

Photochemical [2+2] cycloaddition as a tool to study solid state structural transformation

Mangayarkarasi Nagarathinam, Jagadese J. Vittal*

^aDepartment of Chemistry, National University of Singapore, 3 Science Drive 3, Singapore 117543. Fax: 65 6779 1691; Tel: 65 6516 2975; E-mail: chmjv@nus.edu.sg

Supporting information

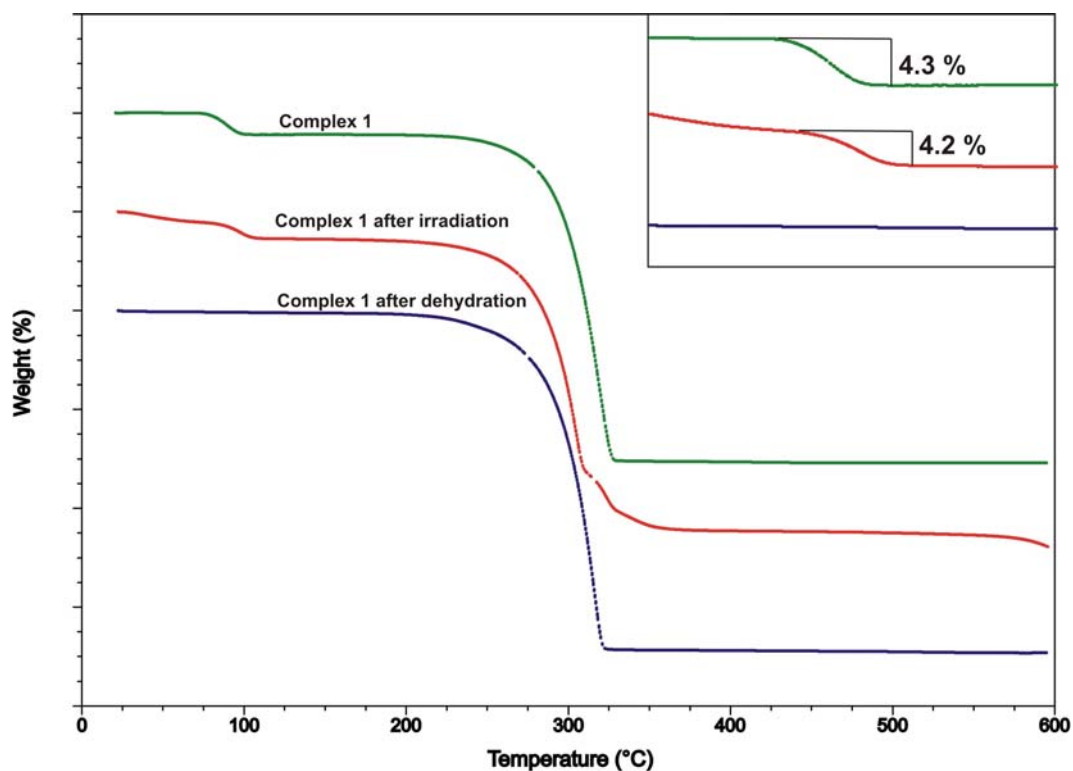


Fig: S1. The TGA of the crystals of complex **1** (—), irradiated crystals of **1** (—) and dehydrated crystals of **1** (—). The inset showing magnified picture at the point of water removal.

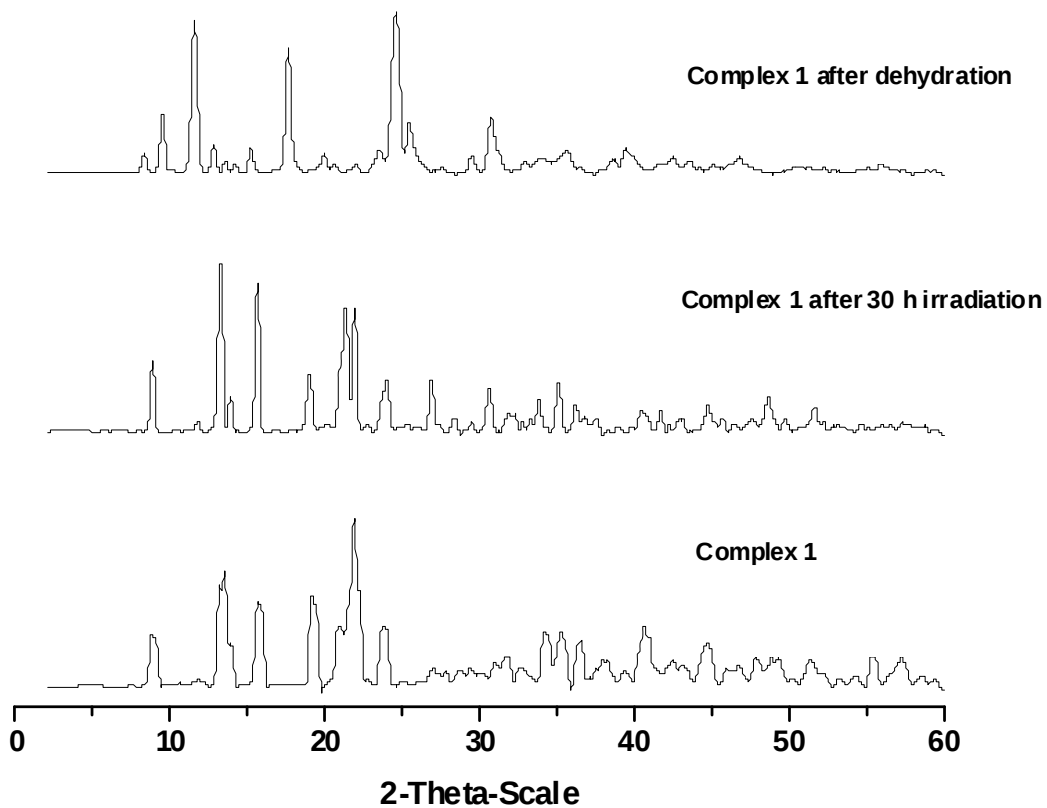


Fig: S2. The powder pattern of the crystals of complex **1**, complex **1** after irradiation and complex **1** after dehydration

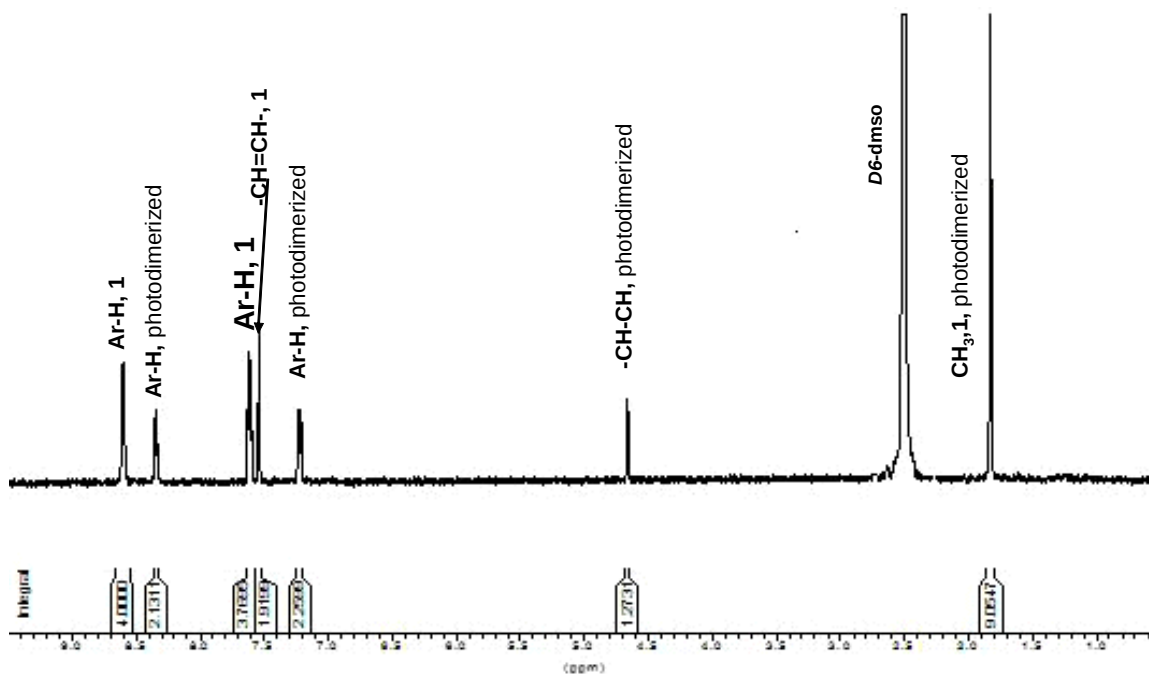


Fig. S3. The ^1H NMR spectrum of the crystals of complex **1** after irradiation for 30 h which shows the mixture of unreacted complex **1** and the photodimerized product

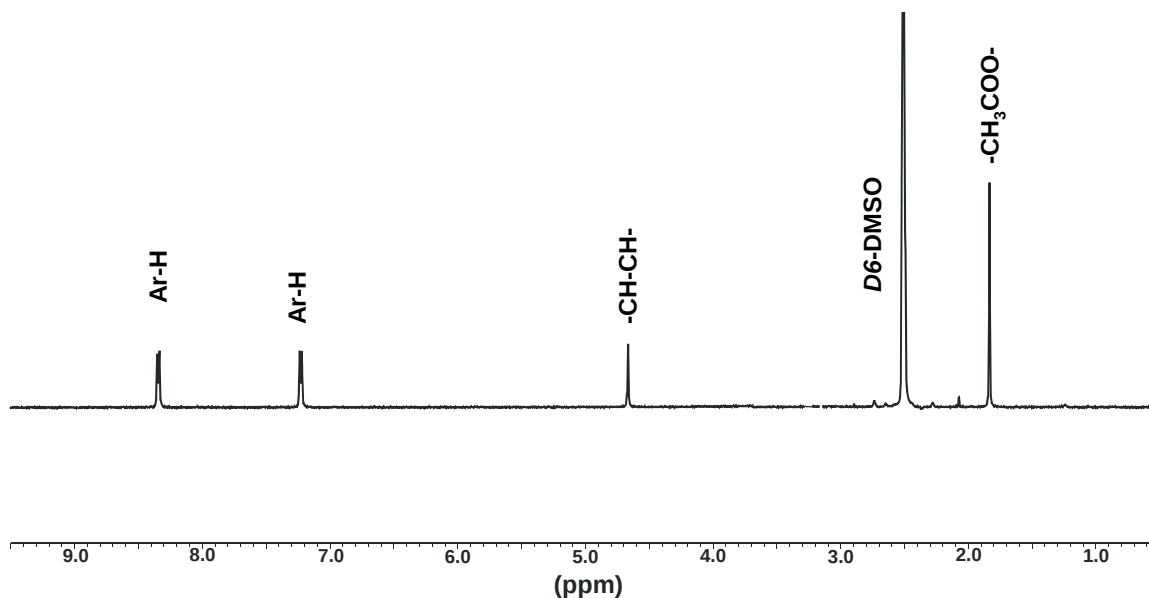


Fig. 4. The ^1H NMR spectrum of the dehydrated crystals of complex **1** after irradiation for 30 h.

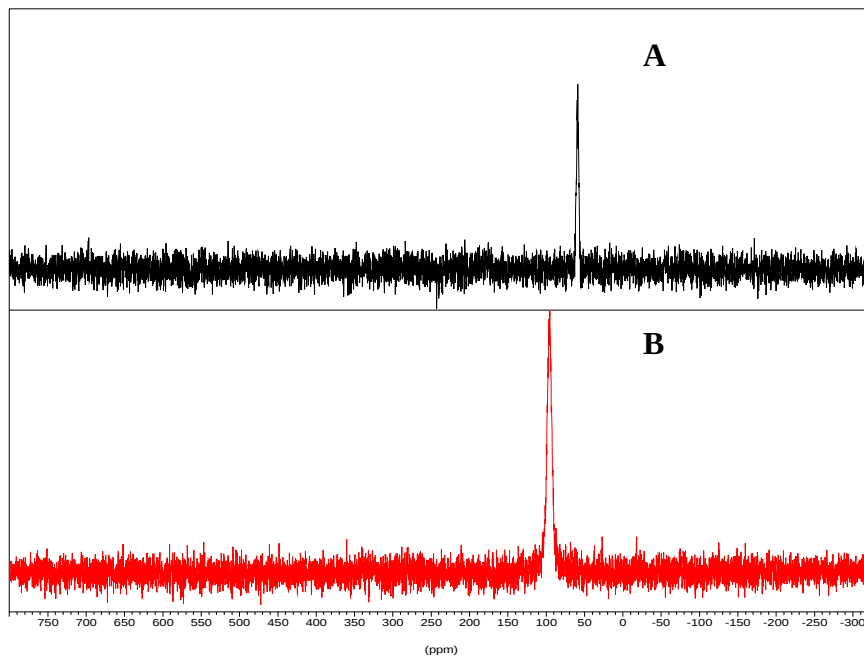


Fig. 5. The ^{113}Cd solid state NMR spectra of complex **1** (A) and its dehydrated product (B)

X-ray crystallography: Both Cd(II) and O of aqua ligand are sitting on twofold symmetry. One H atom of water ligand was located. But DFIX option was used to constraint the position of this atom in the LS refinements. The 2 restraints mention in the CIF arise due to this.