Electronic Supplementary Information for Dalton Transactions

Supporting Information for:

Intramolecular Apical Metal---H-C_{sp3} Interaction in Molybdenum and Silver Complexes

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Contents:

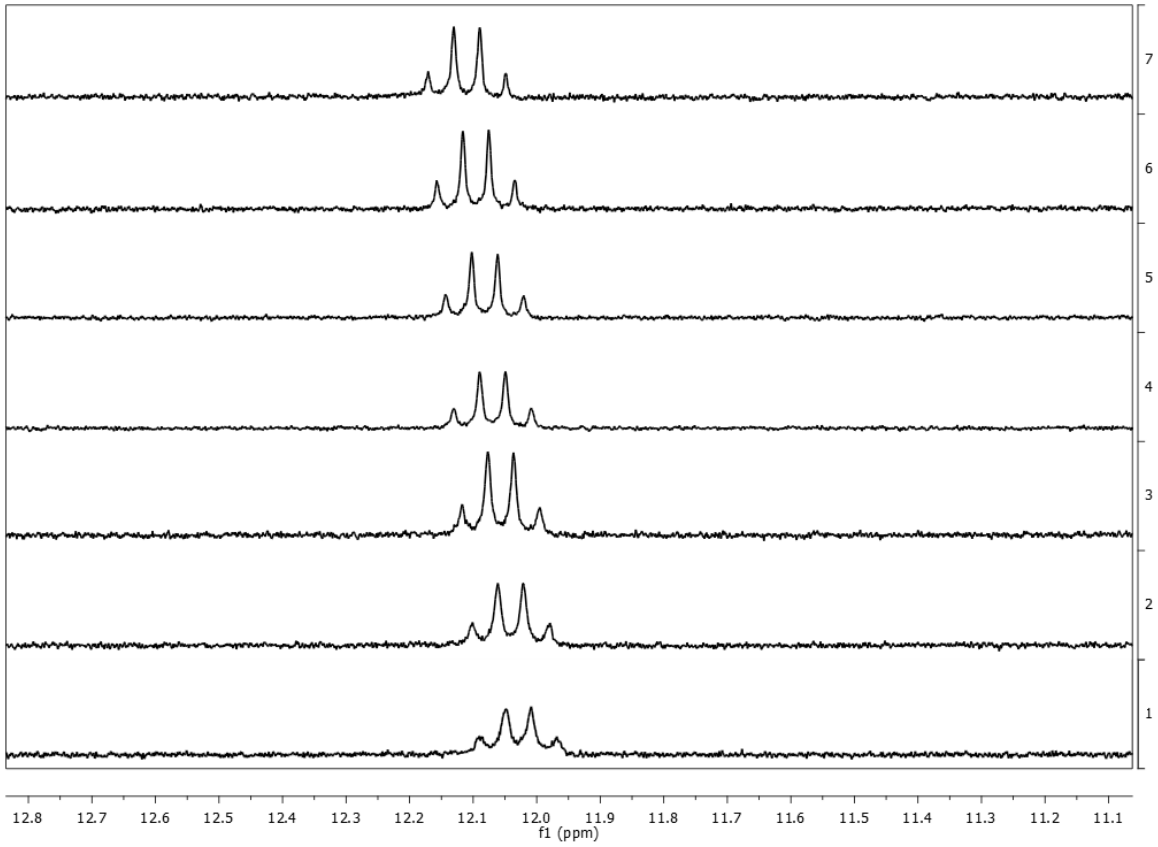

Figure S1: Variable temperature ^{1}H-NMR spectra for Mo complex **4** performed in chloroform in the available temperature range for this solvent. Up to down: +45, +25, +5, -10, -25, -40, and -55 ºC.

Theoretical Methods

Geometry optimization. Stationary points were characterized by frequency analysis. All the calculations were carried out using the Gaussian 03 program package.[1] Due to the large size of the compounds (from 125 to 129 atoms), the optimization of their structures was carried out using the two layer basis set[2] scheme shown in figure S2. For the HTIMP3 ligand, the 6-31g(d) level was used. The B3PW91[3] functional was used to optimize the model systems. In agreement with its NMR spectra, the optimization of the structure of **1** was performed using a C3 symmetric coordination environment.

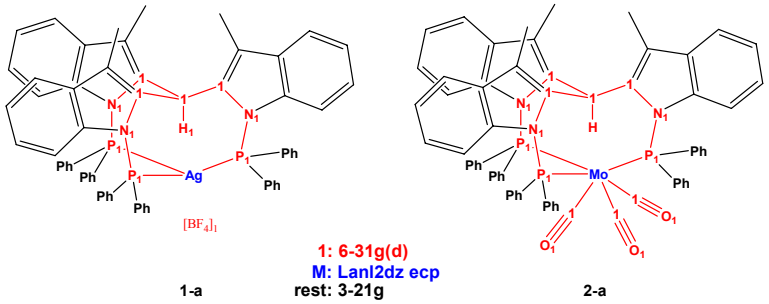

Figure S2

NMR Chemical Shift Calculations. The B3LYP functional together with a locally dense basis set[2] scheme were used to calculate the ^{1}H-NMR chemical shielding.[4] ^{1}H-NMR-GIAO calculations were carried out using the three layer basis set scheme shown in the figure S3. TMS B3LYP/6-311++g(2d,2p) was used as ^{1}H-NMR reference.

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

[2] Basis Set Exchange: A Community Database for Computational Sciences Schuchardt, K.L.; Didier, B.T.; Elsethagen, T.; Sun, L.; Gurumoorthi, V.; Chase, J.; Li, J.; Windus, T.L. *J. Chem. Inf. Model.*, **2007**, 10.1021/ci600510j.

[3] Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. Perdew, J. P.; Wang, Y. *Phys. Rev. B. Condens. Mater. Phys.* **1992**, *45*, 13244.

[4] Zhang, Y.; Lewis, J. C.; Bergman, R. G.; Ellman, J. A.; Oldfield, E. *Organometallics* **2006**, *25*, 3515, and reference 18 within.

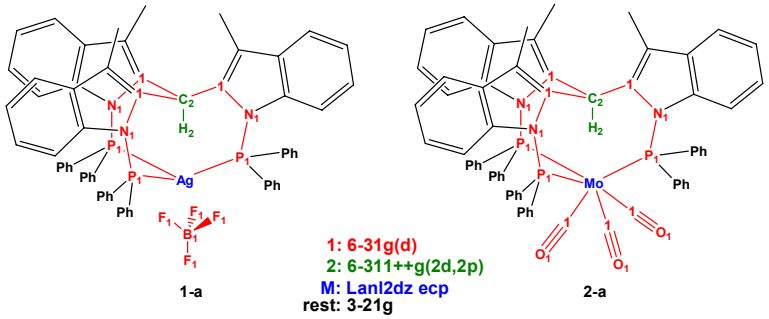


Figure S4

AIM analysis.[5] The electron density $\rho(\mathbf{r})$ parameter was analysed by using the model compounds shown in figure S4.

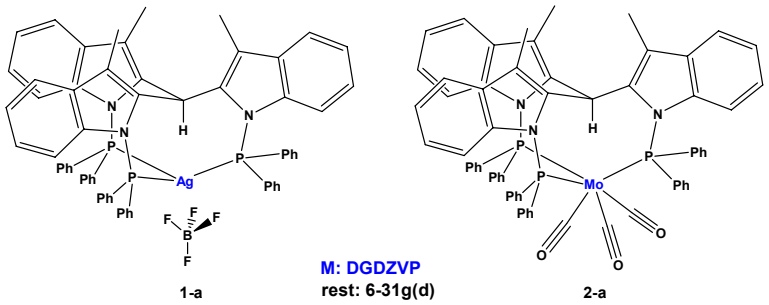


Figure S3

In AIM analysis, the topological properties of the electron density $\rho(\mathbf{r})$ are explored to define the bond path between bonding (o interacting) atoms. A critical point (CP) is defined when the gradient field $\nabla\rho(\mathbf{r})=0$ and classified according to the eigenvalues of the Hessian matrix. The critical points are defined by rank and signature. For rank = 3 (number of non-zero eigenvalues of the Hessian matrix), the critical points have 4 different values of signature (algebraic sum of signs of eigenvalues). At the (3,-3) CP, local maximum, all curvatures of $\rho(\mathbf{r})$ are negative; it corresponds to a nucleus. At the (3,-1) CP, two curvatures are negative (maximum) and one is positive (minimum); it corresponds to a bond critical point (BCP). The trajectory that belongs to the positive curvature is the bond path connecting the two bonded atoms. Two nuclei are considered to be linked by a chemical bond if they have the corresponding (3,-1) BCP. The points

[5] Bader, R. F. W. *Atoms in Molecules: A Quantum Theory*, Oxford: New York, **1990**. Bader, R. F. W. *J. Phys. Chem. A,* **1998**, *102*, 7314. Bieger-king, F. AIM2000, Version 1.0; University of Applied Science: Bielefeld, Germany. For a detailed discussion of AIM see the Supporting Information.

(3, +1) (3,+3) are defined as the ring critical point (RCP) and the cage critical point (CCP), respectively.

The nature of the bond can be characterized by the analysis of the BCP. The electron density, ρ_b, the Laplacian $\nabla^2\rho_b$ and the electronic energy density, (kinetic, potential and total energy density, G_b, V_b and H_b respectively) at the critical point give the properties of the bonding interaction.

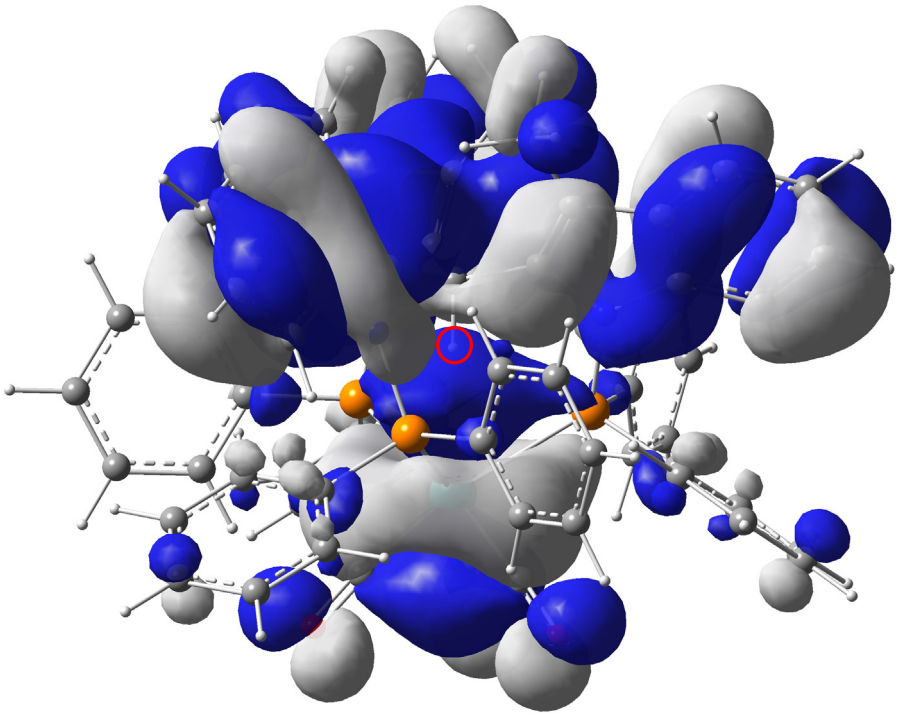
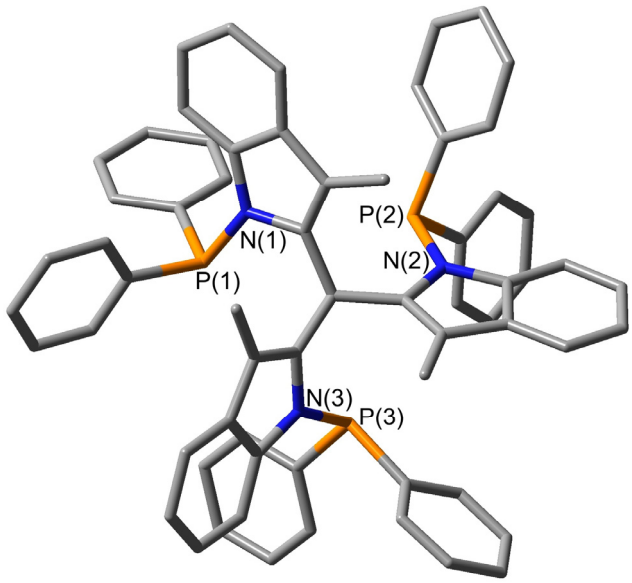


Figure S5. HOMO-5 in complex **4** (isovalue 0.01 a.u.). The hydrogen atom involved in the M---H interaction is highlighted in a red cycle.

Optimized coordinates for compound 1



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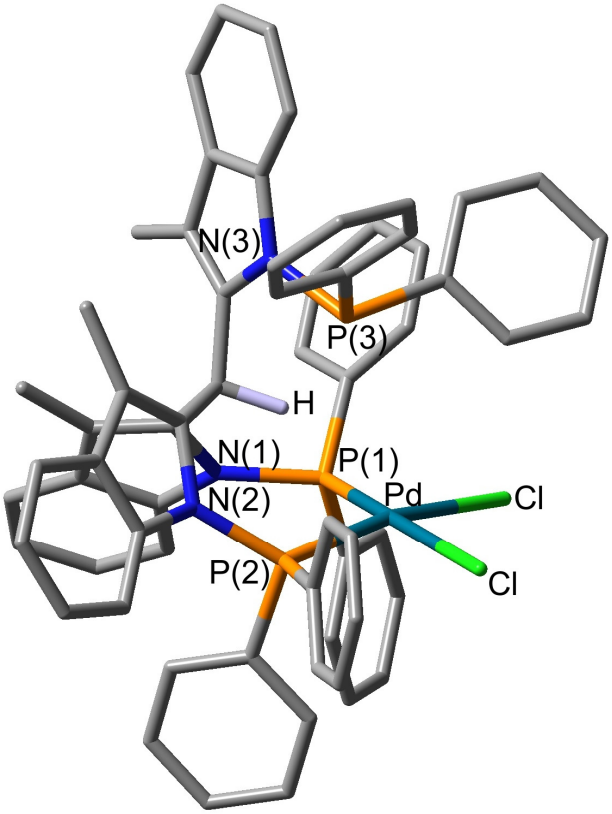

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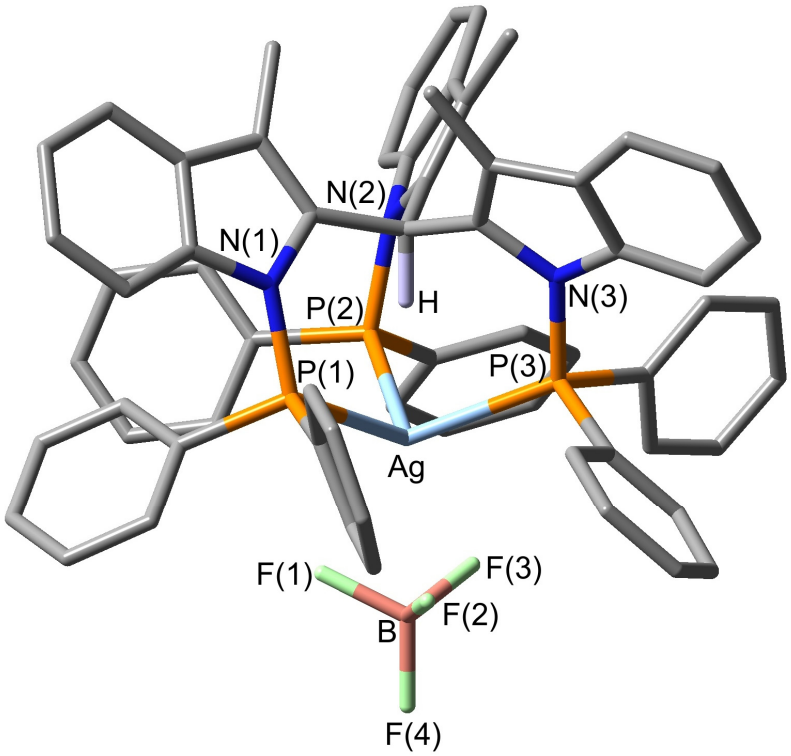
Optimized coordinates for compound 3



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F	0.59923100	1.19926800	-3.65592400
F	-1.32774200	-0.06751400	-3.65833000
B	0.00163800	0.01031400	-4.21759900
P	-1.32208700	1.97536500	-0.41680400
P	-1.05596500	-2.13264700	-0.42068500
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H	6.00296300	-3.52851700	-2.85378200

H	6.09573600	-1.12266700	-3.46709700
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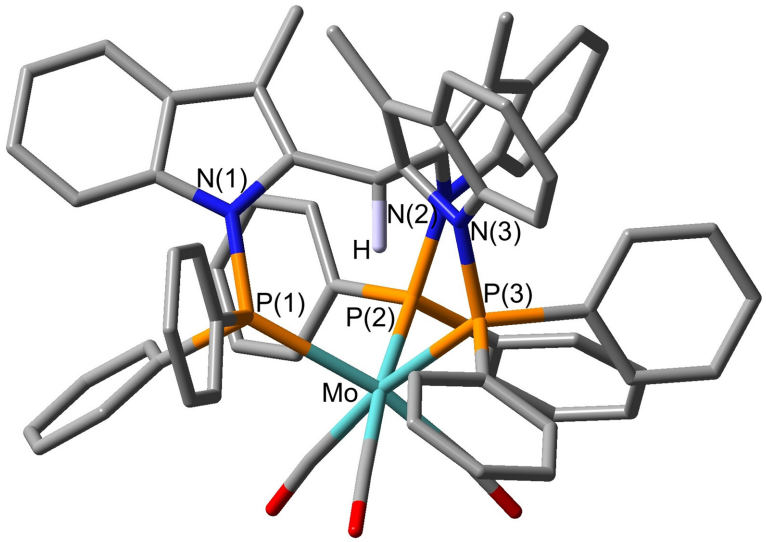
Optimized coordinates for compound 4



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N	1.76034500	-1.68903500	1.12091200
N	0.58270900	2.36307200	1.12061600
N	-2.35092700	-0.66284300	1.10718400
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C	0.75030600	1.25024700	1.98579800
C	-1.46792200	0.02144000	1.98286200
C	-0.00353200	-0.00452400	1.64378600
H	-0.00267200	-0.00095800	0.54270600
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C	2.57832800	3.16966100	-1.24110200
C	2.56757600	5.24770300	3.37388100
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H	-0.71429700	-3.12786300	4.39413900
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H	1.44063900	1.12244500	5.16354100
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H	3.81475500	5.71684000	-3.12575800
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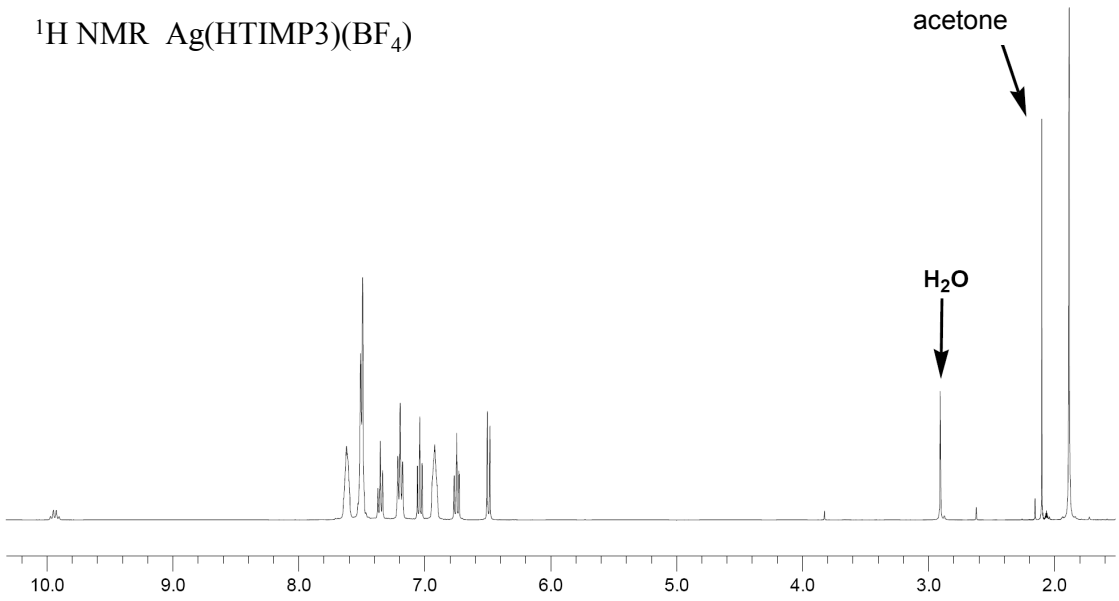
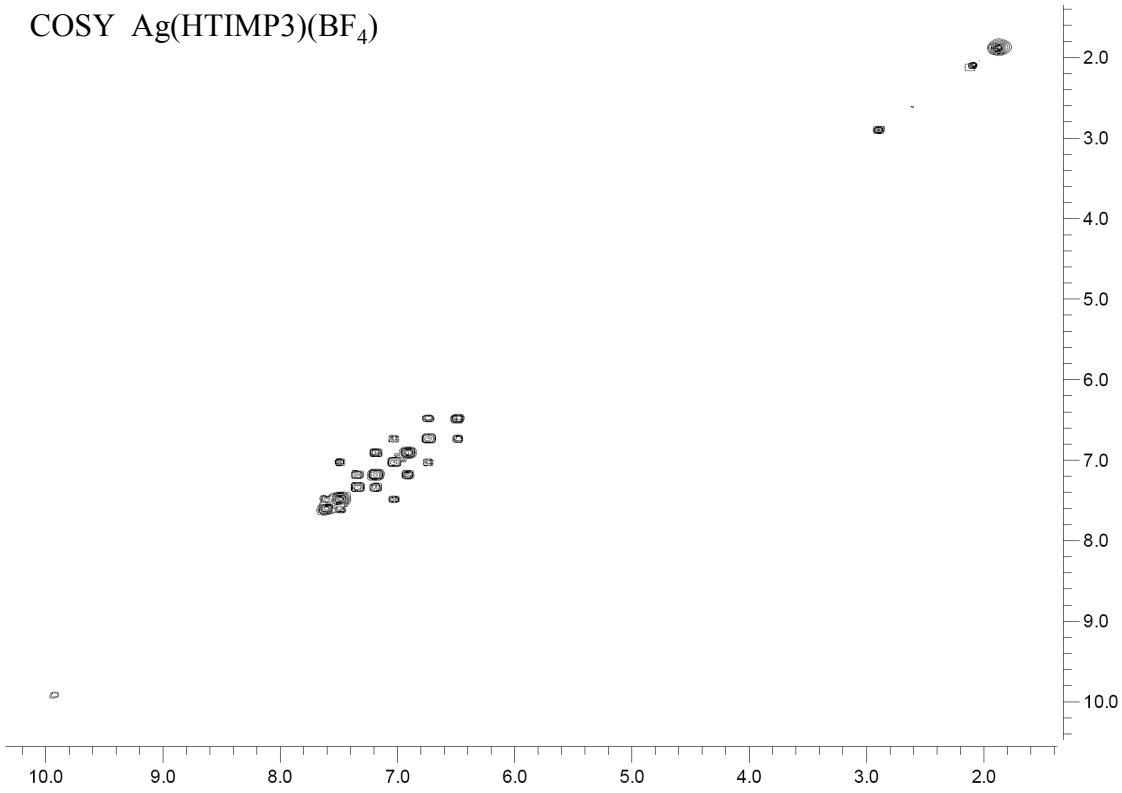
NMR Spectra of Ag(HTIMP3)(BF_4) and Mo($CO)_3$(HTIMP3)

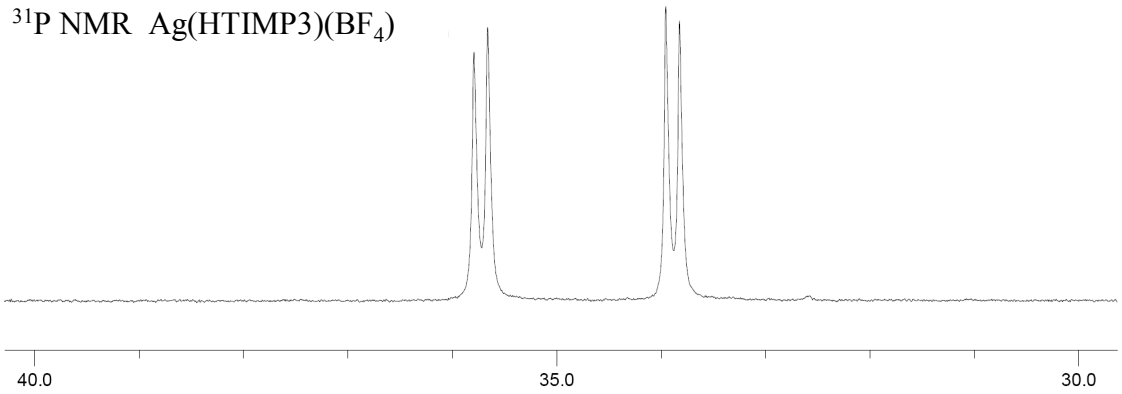
^{1}H NMR Ag(HTIMP3)(BF_4)



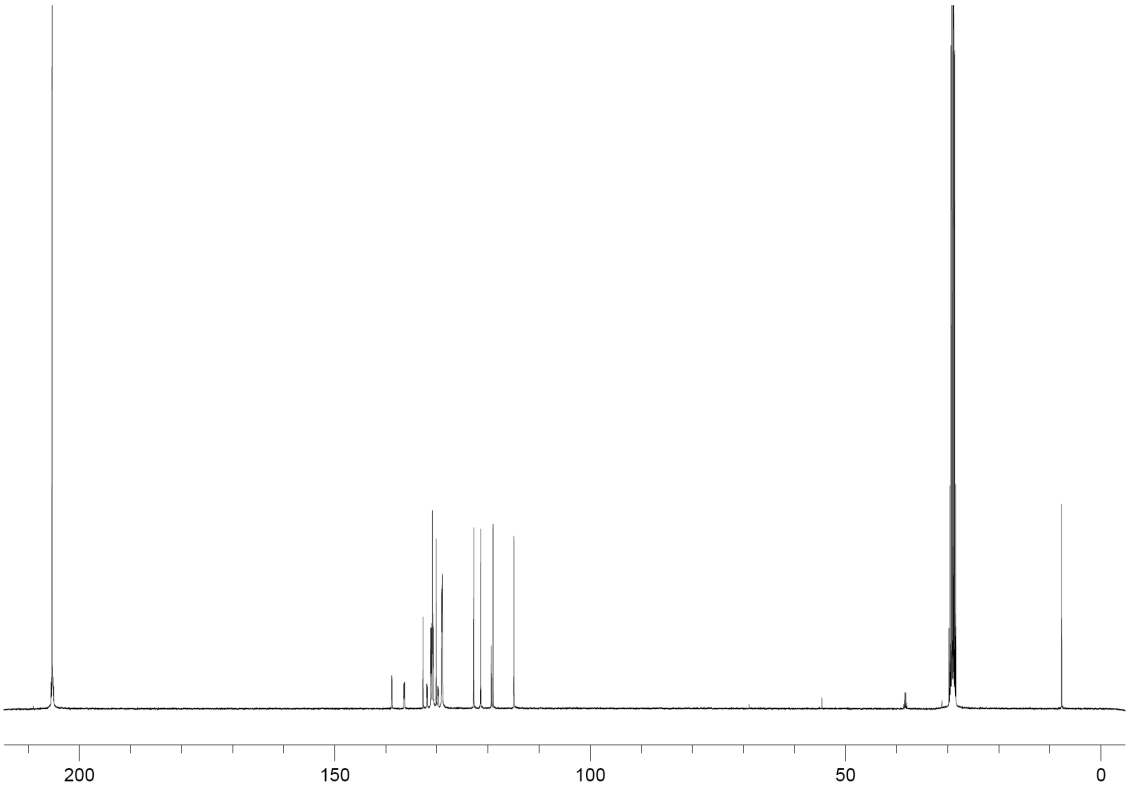
COSY Ag(HTIMP3)(BF_4)

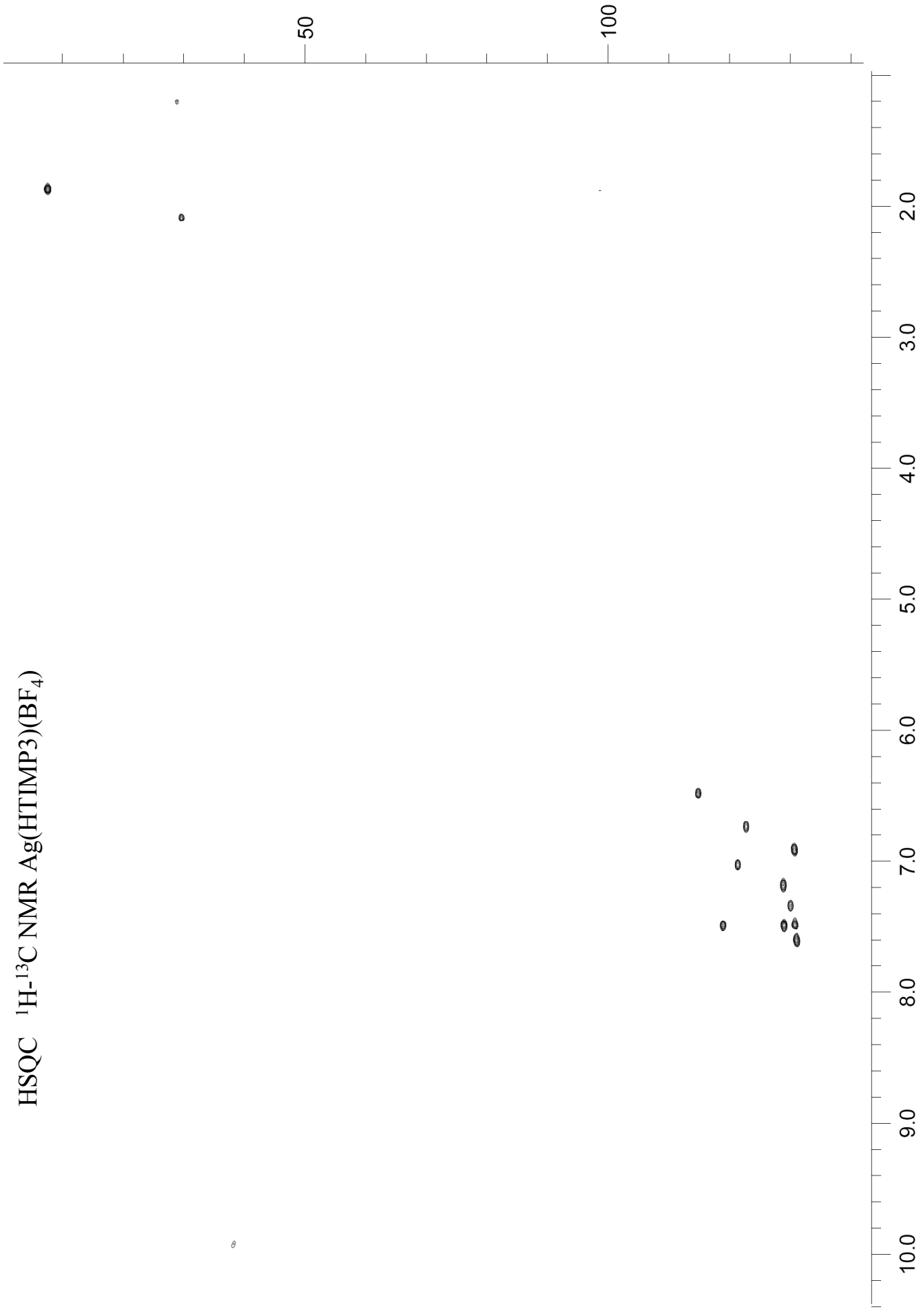


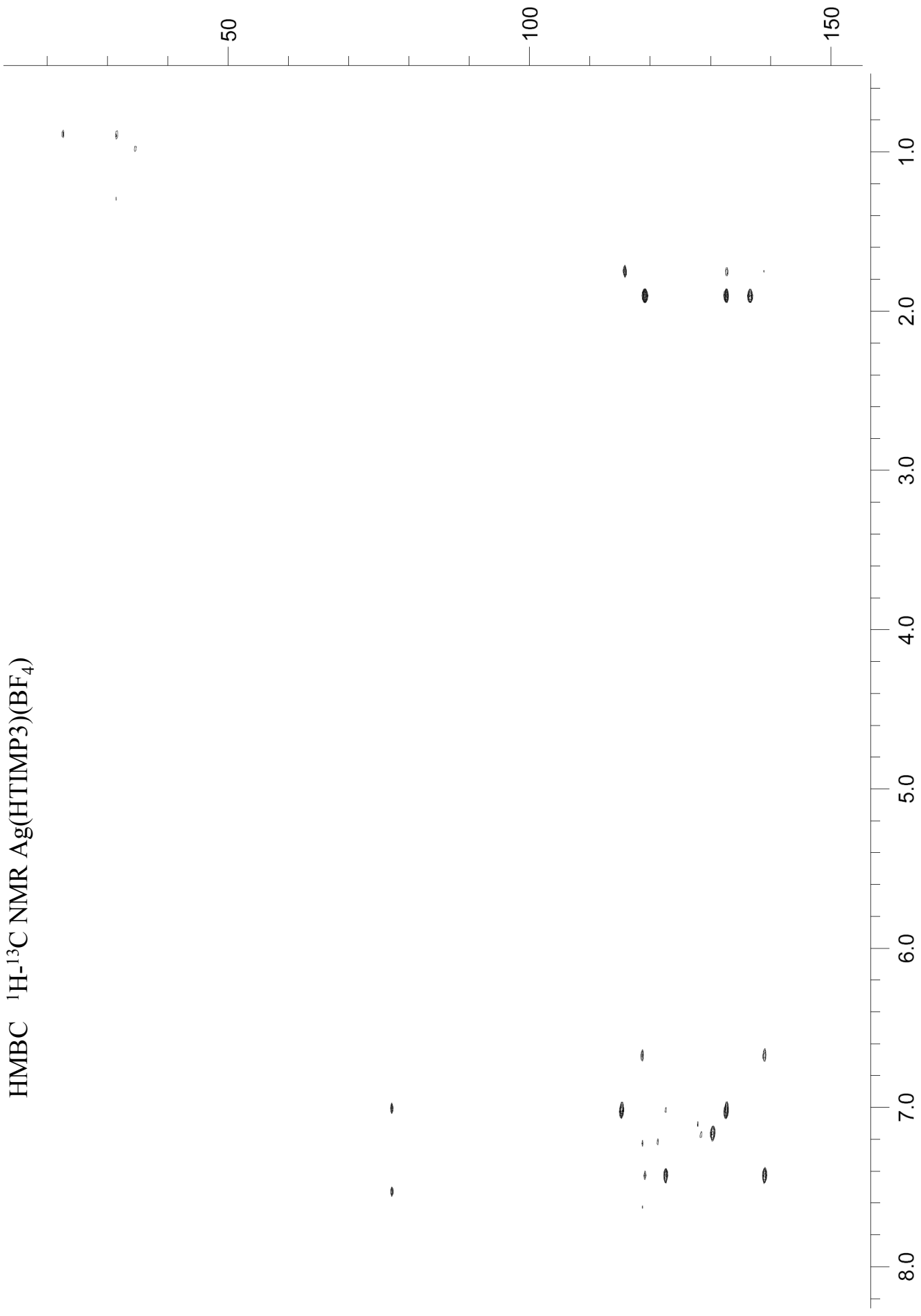
^{31}P NMR Ag(HTIMP3)(BF_4)



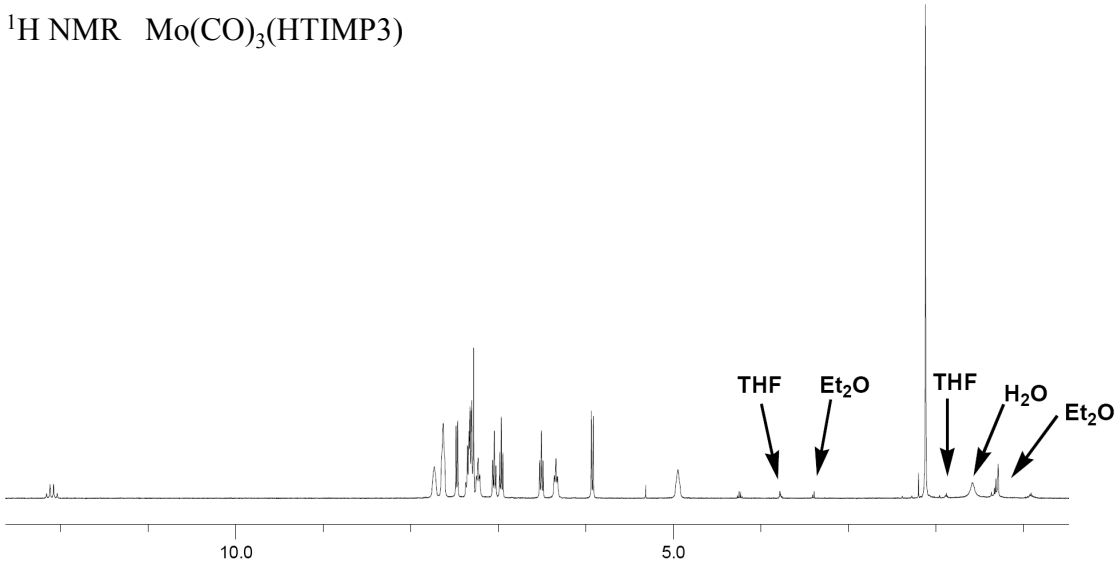
^{13}C NMR Ag(HTIMP3)(BF_4)



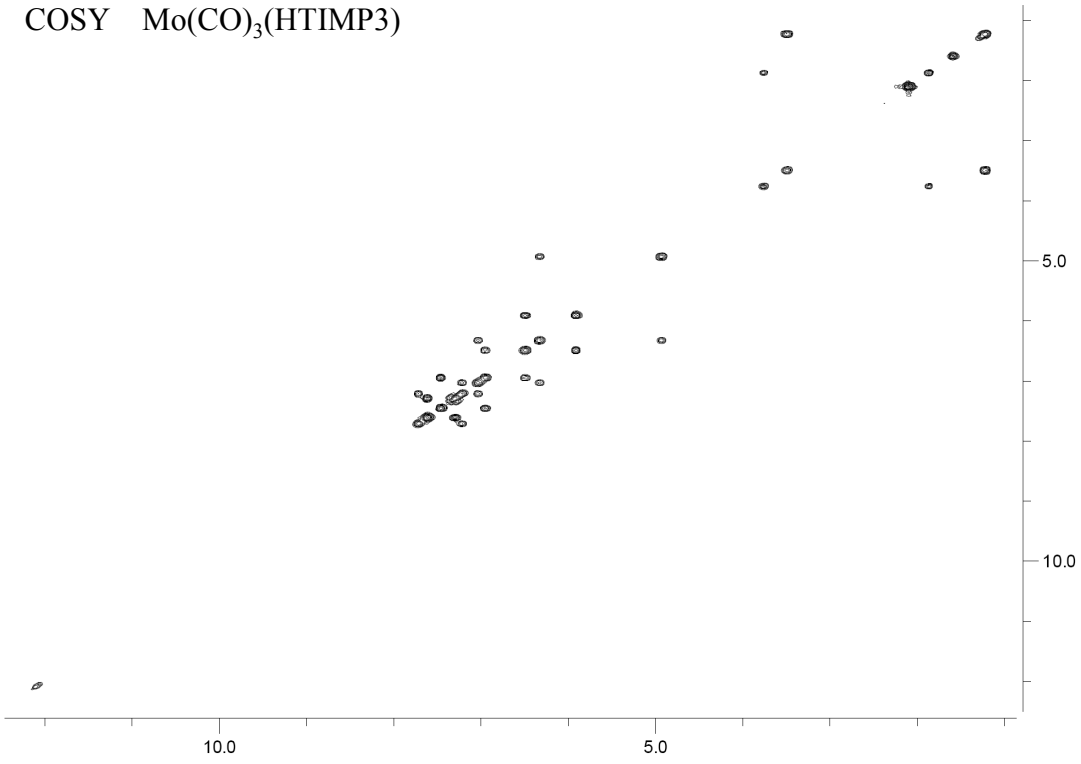




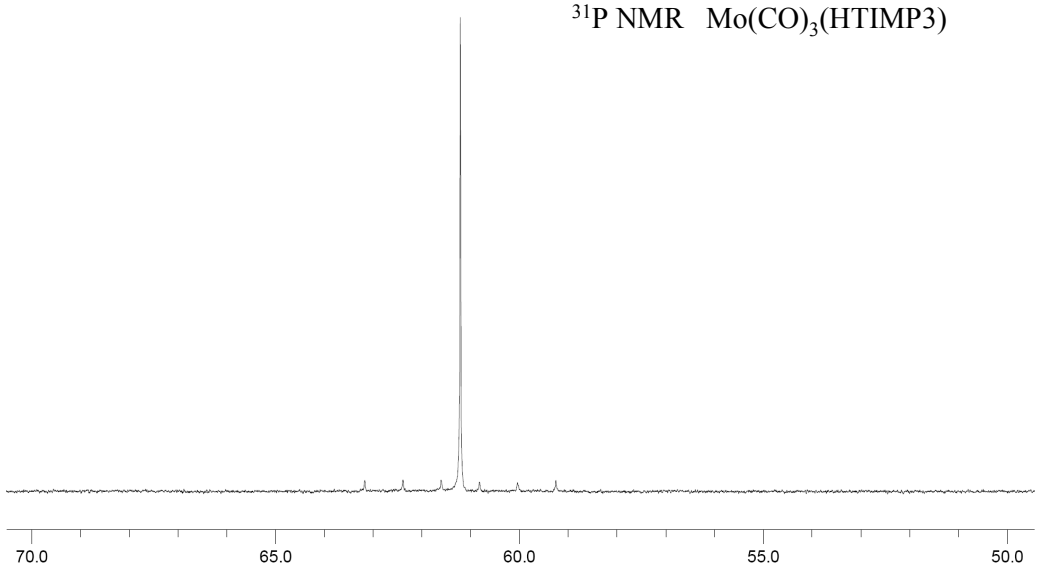
^{1}H NMR $Mo(CO)_3$(HTIMP3)



COSY $Mo(CO)_3$(HTIMP3)



^{31}P NMR Mo(CO)$_3$(HTIMP3)



^{13}C NMR Mo(CO)$_3$(HTIMP3)