

Additions and Corrections

1998, Volume 37

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 (σ)	49.4	34.7	0.2	65.1	50.6	13.3	86.3	0.5
		Mo-P (π)	49.7	0.0	16.9	83.1	50.4	0.0	99.5	0.5
		Mo-P (π)	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 (σ)	47.5	35.0	0.2	64.9	52.5	14.9	84.6	0.5
		W-P (π)	46.7	0.0	16.2	83.8	53.3	0.0	99.5	0.5
		W-P (π)	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 (σ)	25.8	46.9	0.3	52.8	74.2	59.5	40.5	0.0
		Mo-P (π)	61.4	0.0	0.3	99.7	38.6	0.0	99.4	0.6
		Mo-P (π)	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
[W(PS)(NH ₂) ₃]	4	P-S	48.2	40.6	58.7	0.7	51.8	16.0	83.2	0.8
		W-P (σ)	28.0	44.8	0.2	55.0	72.1	58.1	41.9	0.0
		W-P (π)	56.6	0.0	0.5	99.5	43.4	0.0	99.5	0.6
		W-P (π)	56.6	0.0	0.5	99.5	43.4	0.0	99.5	0.6
[Mo(P)(NH ₂) ₃ (NH ₃)]	5	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 (σ)	44.2	41.2	0.3	58.5	55.8	18.2	81.5	0.4
		Mo-P (π)	53.7	0.0	13.4	86.6	46.3	0.0	99.5	0.5
[W(P)(NH ₂) ₃ (NH ₃)]	6	Mo-P (π)	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 (σ)	42.2	41.8	0.3	58.0	57.9	21.8	77.8	0.4
		W-P (π)	48.4	0.0	16.9	83.1	51.6	0.0	99.5	0.5
[Mo(P)(N ₃ N)]	7	W-P (π)	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 (σ)	46.7	37.3	0.4	62.4	53.3	19.2	80.5	0.4
		Mo-P (π)	59.7	0.0	0.2	99.9	40.3	0.0	99.5	0.5
[W(P)(N ₃ N)]	8	Mo-P (π)	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 (σ)	42.8	41.7	0.3	58.0	57.2	23.3	76.4	0.4
		W-P (π)	49.5	0.0	19.6	80.4	50.5	0.0	99.5	0.5
[Mo(PS)(NH ₂) ₃ (NH ₃)]	9	W-P (π)	47.0	0.2	13.0	86.9	53.0	0.0	99.6	0.5
		W-N _{eq} (σ)	16.9	19.5	11.4	69.1	83.2	40.1	59.9	0.0
		Mo-P (σ)	25.4	47.0	0.1	52.9	74.6	63.9	36.1	0.0
		Mo-P (π)	58.1	0.0	11.2	88.8	41.9	0.0	99.5	0.5
[W(PS)(NH ₂) ₃ (NH ₃)]	10	Mo-P (π)	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-P (σ)	27.2	45.1	0.1	54.8	72.8	63.4	36.6	0.0
		W-P (π)	59.2	0.0	0.2	99.8	40.8	0.0	99.5	0.5
		W-P (π)	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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