Supporting Information for

"Dynamical Intramolecular Metal to Metal Ligand Exchange of Phosphine and Thioether Ligands in Derivatives $PtRu_5(CO)_{16}(\mu_6\text{-}C)$"

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Crystal Solution and Refinement Details

Compound **2** crystallized in the orthorhombic crystal system. The systematic absences observed during the collection of the intensity data were consistent with the space groups $Pna2_1$ and *Pnma*. The structure was solved in the space group $Pna2_1$ by a combination of direct methods (SIR92) and difference Fourier syntheses. Efforts to solve the structure in the space group *Pnma* were unsuccessful. The crystal of **2** contains two independent formula units in the asymmetric crystal unit. Because of the large number of atoms, only the platinum, ruthenium, and phosphorus atoms were refined with anisotropic thermal parameters. The hydrogen atoms on the PMe_2Ph ligand were calculated by assuming idealized geometry with the C - H distances at 0.95Å. Their scattering contributions were added to the structure factor calculations, but their positions were not refined. Since the space group $Pna2_1$ is polar, a test for the enantiomorph of the crystal was also performed by inverting the coordinates of all atoms in the final stages of the refinement and refining again. The second refinement was significantly better than the first. This was thus deemed to be the correct enantiomorph and the results of this refinement are the ones reported herein.

Compound **3** crystallized in the monoclinic crystal system. The systematic absences were consistent with either of the space groups $P2_1/m$ or $P2_1$. $P2_1/m$ was selected and the structure was solved by

a combination of direct methods (SIR92) and difference Fourier syntheses. With Z = 2 the molecule contains crystallographic mirror symmetry. All non-hydrogen atoms were refined with anisotropic thermal parameters. The hydrogen atoms on the PMe_2Ph ligand were calculated by assuming idealized geometry with the C - H distances at 0.95Å. Their scattering contributions were added to the structure factor calculations, but their positions were not refined.

Compound **6** crystallized in the monoclinic crystal system. The space group $P2_1/c$ was identified uniquely on the basis of systematic absences observed during the collection of the intensity data. The structure All the nonhydrogen atoms were refined with anisotropic thermal parameters. The structure was solved by a combination of direct methods and difference Fourier syntheses, and refined by full-matrix least-squares on F^2, using the SHELXTL software package.[1]

1. Sheldrick, G. M. SHELXTL Version 6.1; Bruker Analytical X-ray Systems, Inc.,Madison, Wisconsin, USA, 2000.