

Supporting Information for

Intermediate-paramagnetic phases with a half and a quarter spin entities in fluorinated biphenyl-3,5-diyl bis(*tert*-butyl nitroxides)

Takuya Konno, Hiroki Kudo, and Takayuki Ishida*

*Department of Engineering Science, The University of Electro-Communications,
Chofu, Tokyo 182-8585, Japan*

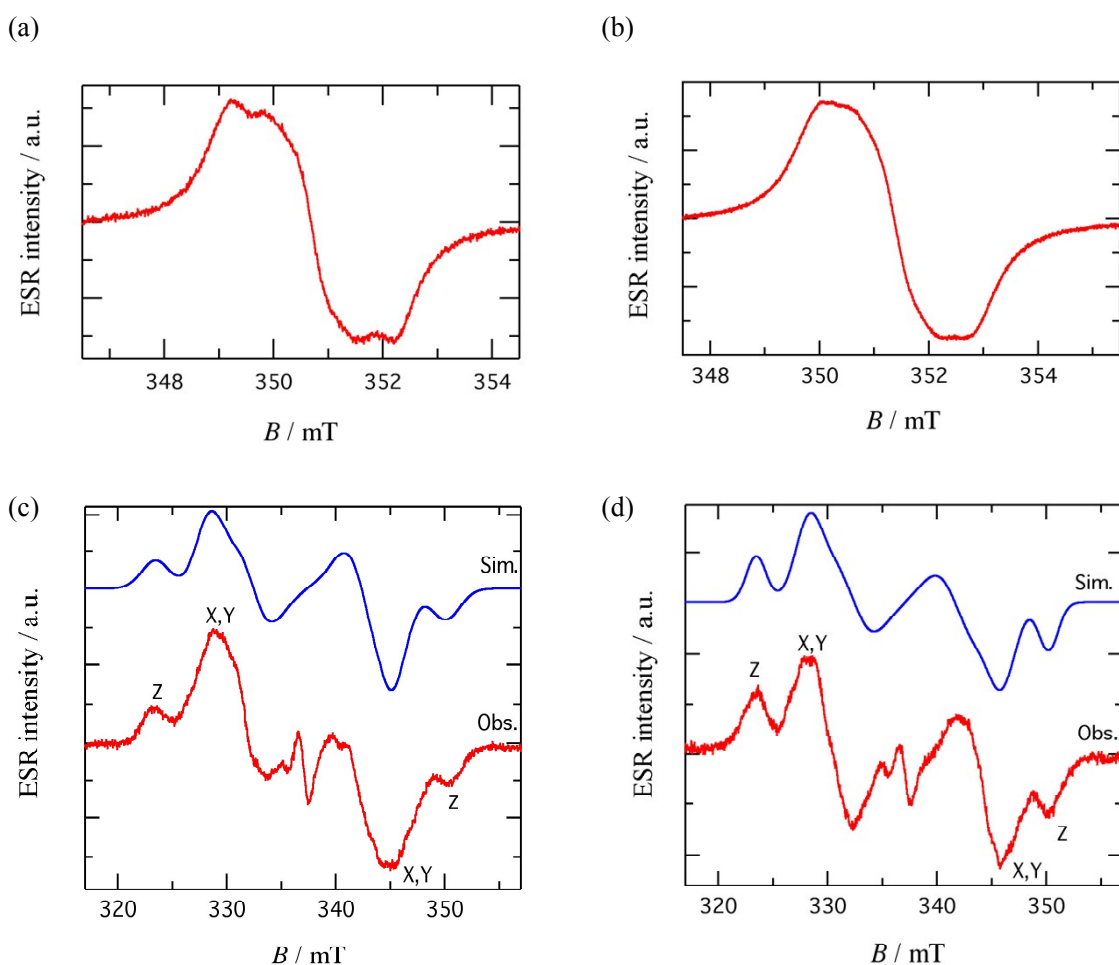


Figure S1. X-band EPR spectra of (a) 3FBPBN and (b) 25FBPBN, measured in a degassed diluted toluene solution (ca. 1×10^{-4} mol/L) at room temperature. Frozen-solution EPR of (c) 3FBPBN and (d) 25FBPBN, measured in a degassed diluted toluene solution at 145 K. The zero-field splitting parameters were determined from these fine structures, giving $|D| = 1.25 \times 10^{-2} \text{ cm}^{-1}$ and $|E| = 1.1 \times 10^{-3} \text{ cm}^{-1}$ for 3FBPBN and $|D| = 1.25 \times 10^{-2} \text{ cm}^{-1}$ and $|E| = 1.3 \times 10^{-3} \text{ cm}^{-1}$ for 25FBPBN. Forbidden signals were hardly observed. Note that the concentrations of doublet impurities are very low.

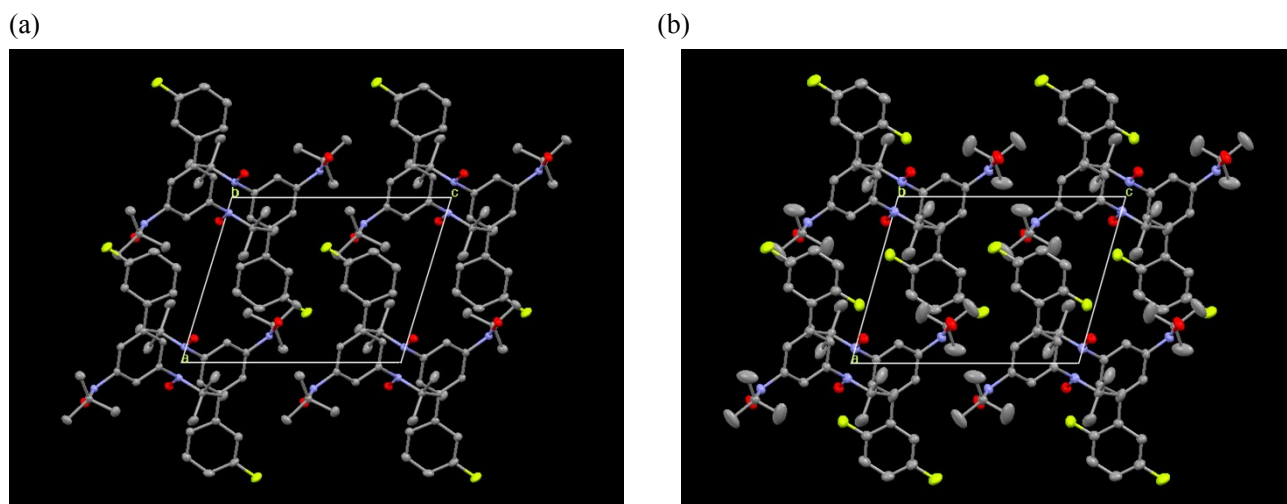


Figure S2. X-ray crystal structures of (a) 3FBPBN (163 K) and (b) the high-temperature phase of 25FBPBN (296 K), viewed along the b axis.

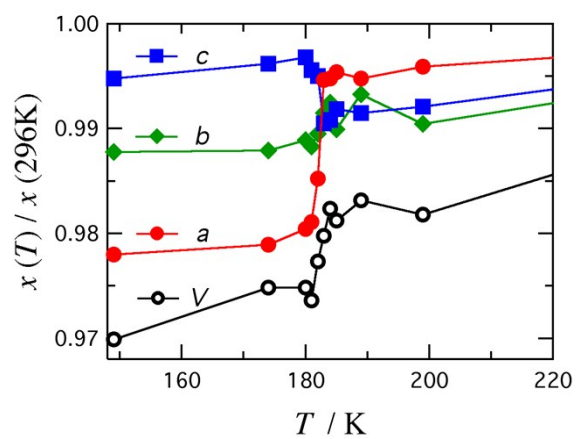


Figure S3. The cell parameters of 25FBPBN as a function of temperature.