

Supporting Information

Slow Magnetic Relaxation in a Homoaxially Phosphine oxide Coordinated Pentagonal Bipyramidal Dy(III) Complex

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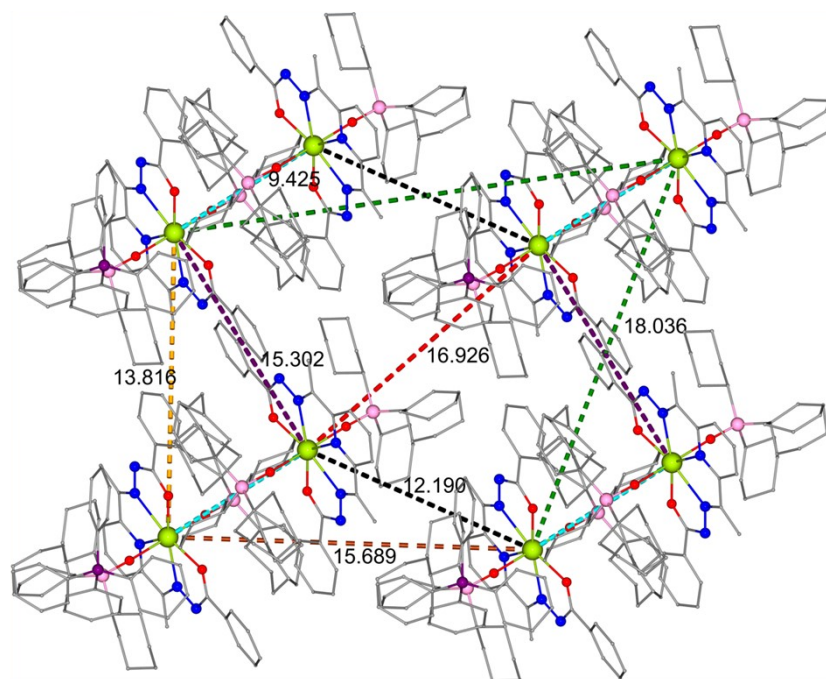


Figure S1. Illustration of intermolecular distances in **1-Dy**.

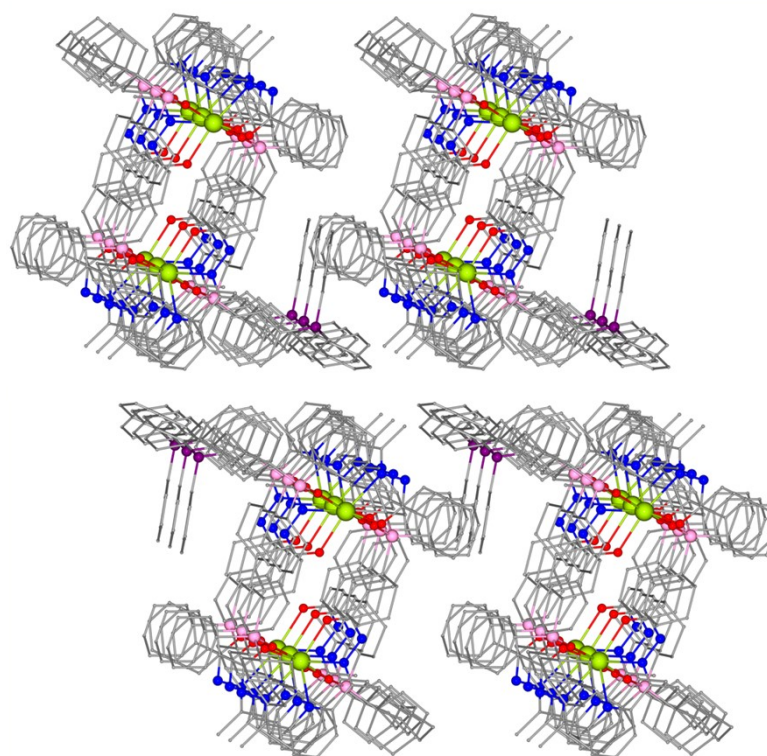


Figure S2. Solid state packing diagram of **1-Dy** viewed along the crystallographic *b* axis.

Table S1. Continuous Shape analysis

Complex	Structure ¹							Ref
	HP-7	HPY-7	PBPY-7	COC-7	CTPR-7	JPBPY-7	JETPY-7	
[(L)Dy(Cy ₃ PO) ₂] ⁺	31.572	20.654	1.396	8.067	6.207	6.487	4.108	This work
[(L)Dy(Cy ₃ PO)Cl]			1.446					[¹]
[(L)Dy(Ph ₃ PO)Cl]			1.505					[¹]
(L')DyCl ₂			1.210					[²]

¹HP-7: Heptagon (D_{7h}); HPY-7: Hexagonal pyramid (C_{6v}); PBPY-7: Pentagonal bipyramid (D_{5h}); COC-7: Capped octahedron (C_{3v}); CTPR-7: Capped trigonal prism (C_{2v}); JPBPY-7: Johnson pentagonal bipyramid J13 (D_{5h}); JETPY-7: Johnson elongated triangular pyramid J7 (C_{3v})

Table S2. Bond angle and distance parameters of **1-Dy**

Bond lengths (Å)		Bond angles (°)			
Dy1–O1	2.241(3)	O1–Dy1–O3	93.17(10)	O1–Dy1–O4	90.55(10)
Dy1–O2	2.222(3)	O1–Dy1–N2	89.88(11)	O1–Dy1–N3	85.95(11)
Dy1–O3	2.282(3)	O1–Dy1–N4	86.28(11)	O2–Dy1–O1	175.33(10)
Dy1–O4	2.262(3)	O2–Dy1–O3	88.74(11)	O2–Dy1–O4	93.28(11)
Dy1–N2	2.444(3)	O2–Dy1–N2	87.06(12)	O2–Dy1–N3	89.56(12)
Dy1–N3	2.467(3)	O2–Dy1–N4	92.92(11)	O3–Dy1–N2	65.11(11)
Dy1–N4	2.466(3)	O3–Dy1–N3	129.81(11)	O3–Dy1–N4	165.84(11)
		O4–Dy1–O3	100.74(9)	O4–Dy1–N2	165.84(11)
		O4–Dy1–N3	129.43(11)	O4–Dy1–N4	65.14(10)
		N2–Dy1–N3	64.71(12)	N2–Dy1–N4	129.00(12)
		N4–Dy1–N3	64.30(12)		

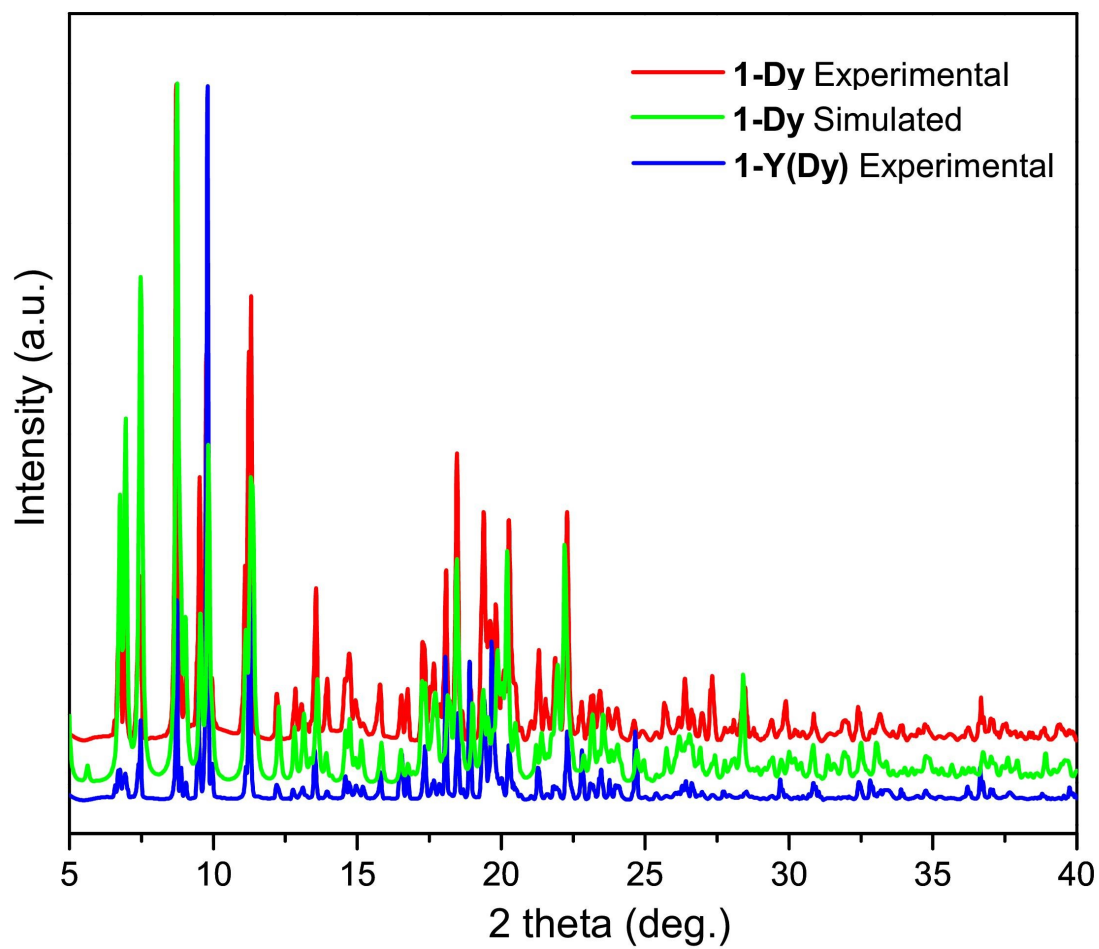


Figure S3. Experimental powder XRD pattern and simulated powder XRD from single crystal data for **1-Dy** along with experimental pattern of **1-Y(Dy)**.

Figure S4. Magnetic behavior for **1-Dy**: (a) $M = f(H)$ for $T = 2, 3, 4,$ and 6 K (full lines are eye guides); (b) $M = f(H)$ at 2 K for **1-Dy** and **1-Y(Dy)**; (c) χ_M' and $\chi_M'' = f(T)$ for AC frequency of 1 kOe in absence and with applied static field (2 kOe); (d) DC field dependence of the relaxation time (τ) at 5 K.

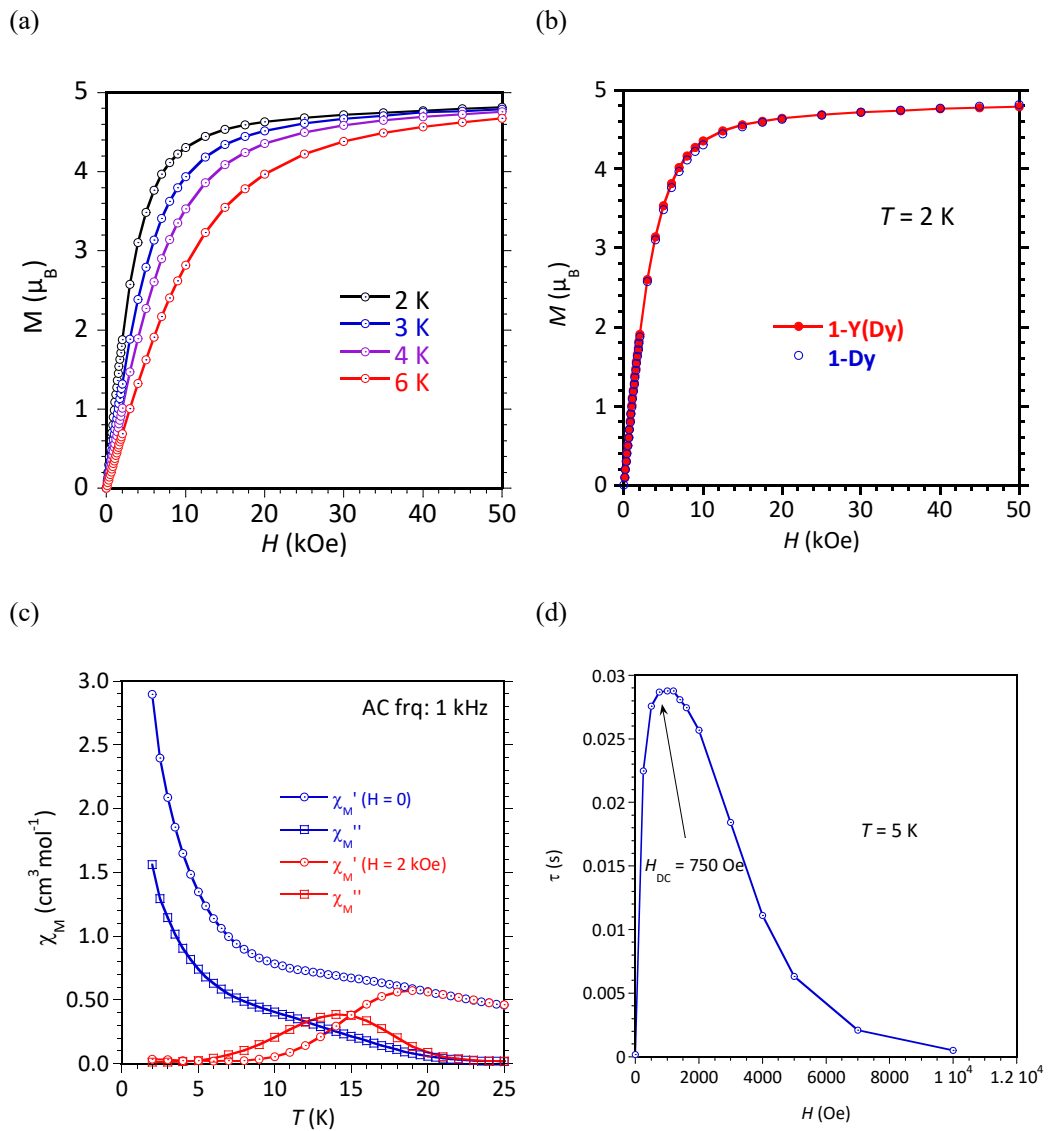


Figure S5. AC susceptibility behaviors for **1-Dy** recorded with $H_{DC} = 750$ Oe

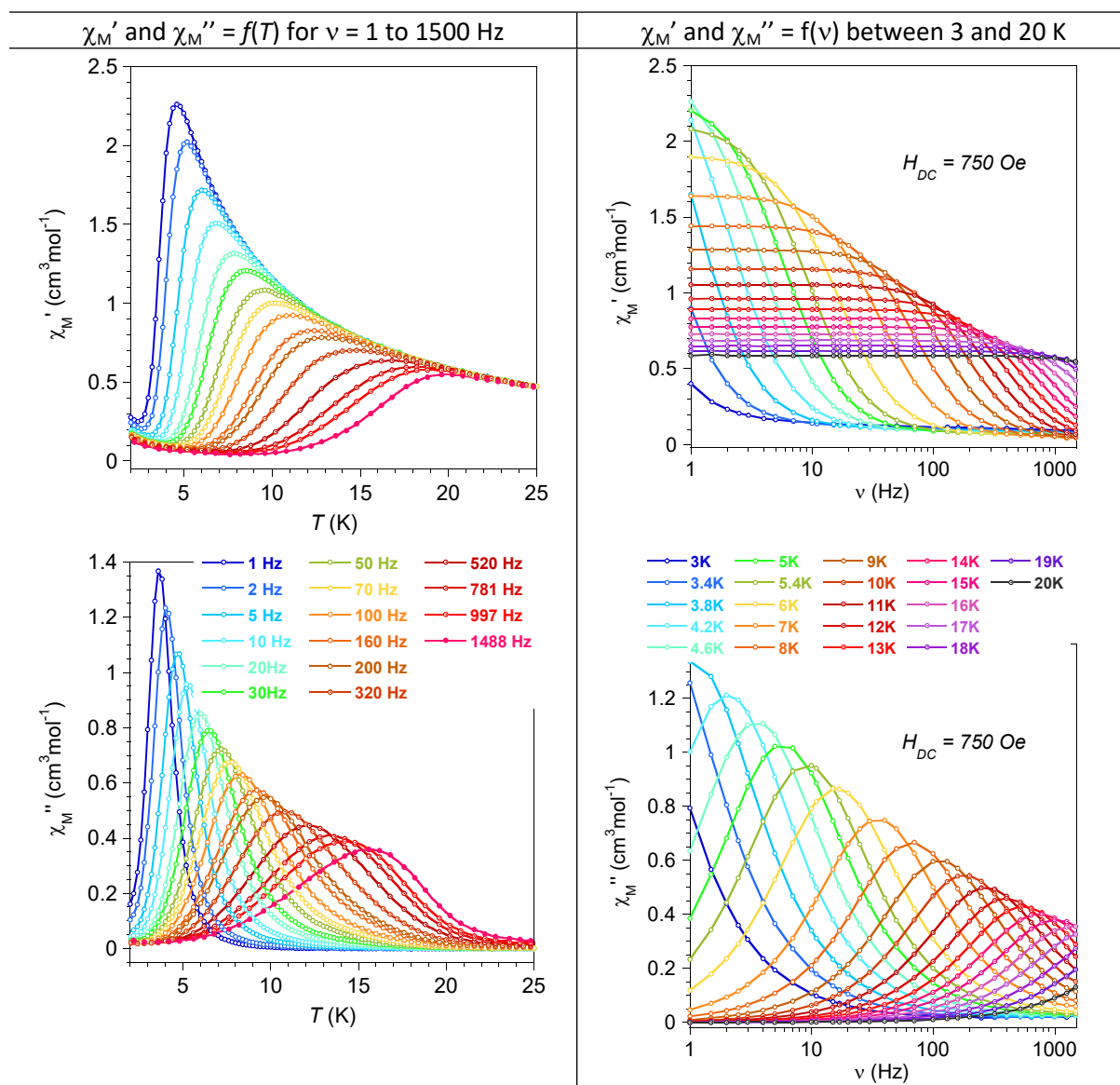
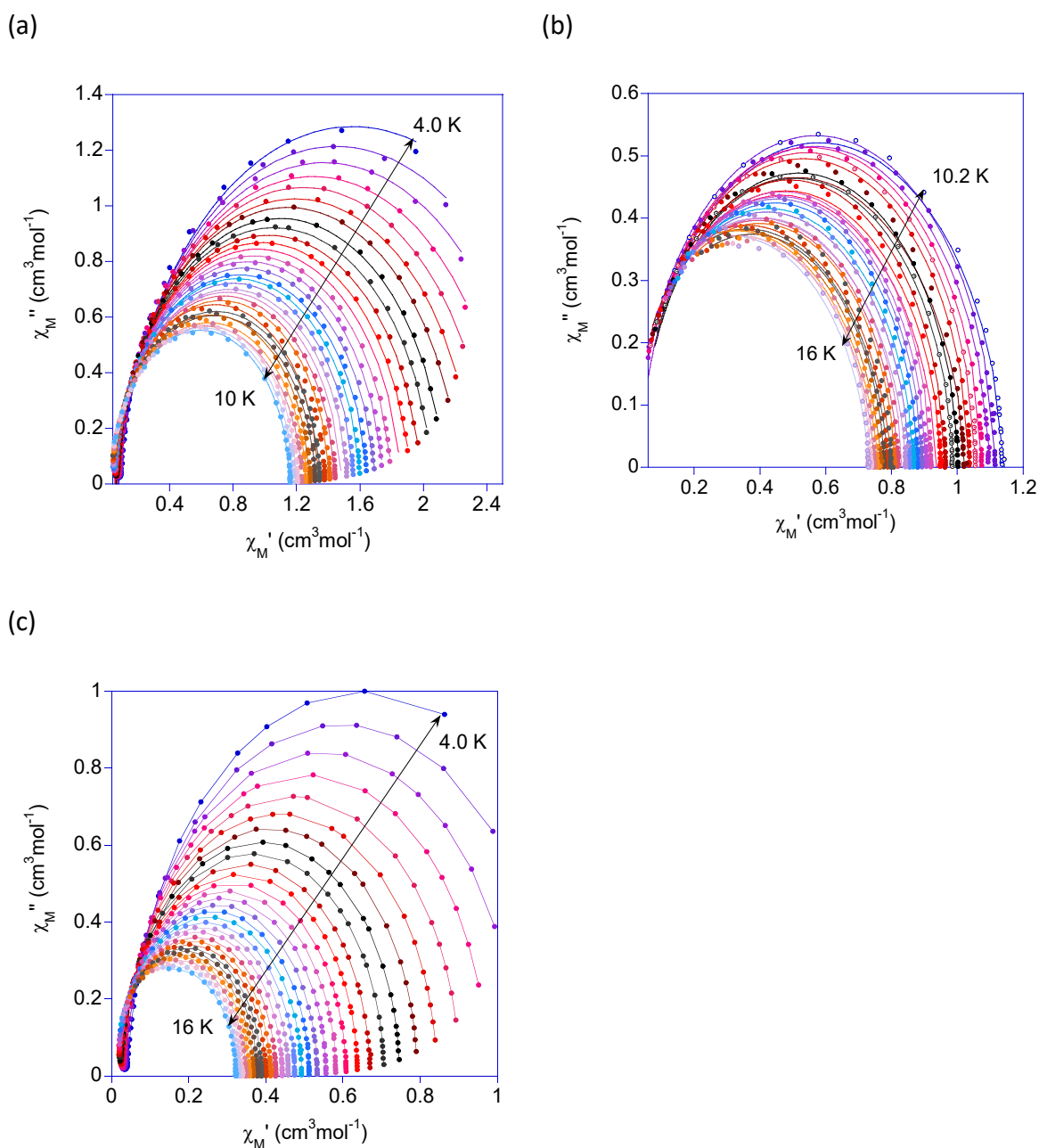


Figure S6. 1-Dy: Cole-Cole plot; (a, b) solid lines are the best-fits of the assessments of the distribution width (α) of the relaxation time for the different temperatures; (c) normalized plot (the lines are just eye-guides). (*Below*) the α values for the temperatures between 4.0 and 16.0 K.



T (K)	α	T (K)	α	T (K)	α
4.0	0.089	7.6	0.037	11.2	0.012
4.2	0.079	7.8	0.029	11.4	0.066
4.4	0.078	8.0	0.025	11.6	0.016
4.6	0.072	8.2	0.027	11.8	0.021
4.8	0.063	8.4	0.026	12.0	0.016
5.0	0.054	8.6	0.040	12.2	0.043
5.2	0.055	8.8	0.042	12.4	0.050
5.4	0.054	9.0	0.019	12.6	0.012
5.6	0.053	9.2	0.043	12.8	0.016
5.8	0.050	9.4	0.045	13.0	0.012
6.0	0.046	9.6	0.018	13.2	0.013
6.2	0.043	9.8	0.018	13.4	0.038
6.4	0.041	10.0	0.014	13.6	0.038
6.6	0.038	10.2	0.049	13.8	0.072
6.8	0.039	10.4	0.014	14.0	0.037
7.0	0.043	10.6	0.019		
7.2	0.035	10.8	0.012		
7.4	0.032	11.0	0.012		

Table S3: best-fit parameters for the analysis of $\chi_M'' = f(\text{freq})$ by the extended Debye model.

T (K)	X _T	X _S	Tau (s)	alpha
3.8	3.39	0.71	0.144	0.075
4.0	3.33	0.77	0.105	0.079
4.2	3.38	0.72	0.0778	0.054
4.4	3.32	0.78	0.0586	0.054
4.6	3.26	0.83	0.0447	0.053
4.8	3.21	0.88	0.0346	0.051
5.0	3.17	0.93	0.02723	0.050
5.2	3.13	0.97	0.02170	0.049
5.4	3.08	1.02	0.01747	0.047
5.6	3.05	1.05	0.01425	0.046
5.8	3.01	1.09	0.01174	0.045
6.0	2.92	1.17	0.00980	0.066
6.2	2.95	1.15	0.00824	0.042
6.4	2.92	1.17	0.00701	0.040
6.6	2.90	1.20	0.00598	0.039
6.8	2.87	1.22	0.00515	0.039
7.0	2.85	1.25	0.00446	0.038
7.2	2.83	1.27	0.00388	0.037
7.4	2.81	1.29	0.00341	0.036
7.6	2.76	1.34	0.00300	0.052
7.8	2.74	1.36	0.002657	0.051
8.0	2.72	1.38	0.002360	0.051
8.2	2.70	1.39	0.002101	0.050
8.4	2.69	1.40	0.001881	0.048
8.6	2.68	1.42	0.001688	0.047
8.8	2.66	1.43	0.001520	0.046
9.0	2.65	1.45	0.001374	0.046
9.2	2.64	1.46	0.001249	0.043
9.4	2.63	1.47	0.001131	0.044
9.6	2.62	1.48	0.001032	0.042
9.8	2.61	1.49	0.000944	0.042
10.0	2.60	1.50	0.000865	0.038
10.2	2.59	1.51	0.00079506	0.038
10.4	2.58	1.52	0.000731	0.038
10.6	2.57	1.53	0.000676	0.037
10.8	2.56	1.54	0.000622	0.035
11.0	2.55	1.55	0.0005773	0.034
11.2	2.54	1.55	0.000537	0.032
11.4	2.54	1.56	0.000499	0.030
11.6	2.54	1.56	0.000465	0.019
11.8	2.52	1.58	0.000434	0.028
12.0	2.50	1.58	0.000396	0.030
12.2	2.50	1.59	0.0003715	0.029
12.4	2.50	1.60	0.000349	0.022
12.6	2.49	1.60	0.0003270	0.025
12.8	2.49	1.61	0.0003067	0.025
13.0	2.48	1.62	0.000288	0.025
13.2	2.48	1.62	0.0002697	0.026
13.4	2.47	1.63	0.0002553	0.022
13.6	2.46	1.63	0.0002408	0.022

13.8	2.46	1.64	0.0002284	0.0187
14.0	2.45	1.64	0.00021390	0.022
14.2	2.45	1.65	0.0002019	0.017
14.4	2.44	1.66	0.0001896	0.018
14.6	2.44	1.66	0.00017956	0.013
14.8	2.43	1.66	0.0001683	0.017
15.0	2.43	1.67	0.0001583	0.019
15.2	2.42	1.67	0.0001513	0.011
15.4	2.42	1.68	0.0001416	0.014
15.6	2.41	1.68	0.0001334	0.013
15.8	2.41	1.68	0.0001241	0.015
16.0	2.40	1.69	0.0001198	0.009
16.2	2.40	1.70	0.0001110	0.012
16.4	2.40	1.70	0.0001051	0.011
16.6	2.39	1.71	$9.85 \cdot 10^{-5}$	0.015
16.8	2.39	1.70	$9.05 \cdot 10^{-5}$	0.011
17.0	2.38	1.71	$8.78 \cdot 10^{-5}$	0.007

Figure S7. 1-Y(Dy): (a) $\chi_M'' = f(T)$ in zero field (test frequency: 997 Hz, $H_{AC} = 3$ Oe); (b) $\tau = f(H)$ at 5 K.

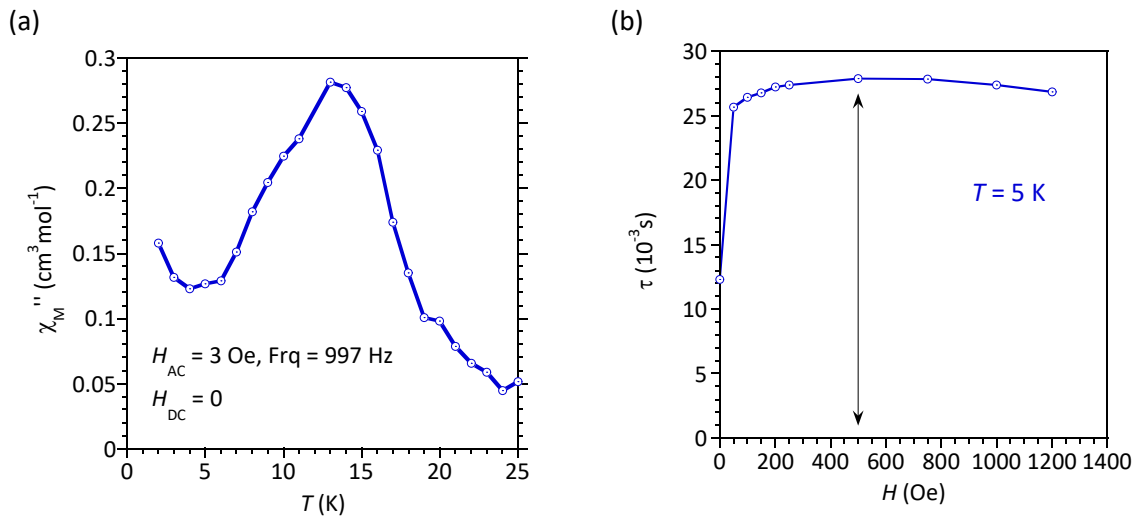


Figure S8. 1-Y(Dy): The temperature and frequency dependencies of χ_M' and χ_M''

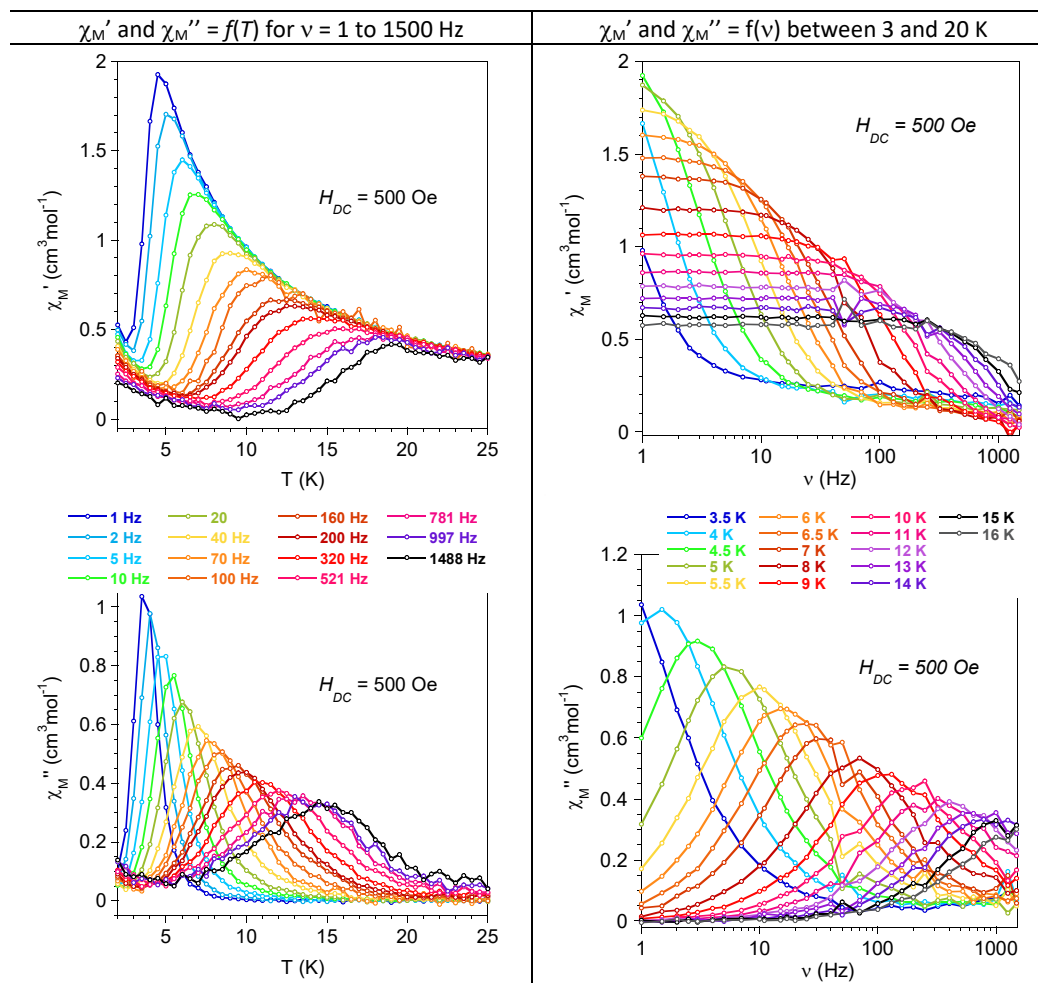
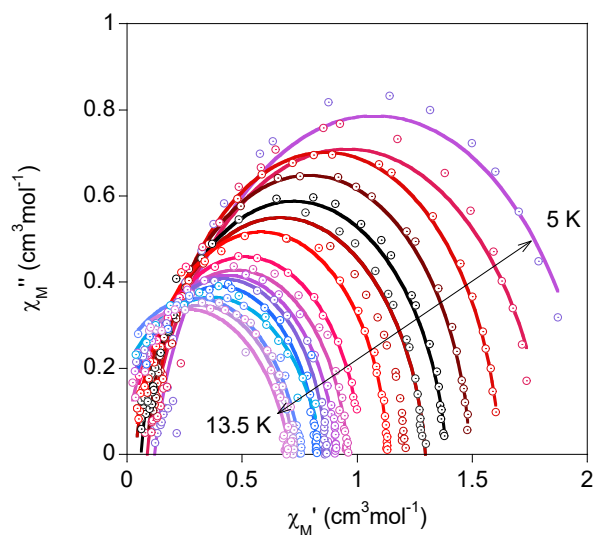


Figure S9. 1-Y(Dy): Cole-Cole plots and best-fit parameters.

The relaxation time distribution width given by parameter α is small suggesting a single or main relaxation process. This is consistent with the observation made for the bulk complex. It can be noticed that from 12 K and above α become larger which could be related to the noise of the data for larger T due to a weaker signal for χ_M'' .



T (K)	X_T	X_S	alpha	R ²
3.5	2.91(9)	0.241(2)	0.077(9)	0.999
4.0	2.61(9)	0.190(3)	0.09(1)	0.995
4.5	2.21(2)	0.165(3)	0.069(8)	0.995
5.0	1.89(3)	0.140(5)	0.08(2)	0.959
5.5	1.78(1)	0.125(5)	0.06(1)	0.979
6.0	1.620(4)	0.103(3)	0.050(7)	0.993
6.5	1.492(3)	0.087(3)	0.051(8)	0.988
7.0	1.389(4)	0.060(3)	0.08(1)	0.972
7.5	1.299(3)	0.036(4)	0.09(1)	0.968
8.0	1.212(2)	0.041(5)	0.07(1)	0.968
8.5	1.132(1)	0.034(3)	0.039(7)	0.988
9.5	1.019(4)	0.007(7)	0.06(1)	0.986
10	0.959(1)	-0.009(8)	0.08(1)	0.971
10.5	0.909(2)	-0.03(1)	0.08(2)	0.970
11.0	0.866(1)	-0.02(1)	0.06(1)	0.972
11.5	0.826(1)	-0.02(2)	0.05(2)	0.955
12.0	0.85(1)	-0.11(3)	0.17(4)	0.925
12.5	0.755(2)	-0.15(3)	0.14(2)	0.976
13.0	0.725(2)	-0.09(3)	0.11(2)	0.967
13.5	0.709(5)	-0.19(8)	0.19(6)	0.885

Table S4. 1-Y(Dy): best-fit parameters for the analysis of $\chi_M'' = f(\text{freq})$ by the extended Debye model

T (K)	X_T	X_S	Tau (s)	alpha	R²
4.0	3.69	1.30	0.12(1)	0.10(3)	0.984
4.5	3.52	1.48	0.053(2)	0.07(2)	0.990
5.0	3.40	1.60	0.0285(7)	0.05(2)	0.988
5.5	3.33	1.67	0.0165(5)	0.06(2)	0.979
6.0	3.26	1.73	0.0102(2)	0.06(2)	0.983
6.5	3.23	1.77	0.0637(2)	0.07(1)	0.995
7.0	3.15	1.84	0.0046(2)	0.08(2)	0.970
7.5	3.13	1.87	0.003208(6)	0.07(1)	0.985
8.0	3.09	1.91	0.00231(5)	0.08(1)	0.988
8.5	3.07	1.93	0.00167(4)	0.07(1)	0.989
9.0	3.04	1.96	0.00129(2)	0.07(1)	0.993
9.5	3.01	1.99	0.00102(2)	0.066(9)	0.995
10	2.97	2.02	0.00082(2)	0.05(1)	0.994
10.5	2.95	2.05	0.00060(3)	0.04(3)	0.957
11.0	2.95	2.05	0.00052(1)	0.07(1)	0.992
11.5	2.93	2.07	0.000448(8)	0.063(1)	0.995
12.0	2.91	2.08	0.000359(5)	0.049(8)	0.998
12.5	2.91	2.09	0.000295(3)	0.06(1)	0.995
13.0	2.89	2.11	0.000245(1)	0.05(1)	0.996
13.5	2.87	2.13	0.000226(4)	0.02(1)	0.997
14.0	2.87	2.13	0.000183(2)	0.051(9)	0.997
14.5	2.85	2.15	0.000165(9)	0.04(3)	0.992
15.0	2.83	2.17	0.000139(8)	0.0016(25)	0.993
15.5	2.86	2.14	0.000111(7)	0.07(2)	0.996
16.0	2.81	2.19	0.000103(5)	0.03(1)	0.998
16.5	2.83	2.17	0.00008(2)	0.05(6)	0.973

Supporting information corresponding to the Computational section

Table S5. Average axial and equatorial bond lengths of the hydrogen-optimised structures of complexes **1-Dy** to **4-Dy**.

	Avg. axial bond lengths	Avg. equatorial bond lengths	Avg. axial/Avg. equatorial
1-Dy	2.231	2.384	0.936
2-Dy	2.644	2.373	1.114
3-Dy	2.431	2.381	1.021
4-Dy	2.449	2.389	1.025

Table S6. CASSCF computed average Mulliken charges on axial and equatorial ligand with the ratio of Avg. axial/Av. equatorial for complexes **1-Dy** to **4-Dy**.

	Avg. axial charges	Avg. equatorial charges	Avg. axial/Avg. equatorial
1-Dy	-0.68	-0.46	1.49
2-Dy	-0.64	-0.40	1.60
3-Dy	-0.65	-0.43	1.51
4-Dy	-0.65	-0.44	1.48

Table S7. SA-CASSCF computed g-tensors, and the angle of deviation from ground state g_{zz} orientation.

1-Dy (CASSCF)

KD	Energy(cm^{-1})	g_{xx}	g_{yy}	g_{zz}	angle(θ)
1	0.00	0.0188	0.0458	19.6246	0.0
2	198.68	0.8490	1.9219	13.8939	84.5
3	223.33	0.1202	1.6347	17.1980	85.6
4	280.74	0.2725	1.9874	10.9564	98.4
5	411.46	2.1261	3.6089	14.3862	91.6
6	472.47	0.9187	4.5448	11.9883	100.6
7	583.01	1.8480	3.3185	12.8051	139.3
8	746.22	0.2213	0.6051	17.8228	108.6

1-Dy (NEVPT2)

KD	Energy(cm^{-1})	g_{xx}	g_{yy}	g_{zz}	angle(θ)
1	0.00	0.0088	0.0230	19.6418	0.0
2	194.87	0.4955	0.9394	15.7256	70.1
3	244.14	0.0014	4.7147	13.9352	94.9
4	284.71	1.1646	1.8235	9.4301	98.3

5	416.31	2.0522	3.0489	14.7338	94.7
6	494.48	0.9301	5.2964	11.1302	96.5
7	605.30	1.7104	3.7895	12.5347	138.9
8	801.31	0.1174	0.3961	17.9771	115.1

2-Dy

KD	Energy(cm ⁻¹)	g _{xx}	g _{yy}	g _{zz}	angle(θ)
1	0.00	0.0031	0.0078	19.6887	0.0
2	148.90	0.3756	0.8604	14.1140	15.0
3	192.83	0.2222	0.4478	12.1927	18.8
4	300.67	1.8118	2.8095	15.3869	97.0
5	361.33	0.1799	5.1511	10.4599	90.6
6	450.07	2.2929	7.8667	9.4345	89.9
7	513.02	2.7867	3.4535	10.6635	10.1
8	624.07	0.2280	0.6332	16.8148	81.9

3-Dy

KD	Energy(cm ⁻¹)	g _{xx}	g _{yy}	g _{zz}	angle(θ)
1	0.00	0.0149	0.0301	19.6617	0.0
2	178.97	0.6810	1.4904	14.4313	13.0
3	233.56	0.9231	2.2326	11.5176	90.9
4	277.55	0.0523	1.3998	14.8883	90.2
5	397.43	1.0544	3.9352	12.2836	97.0
6	459.37	2.6627	6.2009	12.8846	95.5
7	544.24	0.4176	1.2192	12.7401	109.2
8	688.73	0.1467	0.7009	17.4863	94.3

4-Dy

KD	Energy(cm ⁻¹)	g _{xx}	g _{yy}	g _{zz}	angle(θ)
1	0.00	0.0187	0.0366	19.6582	0.0
2	176.84	0.7561	1.9505	14.2340	5.9
3	233.84	0.4796	1.1534	12.0909	21.5
4	309.02	1.0782	1.1817	17.2299	90.9
5	392.36	1.2285	3.9939	12.5905	85.6
6	469.32	2.1355	6.6849	11.3244	88.5
7	552.22	1.2110	2.3757	12.2015	38.3
8	682.11	0.1316	0.8064	17.2490	78.9

5-Dy

KD	Energy(cm ⁻¹)	g _{xx}	g _{yy}	g _{zz}	angle(θ)
1	0.00	0.0060	0.0113	19.7253	0.0
2	170.90	0.4082	0.9808	14.6569	9.4
3	222.56	0.3105	0.5120	12.5881	7.7
4	324.72	1.6795	2.4429	15.6241	84.5
5	385.35	0.1892	5.2974	10.7733	78.5
6	472.26	2.7109	8.4297	9.4364	77.8
7	544.73	1.6203	2.3779	11.8237	9.9
8	675.37	0.0987	0.4886	17.2425	85.9

Table S8. SINGLE_ANISO computed crystal field parameters for **1-Dy**, **2-Dy**, **3-Dy**, **4-Dy**.

$$H_{CF} = \sum_{k=-q}^q B_k^q O_k^q \quad \text{and}$$

The CF parameters were computed using the following equation,

here B_k^q and O_k^q are the crystal field parameters and Steven's operator, respectively.

k	q	B_k^q	B_k^q	B_k^q	B_k^q
		1-Dy	2-Dy	3-Dy	4-Dy
2	-2	-5.24E-01	3.88E-01	1.62E-01	9.19E-02
	-1	-3.44E+00	-7.46E-06	-4.87E+00	7.85E-01
	0	-4.04E+00	-5.80E+00	-2.03E+00	-6.18E+00
	1	-6.62E-01	-4.75E-06	2.02E+00	-1.99E+00
	2	-6.03E-01	-1.15E+00	-1.31E+00	8.15E-03
4	-4	4.27E-03	9.43E-02	8.58E-03	2.21E-01
	-3	-3.50E-02	-7.61E-07	4.64E-02	1.66E-02
	-2	-2.83E-03	7.58E-02	-4.67E-03	-2.47E-01
	-1	5.03E-02	-2.14E-07	1.96E-02	4.31E-03
	0	1.80E-03	-8.81E-03	-1.37E-02	-1.11E-02
	1	-1.78E-03	-1.10E-07	-8.59E-03	1.29E-02
	2	3.69E-02	-2.82E-01	4.90E-03	1.82E-01
	3	3.10E-03	6.77E-08	-1.44E-02	1.49E-02
6	-6	1.50E-05	-1.11E-03	-3.30E-05	2.53E-04
	-5	-3.04E-04	2.17E-08	-2.67E-04	-1.18E-03
	-4	2.30E-05	-3.38E-04	-3.67E-05	6.82E-04
	-3	1.59E-04	3.10E-08	3.33E-04	7.99E-04
	-2	3.27E-05	-2.99E-03	3.10E-05	7.41E-03
	-1	-6.87E-04	2.14E-09	3.58E-04	-1.44E-03
	0	-1.69E-05	-1.24E-03	2.03E-05	-1.32E-03
	1	8.72E-05	3.84E-08	-1.69E-04	-2.21E-04
	2	-2.25E-04	1.05E-02	-2.61E-04	-6.97E-03

	3	-1.20E-04	-1.05E-08	-3.77E-05	-1.25E-03
	4	-1.53E-04	5.91E-04	6.17E-05	-3.92E-04
	5	8.65E-06	2.87E-08	1.71E-05	-1.40E-03
	6	3.22E-05	1.06E-03	5.88E-06	-1.01E-03

Table S9. SINGLE_ANISO computed wave function decomposition analysis for the Dy(III) centre. The major dominating values are kept in bold.

$\pm mJ$	<i>wave function decomposition analysis 1-Dy</i>
KD1	96.5 % $ \pm 15/2\rangle$
KD2	49.1 % $ \pm 13/2\rangle$ + 27.2% $ \pm 9/2\rangle$ + 11.9% $ \pm 5/2\rangle$
KD3	25.1 % $ \pm 1/2\rangle$ + 20.8 % $ \pm 3/2\rangle$ + 19.6 % $ \pm 7/2\rangle$
KD4	44.6 % $ \pm 11/2\rangle$ + 27.3% $ \pm 7/2\rangle$ + 9.0% $ \pm 3/2\rangle$
KD5	37.6 % $ \pm 9/2\rangle$ + 30.8% $ \pm 13/2\rangle$ + 10.9% $ \pm 7/2\rangle$ + 10.8% $ \pm 11/2\rangle$
KD6	22.9 % $ \pm 5/2\rangle$ + 22.9% $ \pm 11/2\rangle$ + 20.9% $ \pm 7/2\rangle$ + 16.2% $ \pm 9/2\rangle$
KD7	32.9 % $ \pm 3/2\rangle$ + 27.7% $ \pm 5/2\rangle$ + 15.6% $ \pm 7/2\rangle$ + 12.2% $ \pm 11/2\rangle$
KD8	59.7 % $ \pm 1/2\rangle$ + 27.7% $ \pm 3/2\rangle$

$\pm mJ$	<i>wave function decomposition analysis 2-Dy</i>
KD1	97.2 % $ \pm 15/2\rangle$
KD2	51.3 % $ \pm 13/2\rangle$ + 39.2% $ \pm 9/2\rangle$
KD3	52.2 % $ \pm 11/2\rangle$ + 43.7% $ \pm 7/2\rangle$
KD4	39.8 % $ \pm 5/2\rangle$ + 28.4% $ \pm 3/2\rangle$ + 18.8% $ \pm 1/2\rangle$
KD5	36.4 % $ \pm 9/2\rangle$ + 36.1% $ \pm 13/2\rangle$ + 12.1% $ \pm 1/2\rangle$
KD6	46.5 % $ \pm 7/2\rangle$ + 41.4% $ \pm 11/2\rangle$
KD7	42.3 % $ \pm 5/2\rangle$ + 33.5% $ \pm 3/2\rangle$ + 17.6% $ \pm 9/2\rangle$
KD8	65.4 % $ \pm 1/2\rangle$ + 25.7% $ \pm 3/2\rangle$

$\pm mJ$	<i>wave function decomposition analysis 3-Dy</i>
KD1	96.8 % $ \pm 15/2\rangle$
KD2	53.1 % $ \pm 13/2\rangle$ + 35.5% $ \pm 9/2\rangle$
KD3	46.4 % $ \pm 7/2\rangle$ + 43.1% $ \pm 7/2\rangle$
KD4	32.6 % $ \pm 3/2\rangle$ + 28.4% $ \pm 5/2\rangle$ + 23.8% $ \pm 1/2\rangle$
KD5	41.8 % $ \pm 9/2\rangle$ + 40.8% $ \pm 13/2\rangle$ + 9.7% $ \pm 5/2\rangle$
KD6	39.4 % $ \pm 7/2\rangle$ + 33.4% $ \pm 11/2\rangle$ + 14.8% $ \pm 5/2\rangle$
KD7	38.4 % $ \pm 3/2\rangle$ + 35.1 % $ \pm 5/2\rangle$
KD8	65.3 % $ \pm 1/2\rangle$ + 26.5% $ \pm 3/2\rangle$

$\pm mJ$	<i>wave function decomposition analysis 4-Dy</i>
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KD1	96.8 % $ \pm 15/2\rangle$
KD2	54.5 % $ \pm 13/2\rangle$ + 35.7% $ \pm 9/2\rangle$
KD3	50.6 % $ \pm 11/2\rangle$ + 43.1% $ \pm 7/2\rangle$
KD4	32.6 % $ \pm 3/2\rangle$ + 32.5% $ \pm 5/2\rangle$ + 24.4% $ \pm 1/2\rangle$
KD5	41.6 % $ \pm 9/2\rangle$ + 38.2% $ \pm 13/2\rangle$
KD6	38.4 % $ \pm 7/2\rangle$ + 32.0% $ \pm 11/2\rangle$ + 13.9% $ \pm 5/2\rangle$
KD7	37.8 % $ \pm 3/2\rangle$ + 35.8 % $ \pm 5/2\rangle$
KD8	65.5 % $ \pm 1/2\rangle$ + 25.7% $ \pm 3/2\rangle$

$\pm mJ$ wave function decomposition analysis 5-Dy

KD1	99.9 % $ \pm 15/2\rangle$
KD2	99.0 % $ \pm 13/2\rangle$
KD3	78.0 % $ \pm 11/2\rangle$ + 15.6% $ \pm 7/2\rangle$
KD4	36.6 % $ \pm 3/2\rangle$ + 30.1% $ \pm 1/2\rangle$ + 15.4% $ \pm 11/2\rangle$
KD5	35.9 % $ \pm 9/2\rangle$ + 33.7% $ \pm 1/2\rangle$ + 12.6% $ \pm 7/2\rangle$
KD6	43.8 % $ \pm 5/2\rangle$ + 33.1% $ \pm 3/2\rangle$ + 16.8% $ \pm 9/2\rangle$
KD7	49.9 % $ \pm 7/2\rangle$ + 30.2 % $ \pm 9/2\rangle$ + 13.2% $ \pm 5/2\rangle$
KD8	26.9 % $ \pm 5/2\rangle$ + 17.4% $ \pm 3/2\rangle$ + 12.2% $ \pm 1/2\rangle$

Table S10. CASSCF/NEVPT2 computed low-lying 21 sextets (in red) and 224 quartet states (in black) along with spin-orbit coupled states (in blue, Kramer doublets). All the values are reported here in cm^{-1} .

1-Dy						
CASSCF						
0.0	24117.3	25907.1	33920.0	56677.6	76469.3	105351.6
11.2	24124.3	25967.1	33949.3	56688.8	76508.1	105407.0
92.9	24156.8	26024.8	33984.3	56749.9	76517.7	105508.6
252.8	24200.8	26117.1	34040.0	56808.9	76561.6	105543.4
305.0	24216.4	29061.5	34123.9	56826.7	76571.5	
346.9	24238.0	29063.2	34140.2	56850.2	76591.9	
415.3	24269.4	29123.4	34147.4	56878.1	76594.1	
464.7	24284.9	29142.5	34166.5	57012.4	77830.2	
698.2	24363.0	29154.4	36907.4	57045.9	77856.0	
904.0	24475.8	29161.7	36921.1	57060.2	77879.0	
927.5	24503.8	29270.6	37046.8	57104.1	78044.0	
7490.9	24525.3	29272.6	37061.2	57117.5	78168.0	
7589.1	24541.2	29322.2	37164.3	57127.3	78235.1	
7703.0	24587.0	29338.4	37194.1	57137.9	78277.2	
7790.1	24604.7	29342.0	37296.8	57185.8	84467.2	
7830.9	24616.6	29355.3	37357.8	57191.4	84530.0	
7898.0	24670.9	29362.5	37431.0	61478.4	84662.7	
8013.9	24682.6	29435.2	37474.2	61479.1	84954.4	

34270.1	24705.3	29436.4	37500.2	61534.2	84967.3	
34702.6	24707.0	30468.7	37586.8	61545.4	87225.7	
34864.7	24719.1	30481.1	42560.5	61590.2	87247.8	
	24730.1	30483.3	42831.8	61606.6	87330.3	
	24763.4	30496.0	42953.1	61628.3	87357.8	
	24788.2	30514.8	43107.3	61702.5	87373.1	
	24807.5	30534.3	43156.3	61711.9	87392.8	
	24875.7	30543.6	43222.5	61858.1	87429.1	
	24881.8	30565.5	43323.9	61862.1	87675.3	
	24908.2	30607.8	44310.0	61953.7	87681.2	
	24978.1	30622.2	44314.6	61954.7	87857.0	
	25019.9	30636.7	44385.0	62069.3	87859.3	
	25048.8	30730.6	44390.4	62070.3	87988.0	
	25057.7	30745.1	44466.7	66592.6	87993.3	
	25072.0	30747.3	44483.6	66733.6	97736.6	
	25080.4	30748.6	44534.0	67138.0	97909.0	
	25122.5	30751.0	44546.2	72284.2	98011.1	
	25186.0	30760.7	44592.2	72335.3	98085.2	
	25193.3	32324.5	44706.5	72682.9	98340.7	
	25262.8	32387.3	44728.2	72757.0	98481.4	
	25264.3	32550.3	44860.9	72845.1	98501.0	
	25751.6	32587.3	44865.8	76162.5	105074.0	
	25765.3	32624.3	56609.7	76439.3	105114.2	
	25844.9	33860.4	56634.7	76448.8	105154.6	
	25876.0	33874.0	56649.0	76460.5	105162.4	
	25897.6	33911.1	56669.6	76466.4	105251.8	

0.00	14087.45	28814.71	33955.53	37655.93
198.68	14881.19	28836.50	33967.27	37680.28
223.33	14901.52	28865.42	33992.04	38002.02
280.74	15357.65	28897.17	34019.16	38040.62
411.46	24381.73	28966.74	34077.88	38072.57
472.46	24447.74	29357.97	34104.92	38130.83
583.01	24555.01	29371.98	34131.79	38156.63
746.22	24669.01	29410.94	34154.14	38210.60
3139.91	24891.40	29463.21	34169.34	38232.41
3200.83	26529.92	29537.24	34185.95	38356.16
3340.54	26692.84	29561.39	34221.08	38381.08
3389.82	26737.65	29590.03	34249.42	38419.14
3452.62	26778.55	29598.35	34294.55	38440.94
3500.96	26836.19	29616.65	34308.20	38520.72
3551.62	26887.32	30319.78	34331.04	38680.65
5413.18	26909.06	30412.51	34344.61	38741.20
5449.53	26956.81	30487.82	34359.89	38773.07
5561.10	27096.74	30547.70	34373.91	38877.46
5644.25	27136.32	30590.89	35344.00	38892.92
5705.84	27180.44	30626.79	35361.21	38914.62
5738.75	27198.35	31509.39	35399.47	38925.08
7125.21	27244.32	31554.52	35458.56	38947.04
7187.09	27320.87	31570.90	35508.39	38968.80

7303.47	27425.17	31591.47	35576.19	39043.18
7389.93	27450.93	31625.27	35690.05	39117.60
7444.22	27465.55	31670.55	35758.56	39603.58
8479.86	27527.79	31681.30	35799.04	39610.28
8518.77	27665.30	31722.67	35852.75	39638.55
8691.61	27744.87	31747.88	35919.26	39659.48
8779.87	27771.00	31838.36	35944.51	39668.35
9468.76	27787.44	31879.71	36033.04	39670.16
9634.04	27834.26	31913.76	36240.41	39737.37
9645.34	27943.29	31971.84	36283.19	39749.94
9669.08	28011.44	32001.64	36313.25	39754.91
9688.95	28246.68	32113.64	36802.18	39772.50
9765.69	28281.90	32125.97	36945.15	39860.27
9838.70	28320.39	32174.16	36968.20	39890.97
9861.55	28397.13	32191.21	37039.72	39923.24
9886.51	28439.10	32226.37	37357.86	39949.62
11022.64	28466.48	32252.36	37380.69	39998.17
11110.85	28478.64	32305.13	37469.86	40429.57
11131.61	28508.67	32330.48	37478.24	40452.16
11167.70	28529.40	32341.70	37488.65	40535.45
11189.56	28587.02	32406.40	37513.03	40577.86
12650.94	28609.94	32450.90	37532.80	40595.16
12751.85	28647.06	32806.05	37537.56	40601.90
12814.70	28699.65	32859.74	37546.27	40621.45
12840.99	28739.89	32885.43	37556.35	40632.23
13968.96	28751.49	32963.83	37596.74	40678.72
14061.98	28801.84	33089.64	37620.98	40695.42

40729.37	50210.96	63473.69	73410.55	86080.31	104456.70
40986.67	50248.62	63480.38	74895.56	88976.73	104543.99
41001.92	50289.01	63521.83	75123.12	89370.23	104591.55
41082.92	50372.12	63533.17	75243.45	89440.08	110139.03
41106.58	50456.40	64130.37	75391.90	89896.58	110302.65
42210.15	50536.29	64161.72	78248.71	90008.96	110543.30
42235.32	50600.40	64195.78	78395.56	90089.57	110840.71
42263.11	50701.11	64218.10	78520.19	90943.12	110919.88
42326.77	50854.75	64289.16	79183.83	91111.29	111095.55
42408.52	50882.79	64406.67	79395.26	91228.64	111215.58
42431.90	50971.77	64445.81	80408.11	91397.96	111246.67
42537.45	50989.96	64508.61	81667.59	91574.75	111283.29
42545.74	51036.67	64576.94	81673.68	91660.60	111321.42
42674.09	51082.59	65680.44	81691.28	91710.51	111371.85
42692.26	51187.87	65737.88	81711.82	91760.76	111439.93
42773.35	51246.66	65779.91	81740.01	91851.10	111485.61
42826.92	51417.28	65833.24	81766.21	92002.37	111539.90
43389.98	51436.78	65870.37	81781.06	92227.67	111580.68
43521.89	51526.38	65966.73	81794.45	92332.09	111633.15
43578.54	51657.69	66058.88	81802.52	93015.60	111747.36

43628.35	51778.68	66173.78	81815.78	93082.49	111904.35
44701.32	60361.72	66268.65	81827.00	93150.49	
44755.41	60425.14	66666.94	81850.13	93243.69	
44783.42	60468.54	66714.62	81866.08	93326.01	
45576.69	60502.47	66771.21	81887.50	93501.44	
45650.20	60541.60	66810.85	81912.23	93626.00	
46130.31	60565.64	66891.82	81922.36	93948.44	
46162.42	60698.13	66972.84	81932.59	94030.26	
47059.10	60791.71	67061.36	81976.83	94114.77	
47085.16	60812.47	67165.90	81987.60	94227.30	
47110.21	60856.06	67565.32	81997.61	94366.06	
47591.52	60915.99	67614.65	82008.13	94508.53	
47768.38	60956.30	67670.44	82028.69	94526.13	
47891.57	61008.13	67743.29	82462.25	94578.63	
48693.08	61036.95	67845.03	82531.91	94802.85	
48789.47	61109.26	67914.85	82640.10	94937.97	
48837.11	61174.33	68030.39	82701.50	95090.49	
48856.35	61318.81	68353.41	82728.06	101856.34	
48904.39	61388.32	68400.18	83227.88	102143.90	
48936.70	61552.00	68487.27	83313.31	102668.45	
48957.75	61658.19	68648.85	84957.52	102820.14	
48977.81	61688.93	68706.87	85115.14	102891.74	
49004.14	61809.06	68842.23	85202.21	103523.33	
49071.55	63130.89	69541.78	85268.92	103595.23	
49172.13	63365.78	69650.85	85713.68	103643.93	
49289.40	63396.33	69816.87	85849.46	103797.87	
50130.59	63439.46	70524.15	85937.51	104274.25	
50155.10	63450.12	70816.59	86053.12	104335.27	

1-Dy						
NEVPT2						
0.0	23620.2	26821.0	32566.6	52467.1	70086.0	94804.8
3.8	23696.7	26880.6	32601.2	52486.7	70135.0	94831.2
88.3	23716.5	27119.9	32652.4	52523.2	70149.0	94991.6
263.5	23819.5	27148.7	32716.2	52569.5	70210.3	95018.7
312.5	23845.2	29092.5	32816.8	52633.5	70225.7	
315.4	23845.4	29094.6	32834.3	52637.4	70243.3	
352.4	23871.5	29156.1	32855.1	52660.8	70243.6	
519.8	23945.7	29177.3	32876.6	52681.0	70324.4	
725.2	24003.3	29186.5	33974.3	52705.3	70352.3	
960.1	24016.7	29196.6	34062.3	52712.0	70372.3	
980.0	24022.6	29354.4	34086.0	52742.0	70539.4	
6204.4	24024.3	29358.4	34147.1	52846.1	70703.9	
6355.8	24083.7	29401.0	34191.6	52848.2	70792.4	
6468.7	24113.5	29446.4	34449.2	52893.1	70861.1	
6583.1	24115.7	29452.7	34662.2	52937.0	74995.2	
6604.4	24210.7	29460.2	34677.8	53047.3	75080.6	
6634.3	24210.7	29464.0	34694.9	57839.5	75181.8	

6766.5	24233.7	29531.7	34778.5	57841.7	75515.5	
28897.4	24233.8	29532.1	34878.0	57902.1	75523.1	
29393.1	24246.0	29586.9	34888.8	57905.6	79816.0	
29512.7	24252.8	29638.8	39924.5	57933.8	79836.7	
	24317.5	29833.5	40306.1	57951.4	79923.0	
	24364.8	29834.1	40426.6	57974.2	79955.4	
	24468.4	29868.7	40627.9	58053.3	79977.8	
	24569.2	31203.4	40631.7	58062.0	80005.4	
	24629.4	31211.3	40652.9	58163.8	80022.7	
	24809.1	31226.4	40776.7	58172.2	80230.7	
	24905.5	31243.4	42505.2	58338.4	80236.2	
	24913.2	31254.4	42512.7	58338.6	80506.9	
	24960.4	31262.3	42619.9	58447.7	80507.3	
	25044.9	31289.3	42628.1	58448.4	80622.0	
	25391.4	31307.1	42689.0	60426.8	80624.1	
	25426.1	31346.6	42699.9	60526.9	88091.7	
	25440.9	31370.2	42728.4	61001.5	88290.1	
	25455.0	31379.6	42738.4	65470.0	88330.2	
	25482.3	31467.6	42786.4	65521.0	88444.9	
	25753.1	31482.5	42902.5	65905.4	88725.8	
	25912.4	31483.8	42924.3	65974.1	88874.9	
	26207.6	31488.5	43091.7	66042.8	88889.2	
	26251.6	31492.5	43094.6	68577.3	94514.2	
	26502.2	31504.1	52287.9	70051.7	94590.9	
	26573.1	32495.4	52309.0	70068.1	94635.5	
	26617.0	32509.1	52411.7	70077.3	94657.3	
	26626.1	32543.5	52415.4	70085.6	94727.3	

0.00	12841.77	29658.55	32759.12	36941.36
194.87	13596.36	29698.61	32842.68	37035.08
244.14	13616.67	29765.74	32904.64	37067.21
284.71	14049.10	29815.09	32935.61	37107.04
416.31	23908.78	29883.42	33006.15	37145.93
494.48	23970.70	29922.65	33063.22	37235.53
605.30	24014.97	29968.38	33137.16	37286.31
801.31	24156.41	30000.08	33168.42	37335.11
3139.46	24304.39	30041.63	33360.00	37374.60
3197.49	25266.90	30062.00	34123.25	37392.03
3361.09	25305.71	30081.03	34348.65	37404.56
3414.05	25344.57	30121.23	34473.17	37453.12
3477.08	25390.34	30182.76	34499.53	37472.11
3520.51	25414.13	30222.11	34561.73	37512.62
3581.47	25449.45	30254.15	34585.47	37527.80
5380.27	26517.93	30377.46	34635.40	37634.91
5426.97	26638.21	30460.55	34643.83	38119.31
5548.37	26743.97	30513.63	34676.12	38133.59
5631.30	26827.76	30615.35	34728.15	38149.82
5698.04	26875.50	30736.61	34764.02	38171.66

5739.37	26941.63	31068.11	34807.56	38184.90
7074.06	26992.69	31171.33	34834.37	38224.53
7145.12	27061.17	31188.36	34866.96	38241.78
7267.29	27364.19	31222.07	34878.35	38291.33
7356.67	27656.72	31294.83	34917.22	38298.31
7424.21	27732.50	31309.61	34941.65	38339.79
8332.20	27804.21	31416.74	34959.60	38345.61
8375.78	27843.78	31566.46	34972.39	38377.09
8396.07	27906.35	31668.09	34986.40	38390.11
8422.35	27950.04	31842.32	35027.81	38428.06
8437.33	28017.81	31883.10	35051.06	38437.91
8522.83	28080.32	31913.60	35098.32	38491.07
8603.85	28163.60	31928.35	35134.01	38520.96
8645.21	28214.04	31951.07	35148.91	38597.81
8663.84	28266.62	31976.40	35169.63	38764.69
8762.57	28327.62	32030.94	35282.33	38859.03
9422.81	28379.51	32063.00	35719.80	39401.80
9592.70	28441.47	32150.02	35852.28	39494.48
9767.42	28594.84	32204.01	35947.64	39543.93
9845.01	28657.83	32231.67	35975.47	39583.60
9945.35	28725.34	32282.65	36025.51	39613.64
9961.54	28801.13	32303.89	36094.51	39706.69
9996.16	28886.73	32318.20	36134.94	39761.68
10042.96	29117.62	32377.41	36283.61	39780.50
11442.75	29182.80	32398.01	36692.73	39821.34
11549.93	29304.62	32421.76	36729.78	39888.75
11608.20	29379.76	32501.35	36787.22	39934.26
11639.83	29449.79	32614.98	36806.93	40056.35
12725.97	29510.87	32676.36	36848.85	40142.85
12810.98	29619.19	32746.64	36893.44	40189.19

40217.65	48154.53	59216.41	67201.67	78469.18	94781.03
40226.84	48313.79	59242.60	68035.40	79707.77	94879.24
40245.15	48333.40	59261.03	68276.79	80367.07	94937.30
40251.39	48396.91	59349.98	68393.44	80408.35	99677.04
40273.11	48432.26	59870.17	68537.00	80774.45	99837.70
40304.65	48483.80	59892.02	71465.90	80879.56	100083.92
40331.10	48509.36	59932.38	71612.99	80959.20	100429.85
40350.02	48551.47	59974.32	71747.44	81613.77	100496.65
40389.06	48646.21	60068.92	72259.37	81768.76	100681.35
40400.33	48747.07	60153.89	72451.51	81895.51	100747.79
40822.84	49225.13	60177.27	73585.16	82073.91	100788.30
40955.94	49244.06	60264.86	74997.83	84215.97	100842.67
40980.73	49283.46	60368.84	75057.80	84304.55	100883.22
41101.98	49331.25	62068.34	75144.39	84358.49	100918.76
41152.05	49441.82	62126.89	75205.44	84402.29	100987.08
41164.18	49502.07	62157.48	75250.13	84499.77	101030.60
41191.85	49656.09	62205.31	75300.26	84612.36	101102.90

41204.03	49685.59	62244.02	75330.33	84917.16	101119.98
41261.40	49763.18	62348.89	75342.22	85007.98	101182.26
41271.63	49893.30	62391.40	75357.52	85694.75	101312.26
41296.93	50028.99	62583.33	75371.07	85765.80	101488.08
42230.60	56124.12	62673.53	75397.20	85826.14	
42267.14	56198.49	63034.53	75419.06	85919.88	
42320.22	56220.28	63079.56	75442.20	85985.40	
42411.84	56256.39	63127.91	75451.93	86213.56	
42493.48	56294.00	63168.70	75483.11	86338.36	
43318.28	56324.82	63233.95	75500.52	86625.39	
43402.74	56405.69	63260.69	75526.26	86708.07	
43957.17	56508.72	63305.11	75533.92	86784.37	
44101.60	56531.98	63381.07	75551.24	86881.28	
44163.31	56563.88	63449.63	75570.50	87067.74	
44731.76	56618.49	63538.69	75592.74	87174.57	
44899.01	56735.11	63556.15	75599.93	87216.04	
44989.71	56808.70	63928.36	75625.52	87232.14	
46114.05	56838.45	63974.12	75651.61	87425.12	
46270.65	56897.65	64027.50	75663.02	87623.84	
46374.70	56963.04	64105.71	75682.28	87771.49	
46439.54	57125.97	64137.22	75696.00	92244.60	
47037.28	57181.96	64188.03	75949.52	92531.16	
47105.33	57249.22	64296.34	76025.52	93033.57	
47174.93	57345.47	64415.58	77588.84	93194.87	
47200.93	57394.53	64468.11	77754.86	93260.01	
47224.33	57462.45	64720.96	77830.49	93862.33	
47291.71	58801.73	64766.52	77912.90	93944.03	
47392.54	59009.32	64844.36	78064.79	93986.09	
47534.81	59106.92	64982.61	78158.33	94148.07	
47972.58	59143.13	65091.20	78367.30	94601.24	
48059.64	59188.10	65228.36	78418.27	94650.70	

Table S11. CASSCF computed low-lying 21 sextets (in red) and 224 quartet states (in black) along with spin-orbit coupled states (in blue, Kramer doublets). All the values are reported here in cm^{-1} .

2-Dy						
0.7	24093.5	25826.4	33853.3	56641.3	76399.4	105247.7
97.3	24095.9	25894.4	33880.9	56641.7	76411.5	105260.7
193.4	24144.5	25958.1	33886.6	56686.3	76417.5	105390.0
249.3	24151.2	26015.9	33982.0	56705.9	76485.0	105396.8
275.4	24205.5	28990.9	34051.7	56709.5	76491.5	
323.4	24223.3	28994.4	34060.3	56786.7	76500.4	
448.5	24253.2	29065.7	34062.2	56788.8	76501.2	
660.9	24274.1	29067.2	34101.1	56936.6	77750.6	
742.9	24343.4	29087.0	36912.5	56943.6	77792.8	
802.5	24424.6	29103.0	36928.3	57005.0	77825.5	

7435.3	24432.5	29189.8	36957.4	57024.8	77933.5	
7600.4	24449.0	29196.0	36958.2	57032.1	78057.8	
7649.6	24453.9	29254.8	37090.2	57032.5	78104.2	
7714.2	24525.9	29260.3	37132.7	57053.3	78198.8	
7747.5	24567.3	29277.8	37246.6	57085.1	84394.1	
7801.4	24611.2	29278.0	37260.5	57103.5	84495.2	
7906.6	24632.7	29286.9	37366.2	61466.9	84532.2	
34208.8	24639.5	29341.2	37369.5	61467.3	84858.3	
34661.3	24642.6	29344.0	37382.9	61484.2	84872.8	
34750.7	24646.2	30425.5	37443.3	61489.5	87203.0	
	24674.8	30430.3	42506.1	61527.4	87219.7	
	24693.8	30435.4	42880.5	61547.7	87288.4	
	24737.6	30451.7	42890.2	61565.7	87303.6	
	24741.8	30463.3	43020.3	61632.3	87343.9	
	24774.6	30470.8	43045.3	61646.2	87353.2	
	24790.7	30492.0	43098.6	61652.0	87360.2	
	24808.9	30501.9	43199.5	61654.9	87432.6	
	24849.4	30537.8	44225.1	61873.8	87451.6	
	24881.7	30547.8	44232.2	61876.1	87759.5	
	24938.4	30554.4	44393.2	61965.5	87766.3	
	24940.2	30635.8	44395.7	61966.3	87881.6	
	24970.3	30645.1	44435.2	66557.8	87885.8	
	24990.2	30646.3	44440.7	66627.6	97758.6	
	24991.0	30650.9	44451.2	67042.4	97822.5	
	25014.1	30660.2	44460.0	72232.0	97904.2	
	25083.2	30662.0	44478.5	72277.5	98018.5	
	25085.1	32296.5	44588.8	72577.1	98144.0	
	25161.9	32336.7	44608.5	72689.7	98382.1	
	25162.7	32485.3	44750.4	72732.3	98422.8	
	25670.4	32487.8	44752.2	76074.6	104979.0	
	25686.9	32521.7	56577.9	76375.1	105006.6	
	25762.5	33809.9	56578.6	76386.3	105128.1	
	25788.5	33815.8	56586.8	76389.1	105133.5	
	25807.3	33846.7	56608.0	76390.9	105163.3	

0.00	14028.04	28735.06	33943.30	37599.85
148.93	14828.59	28774.86	33949.29	37622.34
192.83	14840.46	28781.15	33975.39	37960.58
300.67	15301.31	28808.58	33987.18	37987.40
361.33	24378.14	28891.94	34032.45	38007.63
450.07	24429.66	29303.62	34061.11	38079.65
513.02	24528.99	29320.99	34083.19	38095.68
624.07	24601.98	29382.84	34102.08	38147.84
3101.86	24803.83	29415.26	34110.77	38162.59
3161.31	26521.93	29466.59	34120.61	38312.69
3341.37	26647.49	29504.05	34140.71	38330.96
3387.99	26675.79	29510.53	34166.76	38358.24
3406.95	26755.67	29526.23	34224.84	38365.84

3426.53	26810.25	29530.33	34230.80	38486.57
3457.86	26851.05	30279.84	34259.01	38622.34
5391.24	26867.43	30362.10	34268.93	38680.27
5403.95	26911.18	30484.04	34284.28	38726.01
5539.78	27070.23	30500.78	34301.63	38825.99
5588.64	27103.03	30532.79	35314.53	38838.96
5644.02	27124.56	30537.09	35320.11	38853.75
5690.12	27145.39	31457.77	35356.34	38863.70
7121.70	27185.90	31531.43	35408.05	38892.01
7135.46	27255.60	31533.55	35446.97	38909.94
7259.46	27422.64	31552.41	35502.93	38965.37
7318.74	27439.57	31588.02	35640.32	39041.41
7406.27	27449.09	31610.05	35713.58	39554.99
8461.63	27527.17	31626.65	35724.68	39557.42
8486.31	27567.40	31656.16	35814.22	39579.40
8612.40	27674.92	31675.98	35867.95	39598.09
8747.60	27722.24	31822.81	35889.15	39607.77
9426.58	27729.22	31840.83	35954.75	39624.47
9590.28	27748.49	31875.57	36193.31	39678.06
9628.61	27860.66	31918.94	36225.94	39693.06
9636.46	27939.53	31920.97	36248.48	39696.20
9656.75	28240.80	32072.35	36775.98	39712.27
9712.45	28248.03	32092.04	36897.51	39808.37
9763.43	28297.19	32128.39	36903.11	39836.22
9775.57	28364.89	32137.60	36976.23	39858.67
9809.16	28414.72	32160.42	37313.94	39892.04
10982.10	28436.78	32189.86	37339.15	39925.00
11057.59	28449.31	32258.23	37421.36	40367.64
11082.52	28487.49	32270.34	37423.47	40423.93
11106.91	28504.94	32293.21	37433.56	40463.29
11120.48	28540.03	32327.81	37461.76	40512.61
12615.30	28560.62	32373.18	37471.54	40544.04
12696.97	28586.53	32748.22	37481.48	40547.56
12754.95	28631.29	32798.61	37485.87	40565.83
12776.20	28652.98	32822.07	37509.49	40572.44
13928.89	28670.56	32918.04	37517.80	40614.71
14004.26	28727.67	33004.23	37561.51	40625.53

40655.73	50159.58	63412.30	73344.81	86000.96	104323.84
40926.35	50200.04	63424.71	74842.85	88906.72	104455.67
40949.41	50227.02	63440.93	75063.85	89320.13	104519.40
41013.54	50300.34	63471.92	75206.79	89346.96	110070.28
41046.82	50392.20	64071.42	75271.89	89846.86	110233.26
42184.71	50471.50	64102.15	78193.10	89914.90	110451.84
42196.26	50587.58	64134.05	78346.25	90011.94	110775.91
42225.53	50631.16	64155.51	78436.07	90932.55	110852.64
42261.32	50771.96	64221.56	79125.64	90999.04	111010.12
42300.09	50776.69	64348.08	79314.77	91144.81	111142.40

42373.74	50891.62	64384.86	80340.69	91330.58	111191.90
42466.74	50963.96	64442.05	81611.38	91574.50	111219.74
42506.74	50982.25	64508.39	81617.46	91620.03	111280.95
42606.56	51027.47	65687.81	81640.48	91691.50	111311.34
42643.18	51114.64	65696.37	81656.10	91702.07	111360.01
42707.39	51181.99	65750.81	81689.15	91767.28	111381.25
42737.87	51329.74	65761.30	81704.82	91780.75	111430.75
43338.44	51425.12	65818.47	81712.85	92147.24	111485.92
43488.36	51463.28	65861.81	81725.51	92232.19	111500.16
43492.16	51560.27	65908.96	81736.51	93026.73	111649.34
43557.20	51684.89	66107.67	81749.18	93031.33	111792.33
44651.79	60309.71	66176.28	81767.82	93096.25	
44689.19	60369.23	66658.79	81785.71	93120.44	
44724.52	60409.72	66668.11	81794.22	93192.75	
45525.16	60447.95	66714.55	81815.00	93427.11	
45590.46	60480.74	66757.75	81836.34	93532.38	
46075.78	60508.16	66799.74	81858.60	93947.66	
46096.98	60645.24	66838.86	81865.56	93975.16	
47003.05	60733.61	66998.18	81902.02	94032.17	
47022.56	60750.15	67075.03	81914.84	94079.60	
47044.11	60817.40	67548.20	81917.81	94293.60	
47552.87	60855.50	67564.85	81925.01	94421.02	
47697.76	60929.40	67619.40	81949.13	94517.90	
47815.43	60959.49	67681.00	82402.10	94532.32	
48631.60	60991.89	67693.40	82456.35	94615.66	
48722.25	61000.66	67853.31	82561.59	94855.00	
48789.51	61055.46	67941.42	82610.87	94999.95	
48841.69	61255.43	68336.37	82627.54	101819.87	
48861.94	61317.81	68355.85	83160.37	102054.55	
48881.92	61501.71	68439.79	83241.89	102619.02	
48898.16	61602.09	68483.57	84913.42	102740.15	
48933.26	61614.65	68644.84	85040.94	102804.02	
48944.34	61749.36	68754.38	85113.50	103466.02	
48989.72	63077.48	69485.64	85197.66	103544.15	
49082.99	63323.68	69602.57	85650.73	103564.97	
49204.47	63340.43	69733.95	85780.53	103697.76	
50055.78	63371.44	70458.08	85868.35	104237.83	
50131.05	63384.61	70737.05	85970.76	104254.85	

Table S12. CASSCF computed low-lying 21 sextets (in red) and 224 quartet states (in black) along with spin-orbit coupled states (in blue, Kramer doublets). All the values are reported here in cm^{-1} .

3-Dy						
0.0	24110.6	25874.9	33889.1	56661.6	76435.3	105300.1
8.6	24115.9	25928.3	33922.8	56668.9	76460.4	105335.1
108.0	24159.5	25993.8	33938.6	56727.7	76468.7	105449.0
270.8	24186.5	26068.1	34013.3	56769.8	76527.0	105469.0

291.1	24220.8	29032.1	34089.6	56771.9	76535.3	
297.7	24223.9	29033.3	34101.8	56804.0	76548.3	
355.9	24277.5	29099.1	34109.9	56824.1	76550.0	
456.5	24282.8	29115.1	34136.5	56993.2	77802.0	
676.8	24357.5	29121.4	36916.6	57003.1	77818.7	
833.2	24455.5	29129.3	36923.7	57047.6	77845.7	
865.4	24473.0	29234.0	37005.1	57075.1	77991.2	
7467.4	24493.7	29238.1	37014.1	57076.6	78115.8	
7599.4	24500.0	29299.1	37147.0	57092.7	78180.3	
7681.4	24572.0	29308.9	37156.1	57101.1	78230.9	
7756.5	24587.3	29312.6	37279.6	57117.2	84435.0	
7797.9	24620.1	29317.3	37304.0	57122.0	84530.8	
7849.3	24660.5	29319.7	37402.5	61482.2	84579.2	
7963.9	24667.6	29391.3	37430.1	61486.5	84909.3	
34238.8	24678.2	29391.5	37437.8	61500.6	84919.3	
34734.9	24685.3	30450.9	37516.2	61512.3	87218.5	
34765.6	24687.5	30459.4	42537.3	61562.2	87240.1	
	24719.8	30463.3	42856.9	61585.7	87315.2	
	24759.1	30478.2	42925.7	61588.9	87330.1	
	24766.3	30492.6	43067.5	61670.8	87355.5	
	24797.9	30504.8	43109.7	61681.6	87366.7	
	24835.7	30522.2	43157.7	61754.0	87396.2	
	24856.2	30537.0	43265.2	61757.7	87553.8	
	24870.3	30577.0	44272.3	61920.1	87563.6	
	24934.3	30588.2	44278.8	61921.5	87814.9	
	24983.1	30598.1	44392.9	62019.5	87818.1	
	25005.7	30687.6	44395.8	62019.8	87933.9	
	25016.4	30698.7	44454.1	66612.5	87938.0	
	25027.7	30701.9	44467.8	66645.0	97747.5	
	25030.6	30702.8	44490.9	67095.3	97911.6	
	25072.4	30706.5	44514.3	72260.2	97929.5	
	25138.0	30713.0	44526.0	72309.8	98041.9	
	25143.1	32315.9	44651.2	72662.4	98244.2	
	25216.3	32363.9	44672.1	72697.6	98435.0	
	25217.0	32524.1	44808.6	72786.8	98456.7	
	25718.0	32539.4	44812.0	76120.0	105029.9	
	25723.9	32576.1	56599.3	76411.2	105065.4	
	25807.7	33840.3	56613.7	76421.9	105138.7	
	25840.7	33845.7	56621.3	76425.4	105144.3	
	25852.9	33885.4	56640.0	76427.0	105206.1	

0.00	14059.72	28777.00	33953.08	37630.73
178.97	14856.84	28804.99	33960.15	37651.72
233.56	14872.64	28822.74	33984.59	37982.21
277.55	15331.35	28851.48	34005.70	38016.84
397.43	24382.91	28931.87	34057.85	38041.46
459.37	24443.20	29336.03	34085.86	38109.20
544.24	24544.08	29346.00	34107.57	38124.58

688.73	24638.99	29402.56	34133.07	38182.66
3124.85	24848.17	29434.91	34140.20	38195.90
3181.68	26526.70	29504.58	34153.05	38339.06
3354.80	26675.52	29532.14	34183.55	38357.19
3385.78	26713.92	29552.80	34207.39	38390.25
3433.04	26772.27	29561.25	34264.81	38401.40
3473.96	26826.29	29575.22	34268.04	38505.26
3497.93	26873.79	30301.83	34298.49	38654.92
5412.86	26890.30	30388.66	34307.64	38722.53
5421.12	26929.03	30493.37	34319.91	38738.10
5554.85	27101.74	30521.56	34337.48	38853.02
5630.28	27109.98	30568.16	35332.36	38867.16
5676.58	27156.04	30580.15	35342.33	38886.50
5707.92	27174.81	31485.46	35380.42	38895.12
7128.19	27214.10	31546.20	35435.54	38920.76
7161.57	27291.28	31553.93	35479.48	38940.44
7291.66	27425.43	31573.82	35540.16	39004.09
7356.04	27448.13	31609.78	35666.21	39080.62
7423.81	27457.92	31642.08	35738.30	39581.05
8479.08	27529.14	31654.90	35764.97	39585.37
8500.09	27620.61	31693.81	35834.13	39611.21
8659.21	27728.02	31711.82	35901.39	39631.90
8763.19	27740.26	31839.96	35911.36	39638.48
9451.88	27750.46	31857.05	35994.14	39646.39
9617.78	27790.24	31894.09	36218.17	39709.94
9642.24	27906.70	31947.90	36257.45	39723.94
9650.39	27976.96	31964.45	36281.28	39725.59
9674.14	28247.60	32095.88	36790.73	39742.70
9739.81	28267.12	32112.32	36927.73	39835.50
9805.90	28311.06	32154.07	36934.24	39865.80
9818.25	28384.03	32164.72	37010.19	39892.07
9849.07	28431.54	32193.04	37338.61	39920.62
11004.73	28457.29	32222.67	37360.51	39962.84
11086.87	28465.37	32285.74	37448.32	40401.59
11108.06	28504.89	32302.00	37452.40	40437.42
11139.72	28512.53	32317.80	37461.60	40500.61
11156.33	28566.58	32368.74	37489.72	40546.59
12635.57	28585.48	32410.08	37504.84	40570.51
12726.97	28621.18	32776.78	37512.99	40575.97
12786.15	28667.53	32832.99	37517.48	40594.67
12810.26	28701.57	32856.65	37535.41	40602.92
13951.43	28709.94	32939.95	37554.69	40647.59
14034.86	28764.72	33047.59	37589.13	40661.60

40693.23	50187.44	63442.95	73377.70	86038.53	104386.17
40958.52	50220.13	63452.51	74867.94	88941.40	104497.60
40975.38	50256.07	63478.01	75098.92	89352.25	104550.84
41051.62	50339.48	63503.17	75224.73	89384.28	110108.43

41075.53	50426.56	64104.04	75327.29	89877.18	110259.70
42202.31	50506.30	64130.48	78221.56	89957.09	110497.09
42216.14	50592.99	64165.54	78374.02	90046.89	110826.47
42242.61	50664.19	64185.34	78474.34	90941.27	110864.91
42294.83	50819.23	64256.17	79157.03	91056.25	111049.78
42356.05	50826.36	64382.96	79352.11	91178.79	111186.99
42404.03	50941.73	64409.07	80373.90	91364.72	111222.60
42503.87	50973.86	64474.74	81641.38	91579.33	111248.13
42527.27	51004.60	64543.46	81646.26	91637.46	111292.40
42641.81	51053.45	65694.34	81665.73	91694.01	111342.60
42667.99	51155.36	65706.46	81683.90	91732.50	111396.46
42739.75	51214.88	65768.33	81715.06	91817.02	111433.11
42783.84	51379.31	65797.34	81734.89	91878.84	111486.28
43365.42	51425.70	65840.68	81752.19	92192.73	111532.30
43505.03	51492.67	65938.87	81753.99	92277.44	111546.05
43536.89	51610.59	65957.62	81770.89	93029.78	111696.34
43593.71	51732.25	66145.17	81780.13	93047.08	111848.40
44677.60	60335.89	66221.83	81795.12	93124.95	
44723.91	60397.85	66667.14	81816.43	93197.35	
44754.24	60440.55	66686.77	81829.49	93235.16	
45552.61	60477.27	66746.38	81851.57	93466.46	
45620.85	60515.21	66780.50	81871.28	93578.40	
46104.33	60535.10	66865.28	81891.41	93949.75	
46130.40	60671.75	66883.22	81898.40	94001.34	
47032.30	60768.01	67032.89	81938.65	94084.52	
47054.82	60780.30	67121.01	81952.81	94134.60	
47077.63	60837.63	67559.29	81960.14	94330.63	
47572.99	60887.77	67587.41	81965.08	94466.03	
47738.52	60944.55	67644.49	81988.54	94526.00	
47849.24	60991.96	67717.40	82429.24	94546.24	
48664.51	61003.10	67760.20	82490.75	94706.67	
48759.57	61063.90	67886.69	82600.45	94896.27	
48813.30	61101.27	67986.68	82662.62	95044.02	
48861.41	61291.40	68349.33	82669.93	101844.79	
48876.08	61352.24	68372.70	83194.48	102092.73	
48914.27	61527.37	68463.25	83276.58	102648.67	
48936.26	61633.27	68563.15	84934.82	102778.44	
48945.30	61651.22	68678.32	85077.40	102842.18	
48967.62	61779.01	68798.76	85158.78	103505.68	
49030.14	63104.19	69514.77	85230.72	103563.58	
49130.19	63350.75	69634.06	85680.06	103596.39	
49248.26	63368.37	69768.95	85816.95	103746.31	
50103.75	63406.33	70487.49	85901.68	104264.42	
50138.32	63417.73	70778.16	86011.65	104287.80	

Table S13. CASSCF computed low-lying 21 sextets (in red) and 224 quartet states (in black) along with spin-orbit coupled states (in blue, Kramer doublets). All the values are reported here in cm^{-1} .

4-Dy						
0.0	24124.7	25882.7	33901.5	56686.5	76460.2	105331.2
8.6	24129.2	25941.7	33936.3	56692.1	76477.6	105360.3
124.6	24172.5	26005.4	33954.3	56738.3	76484.7	105481.0
272.7	24202.2	26073.8	34027.3	56772.9	76551.5	105497.4
285.3	24237.7	29043.4	34099.4	56775.8	76559.6	
330.9	24242.6	29044.3	34111.5	56830.0	76572.2	
360.6	24304.0	29109.7	34119.9	56846.4	76574.1	
466.2	24304.3	29125.3	34142.9	57012.4	77823.7	
675.4	24374.8	29131.1	36932.6	57021.6	77833.1	
824.0	24465.6	29136.7	36953.0	57084.7	77882.1	
859.0	24482.6	29251.3	37017.7	57098.9	78014.3	
7476.5	24510.7	29254.7	37032.3	57101.1	78131.0	
7610.3	24512.9	29306.4	37156.4	57102.1	78197.5	
7691.5	24586.5	29311.2	37174.2	57107.5	78265.3	
7757.0	24598.4	29313.1	37284.7	57139.0	84451.0	
7804.3	24640.6	29323.8	37308.0	57156.4	84569.7	
7849.2	24682.3	29328.6	37413.4	61503.4	84583.0	
7960.4	24690.0	29396.9	37438.1	61505.2	84942.5	
34239.6	24698.0	29397.5	37444.2	61522.1	84951.9	
34758.2	24702.0	30467.5	37526.6	61529.3	87251.0	
34777.6	24704.5	30475.6	42555.7	61579.4	87268.4	
	24732.9	30481.8	42880.2	61605.6	87338.2	
	24770.0	30494.4	42948.7	61614.6	87355.6	
	24779.7	30507.9	43069.8	61696.9	87392.7	
	24804.4	30520.2	43128.4	61708.4	87402.3	
	24841.0	30534.0	43165.2	61750.3	87420.2	
	24858.7	30550.6	43268.9	61753.7	87554.2	
	24874.0	30588.2	44276.9	61942.2	87566.5	
	24941.7	30598.0	44284.0	61943.3	87846.1	
	24989.2	30607.3	44418.3	62040.1	87848.6	
	25008.8	30694.6	44422.1	62040.3	87961.0	
	25019.7	30705.9	44480.2	66636.6	87964.3	
	25031.7	30706.6	44490.7	66648.9	97789.6	
	25035.5	30709.0	44503.8	67125.6	97925.3	
	25074.8	30712.9	44530.1	72273.7	97950.3	
	25134.2	30718.5	44535.4	72324.2	98073.4	
	25139.5	32331.6	44656.3	72672.5	98253.6	
	25221.6	32380.8	44676.7	72741.9	98472.0	
	25222.2	32533.9	44820.8	72813.0	98492.8	
	25721.0	32548.8	44823.6	76144.3	105051.6	
	25723.1	32579.2	56610.6	76437.9	105085.0	
	25816.0	33854.4	56625.1	76444.5	105178.5	
	25845.0	33860.1	56641.5	76447.4	105187.2	
	25863.2	33896.8	56651.3	76450.0	105241.5	

0.00	14063.57	28782.00	33970.48	37644.63
176.84	14863.36	28811.04	33976.71	37663.54

233.84	14877.44	28825.49	34001.89	37996.49
309.02	15337.55	28852.92	34023.48	38029.45
392.36	24396.55	28934.53	34071.37	38056.09
469.32	24464.79	29348.97	34101.03	38123.34
552.22	24557.94	29359.28	34116.10	38138.07
682.11	24647.18	29416.79	34142.97	38192.59
3123.74	24849.90	29445.78	34153.07	38205.29
3181.75	26539.85	29517.15	34164.08	38353.85
3358.63	26683.77	29539.62	34192.85	38368.67
3403.98	26726.84	29561.55	34215.97	38402.71
3442.59	26786.63	29568.22	34273.10	38413.65
3472.46	26844.91	29582.32	34278.06	38520.28
3501.79	26893.08	30310.56	34305.13	38660.51
5410.99	26906.56	30397.20	34314.65	38731.15
5426.80	26940.91	30511.19	34327.28	38755.67
5567.07	27108.74	30534.65	34345.93	38868.18
5632.88	27127.33	30581.68	35346.90	38879.32
5679.50	27166.30	30588.88	35356.95	38898.60
5716.94	27184.38	31499.06	35394.93	38906.46
7136.29	27222.48	31559.94	35446.73	38933.05
7164.24	27300.10	31566.82	35488.73	38952.53
7301.46	27430.37	31582.18	35550.26	39015.28
7355.13	27474.04	31623.99	35677.17	39087.57
7432.73	27484.22	31652.20	35749.06	39595.65
8485.62	27545.49	31666.60	35775.08	39599.21
8509.43	27625.29	31698.79	35853.34	39623.36
8657.31	27733.68	31719.98	35909.74	39643.17
8775.20	27750.70	31857.02	35924.70	39649.71
9453.36	27759.30	31875.65	36002.41	39660.90
9621.13	27794.88	31909.38	36231.57	39723.71
9652.52	27905.43	31958.99	36268.55	39735.86
9663.44	27985.23	31978.13	36291.47	39737.91
9683.57	28261.33	32106.82	36805.66	39755.41
9746.08	28279.11	32129.02	36939.52	39847.21
9804.73	28327.06	32164.81	36949.18	39878.62
9819.85	28401.06	32173.06	37019.73	39903.98
9851.74	28448.72	32201.18	37353.55	39934.20
11012.02	28472.69	32232.86	37373.74	39973.35
11091.56	28481.68	32295.22	37462.26	40412.20
11113.27	28520.30	32314.61	37467.22	40455.64
11144.60	28530.21	32325.94	37477.17	40511.42
11159.18	28576.42	32378.73	37500.24	40560.95
12644.26	28599.72	32418.13	37520.87	40584.84
12733.60	28632.39	32782.35	37523.53	40589.99
12790.10	28673.71	32843.85	37529.06	40608.78
12813.52	28708.66	32866.61	37548.74	40616.56
13960.08	28719.17	32954.16	37562.21	40659.63
14040.99	28769.39	33054.37	37603.80	40672.58

40702.60	50201.20	63464.34	73398.87	86066.95	104409.05
40968.71	50238.33	63472.49	74880.77	88963.62	104527.67
40990.21	50274.03	63500.30	75118.99	89380.67	104584.30
41061.85	50352.73	63523.52	75261.01	89407.38	110133.09
41090.47	50447.49	64122.47	75346.91	89905.91	110292.72
42216.97	50517.33	64150.33	78239.32	89979.44	110535.75
42229.11	50614.86	64186.58	78400.38	90075.37	110846.63
42264.48	50680.57	64206.01	78498.66	90974.06	110899.32
42307.35	50825.54	64277.57	79177.63	91070.49	111081.54
42358.20	50842.49	64399.88	79377.31	91208.38	111209.85
42421.18	50947.26	64430.22	80399.80	91399.32	111258.54
42518.32	50995.18	64495.27	81664.28	91611.08	111280.09
42546.55	51019.45	64566.22	81668.98	91658.17	111333.42
42653.39	51071.15	65715.30	81691.88	91731.39	111375.16
42680.77	51167.18	65727.17	81708.88	91752.95	111427.74
42750.17	51236.91	65789.87	81741.38	91846.75	111460.53
42796.02	51386.89	65811.34	81760.61	91885.46	111509.64
43383.17	51448.98	65866.82	81771.63	92225.02	111566.91
43517.02	51510.68	65952.62	81777.51	92306.96	111577.98
43551.57	51618.47	65966.30	81794.81	93061.05	111731.13
43603.83	51746.25	66168.11	81804.48	93073.02	111889.10
44691.82	60350.64	66243.91	81820.54	93148.28	
44737.29	60415.63	66690.65	81839.35	93205.86	
44768.33	60457.83	66705.52	81853.58	93263.58	
45567.04	60497.06	66762.24	81871.18	93498.83	
45636.02	60534.18	66805.51	81894.78	93612.80	
46118.96	60557.99	66881.57	81917.75	93982.46	
46144.57	60686.73	66891.89	81924.93	94024.43	
47046.11	60783.92	67056.08	81960.08	94102.79	
47068.42	60799.51	67143.21	81977.49	94152.05	
47090.78	60860.02	67582.74	81983.09	94362.42	
47589.90	60906.43	67605.40	81988.49	94500.74	
47753.25	60965.52	67666.21	82012.63	94554.29	
47863.69	61006.99	67743.48	82449.49	94576.98	
48679.22	61028.80	67761.23	82513.34	94712.42	
48766.69	61070.93	67910.00	82625.74	94925.67	
48828.49	61120.00	68008.84	82688.28	95075.32	
48883.12	61314.68	68370.39	82696.28	101871.92	
48891.56	61375.90	68395.02	83216.16	102117.66	
48928.79	61543.65	68489.87	83301.05	102679.99	
48951.42	61652.36	68564.75	84961.50	102806.50	
48965.63	61670.10	68701.86	85101.23	102869.09	
48986.60	61799.06	68820.52	85177.47	103532.52	
49043.26	63115.59	69529.24	85259.58	103600.70	
49140.04	63374.08	69652.76	85699.95	103625.89	
49265.48	63389.36	69790.23	85842.35	103770.70	
50108.65	63424.51	70504.74	85925.90	104293.32	
50159.58	63437.95	70806.63	86039.27	104315.87	

Table S14. CASSCF computed low-lying 21 sextets (in red) and 224 quartet states (in black) along with spin-orbit coupled states (in blue, Kramer doublets). All the values are reported here in cm⁻¹.

5-Dy						
0.0	24225.8	26622.4	34373.9	56841.5	76703.5	105897.7
18.2	24247.1	26705.7	34431.9	56967.2	76709.7	105902.4
739.3	24463.0	26850.4	34548.3	56980.0	76736.2	106049.7
845.5	24492.0	26885.0	34570.9	57048.9	76753.5	106189.6
931.6	24554.5	29339.6	34617.9	57119.5	76768.2	
995.8	24606.3	29395.8	34657.6	57331.2	77069.7	
1295.6	24647.7	29538.2	34684.4	57388.9	77079.5	
1356.4	24660.1	29551.4	34712.6	57394.0	77805.4	
1509.9	24740.4	29617.5	37174.1	57433.9	78103.7	
1760.7	24841.5	29647.4	37269.3	57503.0	78491.3	
1799.9	24859.3	29710.4	37401.4	57578.8	78550.8	
7973.4	24877.4	29739.5	37480.7	57688.3	78605.6	
8233.2	24933.1	29754.6	37634.1	57947.6	78716.3	
8280.6	24946.1	29766.4	37738.0	57988.2	78890.8	
8445.1	25009.0	29823.6	37786.5	58015.0	84334.7	
8538.7	25030.1	29831.8	37909.6	58023.9	84450.1	
8618.1	25055.5	29985.2	37961.2	61630.9	84805.1	
8719.7	25134.5	30003.8	38053.7	61632.6	85686.2	
34228.3	25141.8	30053.0	38230.4	61784.9	85708.4	
35311.5	25173.2	30994.1	38293.7	61787.6	87208.5	
35814.0	25242.4	31013.5	42538.1	61880.7	87218.0	
	25270.6	31018.8	43308.3	61934.8	87414.3	
	25283.3	31029.4	43349.3	61939.4	87419.9	
	25324.7	31085.8	43627.0	61974.6	87567.9	
	25353.6	31103.3	43690.9	62018.2	87619.0	
	25460.1	31114.7	43773.8	62026.5	87730.7	
	25467.6	31178.0	43911.6	62040.7	87758.2	
	25492.1	31199.7	44437.4	62276.7	87836.2	
	25508.7	31204.4	44438.3	62278.0	88005.8	
	25543.9	31235.9	44543.1	63054.5	88011.7	
	25567.5	31310.4	44622.8	63057.0	89005.1	
	25638.6	31343.1	44733.2	66432.6	89013.6	
	25669.4	31344.9	44885.2	66889.2	97403.6	
	25731.2	31346.4	45041.4	67967.2	97715.8	
	25765.8	31349.9	45226.4	72062.9	97923.9	
	25831.0	31366.3	45247.3	72173.1	98013.2	
	25848.9	32812.2	45329.9	73049.2	98209.5	
	25873.1	32814.9	45351.3	73411.7	99150.2	
	25878.6	32963.2	45512.6	73496.7	99277.5	
	26017.4	33061.5	45517.5	76555.4	104970.6	
	26091.3	33137.9	56412.7	76558.7	104986.4	
	26366.5	34243.2	56440.6	76647.0	105148.4	

	26398.3	34252.9	56725.6	76666.3	105462.6	
	26588.4	34332.7	56730.8	76669.2	105543.0	

0.00	14733.56	29370.93	34343.57	38258.31
483.01	15495.29	29438.33	34398.81	38356.42
898.30	15537.29	29458.51	34437.83	38414.50
993.99	15982.75	29486.71	34459.90	38446.54
1157.38	24816.31	29514.23	34526.42	38524.41
1229.84	24841.38	29902.12	34557.34	38594.38
1331.67	24955.60	29948.94	34571.09	38623.62
1608.07	25065.65	29976.87	34605.50	38694.67
3312.02	25409.36	30095.98	34644.20	38735.64
3704.24	26760.20	30117.78	34658.15	38773.96
3895.88	26893.64	30144.90	34706.12	38785.91
4013.41	26913.20	30182.72	34736.36	38890.23
4108.06	27089.55	30222.45	34814.11	38918.68
4248.96	27246.34	30238.51	34840.27	39038.15
4436.35	27302.75	30455.12	34885.11	39107.35
5803.34	27407.36	30870.32	34910.78	39139.33
5920.85	27465.41	31019.44	34939.13	39258.12
6044.41	27565.65	31045.35	35031.82	39312.67
6221.74	27613.76	31120.62	35689.39	39331.72
6401.40	27698.74	31237.33	35729.00	39345.45
6633.47	27727.93	31891.36	35786.56	39395.28
7567.55	27788.63	31898.09	35804.95	39428.58
7660.53	27806.89	31918.66	35885.20	39458.07
7810.25	27873.37	32002.72	36077.56	39555.59
8005.10	27903.04	32013.04	36136.61	39695.03
8299.74	27971.15	32034.93	36163.90	40043.64
8920.96	28060.32	32105.18	36293.79	40051.84
9017.36	28092.15	32117.88	36315.90	40057.32
9243.56	28144.50	32215.88	36457.53	40110.85
9593.84	28197.34	32268.10	36477.60	40140.25
10020.68	28261.20	32311.48	36516.41	40167.72
10117.33	28384.80	32365.57	36631.79	40177.88
10201.28	28443.40	32384.15	36696.94	40193.17
10323.42	28528.75	32468.11	36796.03	40227.50
10359.18	28542.81	32518.35	37206.62	40285.21
10403.45	28661.47	32575.17	37381.76	40361.00
10529.67	28710.12	32623.20	37420.13	40393.66
10576.18	28719.47	32672.24	37525.68	40419.98
10645.21	28790.19	32757.25	37732.91	40458.39
11641.70	28852.84	32774.16	37813.70	40510.40
11717.70	28951.89	32867.81	37902.23	40809.76
11756.28	28964.96	32880.20	37924.77	40979.55
11787.92	29084.58	32950.20	37948.79	41053.52
11868.53	29104.82	33027.26	37977.83	41081.06
13237.11	29140.17	33123.26	37998.91	41102.57

13397.23	29198.57	33166.87	38036.62	41116.11
13442.18	29220.23	33286.09	38044.13	41137.52
13482.05	29256.11	33478.42	38051.56	41150.53
14547.33	29273.41	33560.81	38107.77	41187.73
14688.74	29284.91	33640.92	38141.28	41217.15

41250.65	50487.22	63862.09	73684.94	86576.92	104535.95
41373.32	50642.87	63897.27	74653.71	86670.94	104698.05
41536.23	50705.88	64022.20	75378.39	89018.18	104940.50
41548.26	50846.51	64044.29	75693.51	89465.60	105086.22
41636.10	50971.09	64431.98	76017.78	89752.43	109964.59
42592.69	51038.95	64504.79	78257.20	90158.27	110442.73
42646.47	51072.58	64571.14	78597.22	90359.11	110609.47
42668.39	51110.81	64663.88	78925.10	90419.28	111003.31
42743.40	51213.65	64698.01	79300.49	90937.15	111054.38
42784.17	51235.27	64802.22	79812.89	91298.47	111105.48
42819.06	51364.13	64906.26	80837.27	91478.04	111147.48
42949.62	51397.50	64983.87	81580.01	91585.91	111295.62
43069.82	51449.65	65144.89	81779.27	91714.25	111325.39
43160.22	51486.94	65794.59	81828.45	91854.96	111435.22
43219.43	51636.01	65925.07	81857.99	91947.59	111645.78
43299.72	51717.76	66035.40	81926.15	92068.87	111701.01
43482.77	51822.40	66103.62	81935.94	92144.16	111805.14
43836.02	51912.25	66152.38	81966.20	92197.49	111956.00
43931.86	52064.63	66185.75	81985.05	92454.76	112085.68
44115.32	52298.66	66247.74	81998.35	92881.92	112205.30
44164.49	52351.64	66531.97	82008.78	93105.42	112331.29
45151.19	60365.15	66817.49	82030.97	93285.46	112908.43
45183.68	60602.23	66943.18	82046.97	93358.28	
45296.37	60726.99	67041.12	82072.42	93401.56	
45892.43	60744.13	67087.44	82097.06	93523.43	
46140.26	60809.24	67121.49	82141.09	93781.22	
46589.33	60874.08	67163.51	82188.88	93861.71	
46612.02	60932.86	67256.49	82219.45	94099.78	
47364.44	60953.69	67414.94	82250.12	94236.33	
47411.11	61029.30	67736.99	82327.67	94353.04	
47578.11	61172.68	67868.30	82378.97	94449.32	
48064.75	61219.99	67951.31	82431.21	94586.64	
48149.41	61372.15	67999.65	82452.28	94615.91	
48573.18	61406.79	68014.11	82753.60	94780.53	
48902.90	61471.58	68080.19	82903.88	94847.97	
48970.62	61529.38	68234.54	83082.06	95083.19	
49014.25	61597.10	68530.68	83206.35	95440.34	
49122.65	61636.56	68686.90	83333.92	95981.96	
49214.12	61744.22	68773.90	83405.73	101545.27	
49305.34	61897.80	68803.22	83631.14	102155.27	
49321.13	62145.78	68900.51	85075.97	102489.14	
49521.86	62206.70	68973.24	85274.55	102804.24	

49546.99	62270.34	69509.96	85386.37	103033.81	
49741.79	63047.87	69654.16	85793.36	103415.28	
49818.05	63733.03	69711.79	85875.94	103542.69	
49907.44	63777.21	70203.08	86151.18	103950.83	
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50371.00	63794.02	71605.52	86576.92	104143.16	

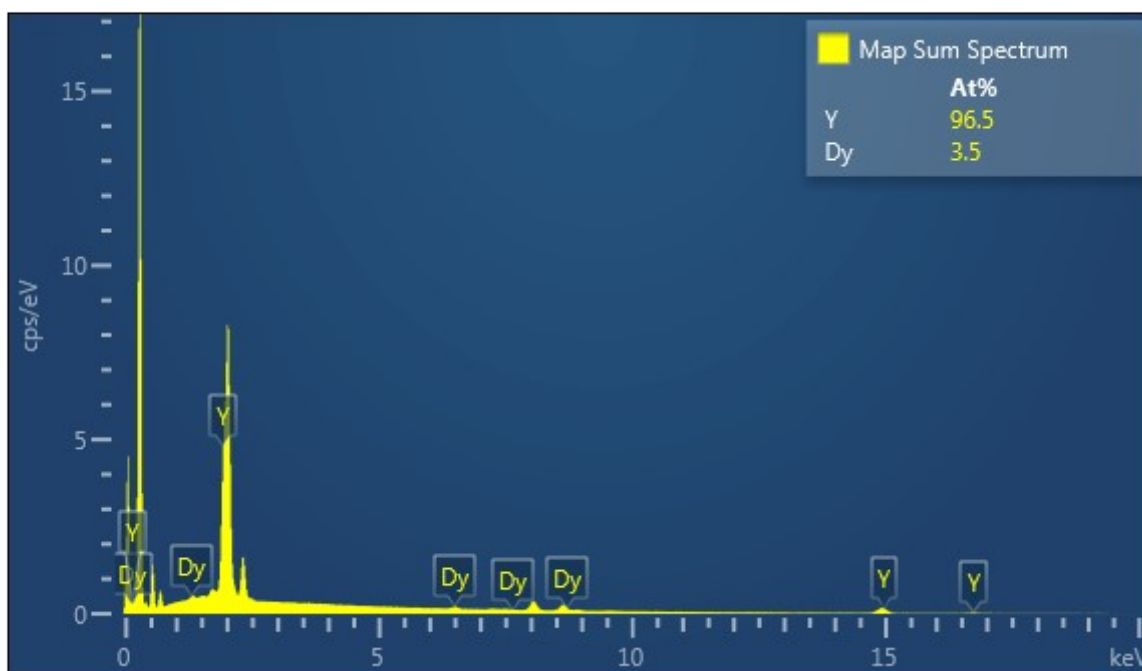


Figure S10. EDS spectrum of **1-Y(Dy)**. The spectrum was analysed by FESEM model JSM 7200F with FEG source.

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