Supplementary Information
Honey-like odor meets single-ion magnet: synthesis, crystal structure, and magnetism of cobalt(II) complex with aromatic trans-cinnamic acid

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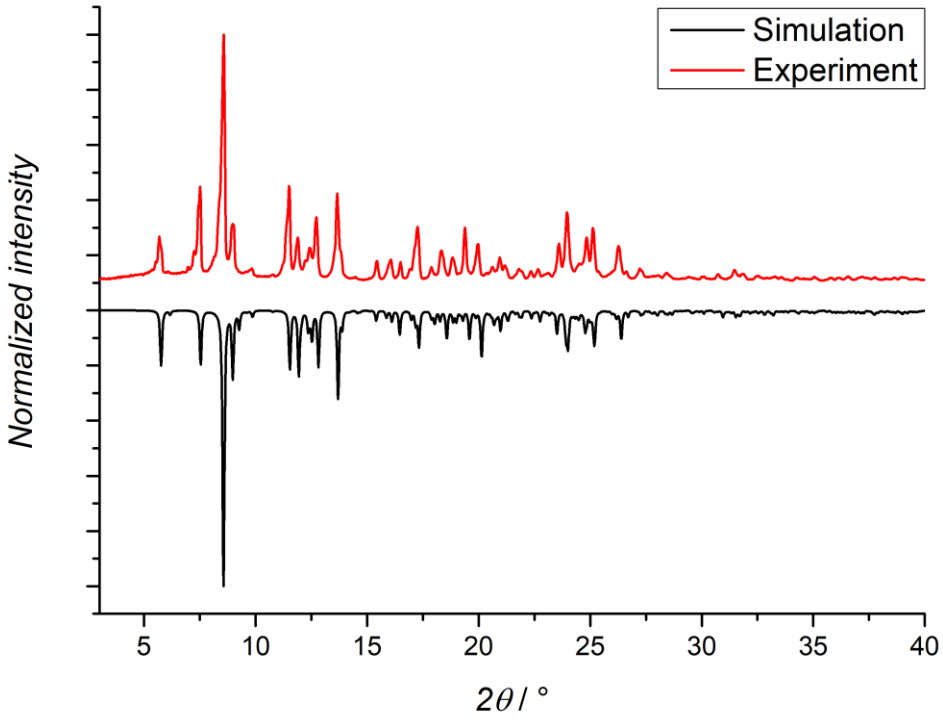

Figure S1. X-ray powder diffraction of compound **1·½Me$_2$CO** measured at room temperature and compared to the simulation calculated from SC-XRD data measured at 293 K.

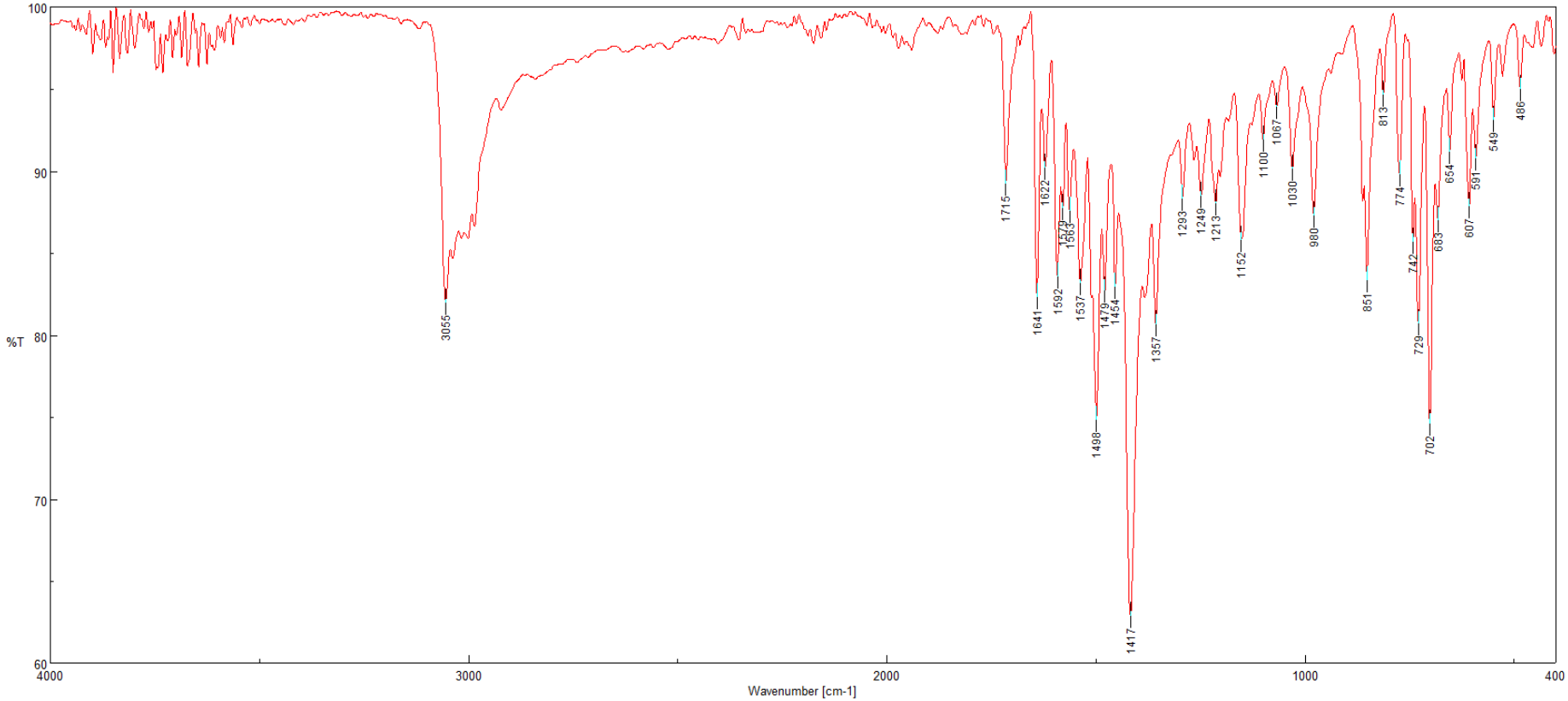

Figure S2. FT-IR spectrum of compound **1·½Me$_2$CO**.

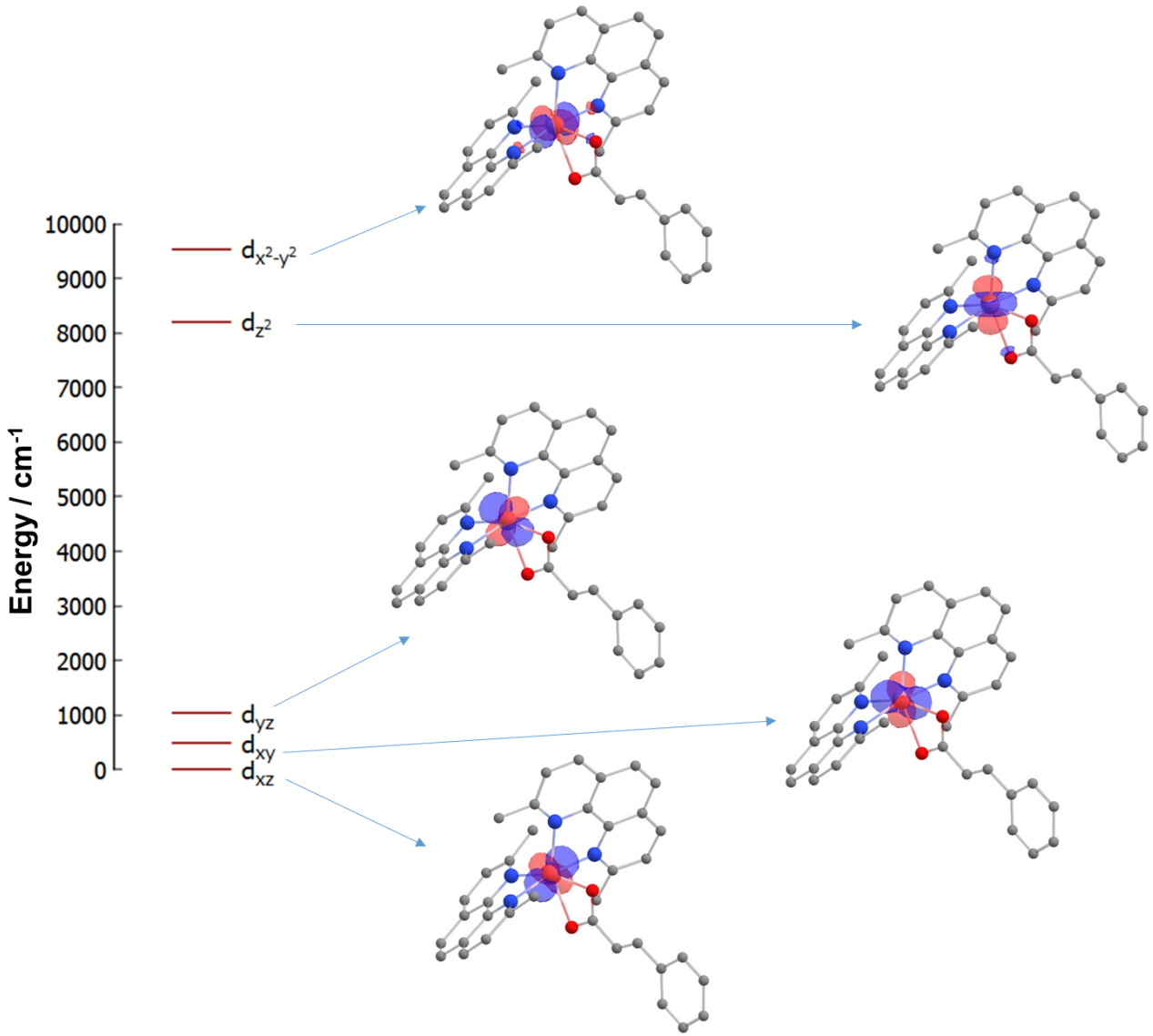

Figure S3. Assignment of energy levels of d-orbitals of compound **1**.

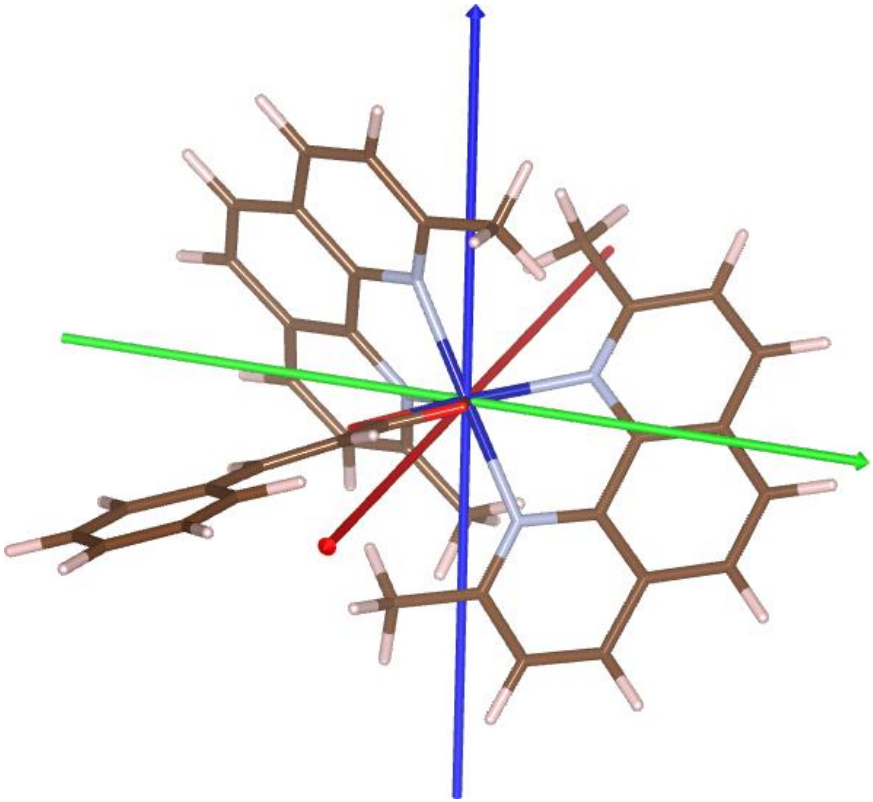

Figure S4. D-tensor (NEVPT2) of compound **1**. Axes: x – red, y – green, z – blue.

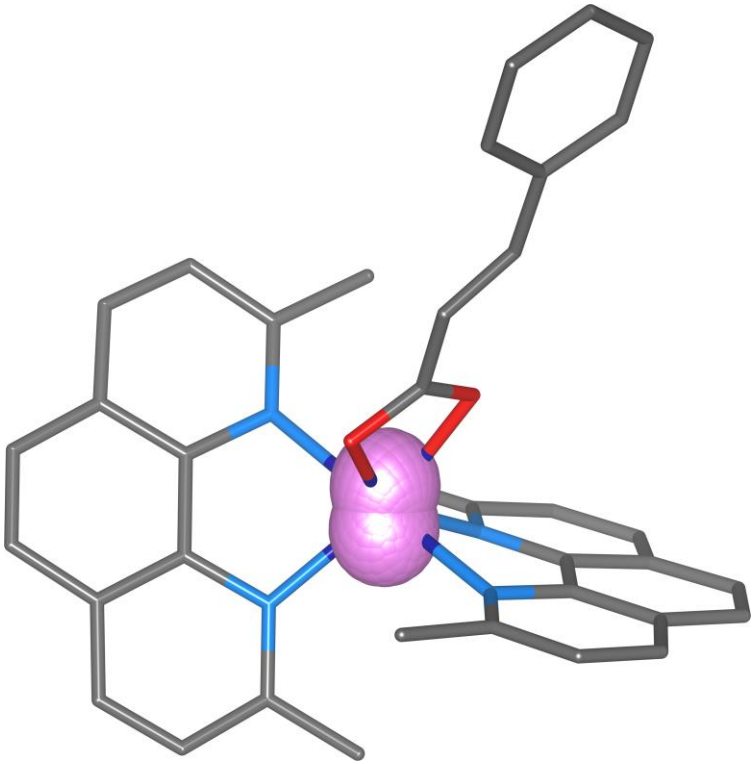

Figure S5. CASSCF/NEVPT2/SINGLE_ANISO calculated the three-dimensional molar magnetization of compound **1** at T = 2 K and B = 0.1 T.

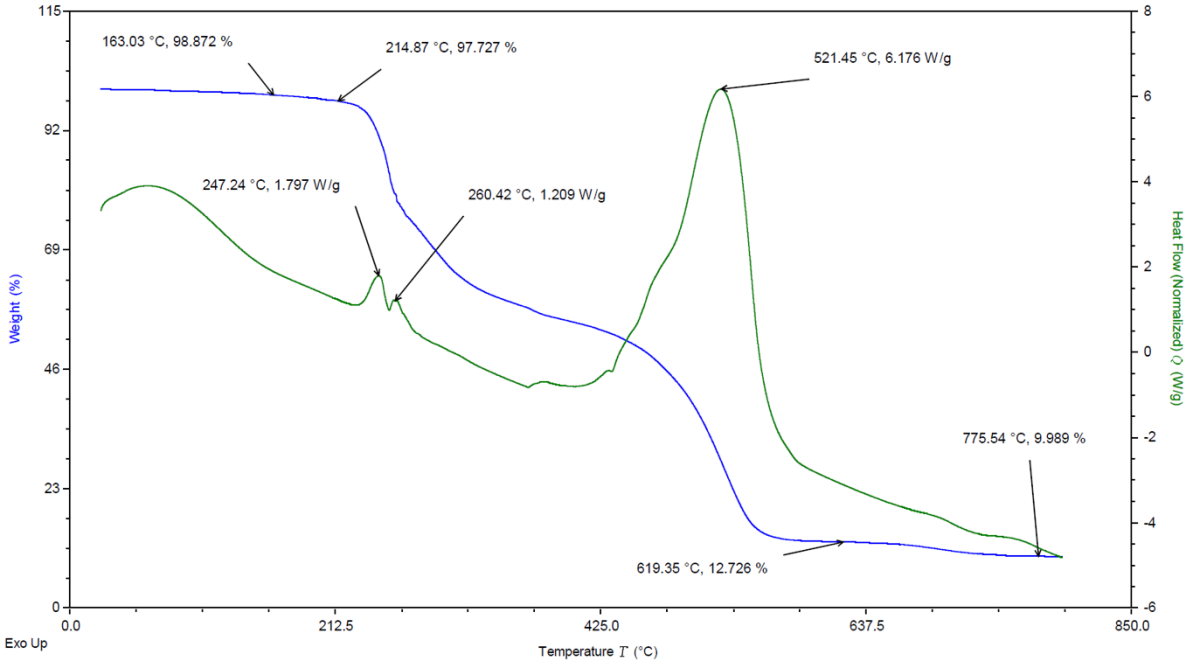

Figure S6. The results of simultaneous TG/DSC thermal analysis of **1·½Me$_2$CO** (5 °C/min, 50 mL/min air atmosphere) are depicted as TG (in blue) and DSC (green) curves; TG = thermogravimetry, DSC = differential scanning calorimetry.

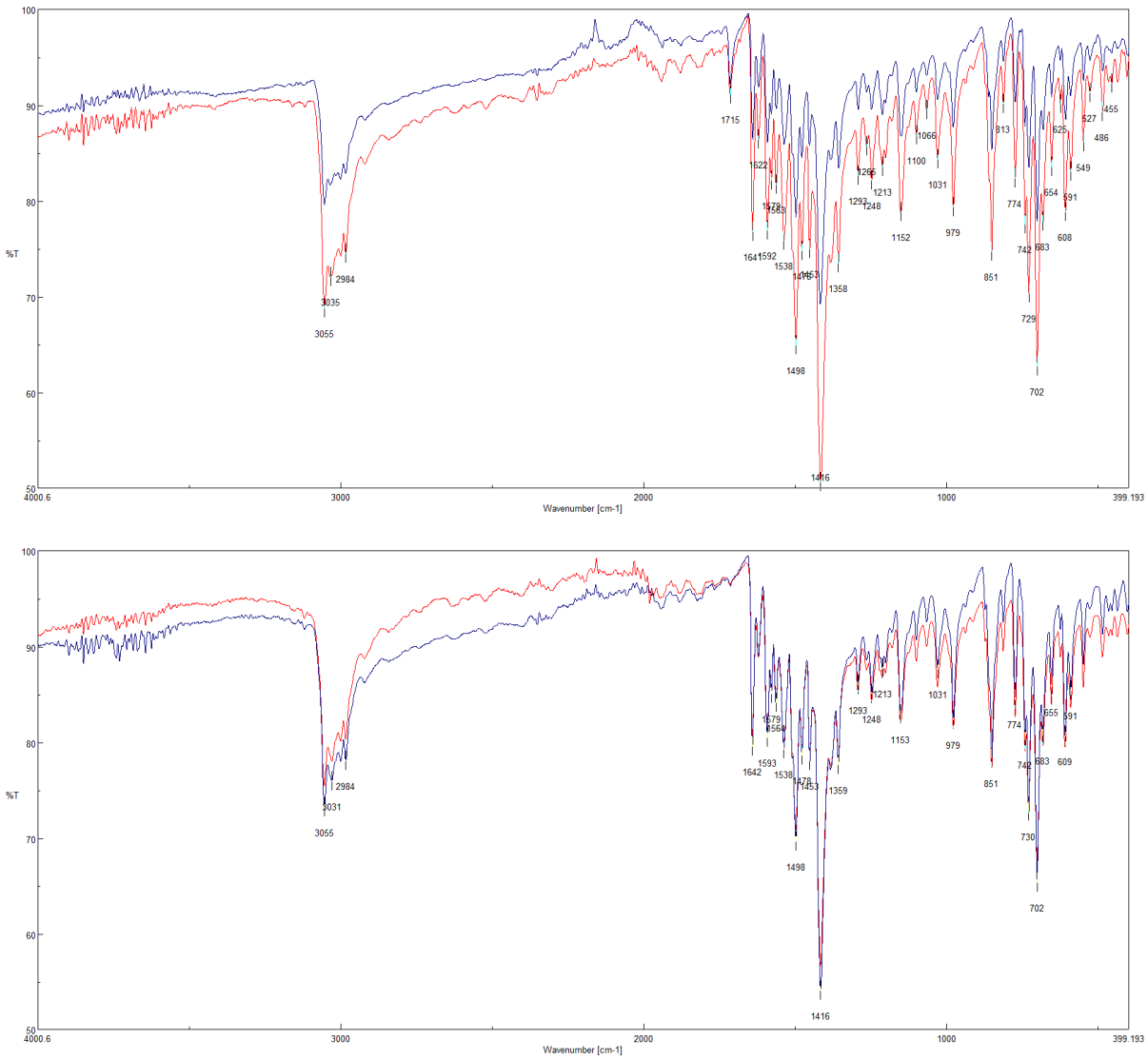

Figure S7. Top – compound **1**·½Me_2CO before (blue) and after (red) irradiation. Bottom – compound **1** before (blue) and after (red) irradiation.

Table S1. The parameters of one-component Debye's model used to analyze the field-dependent AC susceptibility data of **1·½Me$_2$CO**.[a]

B (T)	*T* (K)	c_S (10^{-6} m^{3}mol^{-1})	c_T (10^{-6} m^{3}mol^{-1})	*a*	*t* (10^{-6} s)
0.015	2.00	9.590(0.031)	11.603(0.013)	0.016(0.016)	773.176(19.227)
0.020	2.00	8.045(0.027)	11.609(0.011)	0.037(0.008)	762.189(9.545)
0.030	2.00	5.475(0.017)	11.598(0.007)	0.050(0.003)	810.255(3.901)
0.040	2.00	3.818(0.021)	11.575(0.009)	0.051(0.003)	856.948(3.955)
0.050	2.00	2.780(0.021)	11.542(0.009)	0.054(0.002)	884.414(3.659)
0.060	2.00	2.103(0.026)	11.495(0.012)	0.056(0.003)	896.774(4.456)
0.070	2.00	1.626(0.032)	11.403(0.014)	0.059(0.003)	894.027(5.161)
0.080	2.00	1.299(0.036)	11.340(0.016)	0.064(0.004)	883.041(5.572)
0.090	2.00	1.062(0.044)	11.254(0.019)	0.067(0.004)	865.188(6.602)
0.100	2.00	0.836(0.066)	11.151(0.028)	0.075(0.006)	839.095(9.553)
0.125	2.00	0.480(0.108)	10.867(0.043)	0.092(0.010)	769.056(14.259)
0.150	2.00	0.174(0.195)	10.533(0.070)	0.120(0.017)	693.524(23.661)
0.200	2.00	0.001(0.548)	10.207(0.151)	0.203(0.041)	547.952(58.265)

[a] the standard deviations are reported in parentheses.

Table S2. The parameters of one-component Debye's model used to analyze the temperature-dependent AC susceptibility data of **1·½Me$_2$CO**.[a]

B (T)	*T* (K)	c_S (10^{-6} m^{3}mol^{-1})	c_T (10^{-6} m^{3}mol^{-1})	*a*	*t* (10^{-6} s)
0.090	1.80	1.089(0.117)	12.504(0.045)	0.089(0.011)	1205.769(4.534)
0.090	2.00	1.078(0.111)	11.317(0.037)	0.070(0.011)	862.441(6.745)
0.090	2.20	1.034(0.083)	10.322(0.023)	0.055(0.008)	635.844(9.260)
0.090	2.40	0.995(0.102)	9.561(0.024)	0.048(0.010)	487.527(8.911)
0.090	2.60	0.980(0.098)	8.866(0.019)	0.038(0.009)	379.035(6.751)
0.090	2.80	0.963(0.080)	8.271(0.013)	0.032(0.007)	300.756(4.562)
0.090	3.00	0.989(0.085)	7.749(0.011)	0.023(0.007)	243.077(4.075)
0.090	3.20	1.019(0.147)	7.293(0.015)	0.016(0.012)	199.131(6.089)

0.090	3.40	1.048(0.155)	6.888(0.013)	0.012(0.012)	164.798(5.639)
0.090	3.60	1.093(0.108)	6.530(0.007)	0.008(0.008)	137.332(3.495)
0.090	3.80	1.139(0.166)	6.187(0.008)	0.001(0.012)	115.359(4.807)
0.090	4.00	1.158(0.131)	5.902(0.005)	0.001(0.008)	96.133(3.343)
0.090	4.20	1.156(0.314)	5.639(0.008)	0.001(0.018)	79.653(7.035)
0.090	4.40	1.146(0.301)	5.393(0.005)	0.001(0.015)	65.920(5.836)
0.090	4.60	1.163(0.470)	5.168(0.006)	0.001(0.021)	54.933(7.986)
0.090	4.80	1.268(0.486)	4.964(0.005)	0.001(0.021)	46.694(7.528)
0.090	5.00	0.881(0.805)	4.769(0.004)	0.001(0.024)	34.334(8.519)

[a] the standard deviations are reported in parentheses.