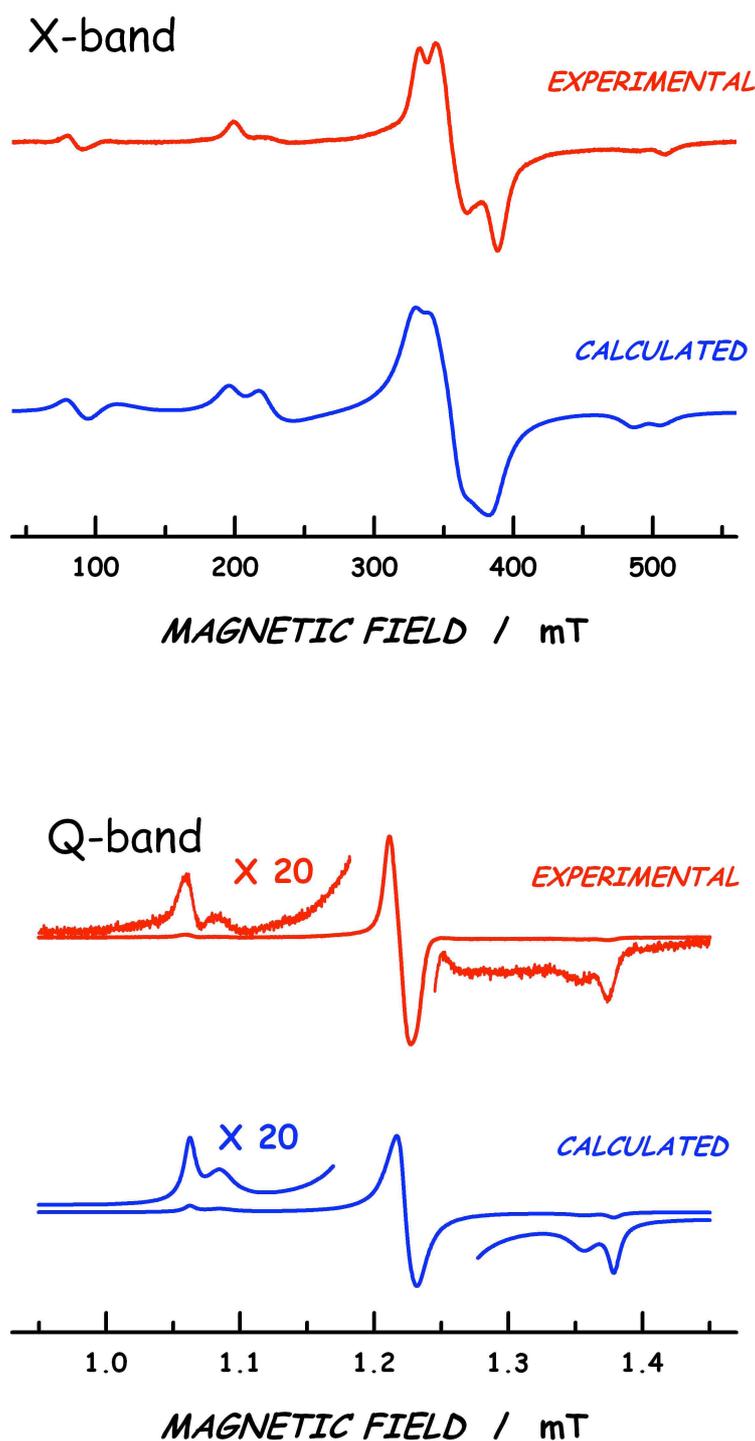


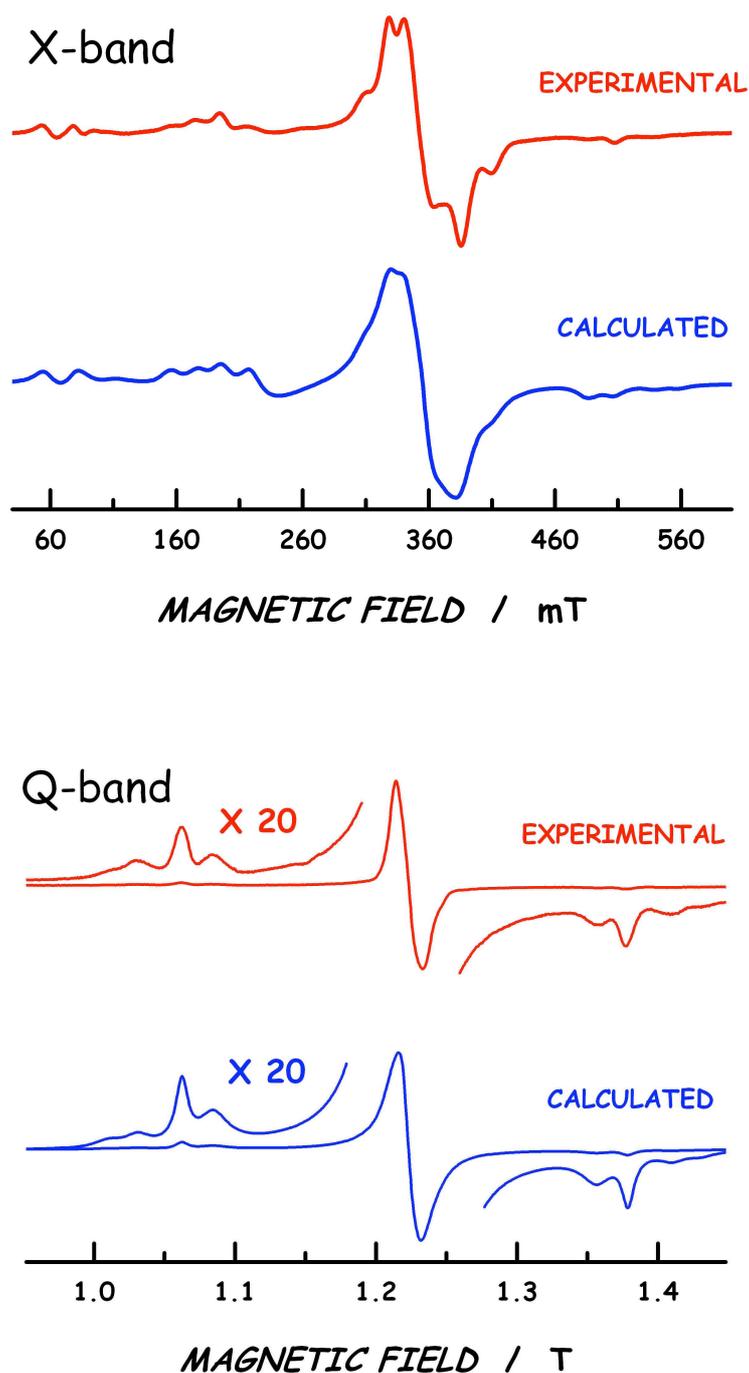
**Supplementary information**  
**for**  
**Synthesis, characterisation and magnetic properties of**  
**octahedral chromium(III) compounds**  
**with**  
**six C-donor ligands**

**Pablo J. Alonso, Ana B. Arauzo, M. Angeles García-Monforte, Inés García-Rubio,**  
**Antonio Martín, Babil Menjón,\* and Conrado Rillo**

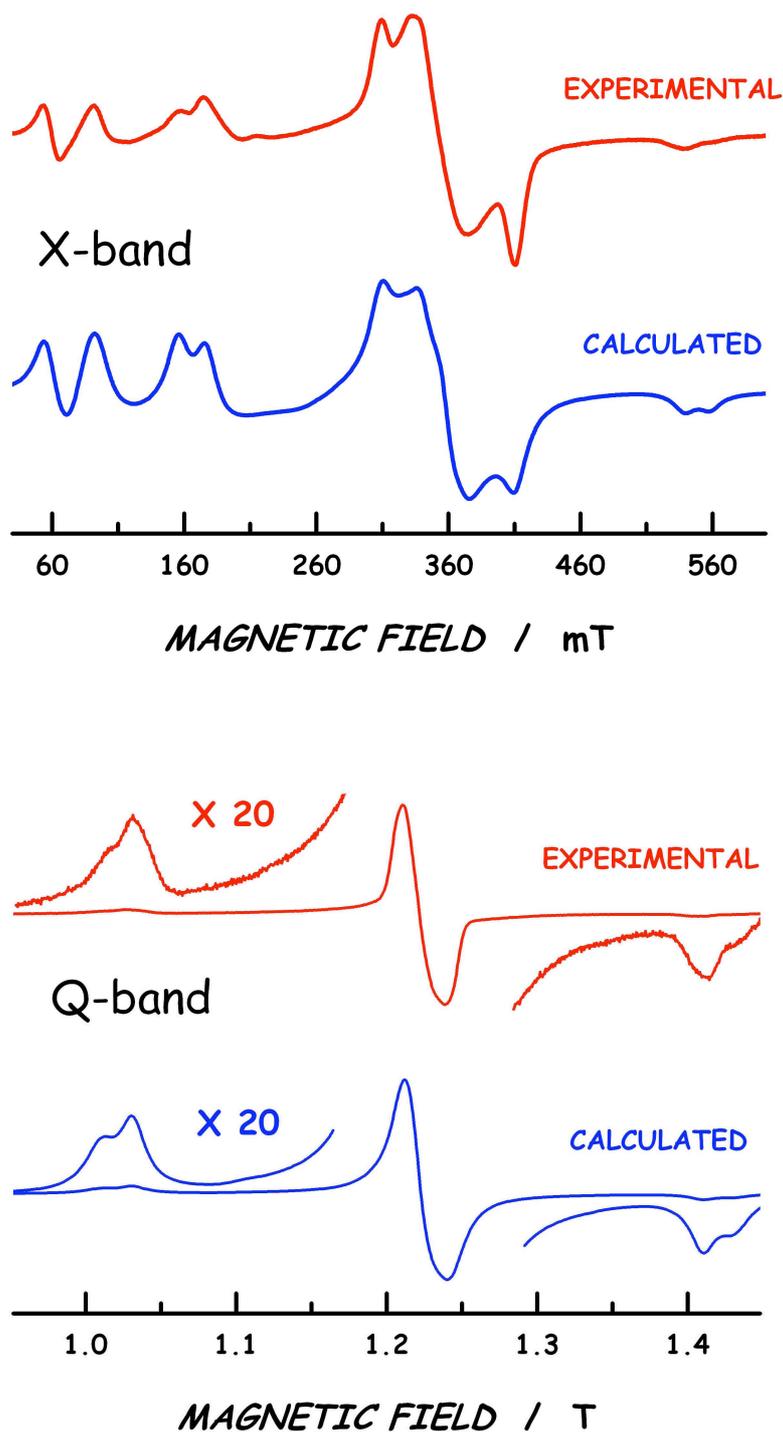
- **Figures S1–S3:** Simulation of EPR spectra registered for  $[\text{NBu}_4][\text{trans-Cr}(\text{C}_6\text{F}_5)_4(\text{CN}^t\text{Bu})_2]$  (**2**) at representative stages of the observed evolution Pages S1–S3
  
- **Figure S4:** EPR spectra of  $[\text{NBu}_4][\text{trans-Cr}(\text{C}_6\text{F}_5)_4(\text{CN-Xy})_2]$  (**3**) compared with typical spectra of **2** Page S4
  
- **Figure S5:** Bulk magnetic properties of **3** Page S5



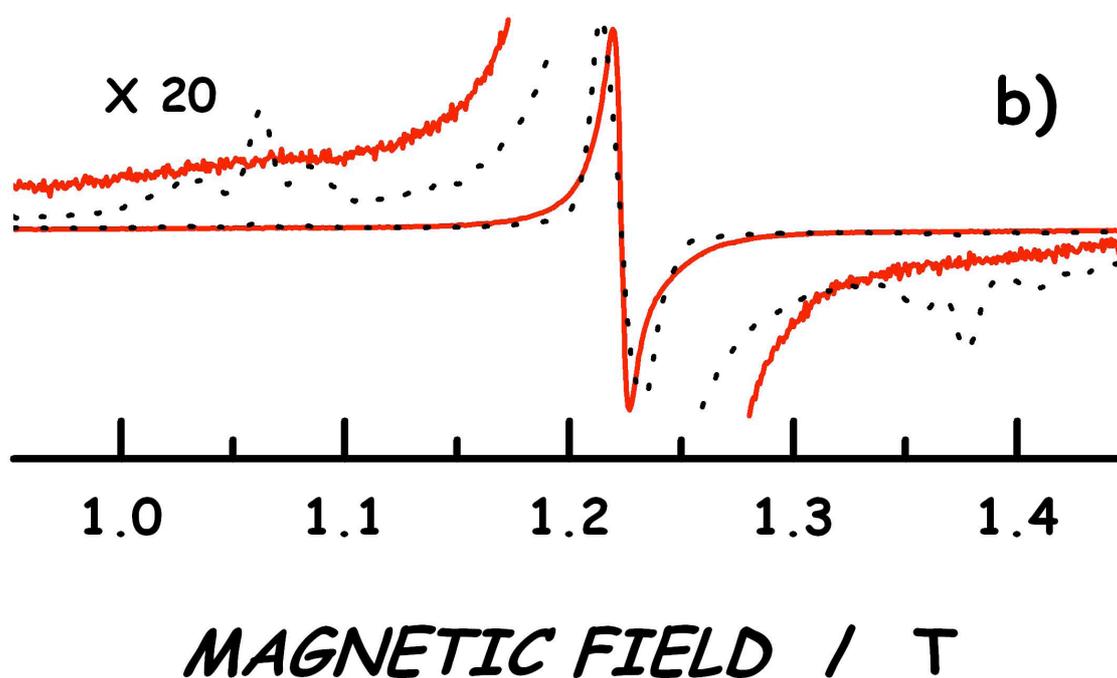
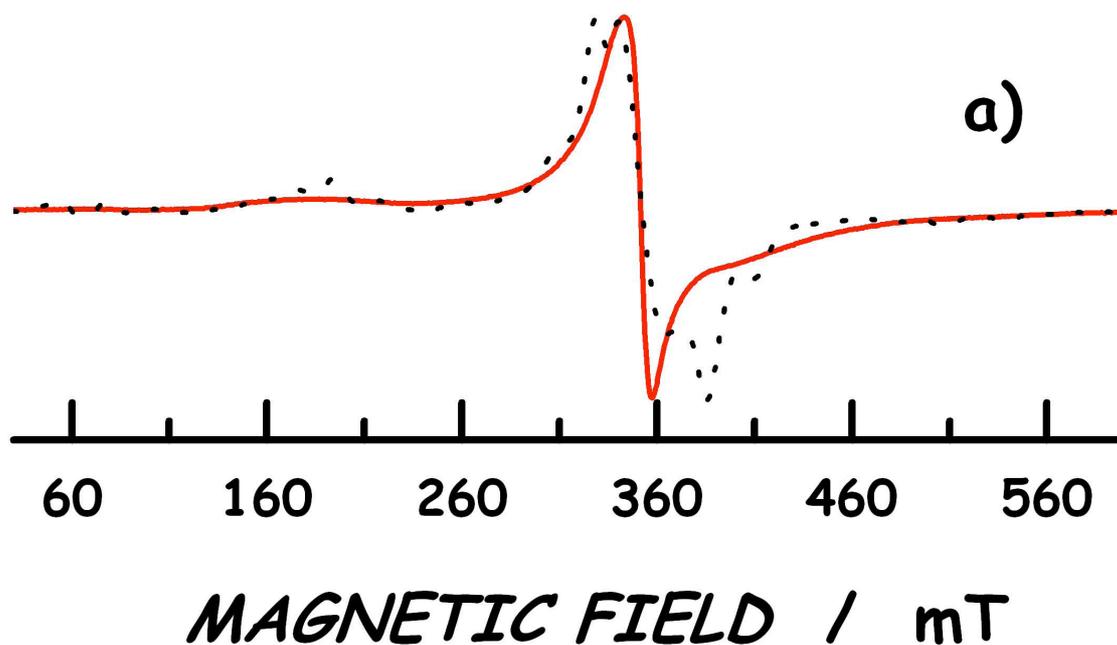
**Figure S1.** Comparison between experimental (red lines) and simulated (blue lines) EPR spectra of a polycrystalline sample of **2** measured at X-band (upper part) and at Q-band (lower part). Experimental spectra correspond to those given in Figures 5c (X-band) and 6c (Q-band). Simulated spectra correspond to type C contribution (Table 3).



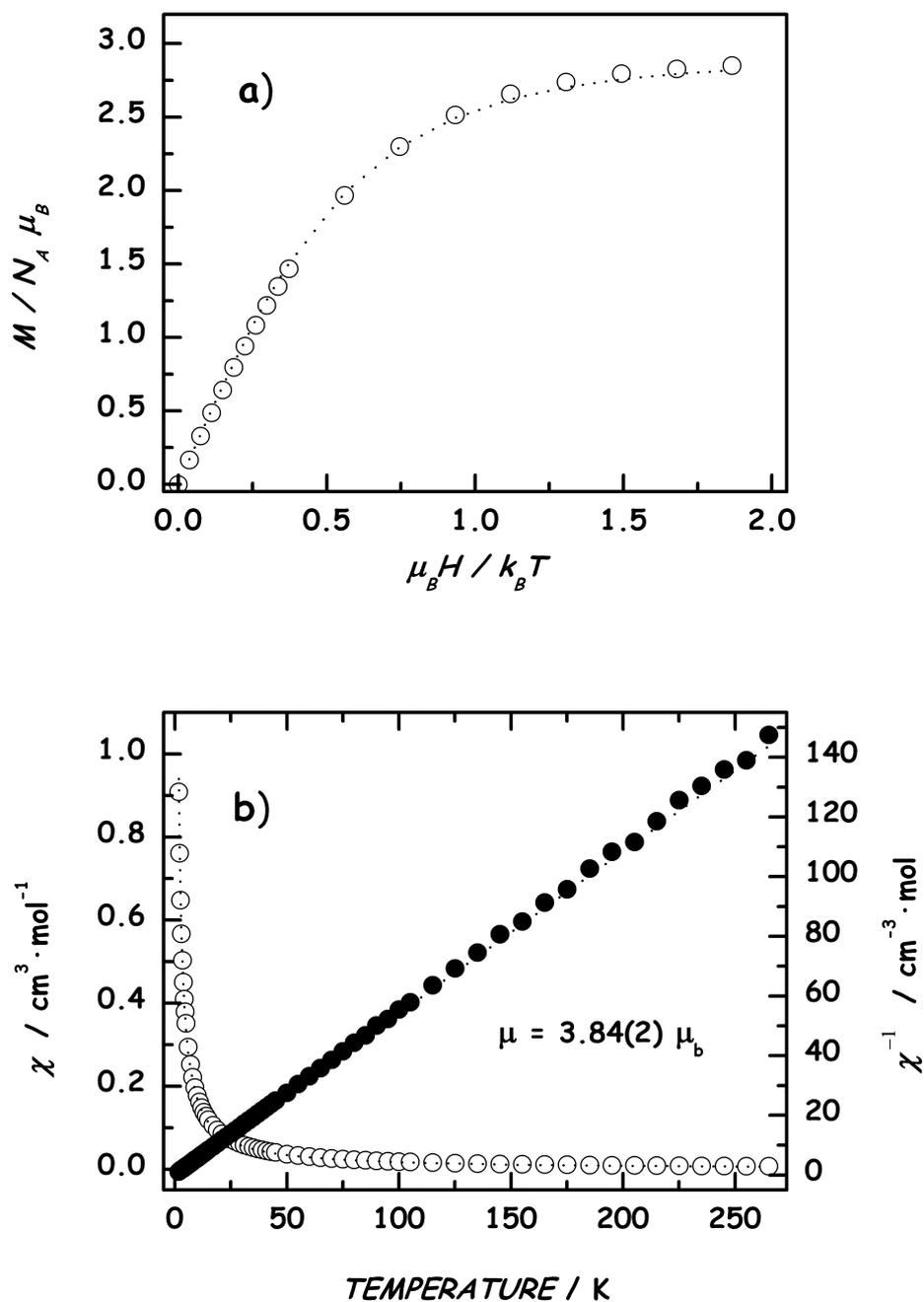
**Figure S2.** Comparison between experimental (red lines) and simulated (blue lines) EPR spectra of a polycrystalline sample of **2** measured at X-band (upper part) and at Q-band (lower part). Experimental spectra correspond to those given in Figures 5d (X-band) and 6d (Q-band). Simulated spectra have been calculated considering coexistence of type C (80%) and type D (20%) contributions (Table 3).



**Figure S3.** Comparison between experimental (red lines) and simulated (blue lines) EPR spectra of a polycrystalline sample of **2** measured at X-band (upper part) and at Q-band (lower part). Experimental spectra correspond to those given in Figures 5e (X-band) and 6e (Q-band). Simulated spectra correspond to type D contribution (Table 3).



**Figure S4.** EPR spectra of **3** (red solid line) compared with typical spectra of **2** (black broken line): a) X-band; b) Q-band..



**Figure S5.** a) Magnetization vs. the reduced applied magnetic field,  $M(\mu_0 H / k_B T)$ , of a powder sample of **3** at 1.8 K (dotted line corresponds to the evolution calculated with a Brillouin function with  $S = 3/2$  and  $g = 1.92$ ); b) Thermal dependence of the magnetic susceptibility,  $\chi$  (empty circles, ordinate scale on the left) and its inverse,  $\chi^{-1}$  (full circles, ordinate scale on the right) of the same sample (dotted lines correspond to the predicted evolution following the Curie law).