Towards rationalizing photoswitchable behavior of $Cu_2^{II}Mo^{IV}$ cyanido-bridged molecule

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$[Cu^{II}(enpnen)]_2[Mo^{IV}(CN)_8]\cdot 7H_2O$ (enpnen = N,N′–bis(2–aminoethyl)–1,3–propanediamine) molecular cluster compound was subject to a series of irradiations with the light of 405 nm. On irradiation isothermal magnetization at 1.8 and 5 K in the field range 0 - 70 kOe as well as magnetic susceptibility in the temperature range of 2 - 300 K were subsequently detected. Both types of magnetic signals were next analyzed assuming that the irradiation triggers two independent processes: the metal to metal charge transfer (MMCT) leading to a state with the Arrhenius-type relaxation and the spin crossover (SC) transition ending in a state whose relaxation displays a threshold behavior. The first mechanism leads to an electron from the spinless Mo(IV) configuration being transferred to one of the Cu(II) ions transforming the trimer into the state Cu(II)-N-C-Mo(V)-C-N-Cu(I), with spin 1/2 on the Mo(V) ion and the spinless Cu(I) ion. The other mechanism gives rise to an excited paramagnetic $Mo(IV)^*$ linked to two paramagnetic Cu(II) centers with a possible superexchange interaction. The spin of the excited $Mo(IV)^*$ species is equal to 1 and associated to a disruption of the 5s-electronic pair. A reasonable result of simultaneous fitting the full series of susceptibility data to the model taking into account both mechanisms corroborates their presence. Moreover, the parameters thus obtained are also consistent with the magnetization data. The presented approach to understanding the behavior of photoswitchable material upon irradiation has never been used before.