# Additions and Corrections

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**Thomas Wegener and Gernot Frenking***: Theoretical Study of Transition Metal Compounds with Molybdenum−and Tungsten−Phosphorus Triple Bonds.

Page 1810. Table 5 is missing data. The complete table appears below.

**Table 5.** Polarization and Hybridization of the Metal−Ligand and P−S Bonds at B3LYP/II Using the NBO Method

| compound | | bond M−L | % M | % s (M) | % p (M) | % d (M) | % L | % s (L) | % p (L) | % d (L) |
|---|---|---|---|---|---|---|---|---|---|---|
| $[Mo(P)(NH_2)_3]$ | **1** | Mo−P ($\sigma$) | 49.4 | 34.7 | 0.2 | 65.1 | 50.6 | 13.3 | 86.3 | 0.5 |
| | | Mo−P ($\pi$) | 49.7 | 0.0 | 16.9 | 83.1 | 50.4 | 0.0 | 99.5 | 0.5 |
| | | Mo−P ($\pi$) | 45.6 | 0.0 | 24.4 | 75.6 | 54.4 | 0.0 | 99.5 | 0.5 |
| | | $Mo-N_{eq}$ | 17.1 | 21.8 | 13.6 | 64.7 | 82.9 | 40.0 | 60.0 | 0.0 |
| $[W(P)(NH_2)_3]$ | **2** | W−P ($\sigma$) | 47.5 | 35.0 | 0.2 | 64.9 | 52.5 | 14.9 | 84.6 | 0.5 |
| | | W−P ($\pi$) | 46.7 | 0.0 | 16.2 | 83.8 | 53.3 | 0.0 | 99.5 | 0.5 |
| | | W−P ($\pi$) | 43.2 | 0.0 | 22.8 | 77.2 | 56.8 | 0.0 | 99.5 | 0.5 |
| | | $W-N_{eq}$ | 15.9 | 21.7 | 12.9 | 65.5 | 84.1 | 41.8 | 58.1 | 0.0 |
| $[Mo(PS)(NH_2)_3]$ | **3** | Mo−P ($\sigma$) | 25.8 | 46.9 | 0.3 | 52.8 | 74.2 | 59.5 | 40.5 | 0.0 |
| | | Mo−P ($\pi$) | 61.4 | 0.0 | 0.3 | 99.7 | 38.6 | 0.0 | 99.4 | 0.6 |
| | | Mo−P ($\pi$) | 61.5 | 0.0 | 0.3 | 99.7 | 38.5 | 0.0 | 99.4 | 0.6 |
| | | $Mo-N_{eq}$ | 23.7 | 17.3 | 0.5 | 82.2 | 76.3 | 25.4 | 74.6 | 0.0 |
| | | P−S | 48.2 | 40.6 | 58.7 | 0.7 | 51.8 | 16.0 | 83.2 | 0.8 |
| $[W(PS)(NH_2)_3]$ | **4** | W−P ($\sigma$) | 28.0 | 44.8 | 0.2 | 55.0 | 72.1 | 58.1 | 41.9 | 0.0 |
| | | W−P ($\pi$) | 56.6 | 0.0 | 0.5 | 99.5 | 43.4 | 0.0 | 99.5 | 0.6 |
| | | W−P ($\pi$) | 56.6 | 0.0 | 0.5 | 99.5 | 43.4 | 0.0 | 99.5 | 0.6 |
| | | $W-N_{eq}$ | 21.3 | 18.2 | 0.4 | 81.4 | 78.7 | 29.2 | 70.8 | 0.0 |
| | | P−S | 49.6 | 41.6 | 57.7 | 0.7 | 50.4 | 15.1 | 84.1 | 0.8 |
| $[Mo(P)(NH_2)_3(NH_3)]$ | **5** | Mo−P ($\sigma$) | 44.2 | 41.2 | 0.3 | 58.5 | 55.8 | 18.2 | 81.5 | 0.4 |
| | | Mo−P ($\pi$) | 53.7 | 0.0 | 13.4 | 86.6 | 46.3 | 0.0 | 99.5 | 0.5 |
| | | Mo−P ($\pi$) | 50.6 | 0.0 | 19.6 | 80.4 | 49.4 | 0.0 | 99.5 | 0.5 |
| | | $Mo-N_{eq}$ | 16.4 | 19.6 | 14.9 | 65.5 | 83.6 | 41.3 | 58.7 | 0.0 |
| $[W(P)(NH_2)_3(NH_3)]$ | **6** | W−P ($\sigma$) | 42.2 | 41.8 | 0.3 | 58.0 | 57.9 | 21.8 | 77.8 | 0.4 |
| | | W−P ($\pi$) | 48.4 | 0.0 | 16.9 | 83.1 | 51.6 | 0.0 | 99.5 | 0.5 |
| | | W−P ($\pi$) | 50.8 | 0.0 | 12.6 | 87.5 | 49.2 | 0.0 | 99.5 | 0.5 |
| | | $W-N_{eq}$ | 15.1 | 19.4 | 13.0 | 67.6 | 84.9 | 56.6 | 43.4 | 0.0 |
| $[Mo(P)(N_3N)]$ | **7** | Mo−P ($\sigma$) | 46.7 | 37.3 | 0.4 | 62.4 | 53.3 | 19.2 | 80.5 | 0.4 |
| | | Mo−P ($\pi$) | 59.7 | 0.0 | 0.2 | 99.9 | 40.3 | 0.0 | 99.5 | 0.5 |
| | | Mo−P ($\pi$) | 57.9 | 5.2 | 0.2 | 94.6 | 42.1 | 0.0 | 99.5 | 0.5 |
| | | $Mo-N_{eq}$ | 21.9 | 27.4 | 0.2 | 72.5 | 78.1 | 30.5 | 69.5 | 0.0 |
| $[W(P)(N_3N)]$ | **8** | W−P ($\sigma$) | 42.8 | 41.7 | 0.3 | 58.0 | 57.2 | 23.3 | 76.4 | 0.4 |
| | | W−P ($\pi$) | 49.5 | 0.0 | 19.6 | 80.4 | 50.5 | 0.0 | 99.5 | 0.5 |
| | | W−P ($\pi$) | 47.0 | 0.2 | 13.0 | 86.9 | 53.0 | 0.0 | 99.6 | 0.5 |
| | | $W-N_{eq}$ ($\sigma$) | 16.9 | 19.5 | 11.4 | 69.1 | 83.2 | 40.1 | 59.9 | 0.0 |
| $[Mo(PS)(NH_2)_3(NH_3)]$ | **9** | Mo−P ($\sigma$) | 25.4 | 47.0 | 0.1 | 52.9 | 74.6 | 63.9 | 36.1 | 0.0 |
| | | Mo−P ($\pi$) | 58.1 | 0.0 | 11.2 | 88.8 | 41.9 | 0.0 | 99.5 | 0.5 |
| | | Mo−P ($\pi$) | 54.3 | 0.0 | 17.1 | 83.0 | 45.8 | 0.0 | 99.5 | 0.5 |
| | | $Mo-N_{eq}$ | 16.3 | 17.4 | 15.2 | 67.4 | 83.8 | 41.9 | 58.0 | 0.0 |
| | | P−S | 46.4 | 36.3 | 62.9 | 0.8 | 53.6 | 17.4 | 81.8 | 0.8 |
| $[W(PS)(NH_2)_3(NH_3)]$ | **10** | W−P ($\sigma$) | 27.2 | 45.1 | 0.1 | 54.8 | 72.8 | 63.4 | 36.6 | 0.0 |
| | | W−P ($\pi$) | 59.2 | 0.0 | 0.2 | 99.8 | 40.8 | 0.0 | 99.5 | 0.5 |
| | | W−P ($\pi$) | 59.2 | 0.0 | 0.2 | 99.8 | 40.8 | 0.0 | 99.5 | 0.5 |
| | | $W-N_{eq}$ | 20.5 | 18.2 | 0.1 | 81.7 | 79.5 | 44.0 | 55.9 | 0.0 |
| | | P−S | 47.7 | 36.5 | 62.8 | 0.7 | 52.3 | 16.7 | 82.5 | 0.8 |

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