

Electronic Supplementary Information for

**5-Hydroxy-2,2,6,6-tetramethyl-4-(2-methylprop-1-en-yl)cyclohex-4-ene-1,3-dione, a novel cheletropic trap for nitric oxide EPR detection**

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**Figure S2:** Details of the central line of the EPR spectrum of **3** showing long range hyperfine couplings, and its superimposed simulation obtained with the following parameters:  $a_N = 14.44$  G,  $a_{HY} = 0.46$  G (*3H*),  $a_{HY} = 0.31$  G (*1H*), and  $g = 2.00404$ . The experimental signal is in black dotted lines, its simulation in red full lines.

**Figure S3:** Details of the central line of the EPR spectrum of **3** showing long range hyperfine couplings, and its superimposed simulation performed by considering an exchange between two conformers with the following parameters: first species (60%),  $a_N = 14.44$  G,  $a_{HY} = 0.43$  G (*3H*),  $a_{HY} = 0.25$  G (*1H*), and  $g = 2.004041$ ; second species (40%),  $a_N = 14.45$  G,  $a_{HY} = 0.42$  G (*3H*),  $a_{HY} = 1.00$  G (*1H*), and  $g = 2.004051$ ; exchange rate constant,  $2.64 \times 10^6$  s<sup>-1</sup>. The experimental signal is in black dotted lines, its simulation in red full lines.

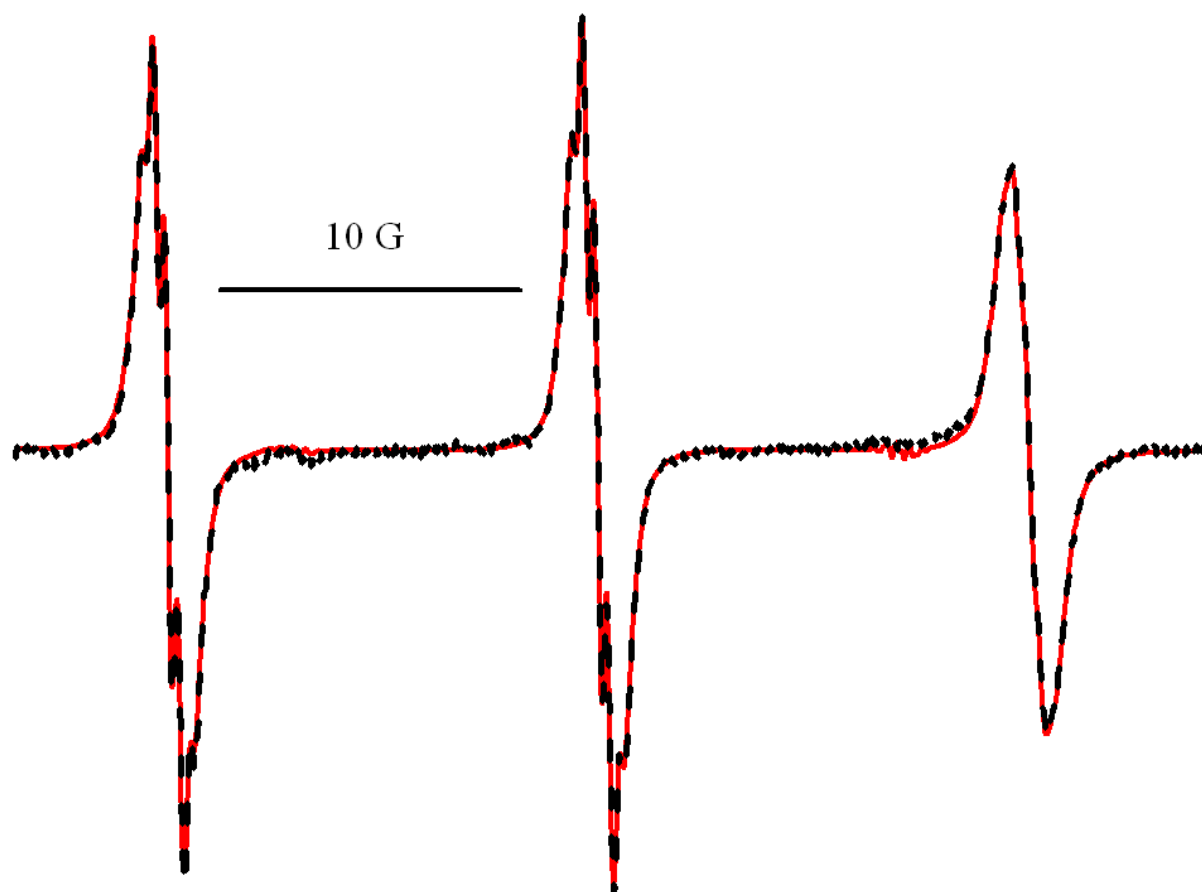
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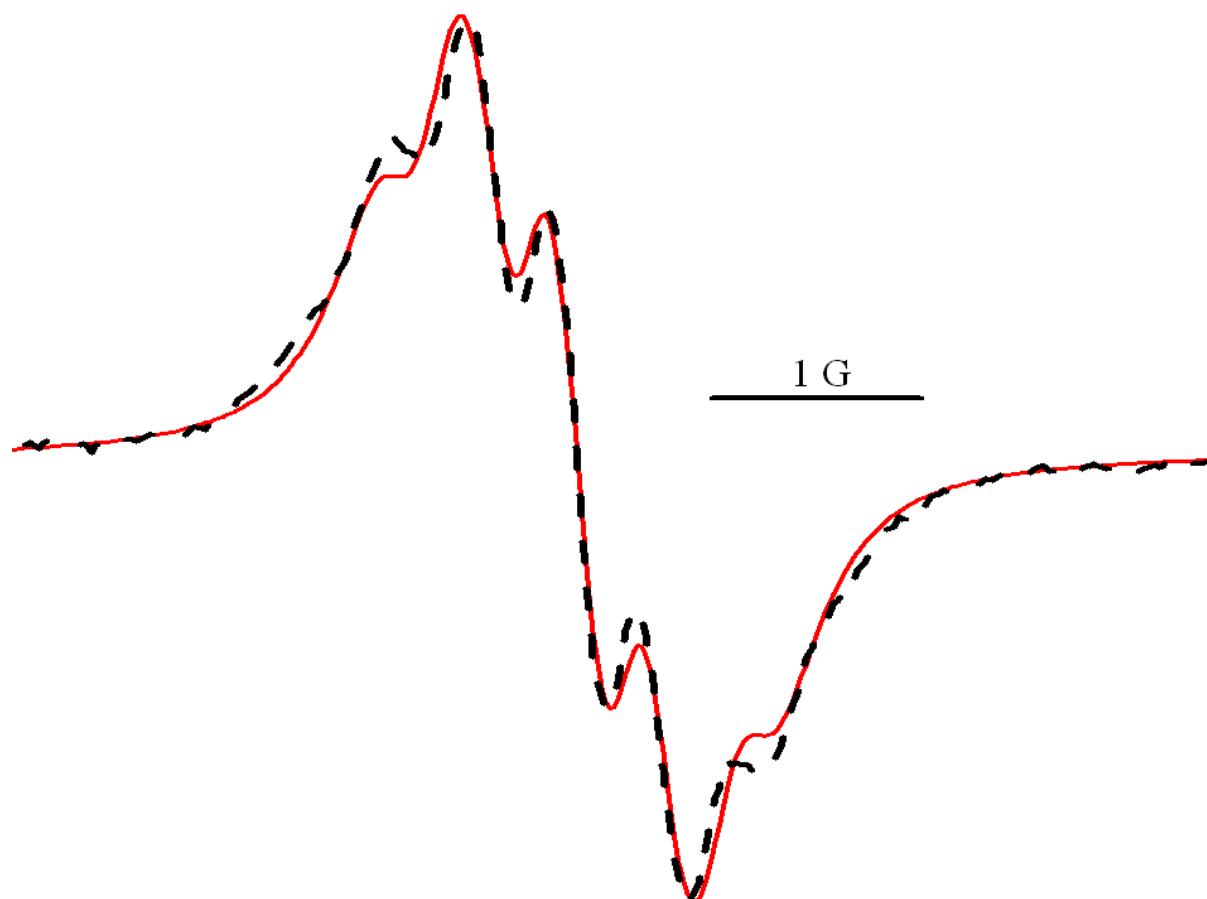
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**Figure S7:** Central line of the EPR spectrum of **4** showing long range hyperfine couplings, recorded with in the following conditions: non saturating microwave power, 20 mW; modulation amplitude, 0.2 G; receiver gain,  $2.5 \times 10^6$ ; time constant, 1.28 ms; scan time, 336 s; 6 scans. Its superimposed simulation was performed by considering an exchange between two conformers with the following parameters: first species (70%),  $a_N = 29.80$  G,  $a_{HY} = 0.21$  G (*3H*),  $a_{HY} = 0.22$  G (*1H*), and  $g = 2.004068$ ; second species (30%),  $a_N = 29.80$  G,  $a_{HY} = 0.21$  G (*3H*),  $a_{HY} = 0.68$  G (*1H*), and  $g = 2.004070$ ; exchange rate constant,  $2.83 \times 10^5$  s<sup>-1</sup>. The experimental signal is in black dotted lines, its simulation in red full lines.

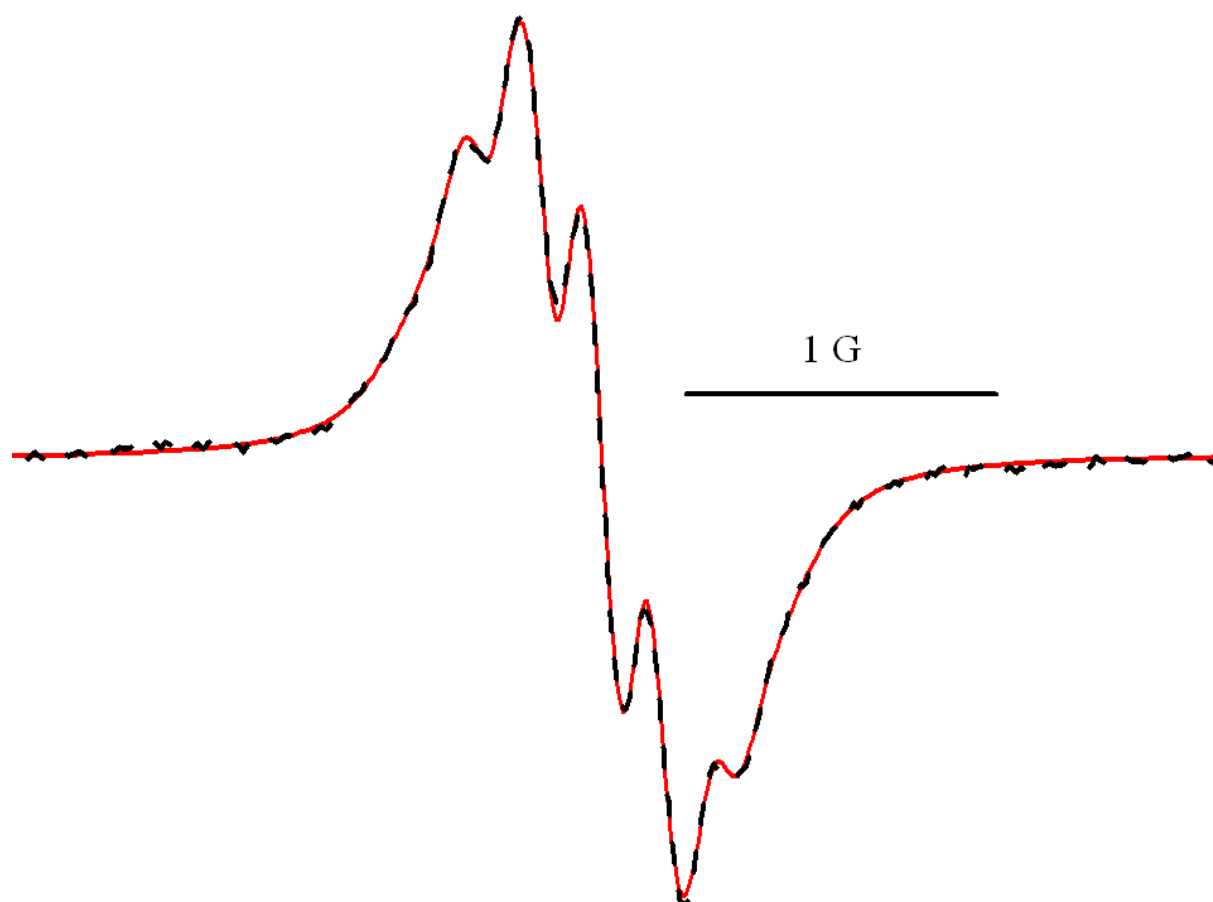
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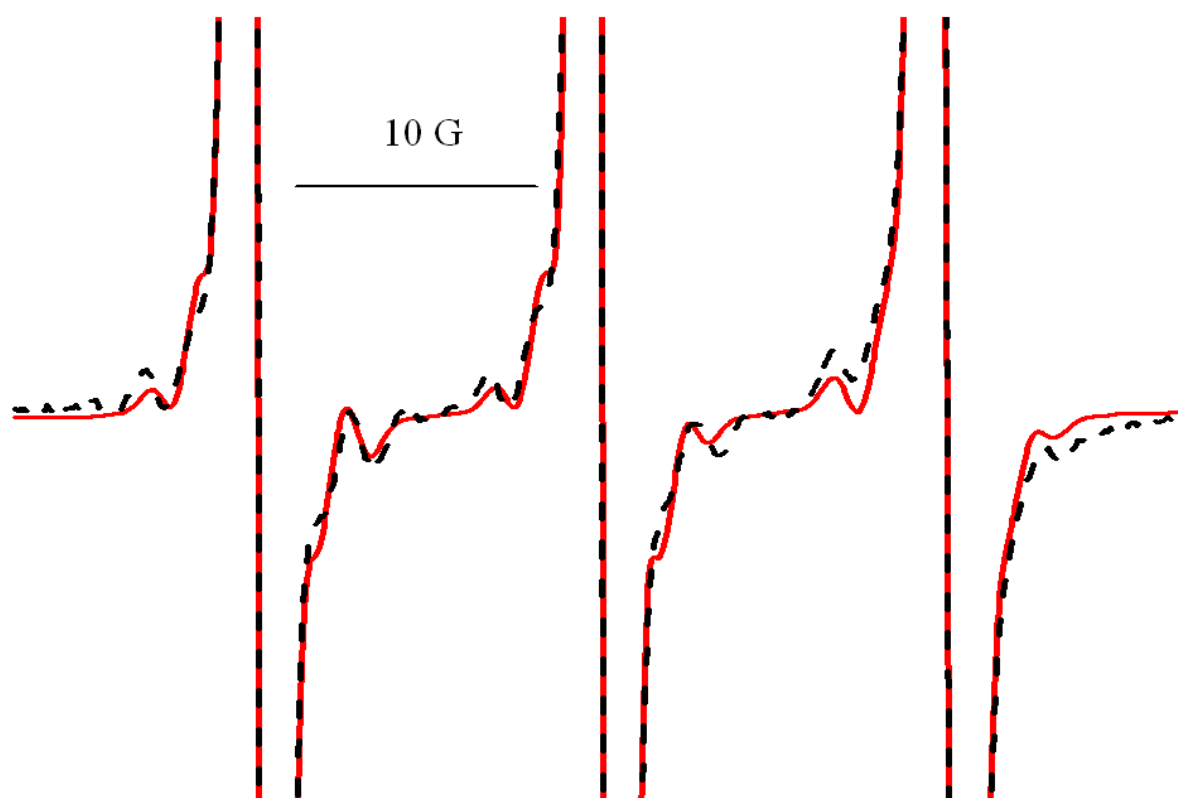
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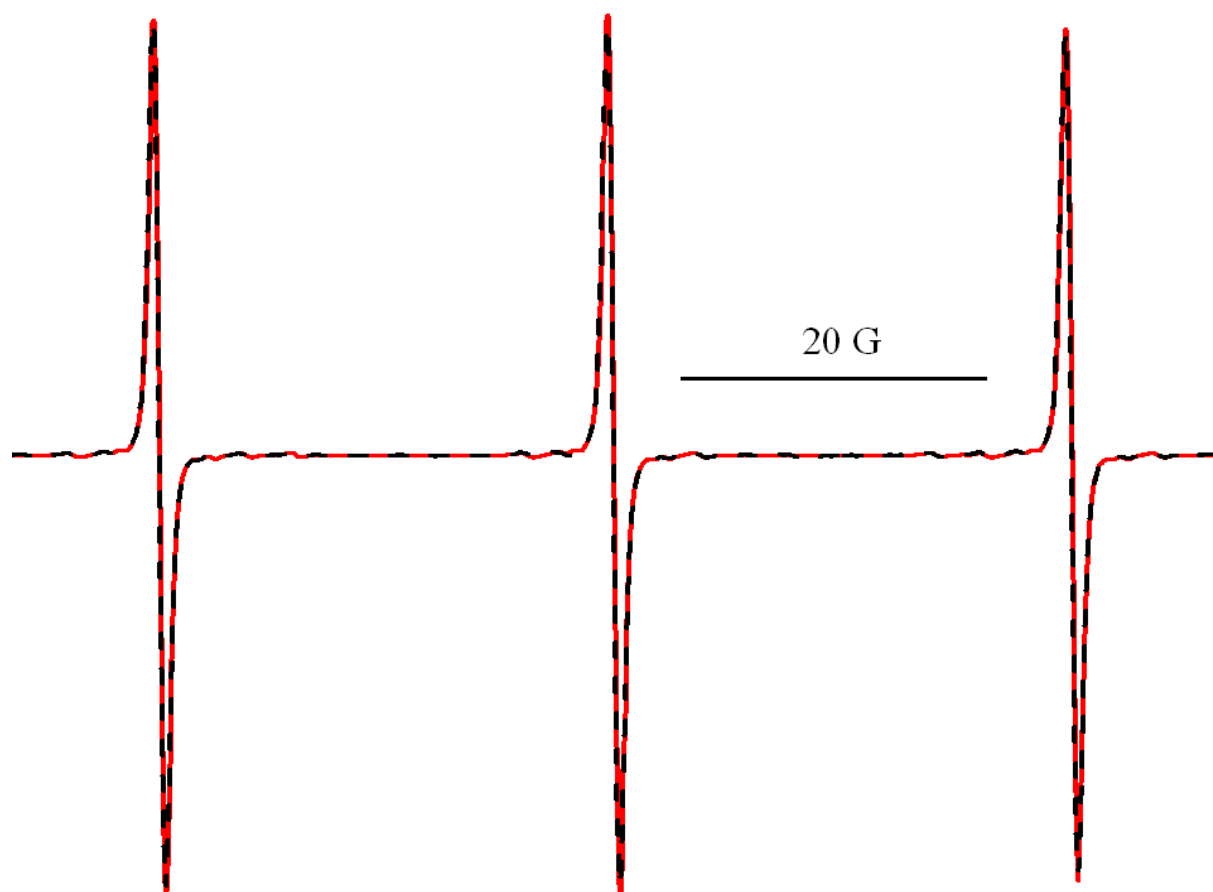
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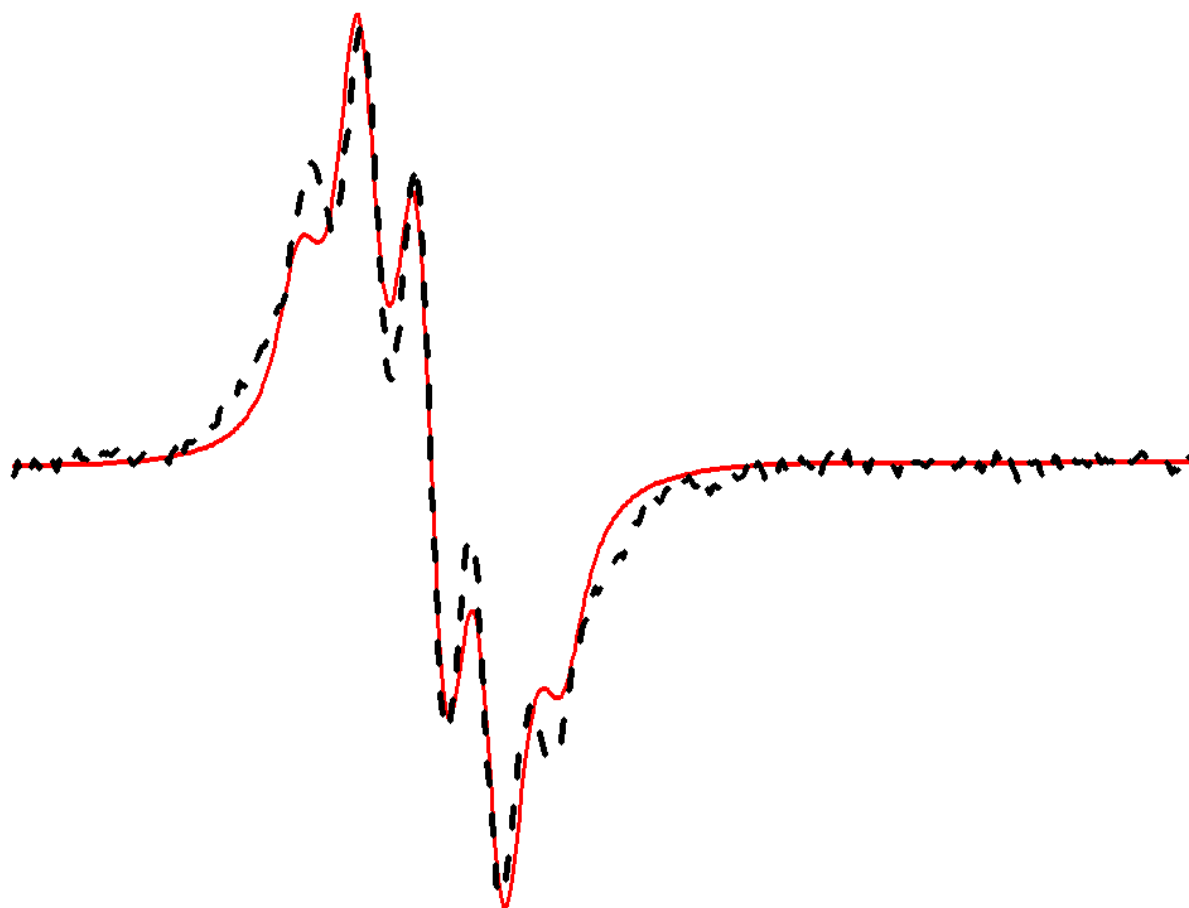
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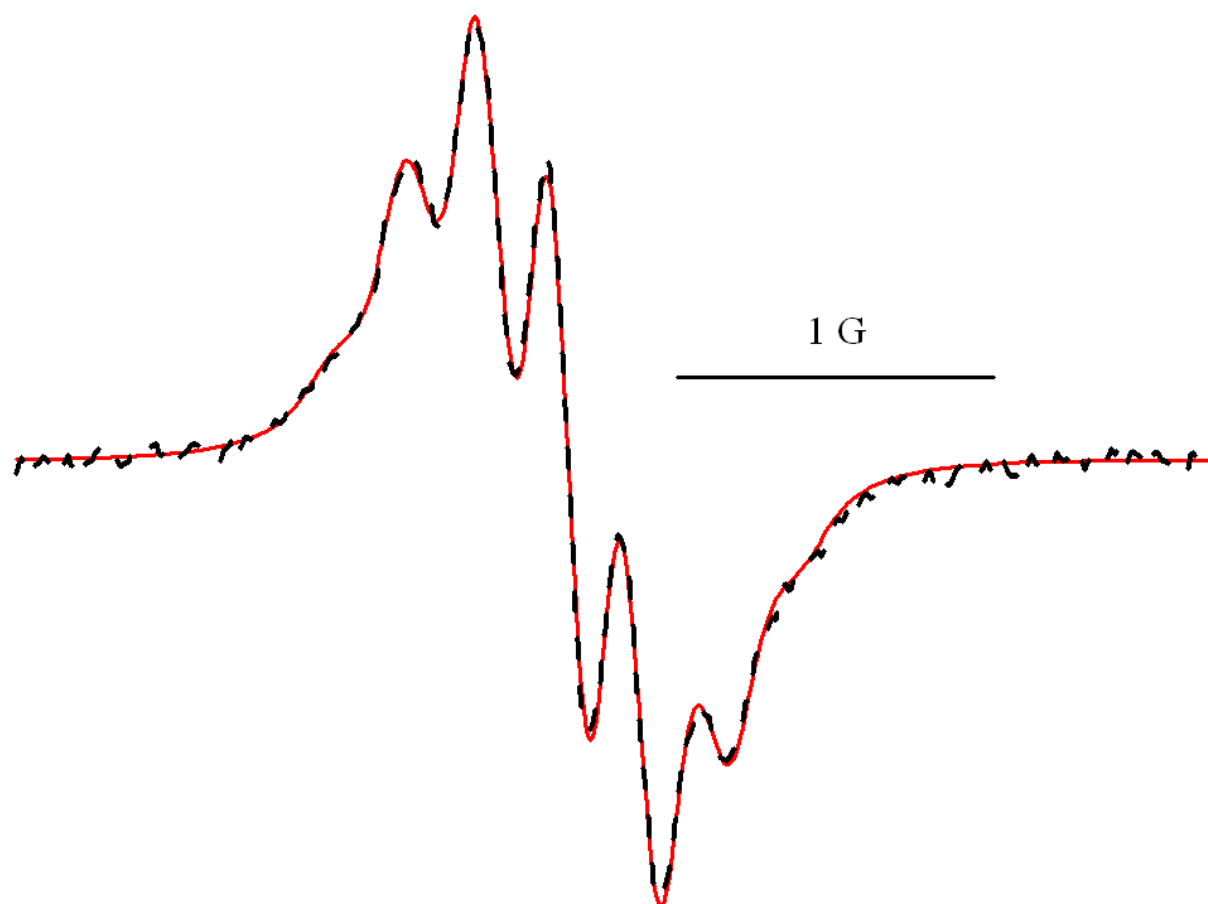


**Figure S5:** Large-scale EPR spectrum of **4** with its superimposed simulation (as shown in figure 2a). The instrument settings were as follows: non saturating microwave power, 20 mW; modulation amplitude, 0.8 G; receiver gain,  $10^5$ ; time constant, 1.28 ms; scan time, 671 s; 9 scans. The experimental signal is in black dotted lines, its simulation in red full lines.

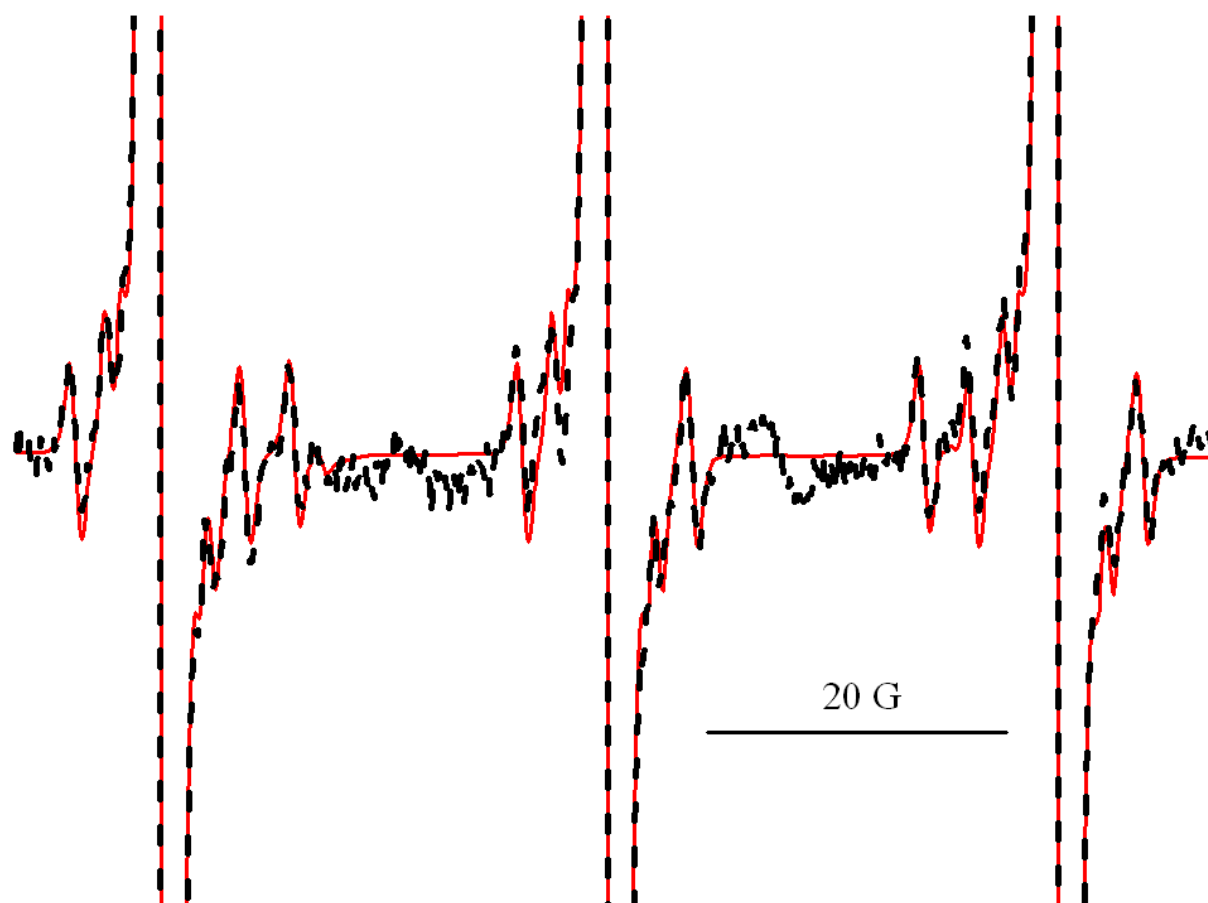


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