Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Temperature-Dependent Dynamics of Endohedral Fullerene $Sc_2@C_{80}(CH_2Ph)$ Studied by EPR Spectroscopy

Yuri E. Kandrashkin[1], *Ruslan B. Zaripov*[1], Fupin Liu,[2] *Bernd Büchner*[2,3], *Vladislav Kataev*[2], *and Alexey A. Popov*[2]

Supporting Information

Table S1. Resonance fields and linewidths of the EPR transitions at T = 250 K.

j	*m*	*B(j,m)*	*ΔB*	*j*	*m*	*B(j,m)*	*ΔB*
0	0	344.77	0.051	5	2	295.54	0.131
1	-1	362.53	0.049	5	3	279.79	0.149
1	0	343.81	0.055	5	4	265.02	0.174
1	1	326.05	0.066	5	5	251.18	0.204
2	-2	380.28	0.056	6	-6	451.30	0.178
2	-1	360.59	0.057	6	-5	427.68	0.164
2	0	341.87	0.063	6	-4	404.96	0.152
2	1	324.12	0.073	6	-3	383.20	0.142
2	2	307.34	0.088	6	-2	362.43	0.136
3	-3	398.04	0.071	6	-1	342.66	0.133
3	-2	377.37	0.069	6	0	323.91	0.135
3	-1	357.67	0.070	6	1	306.18	0.141
3	0	338.94	0.075	6	2	289.48	0.153
3	1	321.20	0.085	6	3	273.78	0.170
3	2	304.42	0.099	6	4	259.07	0.193
3	3	288.62	0.119	6	5	245.31	0.222
4	-4	415.79	0.097	6	6	232.46	0.259
4	-3	394.15	0.09	7	-7	469.06	0.235
4	-2	373.45	0.087	7	-6	444.43	0.218
4	-1	353.73	0.087	7	-5	420.69	0.201
4	0	335.00	0.091	7	-4	397.88	0.187
4	1	317.26	0.100	7	-3	376.05	0.175
4	2	300.50	0.113	7	-2	355.21	0.167
4	3	284.72	0.133	7	-1	335.41	0.163
4	4	269.90	0.158	7	0	316.64	0.163
5	-5	433.55	0.132	7	1	298.93	0.167
5	-4	410.91	0.122	7	2	282.26	0.177
5	-3	389.22	0.114	7	3	266.62	0.193
5	-2	368.49	0.109	7	4	251.99	0.215
5	-1	348.74	0.108	7	5	238.32	0.243
5	0	330.00	0.111	7	6	225.59	0.279
5	1	312.27	0.118	7	7	213.74	0.321

Table S2. The non-zero values of the function $\lambda = \lambda(m,j,j')$.

m	*j*	*J'*	$\lambda(m,j,j')$	*m*	*j*	*J'*	$\lambda(m,j,j')$	*m*	*j*	*J'*	$\lambda(m,j,j')$
0	0	2	7.00	1	2	4	1.28	2	5	7	0.10
0	1	3	2.83	1	3	5	0.75	3	3	5	0.23
0	2	4	1.54	1	4	6	0.37	3	4	6	0.19
0	3	5	0.83	1	5	7	0.12	3	5	7	0.08
0	4	6	0.39	2	2	4	0.64	4	4	6	0.08
0	5	7	0.13	2	3	5	0.53	4	5	7	0.05
1	1	3	1.89	2	4	6	0.29	5	5	7	0.02

Comparison of the EPR Spectra at 140 K, 170 K and 250 K

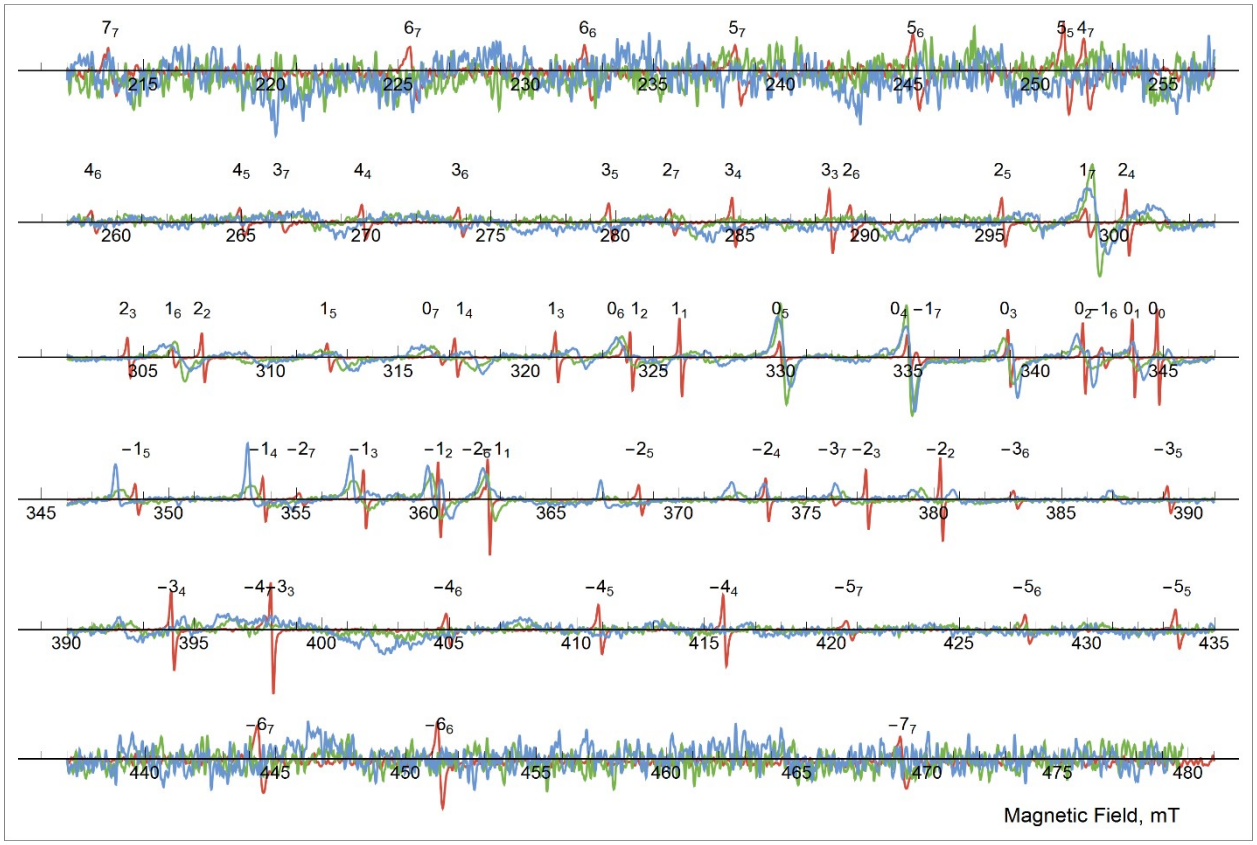

Figure S1. X-Band EPR spectra at several temperatures: 140 K (blue), 170 K (green), and 250 K (red). Due to a large extent of each spectrum they are split in several rows to show in detail all 64 resonance transitions corresponding to the particular states of the nuclear spins. The transitions are labeled as m_j where *j* is the total nuclear spin value and *m* is its projection. The spectra are adjusted to fit the resonance conditions of the EPR line for *j* = 0 and *m* = 0 measured at 250 K.

Experimental and Simulated Spectra at 250 K

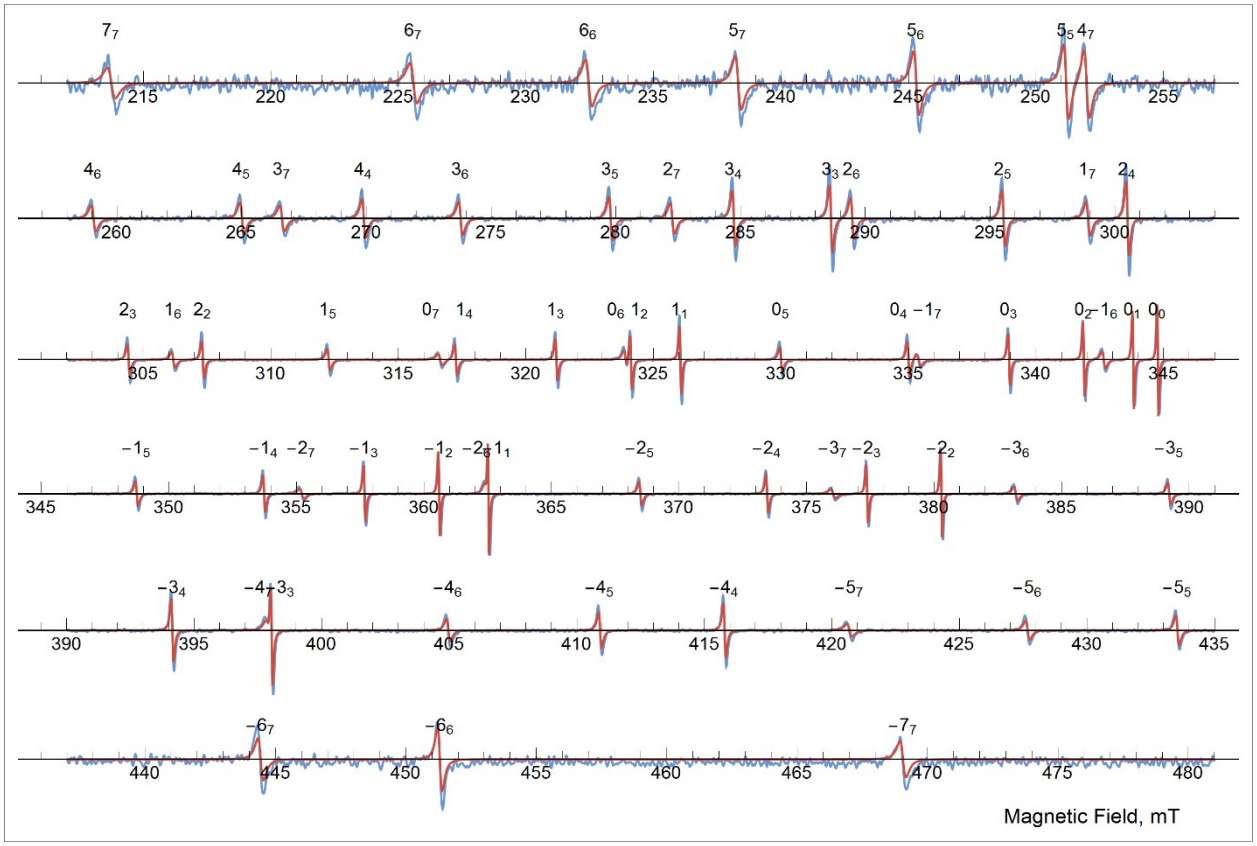

Figure S2. Comparison of the experimental (blue) and modelled (red) EPR spectra at 250 K split in several rows. The transitions are labeled as m_j where j is the total nuclear spin value and m is its projection. The set of the experimental resonance fields, intensities and peak-to-peak linewidths is listed in Appendix I. The details of the simulation are described in the main text. The spin-Hamiltonian parameters equal to g = 1.995 and a = 18.145 mT (see Table 1). The linewidths are modelled according to Eqs. (16)-(20) with the best fit parameters R, Δa, Δg and τ listed in Table 1.

Experimental and Simulated Spectra at Low Temperatures

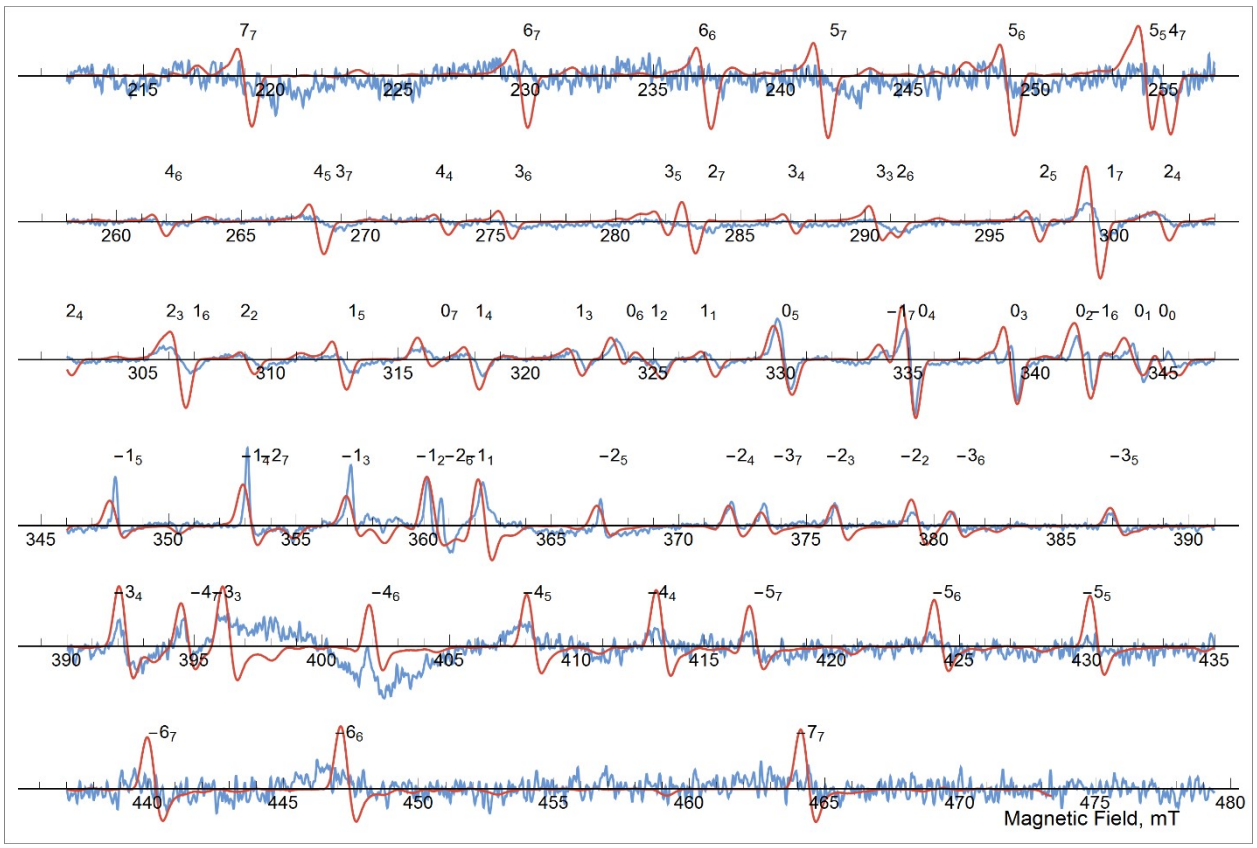

Figure S3. Comparison of the experimental (blue) and modelled (red) EPR spectra at 140 K split in several rows. The transitions are labeled as m_j where j is the total nuclear spin value and m is its projection. The model spectrum is computed with the parameters a = 18.15 mT, $\Delta a = 2.2$ mT, $g = 1.995$, $\Delta g = 0.007$, q = 0.11 mT (same as in Fig. 5).

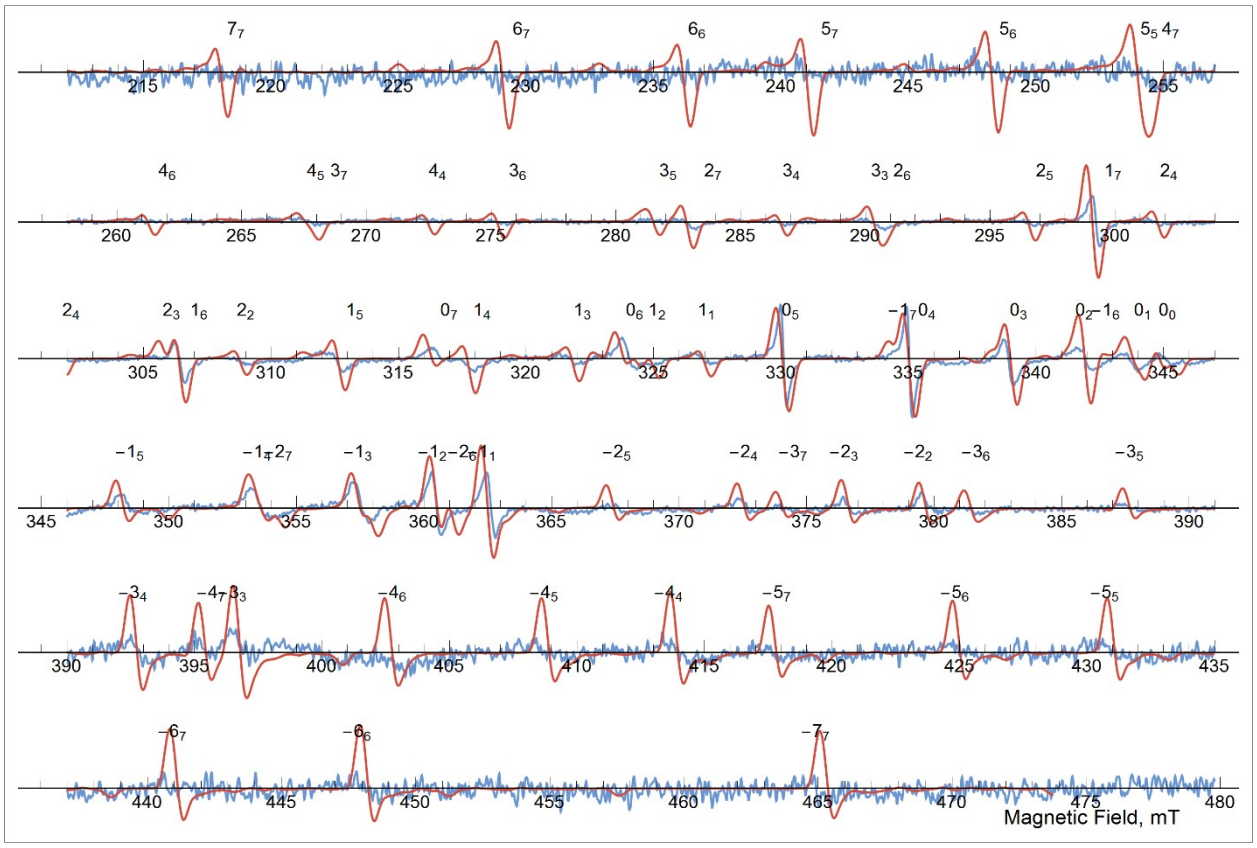

Figure S4. Comparison of the experimental (blue) and modelled (red) EPR spectra at 170 K split in several rows. The transitions are labeled as m_j where j is the total nuclear spin value and m is its projection. The model spectrum is computed with the parameters a = 18.15 mT, $\Delta a = 1.8$ mT, $g = 1.995$, $\Delta g = 0.007$, q = 0.11 mT (same as in Fig. 6).

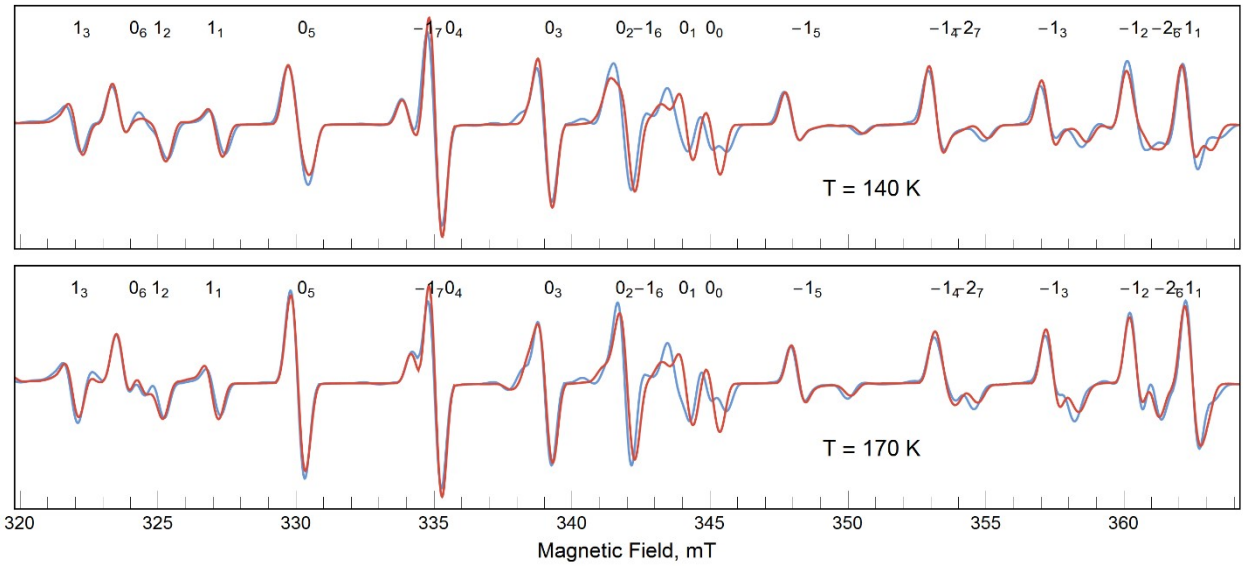

Figure S5. Contribution of the NQI to the broadening of the EPR lines in the central part of the spectrum. The blue color is used for the model spectra shown in Figs. 6 and 7. The red color is used for the model with the same parameters except p = 0.4 MHz (0.014 mT). The transitions are labeled as m_j where j is the total nuclear spin value and m is its projection.