## **Supporting Information**

Ambidentate dimethyl sulfoxide coordination in hydrogen bonded dimethyl sulfoxide, (CH<sub>3</sub>)<sub>2</sub>SO<sup>...</sup>H<sub>3</sub>O<sup>+</sup>, and dichlorobis(dimethyl sulfoxide) palladium(II) and platinum(II) solid solvates by vibrational and sulfur K-edge X-ray absorption spectroscopy.

Emiliana Damian Risberg, János Mink, Alireza Abbasi, Mikhail Yu. Skripkin, Laszló Hajba, Patric Lindqvist-Reis, Éva Bencze and Magnus Sandström

**Figure S1.** Shapes of the unoccupied molecular orbitals for the hydrogen bonded dimethyl sulfoxide molecule corresponding to transitions 1, 2, 3 and 4 in Fig. 6 for model A, and (below) transitions 1, 2 and 3 for the models B and C.



**Figure S2**. The molecular orbitals corresponding to the transitions denoted in the theoretical spectra (cf. Figs. 7A and 7B) of *cis*- and *trans*- isomers of the  $Pt(DMSO)_2Cl_2$  complex, respectively. The following colours depict the atoms: Pt (cyan), S (yellow), O (red), Cl (violet), C (green) and H (white-greyish).



**Figure S3**. The molecular orbitals corresponding to the transitions denoted in the theoretical spectra (cf. Figs. 8A and 8B) of *cis*- and *trans*- isomers of the  $Pd(DMSO)_2Cl_2$  complex, respectively. The following colours depict the atoms: Pd (cyan), S (yellow), O (red), Cl (violet), C (green) and H (white-greyish).

