Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Material for PCCP:

Rotationally Resolved Magnetic Vibrational Circular Dichroism of the Paramagnetic Molecule NO

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Table S1. Spectroscopic parameters used for simulation of NO MVCD.[a]

ground vibrational state ($\nu = 0$):	A = 123.1393 cm^{-1}
	B = 1.696115 cm^{-1}
excited vibrational state ($\nu = 1$):	A = 122.8935 cm^{-1}
	B = 1.678544 cm^{-1}
$h\nu$ = 1875.972 cm^{-1}	
T = 298 K	

[a] J. M. Brown, M. Kaise, C. M. L. Kerr and D. J. Milton, *Mol. Phys.*, 1978, **36**, 553-582.

Table S2. Calculated g_J-values based on Radford's theory (eqn. 9).

	$^2\Pi_{1/2}$		$^2\Pi_{3/2}$	
J	$g_J(v = 0)$	$g_J(v = 1)$	$g_J(v = 0)$	$g_J(v = 1)$
0.5	0.0000	0.0000	4.0000	4.0000
1.5	0.0231	0.0229	0.7769	0.7771
2.5	0.0264	0.0261	0.3165	0.3167
3.5	0.0274	0.0271	0.1631	0.1633
4.5	0.0278	0.0275	0.0934	0.0937
5.5	0.0279	0.0277	0.0560	0.0562
6.5	0.0279	0.0277	0.0336	0.0338
7.5	0.0279	0.0277	0.0192	0.0194
8.5	0.0278	0.0275	0.0094	0.0096
9.5	0.0276	0.0274	0.0025	0.0027
10.5	0.0274	0.0272	-0.0026	-0.0024
11.5	0.0272	0.0270	-0.0064	-0.0062
12.5	0.0270	0.0268	-0.0092	-0.0090
13.5	0.0268	0.0266	-0.0115	-0.0112
14.5	0.0265	0.0263	-0.0132	-0.0130
15.5	0.0263	0.0261	-0.0145	-0.0143
16.5	0.0260	0.0258	-0.0156	-0.0154
17.5	0.0257	0.0255	-0.0164	-0.0162
18.5	0.0254	0.0252	-0.0171	-0.0169
19.5	0.0251	0.0249	-0.0176	-0.0174
20.5	0.0248	0.0246	-0.0180	-0.0178
21.5	0.0245	0.0243	-0.0183	-0.0181
22.5	0.0242	0.0240	-0.0185	-0.0183
23.5	0.0239	0.0237	-0.0186	-0.0185
24.5	0.0235	0.0234	-0.0187	-0.0186
25.5	0.0232	0.0231	-0.0188	-0.0186
26.5	0.0229	0.0228	-0.0188	-0.0187
27.5	0.0226	0.0225	-0.0188	-0.0186
28.5	0.0223	0.0222	-0.0187	-0.0186
29.5	0.0220	0.0219	-0.0186	-0.0185
30.5	0.0217	0.0216	-0.0185	-0.0184

Table S3. Moment analysis results for the NO $^2\Pi_{1/2}$ experimental transitions at 0.2 Tesla.

	ν_0 (cm^{-1})	$\langle A\rangle_0$ (10^{-5})	$\langle \Delta A\rangle_1$ (10^{-8})	$\langle \Delta A\rangle_1/\langle A\rangle_0$ (10^{-3})	g_J (10^{-2})
R(13.5)	1920.7	5.67	22.2	3.92	2.09
R(14.5)	1923.5	4.87	25.0	5.13	2.75
R(15.5)	1926.3	4.78	21.7	4.54	2.44
R(16.5)	1929.0	4.09	18.2	4.45	2.38
R(17.5)	1931.7	3.57	16.9	4.73	2.54
R(18.5)	1934.4	3.18	12.7	3.99	2.13
R(19.5)	1937.0	2.64	-	-	-
R(20.5)	1939.6	2.27	9.95	4.38	2.36
R(21.5)	1942.2	1.90	8.75	4.61	2.46
R(22.5)	1944.7	1.39	6.98	5.02	2.69
R(23.5)	1947.2	1.02	4.12	4.04	2.16
R(24.5)	1949.6	0.85	3.15	3.71	2.00
R(25.5)	1952.0	0.64	2.63	4.11	2.19
P(9.5)	1842.9	7.14	41.0	5.74	3.08
P(10.5)	1839.3	6.91	33.7	4.88	2.62
P(11.5)	1835.5	7.07	31.3	4.43	2.36
P(12.5)	1831.8	6.33	27.1	4.28	2.29
P(13.5)	1828.0	5.16	24.2	4.69	2.52
P(14.5)	1824.2	4.83	22.5	4.66	2.50
P(15.5)	1820.4	4.64	18.0	3.88	2.09
P(16.5)	1816.5	3.83	19.7	5.14	2.76
P(17.5)	1812.6	3.33	13.8	4.14	2.23
P(18.5)	1808.7	2.52	10.8	4.29	2.29
P(19.5)	1804.7	2.71	12.3	4.54	2.43
P(20.5)	1800.7	2.02	13.2	6.53	3.49
P(21.5)	1796.6	1.64	9.31	5.68	3.05