Electronic Supplementary Information

Structure and Dynamics of Heterometallic Clusters Derived from Addition of Metal Carbonyl Fragments to the Unsaturated Hydride $[W_2Cp_2(\mu\text{-}H)(\mu\text{-}PPh_2)(NO)_2]$

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Table S1. B3LYP-DFT optimized structures for compounds **2**, **3** and **7**, with Gibbs free energies at 298 K (in hartree) indicated below

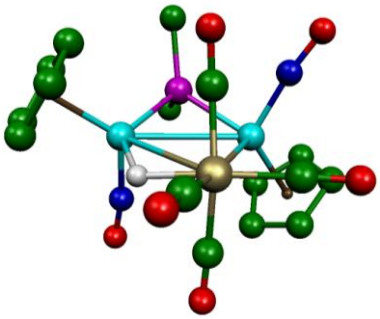
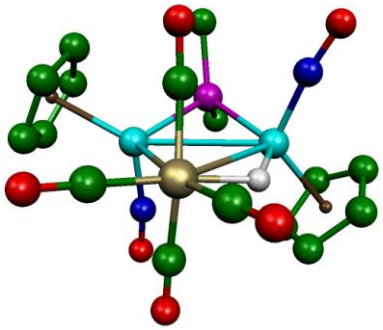
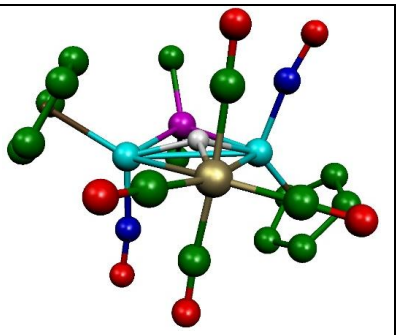
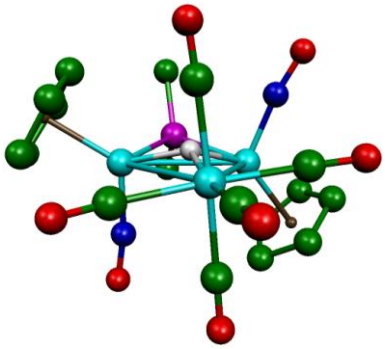
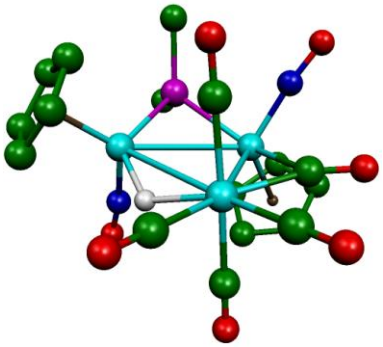
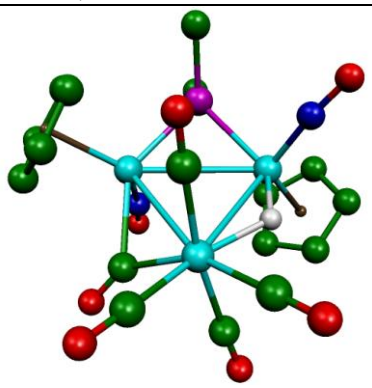
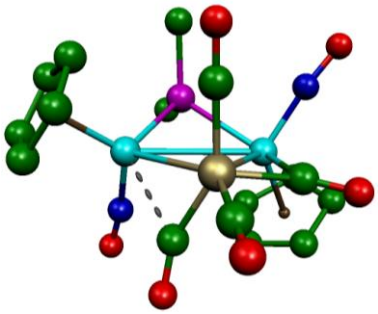
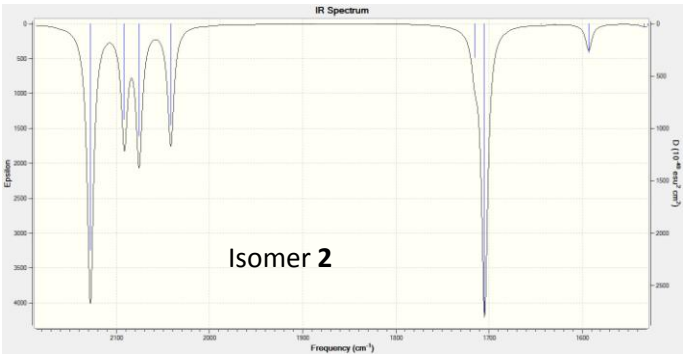
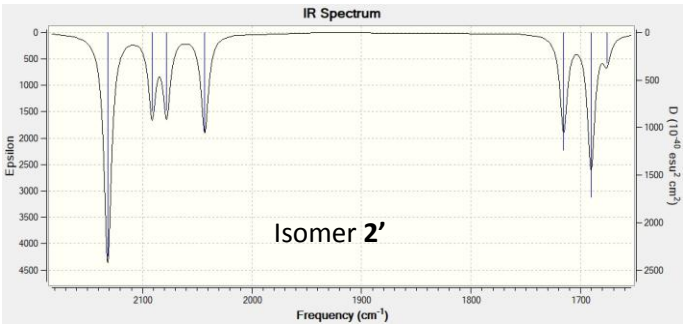
 **2**; G = -2164.413433	 **2'**; G = -2164.412390	 **2F**; G = -2164.411585
 **3**; G = -2222.178117	 **3E**; G = -2222.163867	 **3E'**; G = -2222.158461
 **7**; G = -2185.464009		

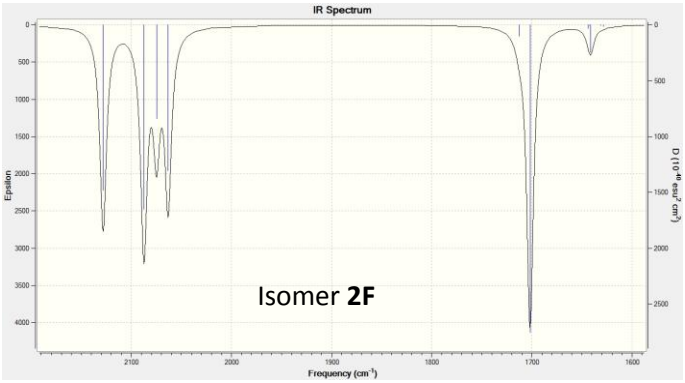
Table S2. Relative Gibbs free energies at 298 K (in kcal/mol) of B3LYP-DFT optimized structures for different isomers of compounds **2** and **3**.

	2	**2'**	**2F**	**3**	**3E**	**3E'**
ΔG	0	0.7	1.2	0	8.9	12.3

Table S3. B3LYP-DFT computed IR spectra of different isomers of compound **2**, with the experimental spectrum (recorded in petroleum ether) shown on the right.







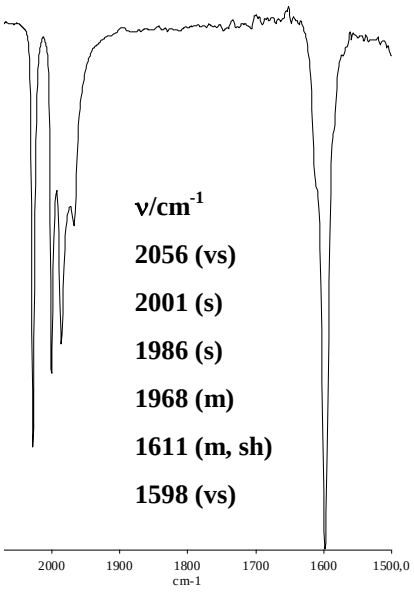


Table S4. B3LYP-DFT computed C–O and N–O stretching frequencies of different isomers of compound **2**, with relative intensities indicated between brackets

Compound	ν (X–O) / cm^{-1}
2	2128(96), 2091(40), 2075(46), 2041(41), 1715(12), 1704(100)
2'	2131(100), 2091(34), 2077(34), 2043(43), 1715(42), 1690(58)
2F	2128(67), 2087(73), 2074(37), 2063(57), 1712(4), 1701(100)

Reference 47:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; *Gaussian 03, Revision B.02*, Gaussian, Inc., Wallingford, CT, 2004.