Supplementary Material for PCCP

SUPPORTING INFORMATION

Spectroscopic CW-EPR and HYSCORE Investigations of Cu^{2+} and O_2^{-} Species in Copper Doped Nanoporous Calcium Aluminate ($12CaO \cdot 7Al_2O_3$)

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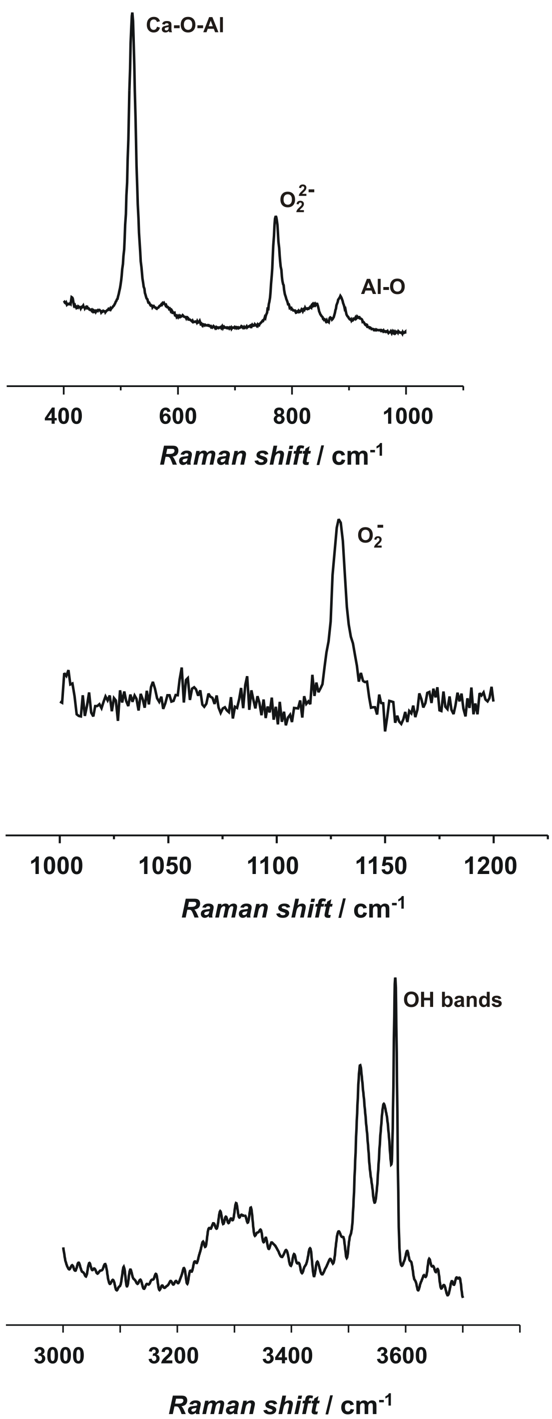

Fig. S1 Raman spectra of copper-doped (1.5 mol%) mayenite sample.

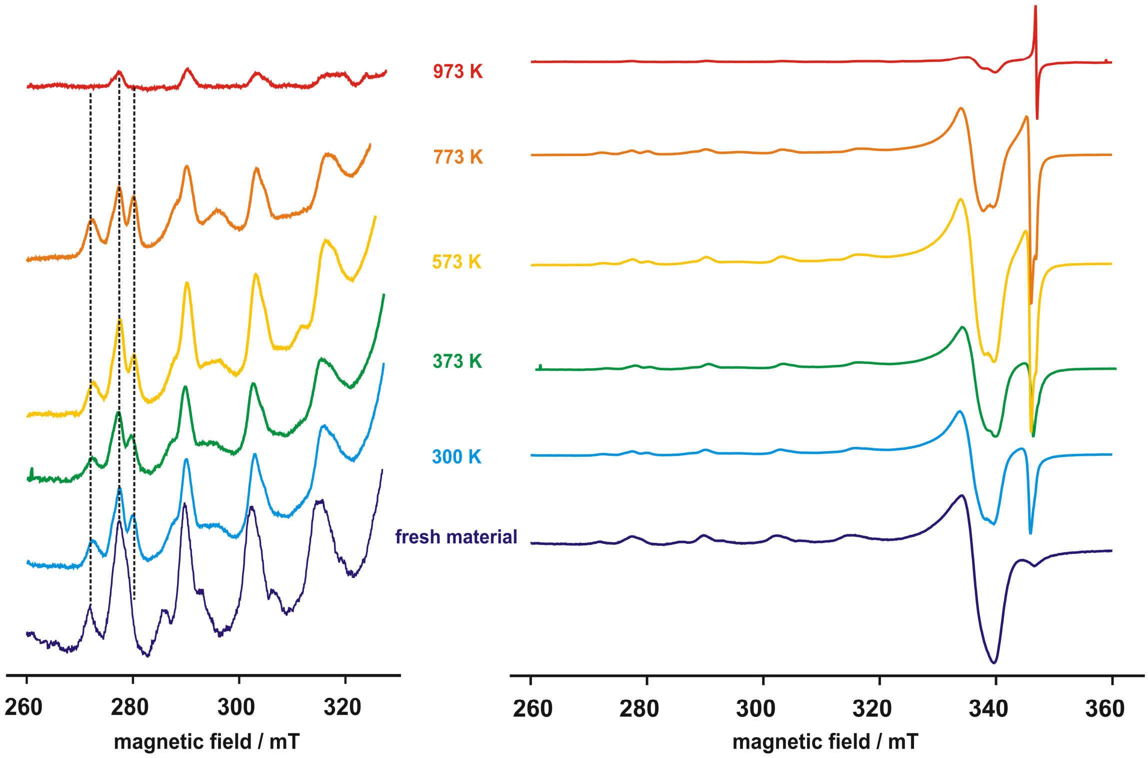

Fig. S2 Evolution of copper(II) EPR signal under thermal treatment in anaerobic conditions of Cu-doped (1.5 mol%) mayenite mixed with carbon black. Three components of the signal are visible in magnified low-field region of the spectra exhibiting “parallel” EPR features.

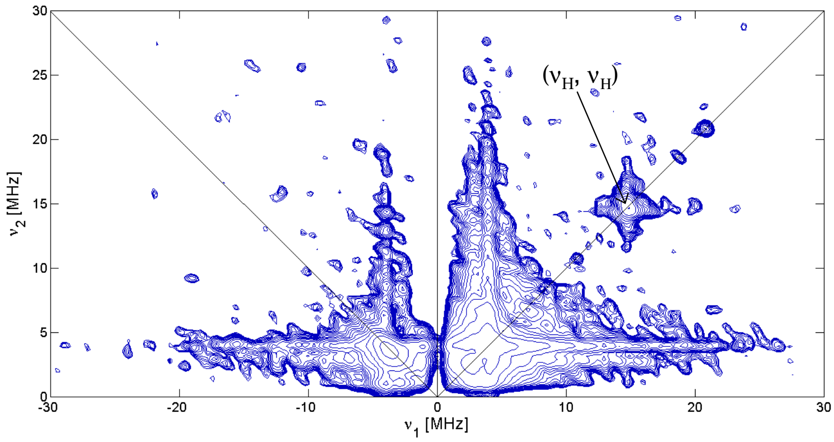

Fig. S3 ^{1}H matched HYSCORE[1] spectrum recorded at B_0 = 347.0 mT and T = 10 K. The experiment was carried out with the sequence $\pi/2-\tau-$(HTA)$-t_1-\pi-t_2-$(HTA)$-\tau-$echo with $\pi/2$ = 16 ns; π = 16 ns. The amplitude of the microwave field of the matching pulses was 15.6 MHz. The length of the high turning angle (HTA) pulse was experimentally determined with a 2D three-pulse experiment where the pulse length of the second and third pulses were increased in steps of 8 ns starting from 8 ns. The optimal length was found to be 72 ns. Two τ values (96, 172) were added together to eliminate blind spot effects.

1 G. Jeschke, R. Rachmatullin, A. Shweiger, *J. Mag. Reson.* **1998**, *131*, 261.

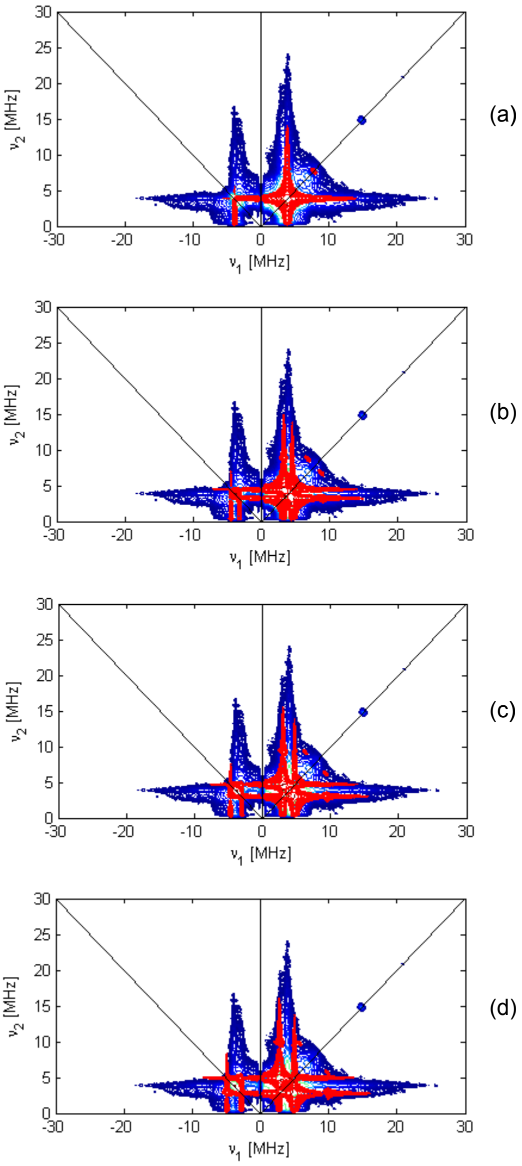

Fig. S4 Effect of increasing a_{iso} on the ^{27}Al HYSCORE spectrum of O_2^-. (a) $a_{iso} = 0$, (b) $a_{iso} = -1$ MHz, (c) $a_{iso} = -1.5$ MHz, (d) $a_{iso} = -2$ MHz. For all spectra $2T = 0.96$ MHz and $e^2qQ/h = 0$.

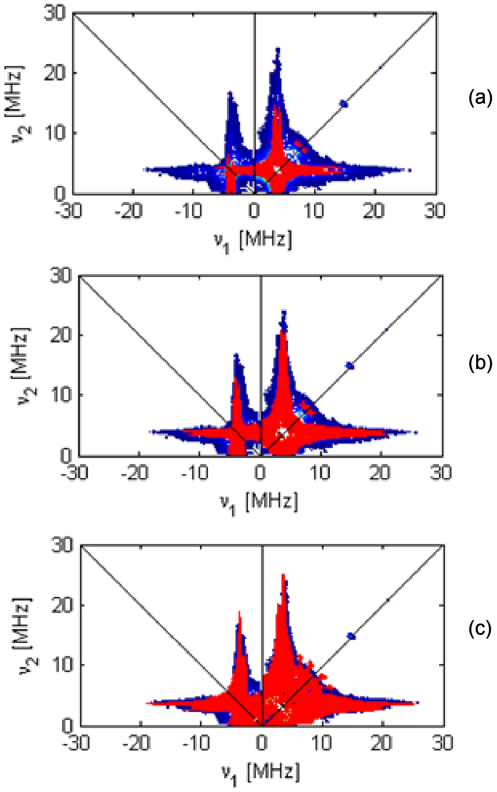

Fig. S5 Effect of increasing quadrupole coupling on the ^{27}Al HYSCORE spectrum of O_2^-. (a) e^2qQ/h = 0; (b) e^2qQ/h = 3 MHz; (c) e^2qQ/h = 11 MHz. For all spectra a_{iso} = – 0.5 MHz and $2T$ = 0.96 MHz.

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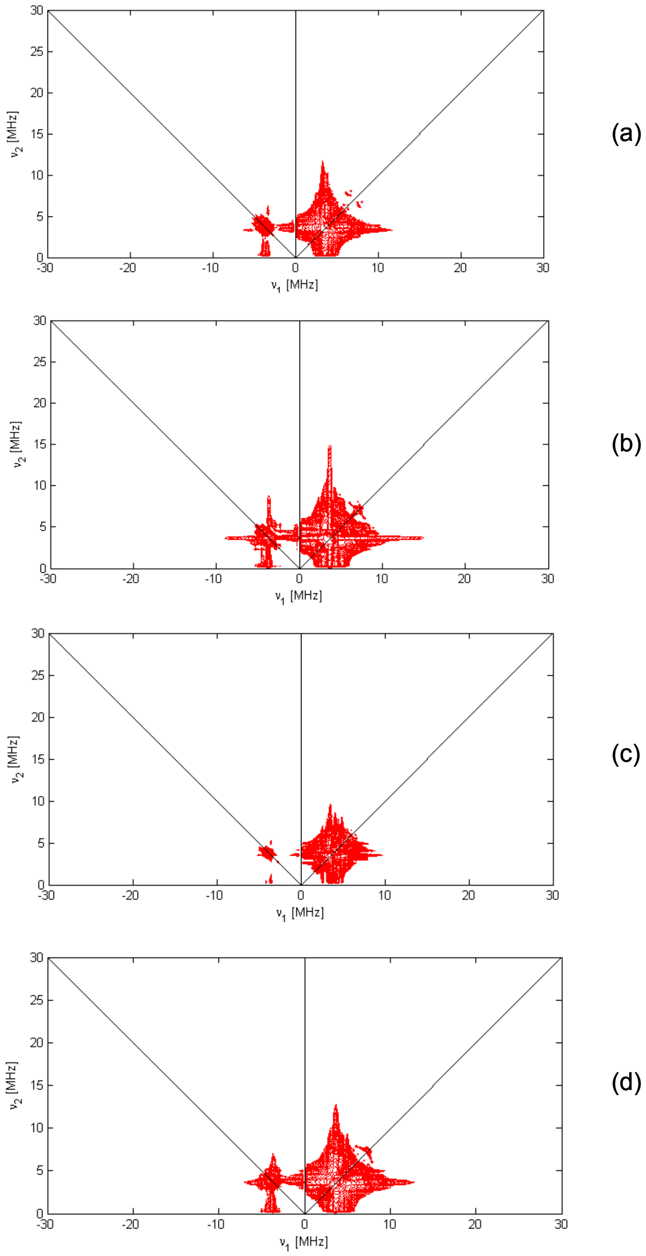

Fig. S6 Angular dependence of the quadrupole coupling on the ^{27}Al HYSCORE spectrum of O_2^-. (a) $\beta = 0$; (b) $\beta = 30°$; (c) $\beta = 60°$; (d) $\beta = 90°$C. For all spectra $a_{iso} = -0.5$ MHz, $2T = 0.96$ MHz.

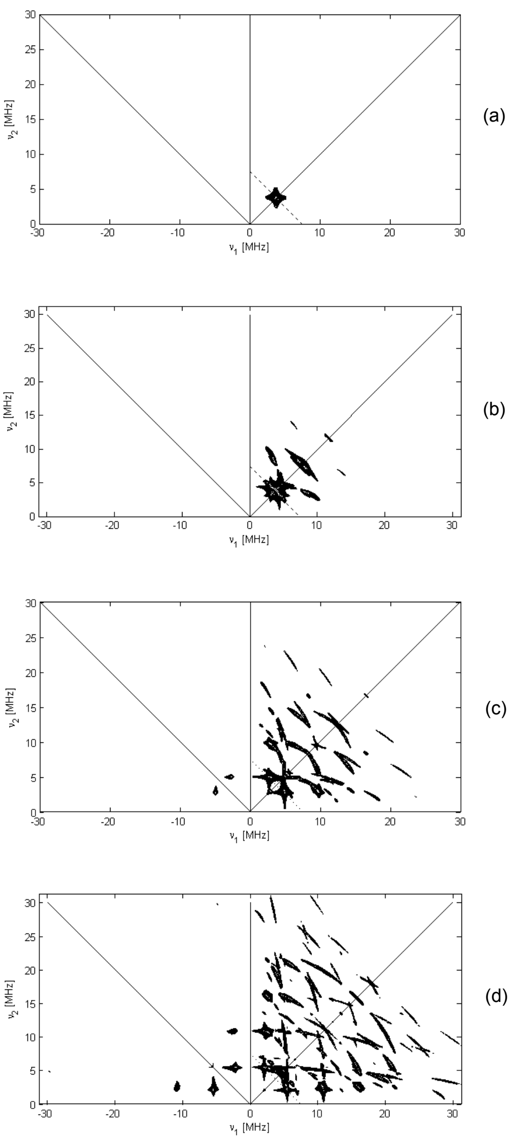

Fig. S7 Effect of increasing dipolar coupling on the ^{27}Al HYSCORE spectrum of Cu^{2+} (B_0 = 337.0 mT). (a) $|T|$ = 0.5 MHz; (b) $|T|$ = 1.5 MHz; (c) $|T|$ = 2.5 MHz; (d) $|T|$ = 3.5 MHz. For all spectra a_{iso} = 0 MHz and e^2qQ/h = 0.