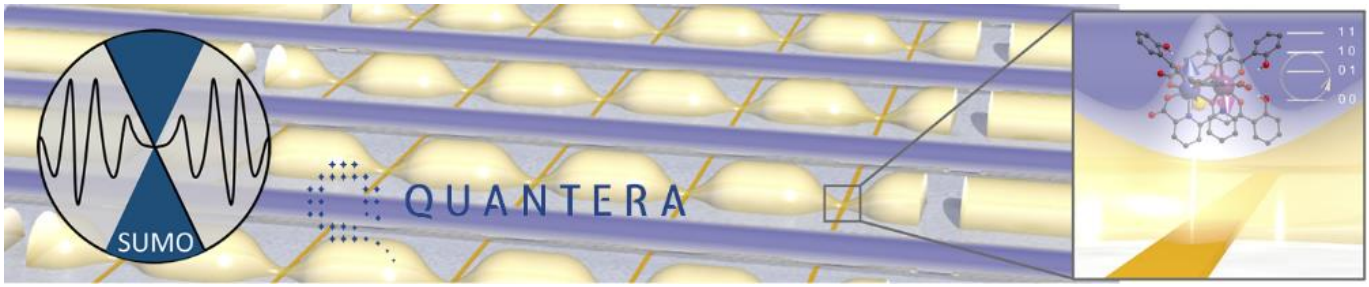

Open data management. Description of available data and metadata related to a publication	
Authors (ORCID codes)	Ivana Borilovic (0000-0002-8485-303X),[1] Pablo J. Alonso (0000-0003-3449-4929),[3] Olivier Roubeau (0000-0003-2095-5843),[3] Guillem Aromí (0000-0001-9821-3650) [1,2]
Date	2020/01/15
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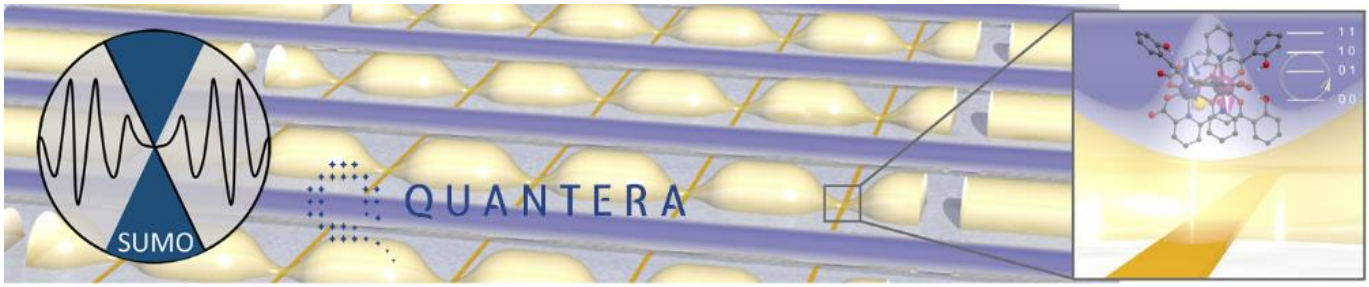
Paper citation	Chem. Commun. **56**, 3139-3142 (2020)
Language	English
Dataset ID	SUMO_CSIC_Roubeau_ChemComm_v1
List of data files available	
Methodology	We synthesized a molecule containing two weakly-coupled vanadyl spins and evaluated the magnetic interaction and the spin lattice and phase-memory times through ac-susceptibility measurements done with commercial Quantum Design MPMS5 SQUID magnetometer and pulsed-EPR using a Bruker Biospin ELEXSYS E 580 spectrometer operating in the X-band. The structure of the compound, its titanyl analogue and the magnetically-dilute phase were determined by single-crystal X-Ray diffraction (SCXRD) data were obtained on either a laboratory Bruker APEX II QUAZAR diffractometer equipped with a microfocus multilayer monochromator with Mo Kα radiation (λ = 0.77073 Å), a Bruker APEX II CCD diffractometer at the Advanced Light Source beamline 11.3.1 at Lawrence Berkeley National Laboratory, from a silicon 111 monochromator (λ = 0.7749 Å) or on the BL13-XALOC beamline[1] of the ALBA synchrotron (λ= 0.77490 Å).
Data processing and software needed	1. SCXRD: Data reduction and absorption corrections were performed by using SAINT and SADABS, respectively. The structures were solved using SHELXT and refined with full-matrix least-squares on F^2 by using SHELXL-2014. The necessary information is inserted into the relevant cif file, deposited at the CCDC. 2. Simulation of the echo-induced EPR spectrum was done with Easyspin (S. Stoll, and A. Schweiger, J. Magn. Reson., 2006, 178, 42)
Access to the data	Contact Olivier Roubeau at roubeau@unizar.es or Guillem Aromí at guillem.aromi@qi.ub.es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