
| MW(1)—CP(25) | 2.40 (2) | MW(2)—CP(45) | 2.30 (2) | MW(3)—CP(65) | 2.27 (3) | MW(4)—CP(85) | 2.29 (2) |
| Fe(1)—C(5) | 1.75 (2) | Fe(2)—C(12) | 1.74 (3) | Fe(3)—C(19) | 1.78 (2) | Fe(4)—C(26) | 1.79 (2) |
| Fe(1)—C(6) | 1.78 (3) | Fe(2)—C(13) | 1.73 (2) | Fe(3)—C(20) | 1.77 (2) | Fe(4)—C(27) | 1.82 (2) |
| Fe(1)—C(7) | 1.80 (2) | Fe(2)—C(14) | 1.80 (3) | Fe(3)—C(21) | 1.78 (2) | Fe(4)—C(28) | 1.76 (3) |

| Molecule 1 | | Molecule 2 | | Molecule 3 | | Molecule 4 | |
|-------------------|------------|-------------------|------------|-------------------|------------|-------------------|------------|
| MW(1)—WM(1)—Te(1) | 40.73 (4) | MW(2)—WM(2)—Te(3) | 40.56 (3) | MW(3)—WM(3)—Te(5) | 40.92 (4) | MW(4)—WM(4)—Te(7) | 40.77 (4) |
| MW(1)—WM(1)—Te(2) | 40.80 (4) | MW(2)—WM(2)—Te(4) | 40.63 (4) | MW(3)—WM(3)—Te(6) | 40.83 (3) | MW(4)—WM(4)—Te(8) | 40.29 (4) |
| MW(1)—WM(1)—Fe(1) | 68.62 (7) | MW(2)—WM(2)—Fe(2) | 68.44 (7) | MW(3)—WM(3)—Fe(3) | 68.79 (8) | MW(4)—WM(4)—Fe(4) | 68.93 (7) |
| Te(1)—WM(1)—Te(2) | 69.35 (4) | Te(3)—WM(2)—Te(4) | 69.01 (5) | Te(5)—WM(3)—Te(6) | 69.49 (5) | Te(7)—WM(4)—Te(8) | 69.01 (5) |
| Te(1)—WM(1)—Fe(1) | 54.91 (7) | Te(3)—WM(2)—Fe(2) | 54.77 (8) | Te(5)—WM(3)—Fe(3) | 54.92 (6) | Te(7)—WM(4)—Fe(4) | 55.25 (7) |
| Te(2)—WM(1)—Fe(1) | 54.96 (7) | Te(4)—WM(2)—Fe(2) | 54.80 (7) | Te(6)—WM(3)—Fe(3) | 55.12 (7) | Te(8)—WM(4)—Fe(4) | 55.18 (8) |
| WM(1)—MW(1)—Te(1) | 39.92 (3) | WM(2)—MW(2)—Te(3) | 39.89 (4) | WM(3)—MW(3)—Te(5) | 40.04 (4) | WM(4)—MW(4)—Te(7) | 39.93 (3) |
| WM(1)—MW(1)—Te(2) | 40.08 (4) | WM(2)—MW(2)—Te(4) | 40.28 (4) | WM(3)—MW(3)—Te(6) | 40.24 (4) | WM(4)—MW(4)—Te(8) | 39.63 (4) |
| WM(1)—MW(1)—Fe(1) | 39.21 (5) | WM(2)—MW(2)—Fe(2) | 39.28 (5) | WM(3)—MW(3)—Fe(3) | 39.26 (4) | WM(4)—MW(4)—Fe(4) | 38.76 (4) |
| Te(1)—MW(1)—Te(2) | 68.12 (6) | Te(3)—MW(2)—Te(4) | 68.20 (6) | Te(5)—MW(3)—Te(6) | 68.30 (6) | Te(7)—MW(4)—Te(8) | 67.79 (5) |
| Te(1)—MW(1)—Fe(1) | 37.48 (6) | Te(3)—MW(2)—Fe(2) | 37.46 (6) | Te(5)—MW(3)—Fe(3) | 37.45 (5) | Te(7)—MW(4)—Fe(4) | 37.41 (6) |
| Te(2)—MW(1)—Fe(1) | 37.60 (5) | Te(4)—MW(2)—Fe(2) | 37.66 (6) | Te(6)—MW(3)—Fe(3) | 37.71 (5) | Te(8)—MW(4)—Fe(4) | 37.16 (5) |
| WM(1)—Te(1)—MW(1) | 99.35 (6) | WM(2)—Te(3)—MW(2) | 99.54 (5) | WM(3)—Te(5)—MW(3) | 99.05 (6) | WM(4)—Te(7)—MW(4) | 99.31 (6) |
| WM(1)—Te(1)—Te(2) | 55.42 (4) | WM(2)—Te(2)—Te(4) | 55.77 (4) | WM(3)—Te(5)—Te(6) | 55.42 (4) | WM(4)—Te(7)—Te(8) | 55.33 (5) |
| WM(1)—Te(1)—Fe(1) | 63.69 (7) | WM(2)—Te(3)—Fe(2) | 63.81 (9) | WM(3)—Te(5)—Fe(3) | 63.73 (7) | WM(4)—Te(7)—Fe(4) | 62.94 (6) |
| MW(1)—Te(1)—Fe(2) | 55.98 (4) | MW(2)—Te(3)—Te(4) | 55.89 (5) | MW(3)—Te(5)—Te(6) | 55.77 (4) | MW(4)—Te(7)—Te(8) | 55.79 (5) |
| MW(1)—Te(1)—Fe(1) | 100.94 (9) | MW(2)—Te(3)—Fe(2) | 101.02 (9) | MW(3)—Te(5)—Fe(3) | 100.94 (9) | MW(4)—Te(7)—Fe(4) | 101.0 (1) |
| Te(2)—Te(1)—Fe(1) | 52.45 (8) | Te(4)—Te(3)—Fe(2) | 52.55 (8) | Te(6)—Te(5)—Fe(3) | 52.55 (8) | Te(8)—Te(7)—Fe(4) | 52.49 (8) |
| WM(1)—Te(2)—MW(1) | 99.13 (5) | WM(2)—Te(4)—MW(2) | 99.11 (6) | WM(3)—Te(6)—MW(3) | 98.94 (5) | WM(4)—Te(8)—MW(4) | 100.08 (6) |
| WM(1)—Te(2)—Te(1) | 55.22 (4) | WM(2)—Te(4)—Te(3) | 55.21 (4) | WM(3)—Te(6)—Te(5) | 55.09 (4) | WM(4)—Te(8)—Te(7) | 55.65 (4) |
| WM(1)—Te(2)—Fe(1) | 63.54 (7) | WM(2)—Te(4)—Fe(2) | 63.42 (8) | WM(3)—Te(6)—Fe(3) | 63.40 (7) | WM(4)—Te(8)—Fe(4) | 63.19 (7) |
| MW(1)—Te(2)—Te(1) | 55.90 (5) | MW(2)—Te(4)—Te(3) | 55.90 (5) | MW(3)—Te(6)—Te(5) | 55.94 (5) | MW(4)—Te(8)—Te(7) | 56.43 (5) |
| MW(1)—Te(2)—Fe(1) | 100.73 (8) | MW(2)—Te(4)—Fe(2) | 100.8 (8) | MW(3)—Te(6)—Fe(3) | 100.75 (8) | MW(4)—Te(8)—Fe(4) | 101.80 (8) |
| Te(1)—Te(2)—Fe(1) | 52.30 (8) | Te(3)—Te(4)—Fe(2) | 52.27 (1) | Te(5)—Te(6)—Fe(3) | 52.15 (6) | Te(7)—Te(8)—Fe(4) | 52.71 (9) |
| WM(1)—Fe(1)—MW(1) | 72.18 (7) | WM(2)—Fe(2)—MW(2) | 72.28 (7) | WM(3)—Fe(3)—MW(3) | 71.96 (7) | WM(4)—Fe(4)—MW(4) | 72.32 (7) |
| WM(1)—Fe(1)—Te(1) | 61.40 (7) | WM(2)—Fe(2)—Te(3) | 61.42 (7) | WM(3)—Fe(3)—Te(5) | 61.36 (7) | WM(4)—Fe(4)—Te(7) | 61.81 (8) |
| WM(1)—Fe(1)—Te(2) | 61.50 (7) | WM(2)—Fe(2)—Te(4) | 61.78 (7) | WM(3)—Fe(3)—Te(6) | 61.48 (7) | WM(4)—Fe(4)—Te(8) | 61.63 (7) |
| MW(1)—Fe(1)—Te(1) | 41.59 (6) | MW(2)—Fe(2)—Te(3) | 41.52 (6) | MW(3)—Fe(3)—Te(5) | 41.62 (6) | MW(4)—Fe(4)—Te(7) | 41.54 (6) |
| MW(1)—Fe(1)—Te(2) | 41.67 (6) | MW(2)—Fe(2)—Te(4) | 41.56 (7) | MW(3)—Fe(3)—Te(6) | 41.55 (6) | MW(4)—Fe(4)—Te(8) | 41.03 (6) |
| Te(1)—Fe(1)—Te(2) | 75.26 (9) | Te(3)—Fe(2)—Te(4) | 75.17 (9) | Te(5)—Fe(3)—Te(6) | 75.30 (9) | Te(7)—Fe(4)—Te(8) | 74.81 (9) |
| WM(1)—C(1)—O(1) | 174 (1) | WM(2)—C(8)—O(8) | 171 (2) | WM(3)—C(15)—O(15) | 177 (2) | WM(4)—C(22)—O(22) | 177 (2) |
| WM(1)—C(2)—O(2) | 172 (2) | WM(2)—C(9)—O(9) | 171 (2) | WM(3)—C(16)—O(16) | 172 (2) | WM(4)—C(23)—O(23) | 175 (2) |
| MW(1)—C(3)—O(3) | 175 (3) | MW(2)—C(10)—O(10) | 176 (2) | MW(3)—C(17)—O(17) | 179 (2) | MW(4)—C(24)—O(24) | 177 (2) |
| MW(1)—C(4)—O(4) | 177 (2) | MW(2)—C(11)—O(11) | 176 (2) | MW(3)—C(18)—O(18) | 176 (2) | MW(4)—C(25)—O(25) | 178 (3) |
| Fe(1)—C(5)—O(5) | 176 (2) | Fe(2)—C(12)—O(12) | 177 (3) | Fe(3)—C(19)—O(19) | 176 (3) | Fe(4)—C(26)—O(26) | 176 (2) |
| Fe(1)—C(6)—O(6) | 176 (2) | Fe(2)—C(13)—O(13) | 177 (3) | Fe(3)—C(20)—O(20) | 174 (2) | Fe(4)—C(27)—O(27) | 175 (2) |
| Fe(1)—C(7)—O(7) | 175 (2) | Fe(2)—C(14)—O(14) | 175 (3) | Fe(3)—C(21)—O(21) | 175 (2) | Fe(4)—C(28)—O(28) | 177 (2) |

$4F_o^2/[\sigma^2(F_o^2) + (0.04F_o^2)^2]$. Final $R = 0.051$, $wR = 0.058$, $S = 1.2$ with final max. shift/e.s.d = 0.03 for 705 variables. The max. and min. heights in the final difference Fourier map were $+1.23$ and -1.35 e Å⁻³. Scattering factors for neutral atoms and f' , f'' were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). All calculations were carried out with programs from the Enraf-Nonius (1982) *VAXSDP Structure Determination Package* on the VAX 11/785 computer.

Final atomic coordinates and B_{eq} values are presented in Table 1* and selected interatomic distances and bond angles in Table 2. A representative molecule is depicted in Fig. 1. No chemically signifi-

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53663 (24 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

cant differences exist between the four independent molecules.

Related literature. The structure of $\text{Cp}_2\text{W}_{1.2}\text{Mo}_{0.8}\text{Fe}(\mu_3\text{-Te})_2(\text{CO})_7$ is similar to that of $\text{Cp}_2\text{Mo}_2\text{Fe}(\mu_3\text{-Te})_2(\text{CO})_7$ (Bogan, Rauchfuss & Rheingold, 1985), in which the average $\text{Te}\cdots\text{Te}$ distances are also short. It may be significant that both clusters have strong $\text{Te}\cdots\text{Te}$ bonding interactions, which contribute to their stabilization.

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Heptacarbonyl- μ -(diphenylphosphanido)- μ -iodo-(triphenylphosphine)dirhenium(I)

BY U. FLÖRKE AND H.-J. HAUPT

Anorganische und Analytische Chemie, Universität-GH Paderborn, Warburgerstrasse 100, D-4790 Paderborn, Germany

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Abstract. $[\text{Re}_2\text{I}\{\text{P}(\text{C}_6\text{H}_5)_2\}(\text{CO})_7\{\text{P}(\text{C}_6\text{H}_5)_3\}]$, $M_r = 1142.8$, monoclinic, $P2_1/n$, $a = 10.526(2)$, $b = 18.381(6)$, $c = 19.457(7)$ Å, $\beta = 100.57(2)^\circ$, $V = 3700.6$ Å³, $Z = 4$, $D_x = 2.051$ g cm⁻³, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 75.8$ cm⁻¹, $F(000) = 2144$, $T = 298(1)$ K, $R = 0.048$, $wR = 0.043$ for 3538 unique observed intensities. The coordination polyhedra of the two Re atoms are distorted octahedra and share μ -I and μ -PPh₂ (Ph = phenyl) as common ligands. The terminal PPh₃ group is *trans* to the μ -PPh₂ bridge. There is no Re–Re bonding in this 36 valence electron cluster.

Experimental. The compound was prepared by reaction of $[\text{Re}_2(\text{CO})_7(\mu\text{-H})(\mu\text{-PPh}_2)(\text{PPh}_3)]$ (Haupt, Balsaa & Flörke, 1988) and iodine in CHCl_3 solution at 293 K for 6 h and recrystallized from CHCl_3 . Yellow crystal, size $0.10 \times 0.11 \times 0.45$ mm. Lattice parameters from 25 reflections $10 \leq 2\theta \leq 25^\circ$. Nicolet *R3m/V* diffractometer, graphite monochromator, Mo $K\alpha$ radiation. ω – 2θ scan; 5731 intensities $3 \leq 2\theta \leq 46^\circ$; $0 \leq h \leq 11$, $0 \leq k \leq 20$, $-21 \leq l \leq 21$; three standard reflections monitored every 400 reflections, steady decrease of 10% in intensities scaled on standards, Lp correction, empirical absorption correction *via* ψ scans, min./max. transmission 0.141/0.163; 5177 unique intensities after merging, $R_{\text{int}} = 0.039$, 3538 with $F > 4\sigma(F)$. Structure solved by direct methods and subsequent ΔF maps; full-matrix least-squares refinement based on F and 383

parameters. All non-H atoms refined anisotropically, H atoms fixed from geometrical considerations with isotropic displacement parameters $U_{\text{iso}} = 0.09$ Å²; phenyl groups treated as rigid bodies (C–C 1.395 Å); $R = 0.0481$, $wR = 0.0436$, $w^{-1} = \sigma^2(F) + 0.000558F^2$, $S = 1.148$; max. $(\Delta/\sigma) = 0.001$; max. height in final ΔF map 1.1 e Å⁻³, min. height in final ΔF map 1.0 e Å⁻³. Scattering factors, structure solution and refinement: *SHELXTL-Plus88* (Sheldrick, 1988). Atomic parameters are given in Table 1,

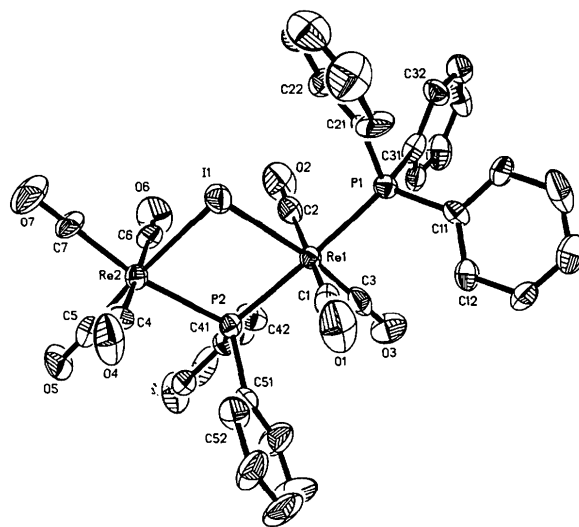


Fig. 1. Molecular structure of the title compound.