

Electronic and structural properties of WO₃:

a systematic hybrid DFT study

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Supporting Information

W valence basis set associated to Hay-Wadt ECP:

0 0 1 2. 1.		
	2.1370000	1.000
0 0 1 2. 1.		
	1.3470000	1.000
0 0 1 2. 1.		
	0.4366000	1.000
0 0 1 2. 1.		
	0.1883000	1.000
0 2 3 6. 1.		
	3.0050000	-0.2405563
	1.2280000	0.7364092
	0.4415000	0.4881487
0 2 1 0. 1.		
	0.4010000	1.000
0 2 1 0. 1.		
	0.20	1.000
0 3 2 0. 1.		
	0.9519000	0.4985265
	0.3270000	0.6111110
0 3 1 0. 1.		
	0.20	1.0000