Electronic Supplementary Information (ESI)

Field-induced slow relaxation of magnetization in pentacoordinate Co(II) compound [Co(phen)(DMSO)Cl_2]

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Table S1 Energy levels (cm^{-1}) of ligand field multiplets in zero magnetic field derived from CASSCF/NEVPT2 calculations for **1** and for **I-V**.

	1	I	II	III	IV	V
0:	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1:	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2:	40.1000	94.6257	232.3152	244.7170	218.9037	86.6385
3:	40.1000	94.6257	232.3152	244.7170	218.9037	86.6385
4:	1863.5883	1446.7049	731.8815	565.5706	554.5198	2210.0992
5:	1863.5883	1446.7049	731.8815	565.5706	554.5198	2210.0992
6:	2056.1053	1577.1244	1017.2286	870.5264	823.8131	2605.8479
7:	2056.1053	1577.1244	1017.2286	870.5264	823.8131	2605.8479
8:	3285.8831	3342.5351	2708.4632	2639.5543	2456.9723	3191.6720
9:	3285.8831	3342.5351	2708.4632	2639.5543	2456.9723	3191.6720
10:	3533.7953	3427.1128	2767.8466	2704.9463	2501.9102	3453.9865
11:	3533.7953	3427.1128	2767.8466	2704.9463	2501.9102	3453.9865
12:	3891.9764	5895.7725	5079.4861	3863.9853	3951.1400	4736.3564
13:	3891.9764	5895.7725	5079.4861	3863.9853	3951.1400	4736.3564
14:	4076.5071	6002.1186	5186.9811	3996.7046	4073.7580	4787.1227
15:	4076.5071	6002.1186	5186.9811	3996.7046	4073.7580	4787.1227
16:	6104.9803	8525.1204	7238.5843	6953.0228	7339.6499	6028.6941
17:	6104.9803	8525.1204	7238.5843	6953.0228	7339.6499	6028.6941
18:	6194.0892	8587.3186	7312.1915	7030.3683	7405.1515	6083.6936
19:	6194.0892	8587.3186	7312.1915	7030.3683	7405.1515	6083.6936
20:	10258.0176	10284.5214	9205.2174	8363.1561	8473.9062	12357.7666
21:	10258.0176	10284.5214	9205.2174	8363.1561	8473.9062	12357.7666
22:	10431.3709	10351.7738	9312.3811	8486.9626	8599.5394	12624.6367
23:	10431.3709	10351.7738	9312.3811	8486.9626	8599.5394	12624.6367
24:	12047.0808	10619.9712	12225.4299	12107.8500	11826.1176	12907.8699
25:	12047.0808	10619.9712	12225.4299	12107.8500	11826.1176	12907.8699
26:	12143.6103	15248.8101	13420.3546	12132.1577	12807.4835	13551.8622
27:	12143.6103	15248.8101	13420.3546	12132.1577	12807.4835	13551.8622
28:	13266.1283	15381.1965	13441.4726	12765.8144	12825.4142	13816.4989
29:	13266.1283	15381.1965	13441.4726	12765.8144	12825.4142	13816.4989
30:	14942.8712	15538.0319	15245.8550	16128.3654	15774.4563	13911.5961
31:	14942.8712	15538.0319	15245.8550	16128.3654	15774.4563	13911.5961
32:	17973.8348	16046.2701	16387.9994	16428.8554	16354.0567	17268.1753
33:	17973.8348	16046.2701	16387.9994	16428.8554	16354.0568	17268.1753
34:	18746.4925	17281.8455	17901.2192	17357.4736	16762.0801	18117.3405
35:	18746.4925	17281.8455	17901.2192	17357.4736	16762.0801	18117.3405
36:	19103.3554	18770.5617	18518.8776	18588.3686	18759.3075	19922.9373

37:	19103.3554	18770.5617	18518.8776	18588.3686	18759.3075	19922.9373
38:	19181.6812	18957.4187	18955.8276	18856.7015	18978.1542	20237.4933
39:	19181.6812	18957.4187	18955.8276	18856.7015	18978.1542	20237.4933
40:	19318.1268	19017.5112	19026.3169	18907.1894	19023.5492	20283.6844
41:	19318.1268	19017.5112	19026.3169	18907.1894	19023.5492	20283.6844
42:	19919.6126	19847.7576	19293.5626	19200.6261	19086.7931	20325.4219
43:	19919.6127	19847.7576	19293.5626	19200.6261	19086.7931	20325.4219
44:	20180.6591	19989.4795	20020.0887	19674.0870	19599.3263	20423.4207
45:	20180.6591	19989.4795	20020.0887	19674.0870	19599.3263	20423.4207
46:	20651.8750	20817.1265	20407.7489	20080.2220	19987.0585	20608.5882
47:	20651.8750	20817.1265	20407.7489	20080.2220	19987.0585	20608.5882
48:	20900.4766	22183.8439	21041.8889	20182.2744	20100.6273	20702.6932
49:	20900.4766	22183.8439	21041.8889	20182.2744	20100.6273	20702.6932
50:	21015.3030	22706.6200	21189.1678	20252.6416	20164.0252	20820.7667
51:	21015.3030	22706.6200	21189.1678	20252.6416	20164.0252	20820.7667
52:	21408.6226	22774.4261	21449.0664	21295.0501	21489.1952	20986.3203
53:	21408.6226	22774.4261	21449.0664	21295.0501	21489.1952	20986.3203
54:	21716.6788	23016.9177	22100.3906	21635.5917	21852.3371	21550.9860
55:	21716.6788	23016.9177	22100.3906	21635.5917	21852.3371	21550.9860
56:	22396.5927	23290.0882	22426.3940	21752.2642	22339.0184	22196.1350
57:	22396.5927	23290.0882	22426.3940	21752.2642	22339.0184	22196.1350
58:	22631.6899	23933.2437	22520.8174	22114.1675	22748.7332	23125.7592
59:	22631.6899	23933.2437	22520.8174	22114.1675	22748.7332	23125.7592
60:	23111.8373	24902.2392	22889.8247	22526.1477	22836.5213	23180.4090
61:	23111.8373	24902.2392	22889.8247	22526.1477	22836.5213	23180.4090
62:	23474.3364	24977.9465	23498.7678	23348.3214	23136.9212	23514.3099
63:	23474.3364	24977.9465	23498.7678	23348.3214	23136.9212	23514.3099
64:	26011.9515	27082.7253	26271.2874	25500.5097	25626.6623	26082.8444
65:	26011.9515	27082.7253	26271.2874	25500.5097	25626.6623	26082.8444
66:	26130.4942	27380.8644	26424.1660	26258.2709	26496.9580	26186.3060
67:	26130.4942	27380.8644	26424.1660	26258.2709	26496.9580	26186.3060
68:	27955.3578	27905.8186	26933.0992	26662.9157	26849.6921	28931.5429
69:	27955.3578	27905.8186	26933.0992	26662.9157	26849.6921	28931.5429
70:	28529.2523	28637.7509	27653.3554	26939.3578	27202.2260	29438.6020
71:	28529.2523	28637.7509	27653.3554	26939.3578	27202.2260	29438.6020
72:	28847.9087	29605.3775	28387.8174	28041.9865	28441.1912	29687.6176
73:	28847.9087	29605.3775	28387.8174	28041.9865	28441.1912	29687.6176
74:	29318.9081	30440.7472	29132.2959	28495.4962	28794.0685	30528.5831
75:	29318.9081	30440.7472	29132.2959	28495.4962	28794.0685	30528.5831
76:	29620.6820	30757.1334	29603.2055	28862.3526	29320.9711	30839.8890
77:	29620.6820	30757.1334	29603.2055	28862.3526	29320.9711	30839.8890
78:	30100.2587	31202.5757	29951.7160	29361.5424	29789.7357	31166.0331
79:	30100.2587	31202.5757	29951.7160	29361.5424	29789.7357	31166.0331
80:	30389.4554	31431.4416	30280.1527	29615.9396	30190.4195	31490.0925
81:	30389.4554	31431.4416	30280.1527	29615.9396	30190.4195	31490.0925
82:	30696.1492	31721.6542	30696.4942	29816.9491	30418.6470	31825.7400
83:	30696.1492	31721.6542	30696.4942	29816.9491	30418.6470	31825.7400
84:	31026.5998	33048.2030	31459.9264	30873.4314	31302.6394	32095.4441
85:	31026.5998	33048.2030	31459.9264	30873.4314	31302.6394	32095.4441
86:	31542.1220	33318.2574	32042.9158	31170.5998	31766.5375	32767.4625
87:	31542.1220	33318.2574	32042.9158	31170.5998	31766.5375	32767.4625
88:	31766.4670	33864.7223	32510.7306	31464.0705	31995.3612	32989.6106
89:	31766.4670	33864.7223	32510.7306	31464.0705	31995.3612	32989.6106
90:	31999.1779	35458.6036	33123.1770	31859.8631	32195.0526	33263.4633
91:	31999.1779	35458.6036	33123.1770	31859.8631	32195.0526	33263.4633
92:	33155.3284	35915.7383	33612.0130	32189.1400	32668.5751	34382.7085
93:	33155.3284	35915.7383	33612.0130	32189.1400	32668.5751	34382.7085
94:	33761.9308	36418.3804	34059.8170	32871.8550	33405.2883	35208.5098
95:	33761.9308	36418.3804	34059.8170	32871.8550	33405.2883	35208.5098
96:	40703.4924	41092.4704	40005.9140	39782.4147	39917.8558	40979.7470

97:	40703.4924	41092.4704	40005.9140	39782.4147	39917.8558	40979.7470
98:	41217.1399	41783.9820	40660.4456	40399.5246	40655.7640	41123.0795
99:	41217.1399	41783.9820	40660.4456	40399.5246	40655.7640	41123.0795
100:	41469.2004	42281.3859	41544.4762	41100.7158	41215.3186	42484.0850
101:	41469.2004	42281.3859	41544.4762	41100.7158	41215.3186	42484.0850
102:	42598.9899	44133.9536	42142.3669	41712.2102	42259.3006	42658.4884
103:	42598.9899	44133.9536	42142.3669	41712.2102	42259.3006	42658.4884
104:	42891.2691	44319.4022	42421.5006	41901.2332	42443.0724	42883.4304
105:	42891.2691	44319.4022	42421.5006	41901.2332	42443.0724	42883.4304
106:	43115.8128	44871.3467	43038.2428	42240.3537	42788.3777	43057.6601
107:	43115.8128	44871.3467	43038.2428	42240.3537	42788.3777	43057.6601
108:	43489.7744	45017.2275	43142.4921	42601.0392	43066.1107	43532.4060
109:	43489.7744	45017.2275	43142.4921	42601.0392	43066.1107	43532.4060
110:	61058.3099	60759.5505	60405.1309	60128.5845	60365.1798	61169.4200
111:	61058.3099	60759.5505	60405.1309	60128.5845	60365.1798	61169.4200
112:	61390.0357	61854.7912	60663.4620	60414.5437	60563.0277	61530.5179
113:	61390.0357	61854.7912	60663.4620	60414.5437	60563.0277	61530.5179
114:	62665.5920	63602.0749	62119.1714	61682.8617	62240.0003	63393.1159
115:	62665.5920	63602.0749	62119.1714	61682.8617	62240.0003	63393.1159
116:	63951.5734	65608.0704	63504.9284	62632.1377	63020.0850	63648.2579
117:	63951.5734	65608.0704	63504.9284	62632.1377	63020.0850	63648.2580
118:	64284.6638	66432.6372	64269.6899	63358.5766	64108.0696	64203.2338
119:	64284.6638	66432.6372	64269.6899	63358.5766	64108.0696	64203.2338

Table S2. Individual contributions to *D*-tensor for **1** calculated by CASSCF/NEVPT2.

Multiplicity	Root	*D*	*E*
4	0	0.000	0.000
4	1	-21.647	-3.526
4	2	-0.019	-0.211
4	3	-5.303	-8.866
4	4	7.957	6.140
4	5	-0.189	-0.113
4	6	0.340	0.244
4	7	0.001	-0.000
4	8	0.047	0.015
4	9	-0.045	-0.012
2	0	-0.153	0.375
2	1	0.554	0.055
2	2	-0.292	-0.183
2	3	0.410	0.266
2	4	0.073	-0.001
2	5	0.100	0.047
2	6	3.647	0.004
2	7	-1.710	1.620
2	8	-2.591	-1.886
2	9	-0.015	-0.007
2	10	0.003	0.019
2	11	0.003	0.003
2	12	-0.008	-0.006
2	13	0.034	0.020
2	14	0.240	0.008
2	15	-0.023	0.122
2	16	0.112	0.083
2	17	0.066	0.002
2	18	-0.001	0.002
2	19	0.030	-0.003
2	20	-0.204	-0.247
2	21	-0.063	-0.081
2	22	-0.546	-0.547
2	23	-0.188	0.046
2	24	-0.550	0.397
2	25	0.687	-0.001
2	26	0.032	0.042
2	27	-0.037	-0.075
2	28	0.143	0.070
2	29	0.116	-0.009
2	30	-0.037	0.026
2	31	-0.073	-0.055
2	32	-0.011	0.015
2	33	-0.008	0.004
2	34	0.001	0.004
2	35	0.001	0.000
2	36	-0.036	-0.022
2	37	-0.007	0.010
2	38	0.012	0.002
2	39	0.014	0.008

Table S3. Individual contributions to *D*-tensor for **I-V** calculated by CASSCF/NEVPT2.

		I		**II**		**III**		**IV**		**V**	
Multiplicity	Root	*D*	*E*	*D*	*E*	*D*	*E*	*D*	*E*	*D*	*E*
4	0	-0.000	-0.000	-0.000	-0.000	0.000	-0.000	0.000	-0.000	0.000	-0.000
4	1	-65.702	0.093	-113.846	-0.131	-123.541	-0.267	-128.718	-0.077	9.009	9.009
4	2	10.128	-10.123	2.132	-3.223	-0.203	-1.171	18.705	-15.975	-0.042	-0.136
4	3	3.032	-3.019	-9.905	-4.074	-11.920	-5.665	0.371	2.422	13.570	13.570
4	4	5.194	5.864	3.595	-6.822	2.760	-6.677	1.314	1.967	13.050	-13.056
4	5	1.308	-1.312	0.017	0.017	0.078	-0.087	4.981	2.850	-0.015	-0.000
4	6	0.159	0.198	0.017	0.017	0.082	-0.009	0.211	0.034	0.005	0.005
4	7	0.004	-0.004	0.089	-0.097	0.076	-0.092	0.021	0.014	0.012	0.012
4	8	0.009	0.037	0.000	0.000	-0.001	-0.001	-0.003	0.012	0.146	-0.147
4	9	0.035	-0.035	-0.090	-0.003	-0.066	-0.008	-0.004	-0.017	0.094	0.094
2	0	0.694	-1.378	-1.211	-1.211	-1.034	-1.038	2.214	0.498	-0.000	-0.000
2	1	-0.217	0.226	-2.322	-2.322	-0.071	-0.163	0.731	-0.041	0.514	0.008
2	2	1.486	-0.135	-0.179	-0.179	-1.695	-1.744	0.036	-0.040	2.960	0.000
2	3	1.781	-0.048	0.269	0.022	0.274	0.058	0.574	0.579	-0.000	-0.000
2	4	-0.115	0.116	-0.000	-0.000	0.009	0.000	0.317	0.123	-0.513	-0.513
2	5	-0.030	0.032	3.114	0.004	3.225	0.018	2.325	-0.119	-1.197	-1.197
2	6	1.847	-0.142	-0.075	0.170	-0.171	0.124	-0.267	0.002	-0.213	0.214
2	7	-1.626	1.619	-1.032	1.087	-1.247	1.272	-1.414	1.446	-0.721	1.223
2	8	-0.091	-0.955	-2.654	-2.654	-2.588	-2.586	-1.027	-1.242	8.750	0.080
2	9	-0.370	-0.370	-0.019	-0.019	0.033	0.002	-0.011	0.089	0.016	0.002
2	10	-0.280	0.282	0.058	0.004	0.029	-0.012	-0.124	0.046	-0.002	-0.002
2	11	-0.039	0.039	0.001	0.017	-0.026	0.030	-0.025	0.025	-0.001	-0.001
2	12	-0.158	0.157	-0.215	0.215	-0.072	0.077	-0.024	0.007	-0.051	0.051
2	13	0.431	0.000	0.295	0.063	0.149	0.009	-0.008	0.078	-0.018	-0.018
2	14	-0.278	0.279	-0.184	0.211	-0.081	-0.028	0.102	-0.007	-0.118	0.127
2	15	-0.089	0.088	-0.050	-0.050	-0.093	0.113	-0.188	0.007	-0.110	-0.110
2	16	-0.014	-0.014	0.029	0.000	-0.134	-0.272	0.257	0.173	-0.055	0.095
2	17	0.143	-0.145	-0.085	-0.085	-0.145	-0.094	0.252	-0.076	-0.001	-0.001
2	18	-0.138	0.134	-0.410	-0.410	0.009	-0.021	-0.028	0.010	0.010	0.049
2	19	0.274	-0.339	-0.002	-0.002	-0.008	0.002	-0.013	-0.071	-0.034	-0.034
2	20	-0.382	0.377	-0.137	0.152	-0.061	0.057	-1.192	-0.057	0.125	0.035
2	21	-1.004	-0.998	-0.560	-0.560	-0.745	-0.615	-0.151	0.139	-0.062	-0.062
2	22	-0.013	0.012	0.327	0.000	0.168	0.002	-0.053	-0.043	1.058	0.000
2	23	0.390	-0.003	-0.001	-0.001	-0.004	0.039	0.383	0.016	-0.007	-0.007
2	24	-0.056	0.056	-0.757	0.855	-0.053	0.028	0.380	-0.160	-0.003	-0.003

2	25	0.019	-0.034	-0.001	-0.001	-0.008	0.583	-0.024	-0.040	0.013	0.074
2	26	-0.006	0.006	-0.044	-0.044	-0.043	0.294	-0.076	-0.119	-0.706	0.706
2	27	0.051	0.000	0.565	0.021	-0.077	-0.077	-0.042	-0.065	-0.480	-0.480
2	28	-0.144	0.144	-0.045	0.073	0.105	0.042	-0.096	0.025	-0.137	0.138
2	29	-0.013	0.013	0.273	0.007	0.147	0.049	0.004	-0.024	-0.226	-0.226
2	30	-0.056	-0.111	-0.002	-0.002	0.007	0.000	0.096	-0.037	-0.011	-0.011
2	31	0.132	-0.008	0.195	0.001	0.159	-0.002	0.007	0.011	-0.071	0.072
2	32	0.034	0.005	-0.003	-0.003	-0.006	0.014	0.001	-0.033	-0.042	-0.042
2	33	-0.015	0.016	-0.070	0.087	-0.073	0.077	-0.023	0.024	0.004	0.004
2	34	0.005	-0.003	-0.003	-0.003	-0.001	-0.003	0.012	0.000	-0.001	-0.001
2	35	0.036	-0.005	-0.031	-0.031	-0.004	-0.006	0.009	0.011	0.087	0.000
2	36	0.000	0.000	0.004	0.000	-0.029	-0.025	0.001	-0.000	-0.001	-0.001
2	37	0.013	-0.005	-0.000	-0.000	0.004	-0.000	0.015	0.002	0.026	0.003
2	38	-0.012	0.012	-0.006	0.007	-0.009	-0.000	-0.008	-0.002	-0.000	-0.000
2	39	0.005	-0.019	-0.062	-0.062	-0.043	-0.042	0.033	0.012	0.066	0.001

Table S4. Parameters of one-component Debye model for **1** derived according Eq.8 in main text.

T/K	χ_S/(10^{-6} m^3mol^{-1})	χ_T/(10^{-6} m^3mol^{-1})	α	τ/(10^{-6} s)
1.9	6.030	9.109	0.359	0.8878
2.2	5.375	8.100	0.343	0.6204
2.5	4.730	7.327	0.304	0.3797
2.8	4.182	6.703	0.300	0.2245

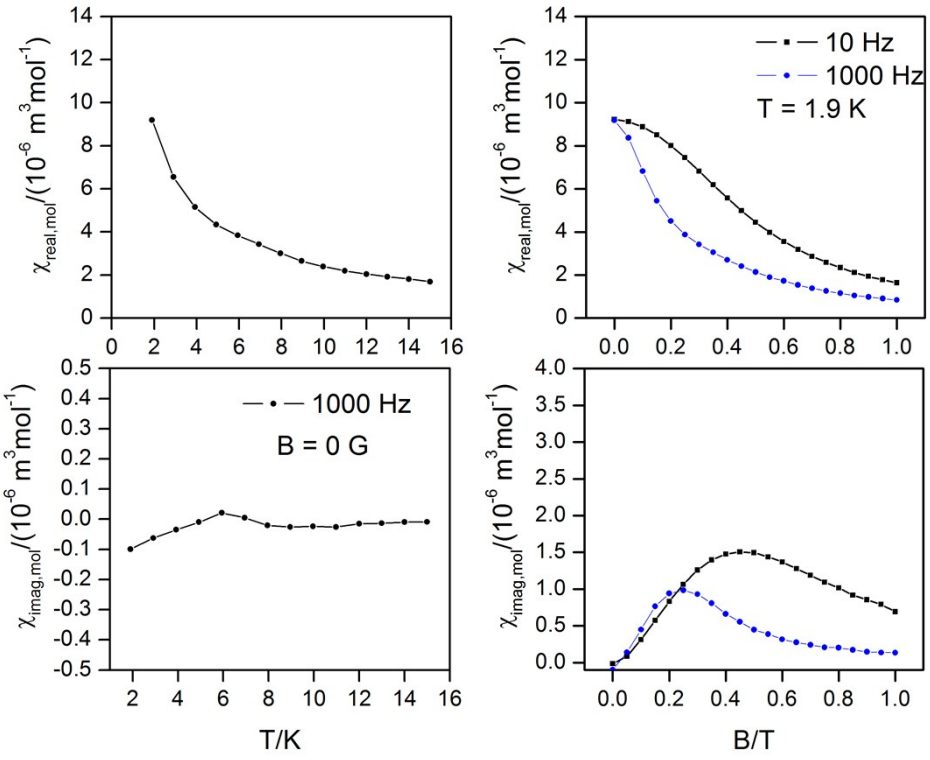

Fig S1 In-phase χ_{real} and out-of-phase χ_{imag} molar susceptibilities for **1** at zero static magnetic field (left) and in non-zero static field (right). Lines serve as guides for the eyes.

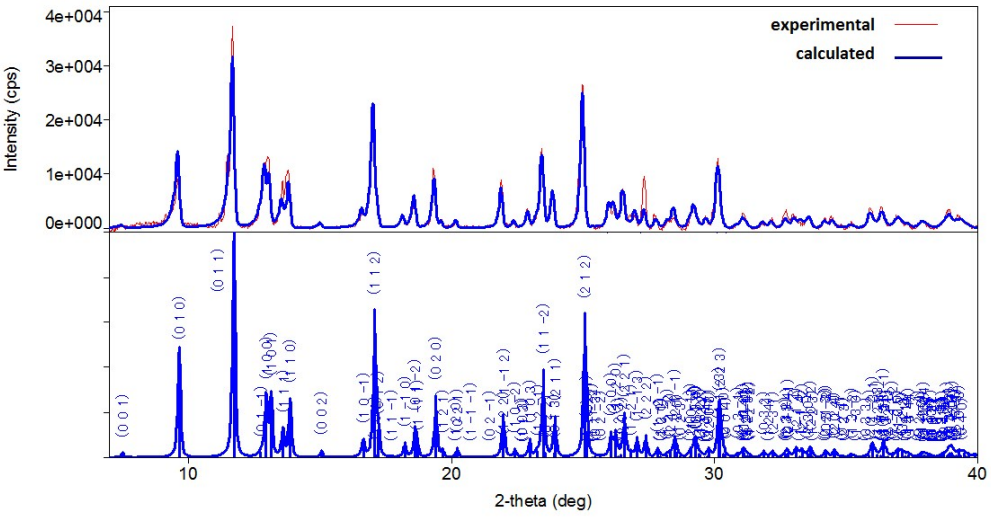

Fig S2 Powder diffraction pattern for **1**. Experimental data are shown as a red line, while calculated ones as a blue line.

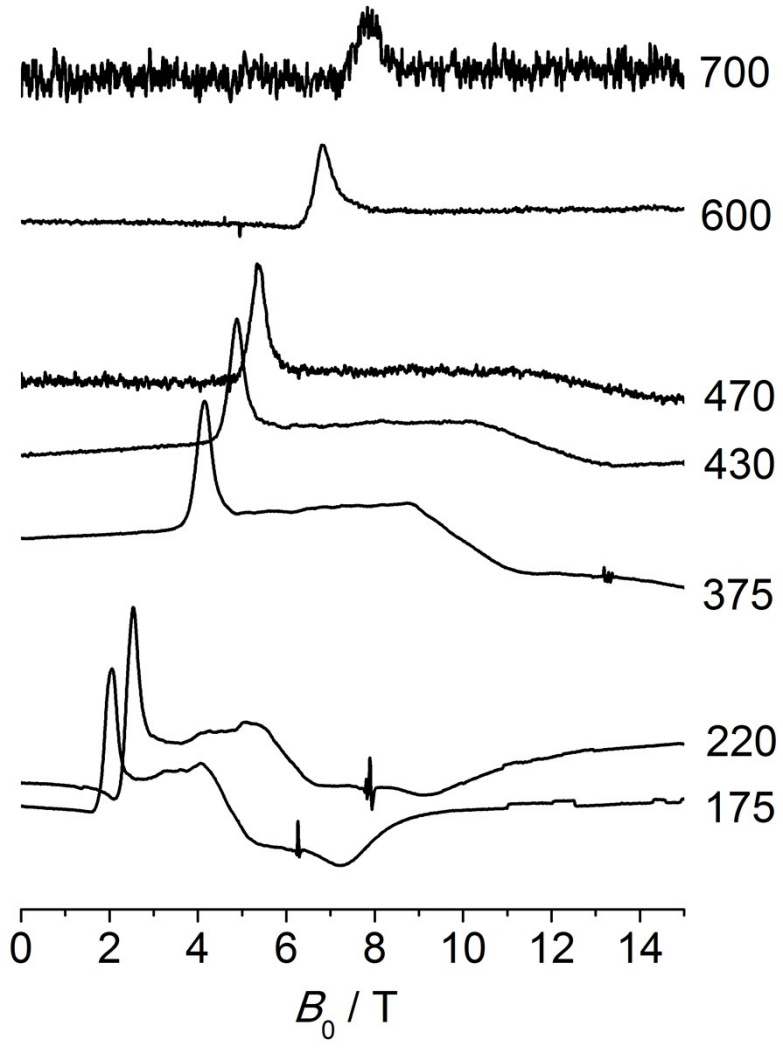

Fig S3 HFEPR spectra recorded on pressed powder pellets of **1** at 5 K and different frequencies as indicated.