Supplementary Material (ESI) for Chemical Communications

Supporting information for:

Binuclear Gadolinium(III) Coordination Complex based on bridging Tetrathiafulvalenecarboxylate Radical Cations

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Physical measurements: Optical spectra were measured using the KBr disk method on Perkin-Elmer 1600 Series FT-IR (resolution 4 cm^{-1}) for infrared (IR) and on a Varian Cary 5000 UV-Visible-NIR spectrometer equipped with an integration sphere for UV-Visible-Near I.R.. EPR spectra were recorded down to 290 K for crystalline powder sample of $[Gd(hfac)_3(\mu\text{-}TTF^{\bullet+}COO^-)]_2$ with a BRUKER EMX X-band ESR spectrometer equipped with an OXFORD cryostat. The dc magnetic susceptibility measurements were performed on solid polycrystalline sample with a Quantum Design MPMS-XL SQUID magnetometer between 2 and 300 K in applied magnetic field of 0.2 T for temperatures of 2-20 K and 1T for temperatures of 20-300 K. These measurements were all corrected for the diamagnetic contribution as calculated with Pascal's constants.

The PART instruction was used for disordered fluorine atoms bound to carbon atoms C20 and C30. These carbon atoms were respectively splitted as C20 - C20A and C30 - C30A as four - CF_3 groups. For C30 and C30A which have close occupancy factors (50%), it works.
However, for C20 and C20A, the constraints reached to meaningless results: very short C20A-F distances as well as a too long C20A-C21 bond length. We decided to use a single C20 atom with occupancy factor of 1.0 and two disordered F_3 groups.

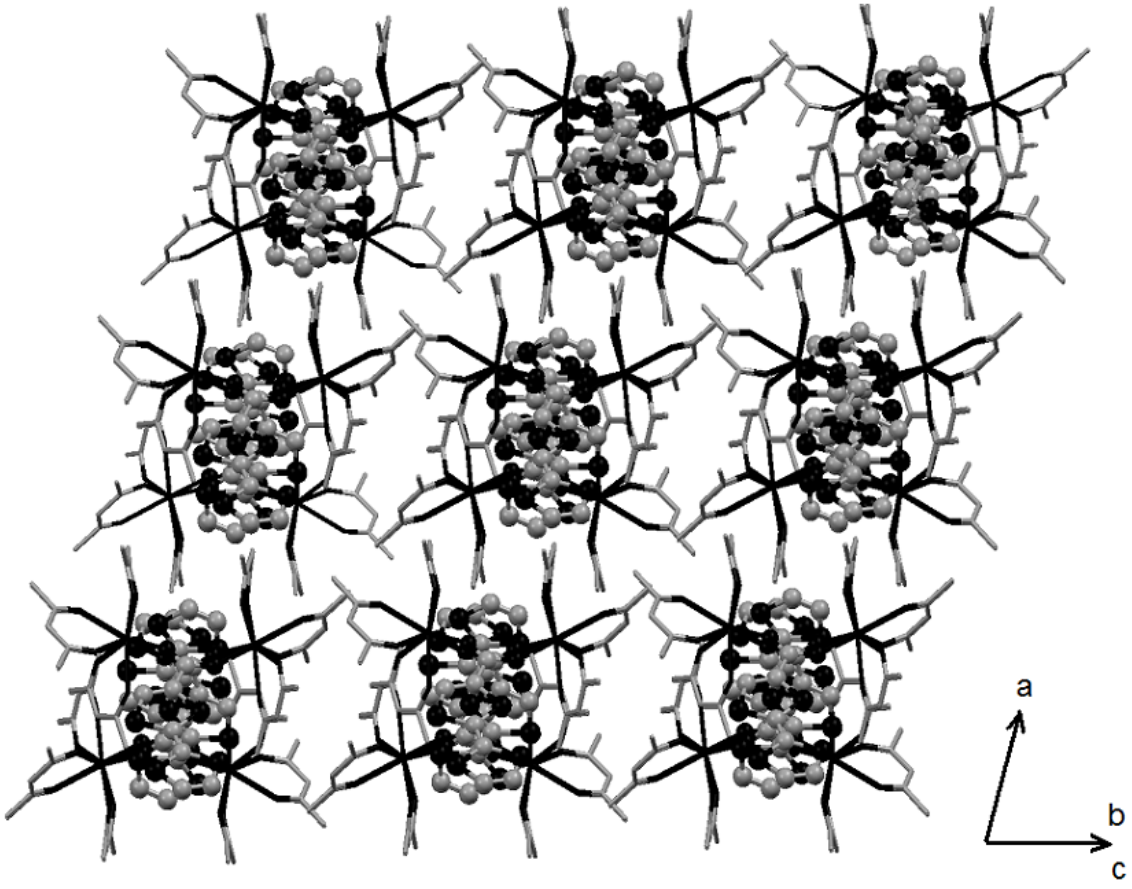

Fig. S1 Packing view of the dinuclear complex $[Gd(hfac)_3(\mu\text{-}TTF^{\bullet+}COO^-)]_2$ highlighting the short contacts between the perfluorated groups.

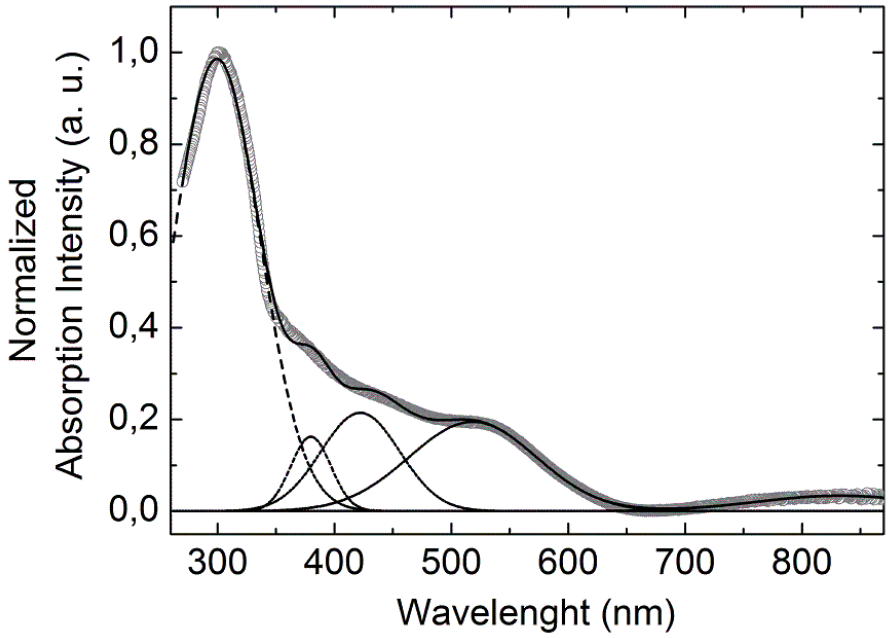

Fig. S2 Experimental solid state (KBr pellet) absorption UV-visible-Near I.R. spectrum of the $[Gd(hfac)_3(\mu\text{-}TTF^{\bullet+}COO^-)]_2$ complex (open gray circles). Deconvolution of the experimental curve (dash black lines) and the best fit R = 0.998 (full black line). The fit is performed between 11500 (870 nm) and 37000 cm^{-1} (270 nm). To highlight the large absorption band centred at 12050 cm^{-1} (830 nm), the absorption spectrum is represented in nanometers.

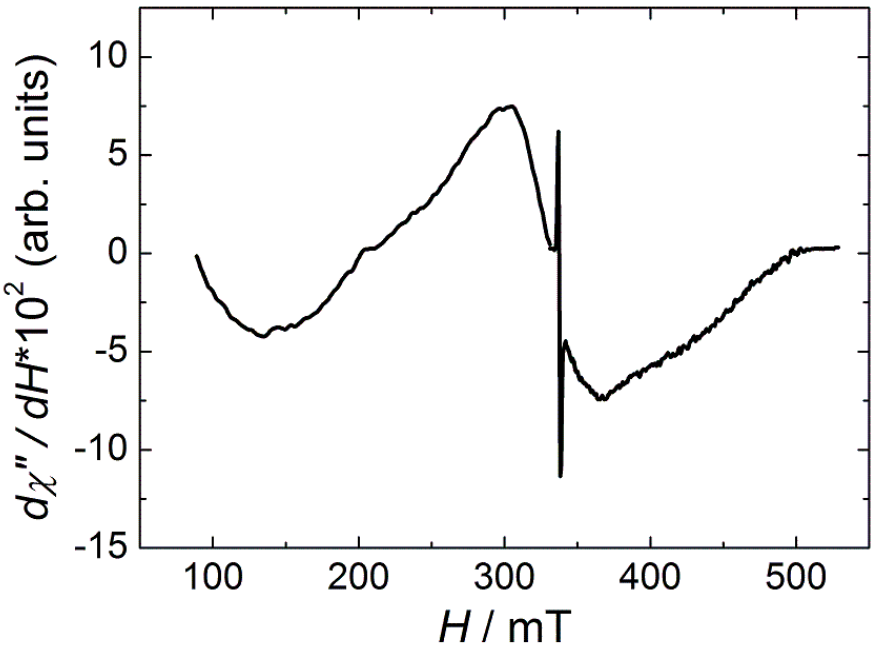

Fig S3 X-band (9.470 GHz) solid state EPR spectrum of crunched single crystals of $[Gd(hfac)_3(\mu\text{-}TTF^{\bullet+}COO^-)]_2$ at 290 K.

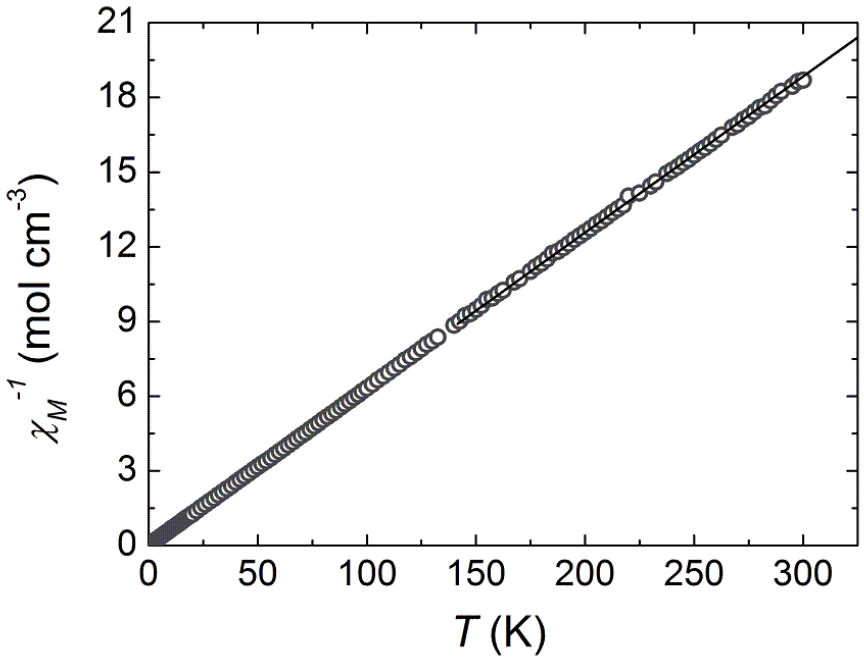

Fig. S4 Thermal variation of the χ_M^{-1} of $[Gd(hfac)_3(\mu\text{-}TTF^{\bullet+}COO^-)]_2$ (gray circles) with a Curie-Weiss fit (full black line) in the range of temperature 140-300 K in an applied field of 1 Tesla.