Electronic supplementary information

Unravelling the Role of Spin-Vibrational Coupling in Designing High-Performance Pentagonal Bipyramidal Dy(III) Single Ion Magnets

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Table S1: The summary of the computed and experimental parameters that are relevant to the performance of PBP SIMs.[1]

Complex	Symmetry	CShM	FC/ZFC T_B (K)	T_H (K)	Sweep rate (T/min)	U_{eff} (cm^{-1})	U_{cal} (cm^{-1})	B_2^0	g_{zz} of KD1	Relaxation via KD	Ref.
$[Zn_2DyL_2(MeOH)]NO_3.3MeOH.H_2O$	D_{5h}	0.660	--	11	0.02	305	290	-1.72	19.87	2nd	2
$[L_2Ln(H_2O)_5][I]_3.L_2.H_2O$ (**5**)	D_{5h}	2.677	12	16	0.0018	453	478	-2.82	19.86	3rd	3
$[Dy(Cy_3PO)_2(H_2O)_5]Cl_3\cdot(Cy_3PO)\cdot H_2O\cdot EtOH$	D_{5h}	0.239	8	11	0.02	328	299	-1.80	19.86	3rd	4
$[Dy(Cy_3PO)_2(H_2O)_5]Br_3\cdot 2(Cy_3PO)\cdot 2H_2O\cdot 2EtOH$	D_{5h}	0.142	11	20	0.02	375	378	-1.85	19.88	4th	4
$[Dy(CyPh_2PO)_2(H_2O)_5]Br_3\cdot 2(CyPh_2PO)\cdot EtOH\cdot 3H_2O$	D_{5h}	0.174	10.5	19	0.02	353	206 207	--	19.88	2nd	5
$[Dy(H_2O)_5(HMPA)_2]Cl_3.HMPA.H_2O$	D_{5h}	0.154	7	6	0.004	320	410	-2.43	19.99	3rd	6
$[Dy(H_2O)_5(HMPA)_2]I_3.2HMPA$	D_{5h}	0.131	7	9	0.004	417	445	-2.58	19.97	3rd	6
$[Dy(OPCy_3)_2(H_2O)_5](CF_3SO_3)_3\cdot 2OPCy_3$	D_{5h}	0.639	8.5	2	0.018	391	509	-3.13	19.97	3rd	7
[Dy(bbpen)Cl]	D_{5h}	2.048	7.5	8	0.02	492	586	-4.00	19.88	3rd	8
[Dy(bbpen)Br] (**1**)	D_{5h}	2.327	9.5	14	0.02	712	721	-4.40	19.88	4th	8
$[Dy(bbpen\text{-}CH_3)Cl]$	D_{5h}	1.824	--	9	0.02	502	634	--	19.88	3rd	9

[Dy(bbpen-CH_3)Cl]	D_{5h}	2.111	12.1	15	0.2 0.02	808	820	--	19.88	4th	9
[Dy(bbpen-F)Cl]	D_{5h}	1.796	--	20	-- 0.02	582	611	--	19.98	3rd	10
[Dy(bbpen-F)Br]	D_{5h}	2.142	--	30	-- 0.02	800	770	--	19.99	4th	10
[Dy(Bpen)$(Cl)_3$]	D_{5h}	1.271	--	--	--	16	37	--	17.29	2nd	11
[Dy(bmbpen-F)Br]	D_{5h}	2.077	--	36	0.002	833	904	--	19.99	5th	12
[Dy(bmbpen-F)Cl]	D_{5h}	1.759	--	26	0.002	733	841	--	19.98	6th	12
[Dy(Bpen)Cl$(OPhCl_2NO_2)_2$]	D_{5h}	1.904	--	--	--	60	307	--	19.83	2nd	11
[Dy(Bpen)$(OPhCl_2NO2)_3$]	D_{5h}	1.780	--	--	--	24	218	--	19.77	2nd	11
[Dy(Bpen)$(OPhNO_2)_3$]	D_{5h}	1.355	--	--	--	19	234	--	19.77	2nd	11
[Dy(O^tBu)$_2(py)_5$][BPh_4]	D_{5h}	0.801	14	4	0.0012	1262	1183	--	19.89	5th	13
[Dy$(L)_2(py)_5$][BPh_4]	D_{5h}	0.759- 0.787	23	22	0.2 0.0010	1130	1086- 1109	-6.26- -6.45	19.89	4th	14
[Dy(^tBuO)Cl$(THF)_5$][BPh_4]·2THF	C_{5v}	--	--	--	--	660	562	--	19.88	3rd	15
[$DyCl_2(THF)_5$][BPh_4]	D_{5h}	0.196	--	--	--	54	42	--	14.83	1st	16
[Dy$(OCMe_3)$Cl$(THF)_5$][BPh_4]	D_{5h}	0.293	7.0	11.0	0.0015	636-652	562	--	19.88	3rd	16
[Dy$(OSiMe_3)$Cl$(THF)_5$][BPh_4]	D_{5h}	0.352	4.5	9.0	0.0015	557	561	--	19.88	3rd	16
[Dy$(OCMe_3)$Br$(THF)_5$][BPh_4] (**2**)	D_{5h}	0.386	4.5	9.0	0.0015	569	558	--	19.88	3rd	16
[Dy$(OSiMe_3)$Br$(THF)_5$]	D_{5h}	0.483	4.5	9.0	0.0015	509	473	--	19.88	3rd	16

$[BPh_4]$ (**3**)											
$[Dy(OPh)Cl(THF)_5][BPh_4]$	D_{5h}	0.456	6.8	9.0	0.0015	512	406	--	19.88	3rd	16
$[Na(THF)_5][Dy(OPh)_2(THF)_5][BPh_4]_2$	D_{5h}	0.556	12.0	18.0	0.0015	924	853	--	19.88	4th	16
$[Dy(OPh)_2(py)_5][BPh_4]$	D_{5h}	0.700	13.0	16.0	0.0015	832-905	826	--	19.88	4th	16
$[Dy(OSiMe_3)_2(py)_5][BPh_4]$	D_{5h}	0.683	15.0	22.0	0.0015	1109	1101	--	19.89	4th	16
$[Dy(OCMe_3)_2(4\text{-}Mepy)_5][BPh_4]$	D_{5h}	0.618	16.0	23.0	0.0015	1041	1072	--	19.89	4th	16
$[Dy(tfpz)Cl(THF)_5][BPh_4]$	C_{5v}	--	--	--	--	--	74	-0.62	19.44	2nd	17
$[Dy(Mepz)Cl(THF)_5][BPh_4]$	C_{5v}	--	--	--	--	143	150	-0.80	19.87	2nd	17
$[Dy(Iprpz)Cl(THF)_5][BPh_4]$	C_{5v}	--	--	--	--	218	186	-1.01	19.88	3rd	17
$[Dy(Me_2pz)Cl(THF)_5][BPh_4]$	C_{5v}	--	--	--	--	250	216	-1.21	19.88	3rd	17
$[Dy(Ipr_2pz)Cl(THF)_5][BPh_4]$	C_{5v}	--	--	--	--	188	180	-0.97	19.87	3rd	17
$[Dy(pz)Cl(THF)_5][BPh_4]$	C_{5v}	--	--	--	--	327	334	-1.91	19.91	4th	17
$[Dy(tfpz)_2(THF)_5][BPh_4]$	C_{5v}	--	--	--	--	264	222	-0.91	19.79	2nd	17
$[Dy(pz)_2(THF)_5][BPh_4]$	C_{5v}	--	4	5	0.0012	362	318	-1.97	19.82	3rd	17
$[Dy(pz)_2(py)_5][BPh_4]\cdot 2py$	C_{5v}	--	3.5	5	0.0012	327	288	-1.28	19.81	3rd	17
$[Dy(pz)_2(NS)_5][BPh_4]$	C_{5v}	--	3	5	0.0012	309	257	-1.37	19.78	3rd	17
$(Et_3NH)[(H_2L)DyCl_2]$	D_{5h}	1.210	--	--	--	49	147	-2.80	19.74	2nd	18, 19
$[(L)Dy(Cy_3PO)Cl]$	D_{5h}	1.446	--	--	--	145	158	-2.18	19.74	2nd	19

[(L)Dy(Ph_3PO)Cl]	D_{5h}	1.505	--	--	--	168	155	-2.32	19.73	2nd	19
[Dy(L^{N5})(Ph_3SiO)$_2$](BPh_4).CH_2Cl_2 (**4**)	D_{5h}	1.293-1.681	5	14	0.01	771	723-731	(-4.96) -(-5.20)	19.98	3rd	20
CShM = Continuous Shape Measures, T_H = The temperature below which opening of magnetic hysteresis is observed, U_{eff} = Experimental blocking barrier,U_{cal} =Calculated blocking barrier, $B_2^0 =$ axial crystal field parameter											

Table S2. A comparison of selected structural parameters (bond lengths are shown in Å and bond angles are shown in degree) between optimized and X-ray crystal structures of **1**.

Structural parameter	Crystal structure	DFT optimized geometry	
		1	**1-CH$_3$**
Dy-O1	2.163	2.163	2.141
Dy-O2	2.163	2.163	2.141
Dy-N1 (Py)	2.594	2.618	2.676
Dy-N2 (Py)	2.594	2.618	2.676
Dy-N3 (Ph)	2.578	2.666	2.948
Dy-N4 (Ph)	2.578	2.666	2.948
Dy-Br	2.851	2.787	2.811
O1-Dy-O2	155.8	154.7	162.9

Table S3. The computed energies (cm^{-1}) along with g tensor of eight $^6H_{15/2}$ KDs of optimized geometry of **1**. The values in parenthesis correspond to the calculations with the X-ray crystal structure.

Complex **1**			
Energy	g_x	g_y	g_z
0.0 (0)	0.001 (0.001)	0.001 (0.001)	19.985 (19.881)
387.3 (394)	0.074 (0.062)	0.095 (0.080)	17.035 (16.985)
624.4 (627)	1.082 (0.868)	1.716 (1.559)	13.585 (13.510)
732.4 (721)	7.813 (4.742)	6.825 (6.038)	5.444 (9.820)
800.4 (780)	0.350	1.523	12.624
815.6 (795)	0.090	0.405	17.454
836.5 (802)	0.201	0.597	12.863
876.5 (876)	0.110	0.290	16.921
Complex **1**$_{Caspt2}$			
0.0	0.000	0.001	19.986
375.7	0.078	0.096	17.045
601.8	1.063	1.679	13.609
701.2	7.303	6.561	5.590
737.6	0.358	0.909	18.335
755.2	0.196	1.794	13.747
786.5	0.065	0.195	11.240
818.2	0.311	1.179	15.076

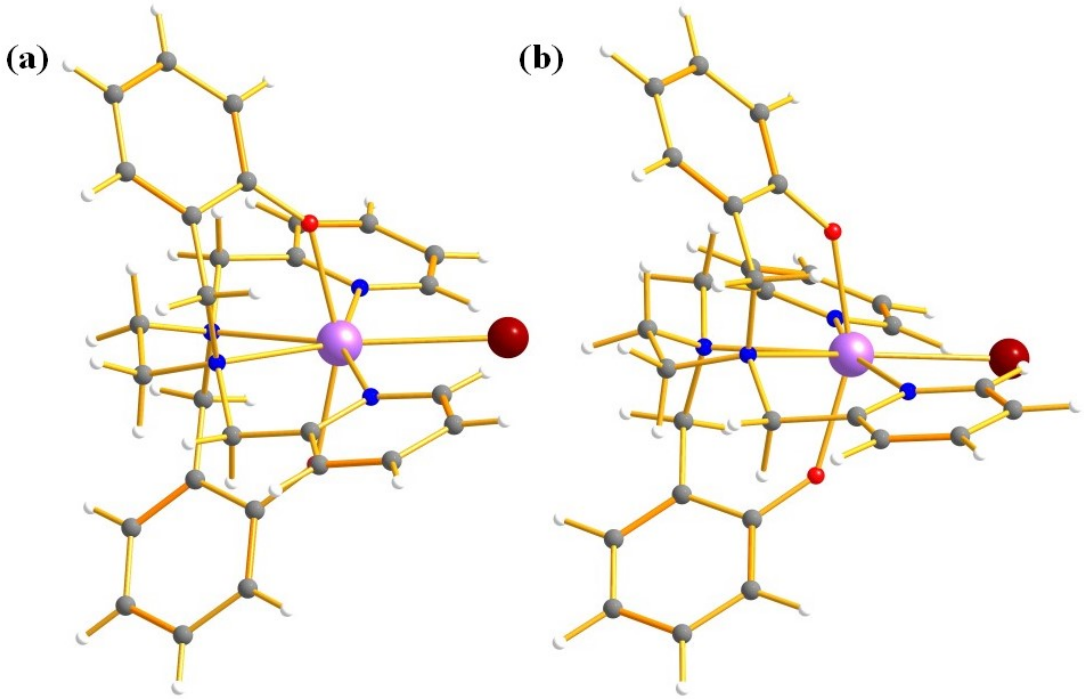


Figure S1. (a) The crystal structure and (b) DFT optimized structure of **1**. Colour code: Dy-blue violet, Br-brown, O-red, N-blue, C-grey and H-white.

Table S4. The computed crystal field (CF) parameters of X-ray geometry of **1**, optimized geometry of **1**, **1-F**, **1-pCH$_3$** and **1-CH$_3$**. Here, the crystal field (CF) parameters have been computed according to Stevens Hamiltonian:

$$H_{CF} = \sum_{k=2,4,6} \sum_{q=-k}^{q=+k} B_k^q \tilde{O}_k^q$$

where B_k^q is the CF parameter and $\tilde{O}_k^q$ is the Stevens operator.

k	q		B_k^q				
		1 (X-ray)	**1** (opt)	**1-F**	**1-pCH$_3$**	**1-pCH$_3$F**	**1-CH$_3$**
2	-2	5.39E-03	1.08E-03	-2.67E-03	-4.52E-02	9.63E-03	-6.42E-03
	-1	5.13E-03	4.19E-03	-3.28E-02	-2.46E-02	2.72E-02	-1.18E-02
	0	-4.30E+00	-4.57E+00	-4.92E+00	-4.83E+00	-5.05E+00	-7.28E+00
	1	-3.85E-01	-3.68E-01	2.20E-01	1.16E-01	-1.43E-01	-3.22E+00
	2	9.68E-01	8.13E-01	1.30E+00	7.27E-01	1.19E+00	-6.75E-01
4	-4	-5.92E-05	-1.01E-04	7.10E-05	2.69E-04	9.98E-05	-2.57E-04
	-3	-2.95E-04	-1.38E-04	-1.12E-04	-3.30E-04	-8.34E-05	5.30E-05
	-2	-7.57E-05	-7.57E-05	2.59E-05	-1.79E-04	1.18E-04	-5.21E-05
	-1	7.86E-05	4.82E-05	-1.98E-04	-3.90E-05	-5.28E-05	4.33E-05
	0	-1.03E-02	-9.60E-03	-9.56E-03	-9.41E-03	-9.54E-03	-9.85E-03
	1	4.99E-03	4.76E-03	-4.20E-03	-3.33E-03	3.82E-03	2.18E-02
	2	4.08E-03	5.41E-03	5.14E-03	5.38E-03	4.69E-03	5.07E-03
	3	-2.18E-02	-1.73E-02	1.93E-02	1.83E-02	-1.87E-02	-2.68E-03
	4	-3.36E-03	-9.94E-03	-8.56E-03	-9.06E-03	-8.87E-03	-1.49E-02
6	-6	7.01E-06	3.92E-06	-2.06E-06	-2.85E-06	-1.24E-05	4.48E-06
	-5	2.12E-06	6.79E-07	1.40E-06	2.02E-08	-6.96E-06	7.78E-06
	-4	-5.57E-07	-7.42E-07	7.65E-07	9.59E-07	-2.35E-07	-1.23E-06
	-3	-2.22E-06	-1.23E-06	-1.63E-06	6.07E-06	4.17E-06	7.52E-07
	-2	-2.20E-06	-1.91E-06	1.31E-06	7.51E-07	-1.19E-06	-2.31E-06
	-1	-1.09E-07	-1.84E-08	-1.08E-07	3.24E-06	1.55E-06	-4.25E-07
	0	2.98E-06	3.50E-06	5.53E-06	3.82E-06	4.85E-06	3.16E-05
	1	-5.20E-05	-4.76E-05	5.77E-05	5.21E-05	-5.95E-05	-1.13E-05
	2	-9.08E-05	-9.00E-05	-9.21E-05	-8.83E-05	-8.94E-05	-5.08E-05
	3	-1.49E-04	-1.38E-04	1.44E-04	1.27E-04	-1.45E-04	-1.06E-05
	4	8.23E-07	-3.24E-05	-2.77E-05	-2.63E-05	-2.71E-05	-7.12E-05
	5	8.37E-05	2.78E-05	-1.54E-05	-4.63E-05	7.87E-05	3.90E-04
	6	2.61E-04	2.67E-04	2.46E-04	2.48E-04	2.37E-04	1.82E-04

Table S5. The vibrational mode numbers (ω), energy (cm^{-1}), oscilator strength (km mol^{-1}), population (at 100 K), maximum displacement (Q_k) and coupling strength (S_j in cm^{-1}) of the first 35 normal modes of **1**.

Mode number (j)	Energy	oscilator strength	population	Q_k	S_j
1	16.9	2.625	0.126	0.54	0.019
2	35.8	0.014	0.096	0.42	0.081
3	45.4	0.311	0.083	0.26	0.162

4	49.7	0.355	0.078	0.36	0.118
5	50.7	0.296	0.077	0.36	0.034
6	62.8	0.492	0.065	0.32	0.164
7	71.4	0.641	0.057	0.32	0.074
8	78.8	0.474	0.052	0.30	0.125
9	80.2	0.199	0.051	0.32	0.154
10	97.8	0.081	0.039	0.26	0.176
11	99.5	0.219	0.038	0.24	0.082
12	113.0	8.621	0.032	0.24	0.223
13	113.9	0.050	0.031	0.16	0.105
14	136.7	15.157	0.022	0.18	0.069
15	139.6	0.726	0.021	0.24	0.082
16	147.2	0.967	0.019	0.24	0.320
17	148.4	22.879	0.019	0.14	0.037
18	167.9	3.828	0.014	0.22	0.079
19	175.3	36.193	0.013	0.12	0.104
20	192.4	8.225	0.010	0.18	0.108
21	192.4	7.868	0.010	0.20	0.129
22	204.2	0.101	0.008	0.18	0.162
23	211.2	4.490	0.006	0.18	0.160
24	224.8	2.647	0.004	0.18	0.058
25	259.2	0.042	0.003	0.22	0.066
26	275.7	47.365	0.003	0.16	0.293
27	282.3	0.240	0.002	0.16	0.140
28	297.0	12.548	0.002	0.18	0.074
29	303.4	0.395	0.002	0.16	0.062
30	322.2	3.330	0.001	0.18	0.186
31	337.0	4.762	0.001	0.20	0.047
32	338.4	33.902	0.001	0.20	0.149
33	347.8	6.546	0.001	0.16	0.108
34	352.1	1.497	0.001	0.18	0.012
35	363.7	1.010	0.008	0.42	0.234
Total			1.00		

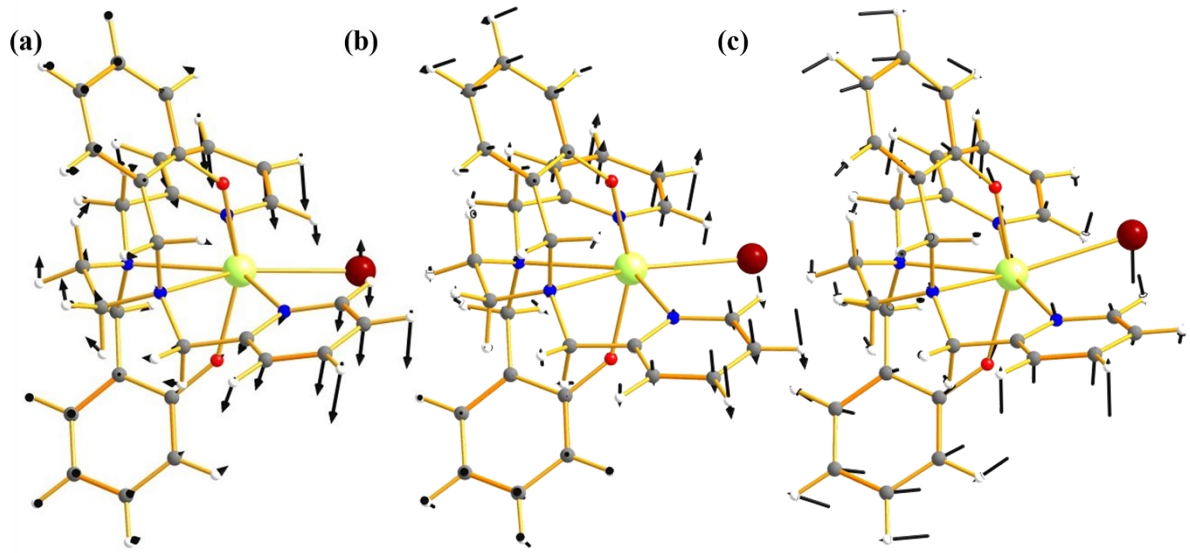


Figure S2. The molecular vibrations of **1** corresponds to (a) $^{\omega_1}$ (b) $^{\omega_2}$ and (c) $^{\omega_3}$ vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

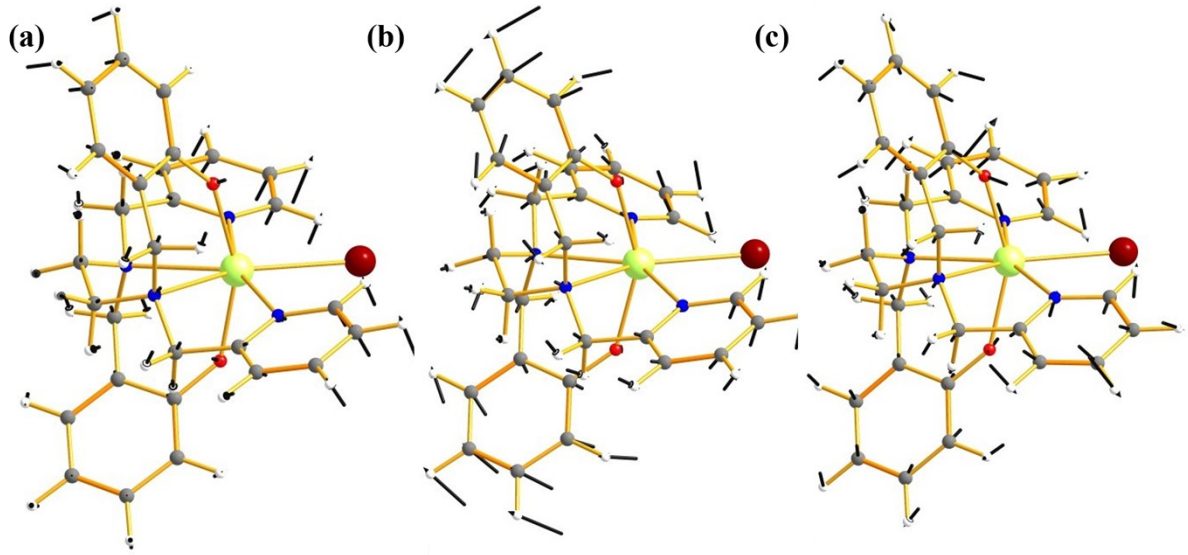


Figure S3. The molecular vibrations of **1** corresponds to (a) $^{\omega_4}$ (b) $^{\omega_5}$ and (c) $^{\omega_6}$ vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

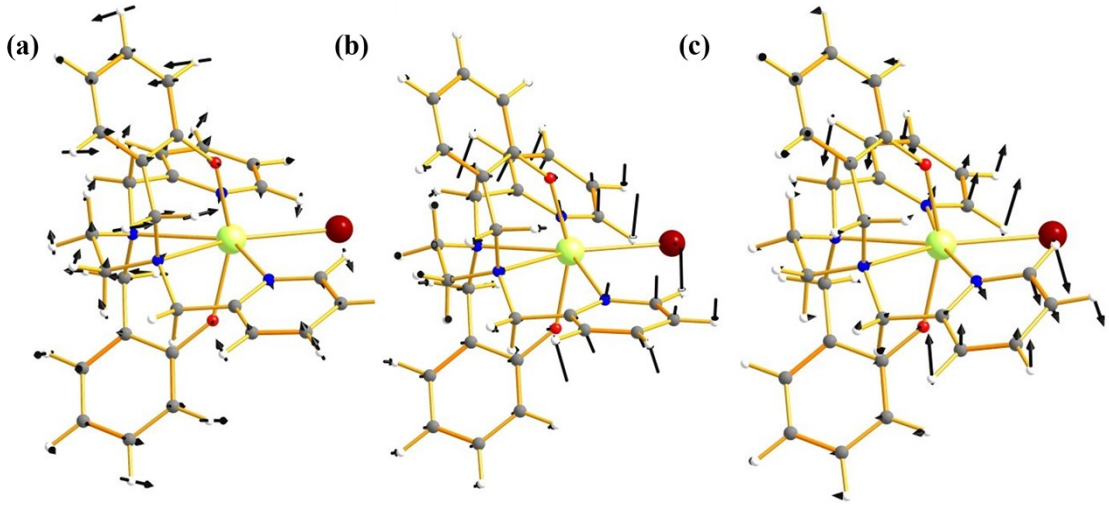
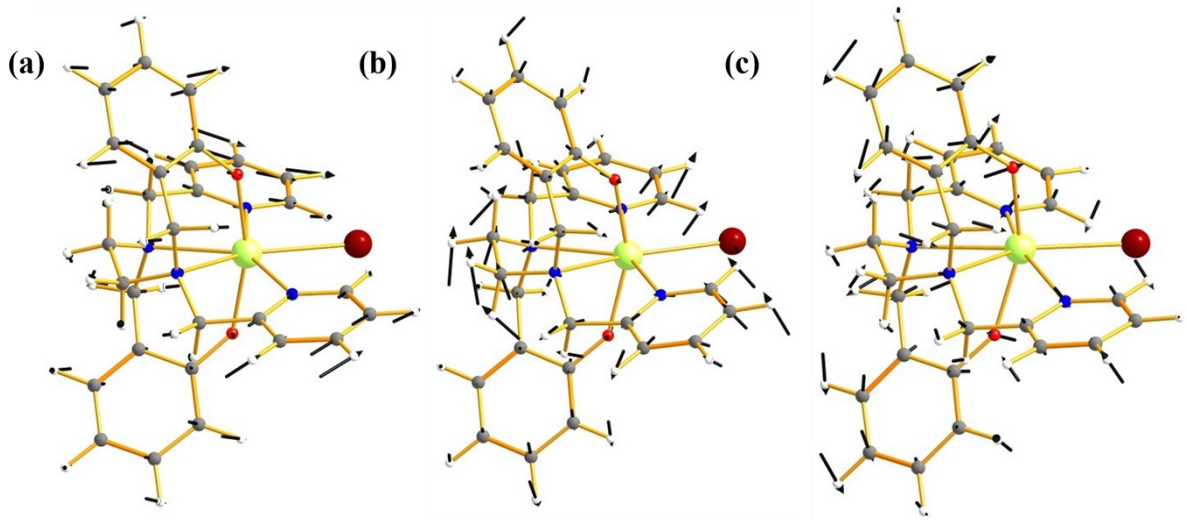


Figure S4. The molecular vibrations of **1** corresponds to (a) $^{\omega_7}$ (b) $^{\omega_8}$ and (c) $^{\omega_9}$ vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.



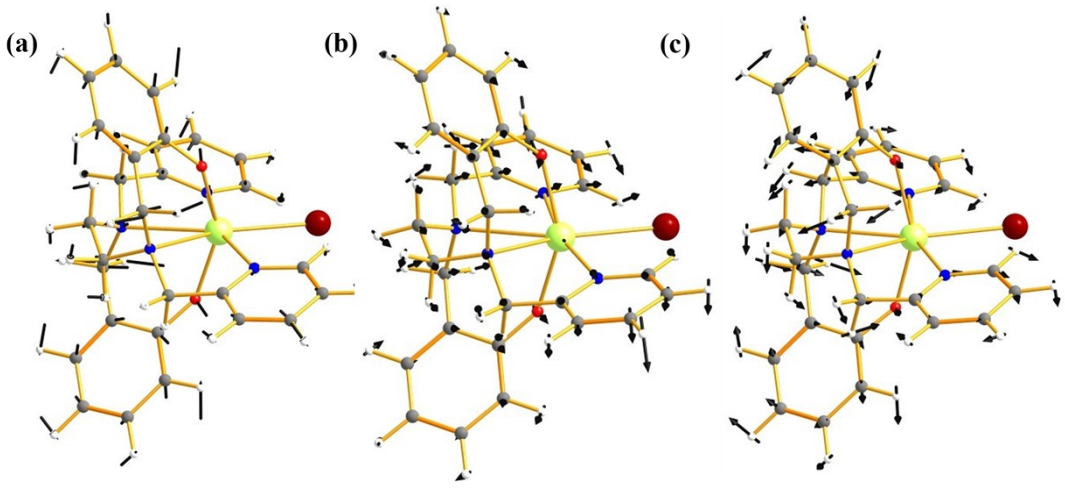


Figure S5. The molecular vibrations of **1** corresponds to (a) ω_{10} (b) ω_{11} and (c) ω_{12} vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

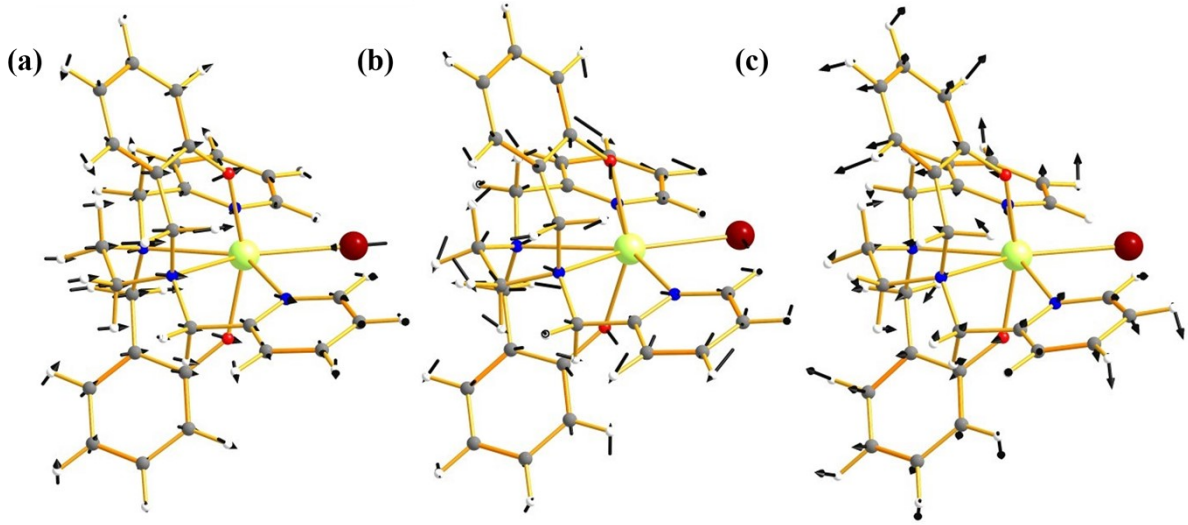


Figure S6. The molecular vibrations of **1** corresponds to (a) ω_{13} (b) ω_{14} and (c) ω_{15} vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

Figure S7. The molecular vibrations of **1** corresponds to (a) ω_{16} (b) ω_{17} and (c) ω_{18} vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

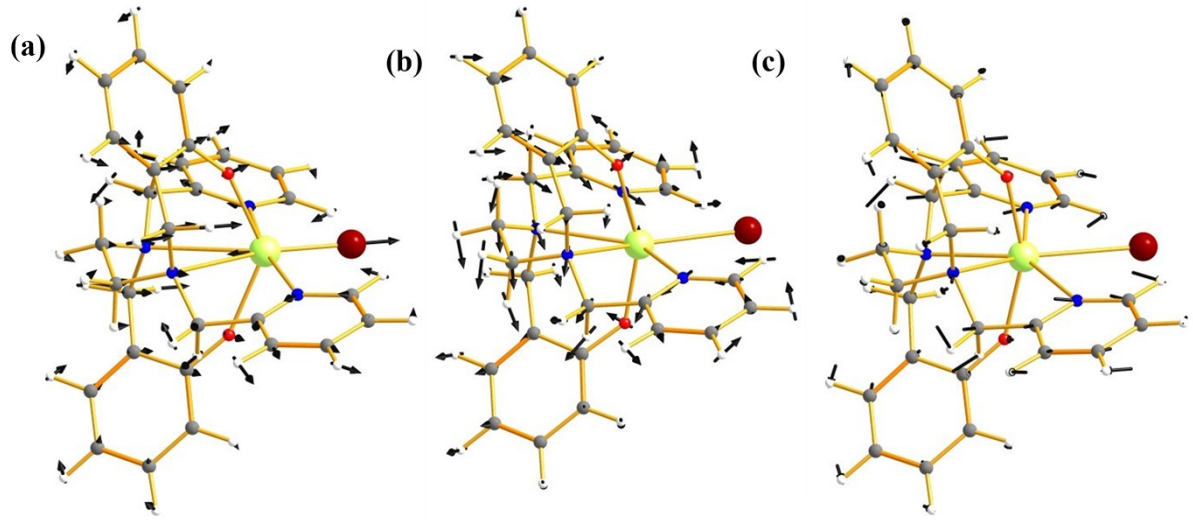


Figure S8. The molecular vibrations of **1** corresponds to (a) ω_{19} (b) ω_{20} and (c) ω_{21} vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

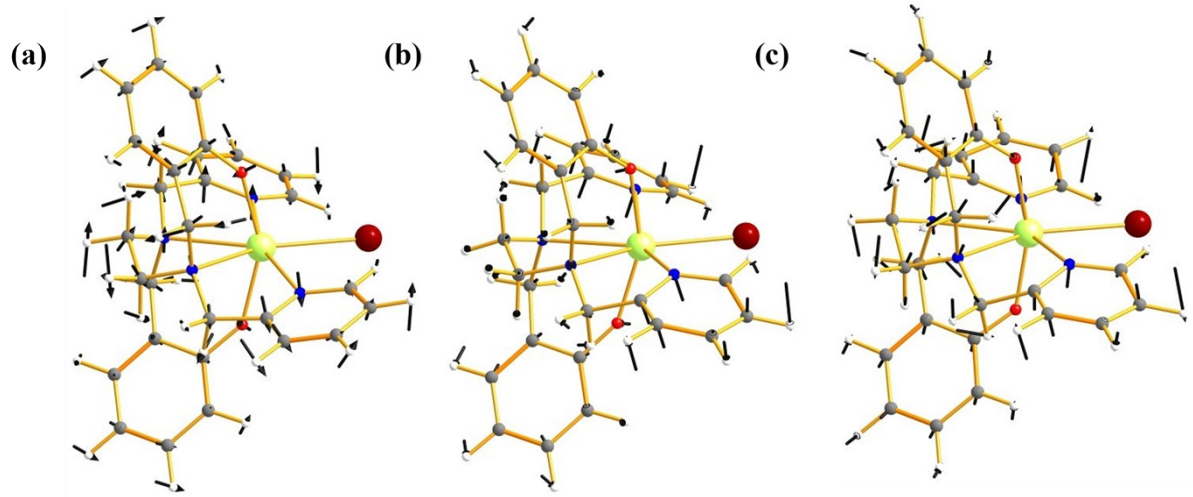


Figure S9. The molecular vibrations of **1** corresponds to (a) ω_{22} (b) ω_{23} and (c) ω_{24} vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

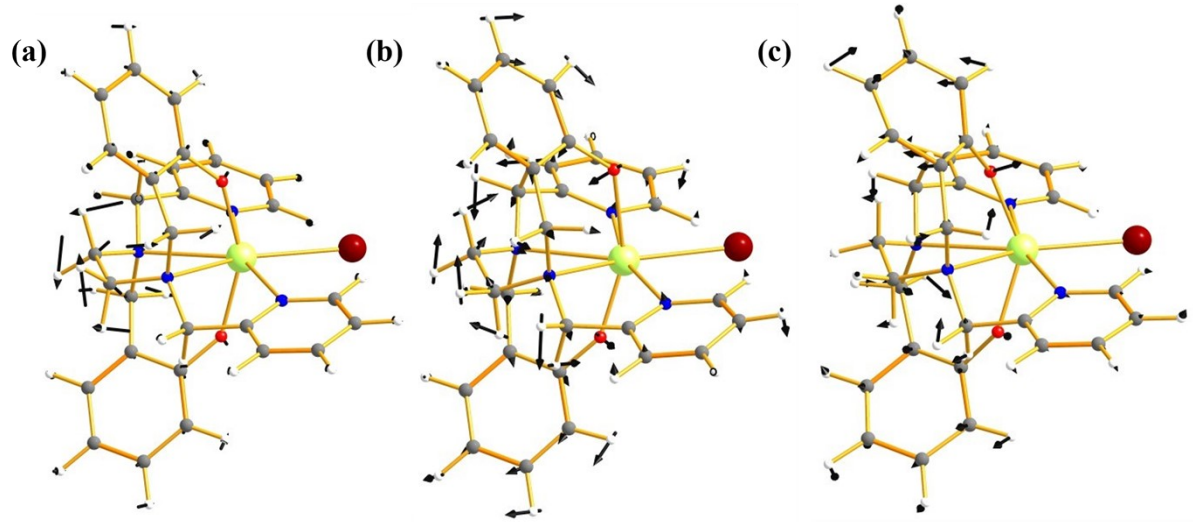


Figure S10. The molecular vibrations of **1** corresponds to (a) ω_{25} (b) ω_{26} and (c) ω_{27} vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

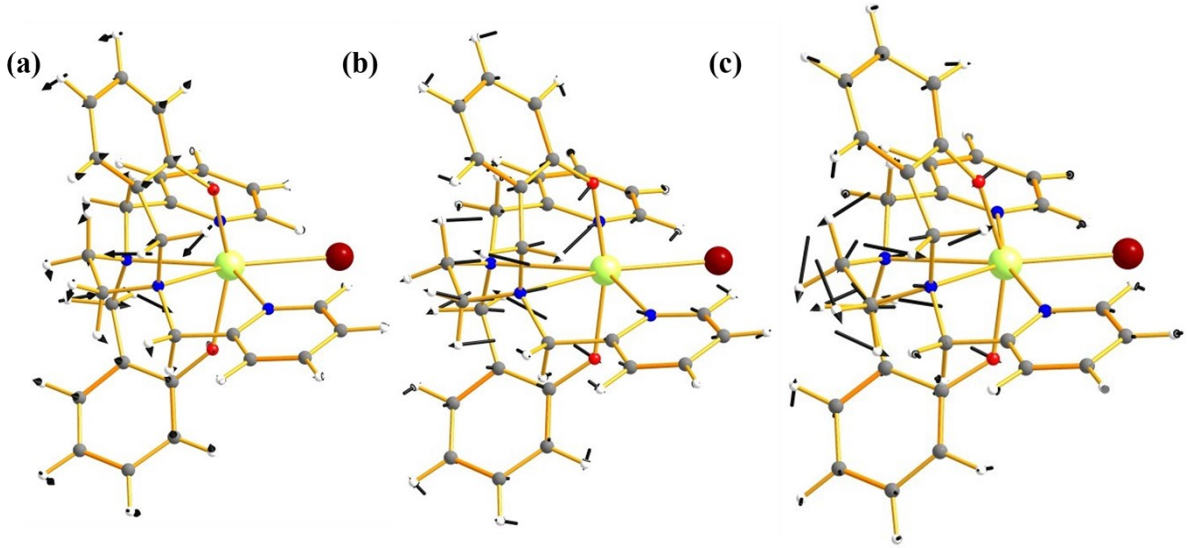


Figure S11. The molecular vibrations of **1** corresponds to (a) ω_{28} (b) ω_{29} and (c) ω_{30} vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

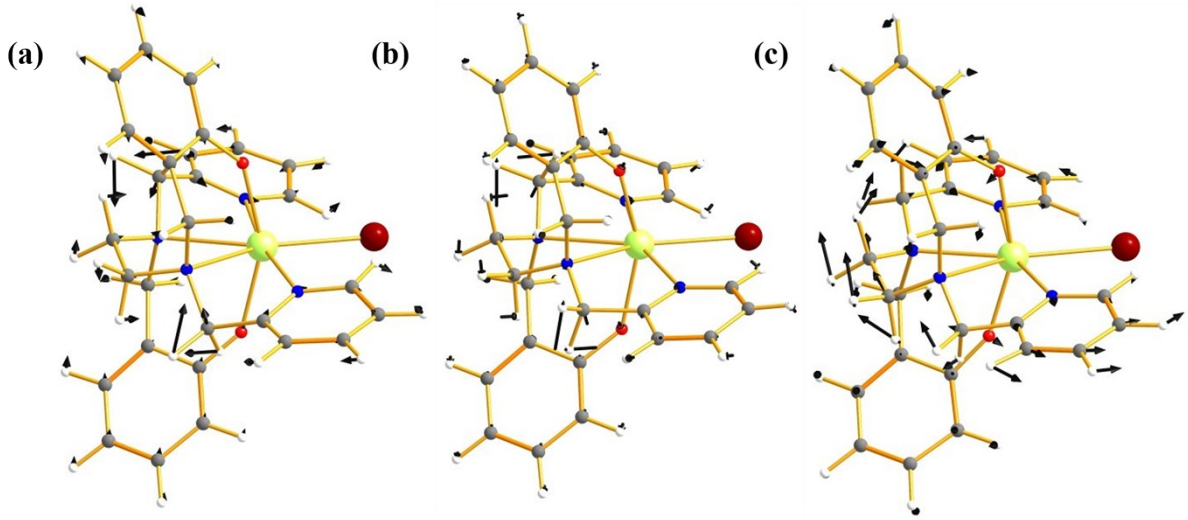


Figure S12. The molecular vibrations of **1** corresponds to (a) ω_{31} (b) ω_{32} and (c) ω_{33} vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

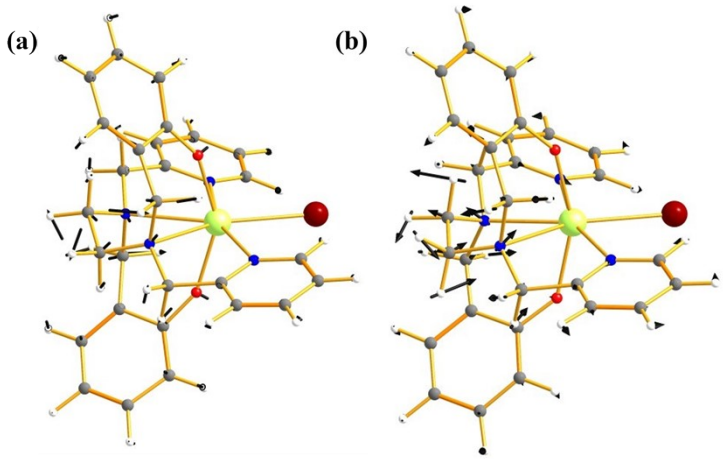
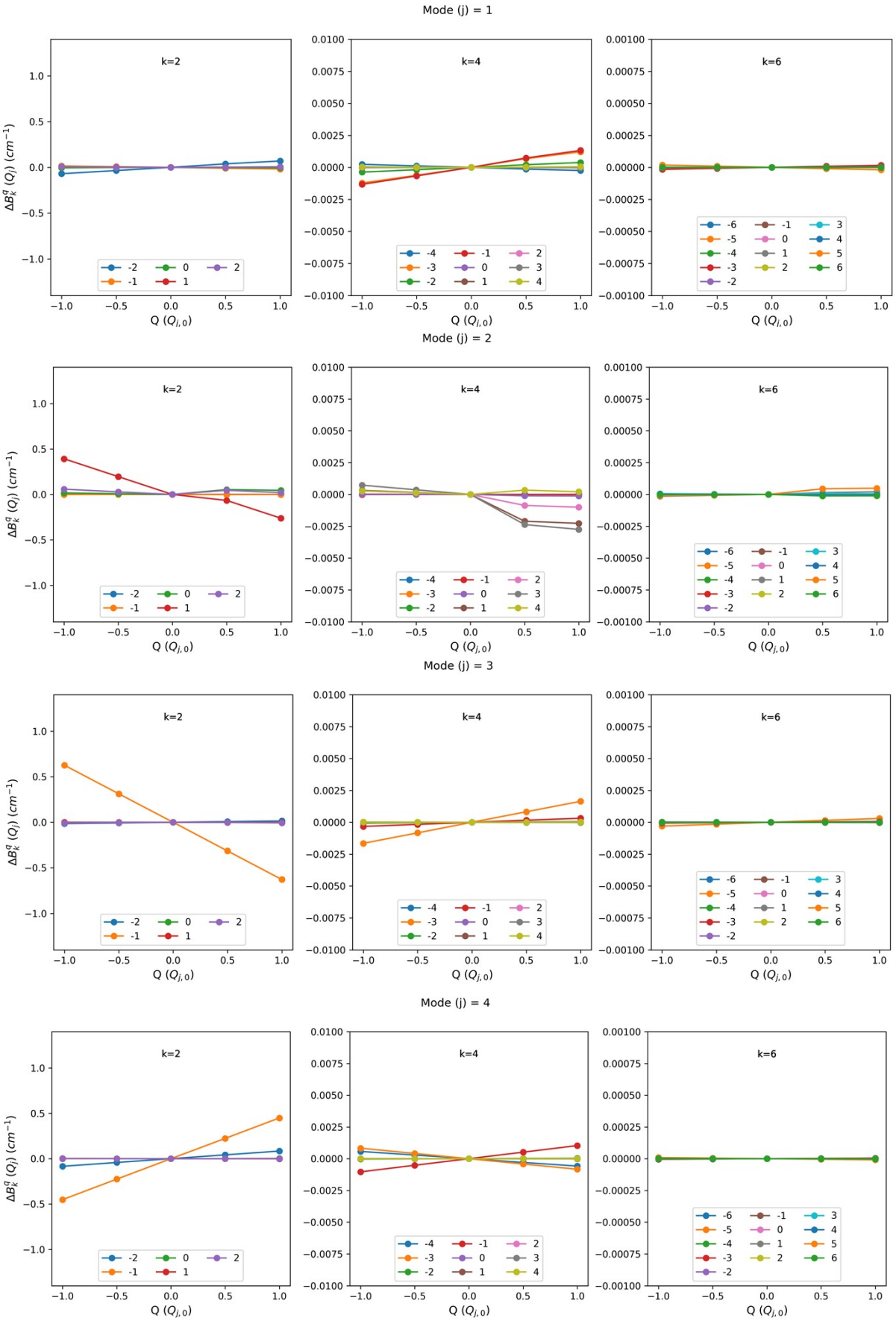
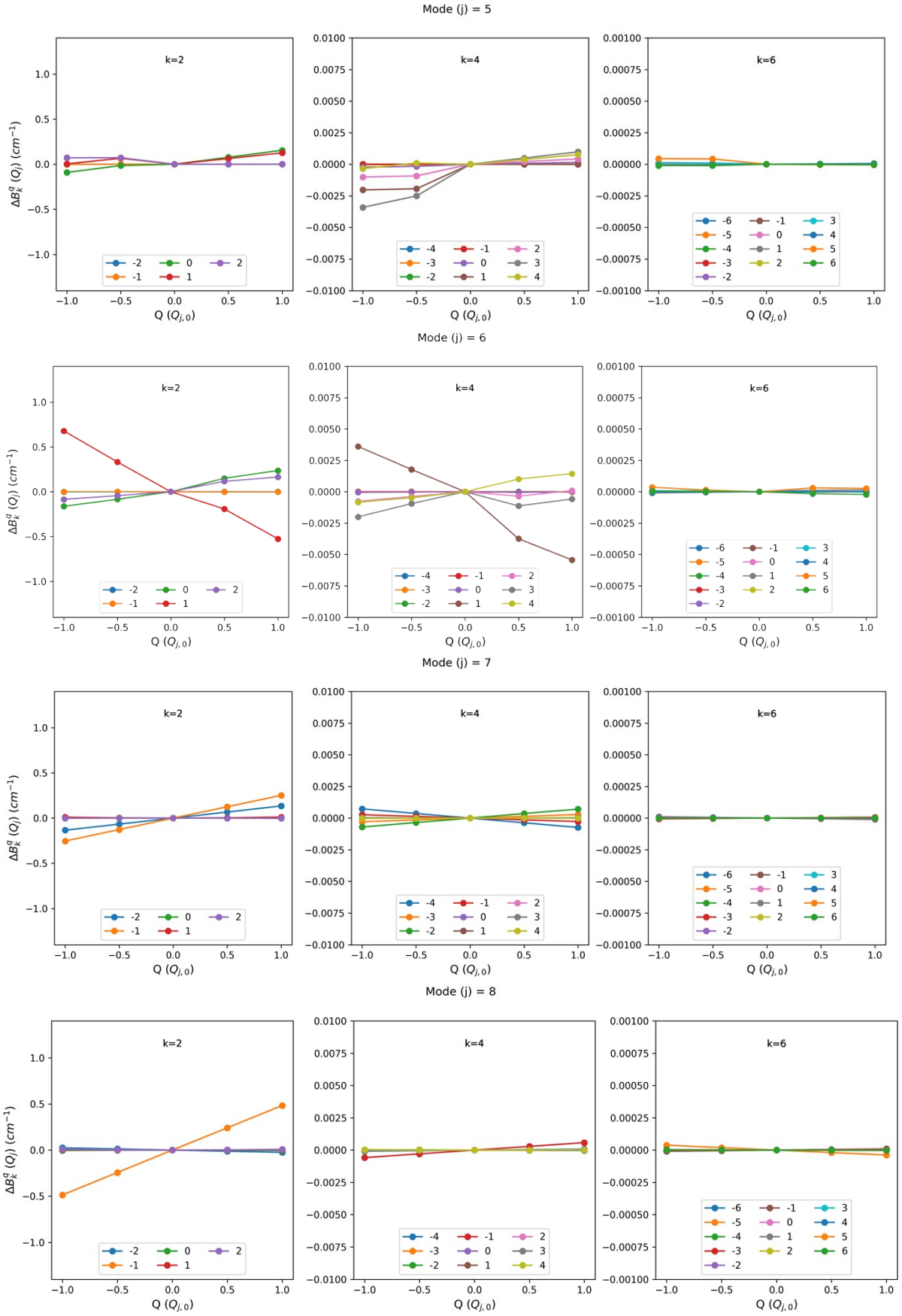
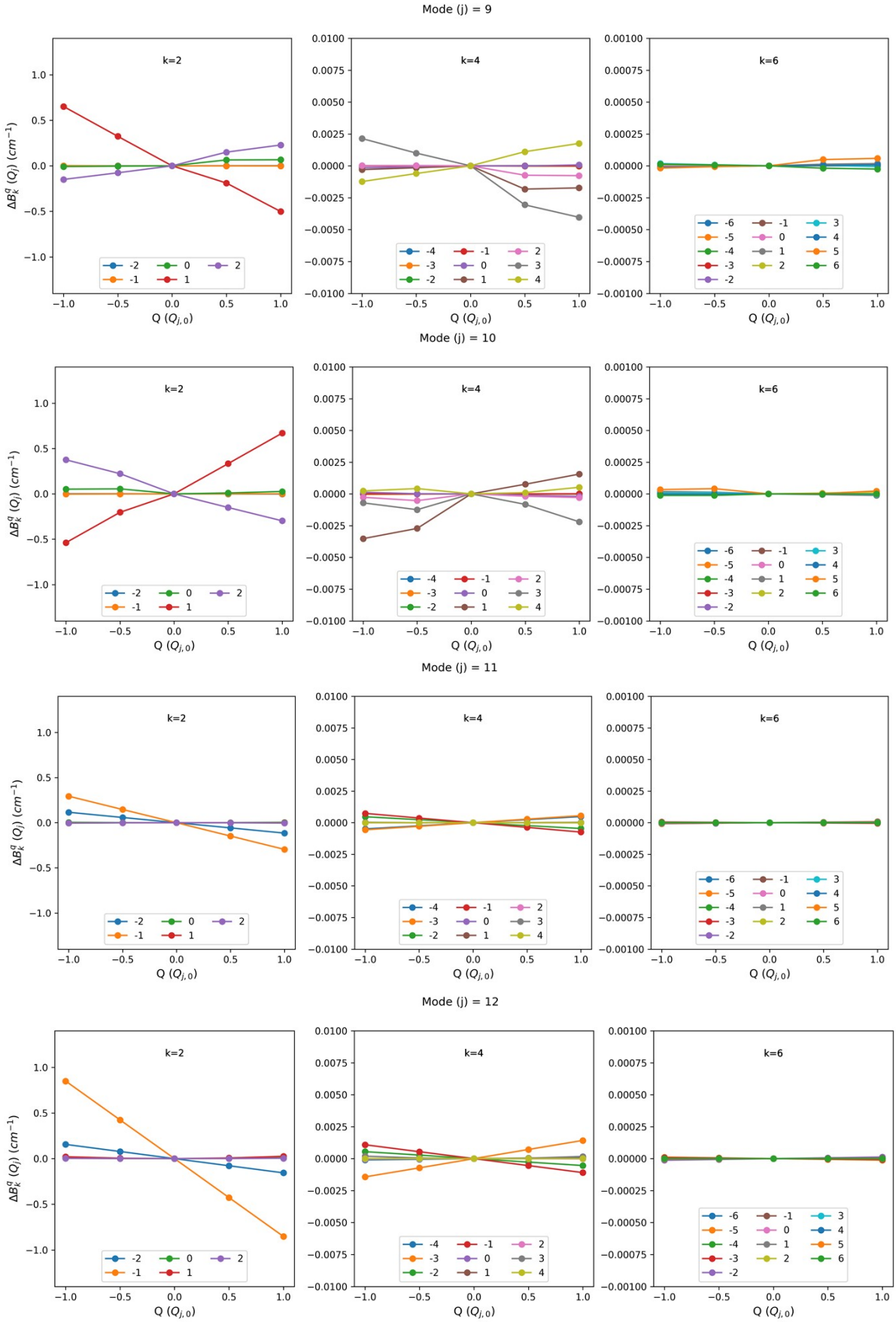


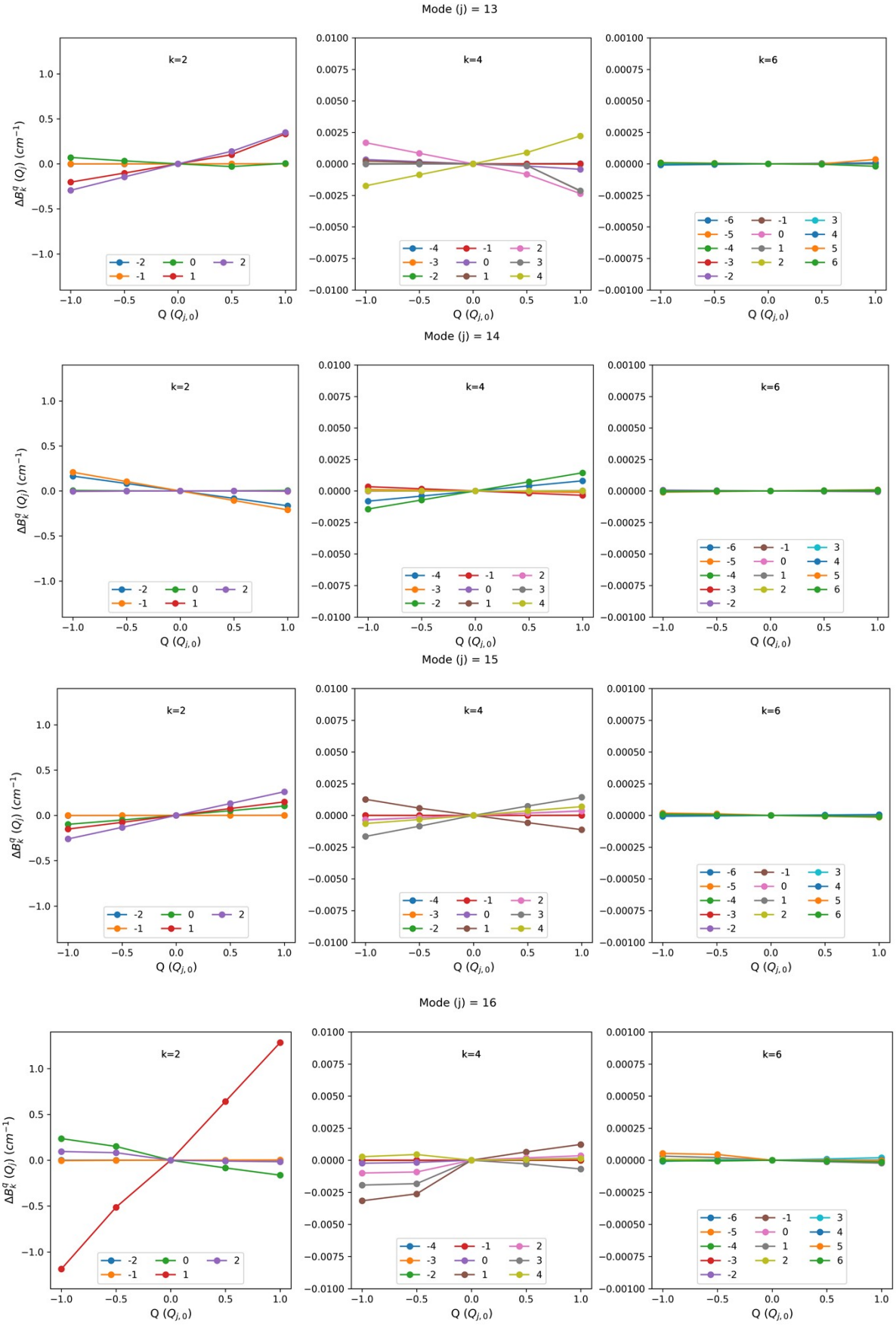
Figure S13. The molecular vibrations of **1** corresponds to (a) ω_{34} and (b) ω_{35} vibrational modes. The black arrow



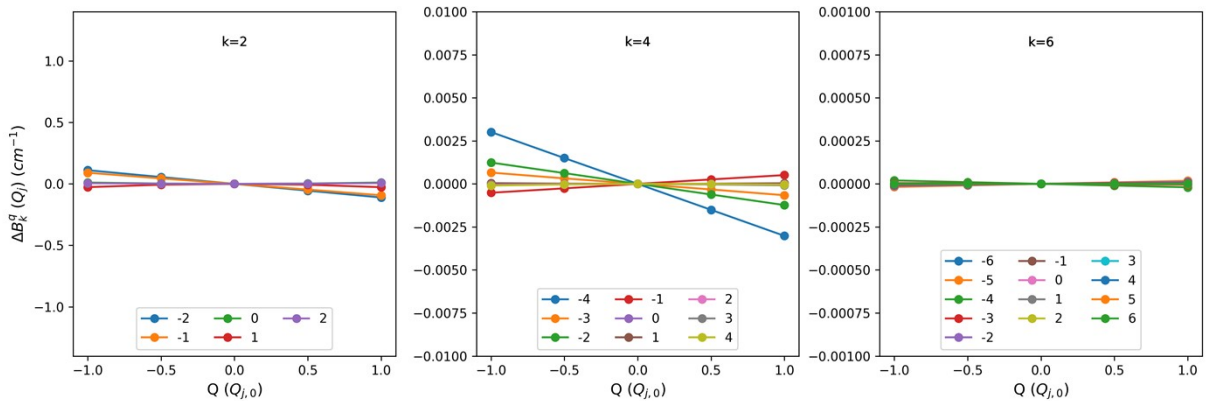
corresponds to the scaled displacement vectors. See Figure S1 for colour code.



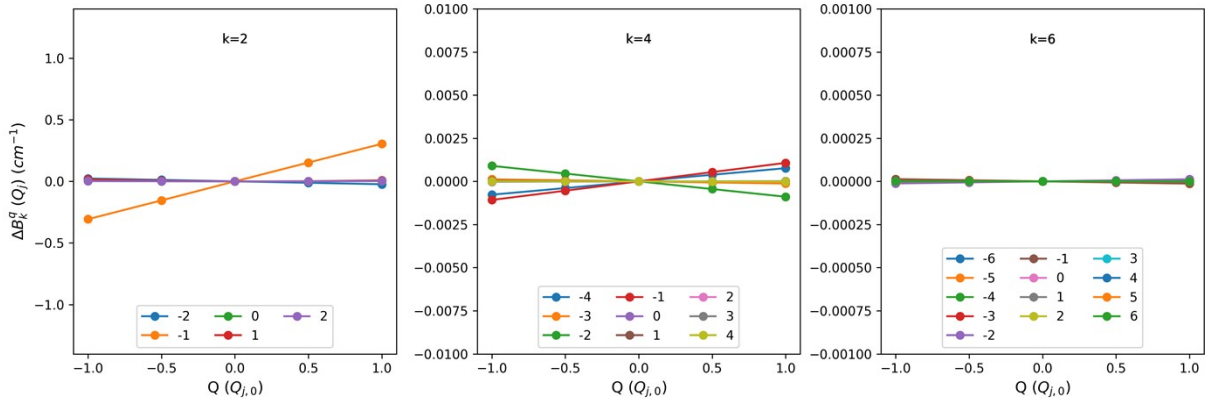

Mode (j) = 9
Mode (j) = 10
Mode (j) = 11
Mode (j) = 12
k=2
k=4
k=6
$\Delta B_k^q(Q_j)\ (cm^{-1})$
Q $(Q_{j,0})$


Mode (j) = 13
Mode (j) = 14
Mode (j) = 15
Mode (j) = 16
k=2
k=4
k=6
$\Delta B_k^q\ (Q_j)\ (cm^{-1})$
Q $(Q_{j,0})$

Mode (j) = 17



Mode (j) = 18



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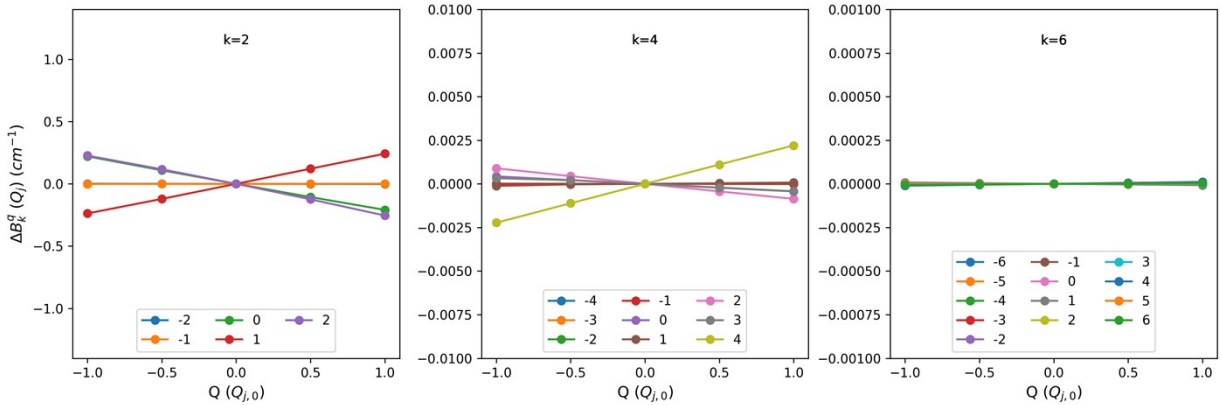

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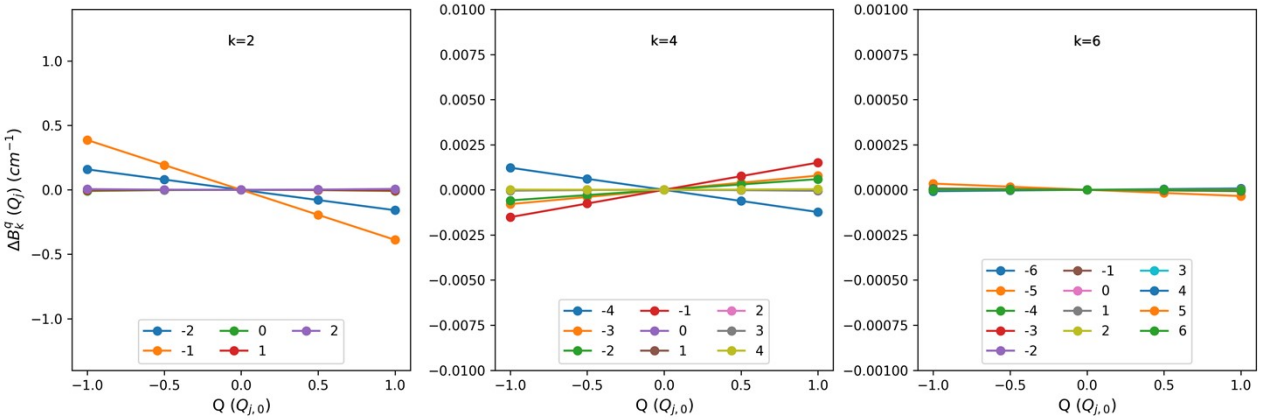

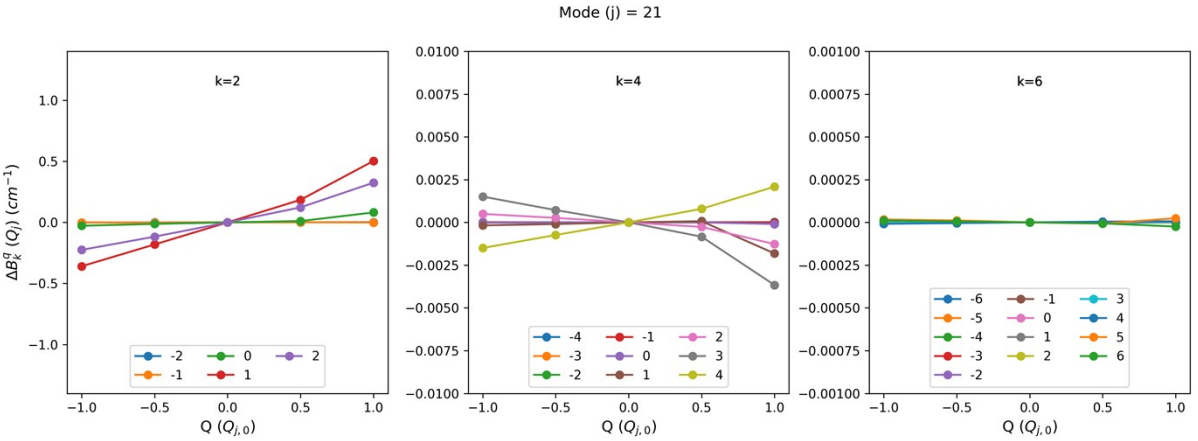
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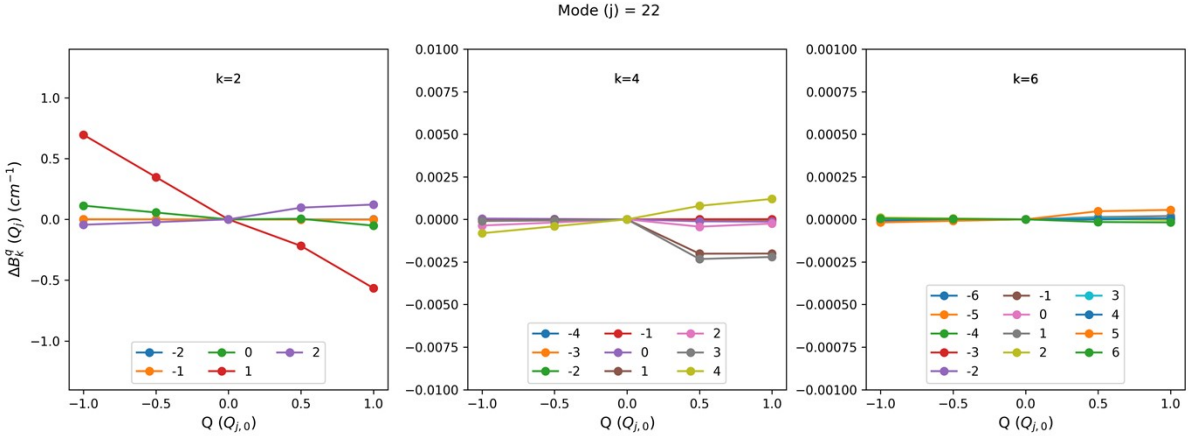
Q ($Q_{j,0}$)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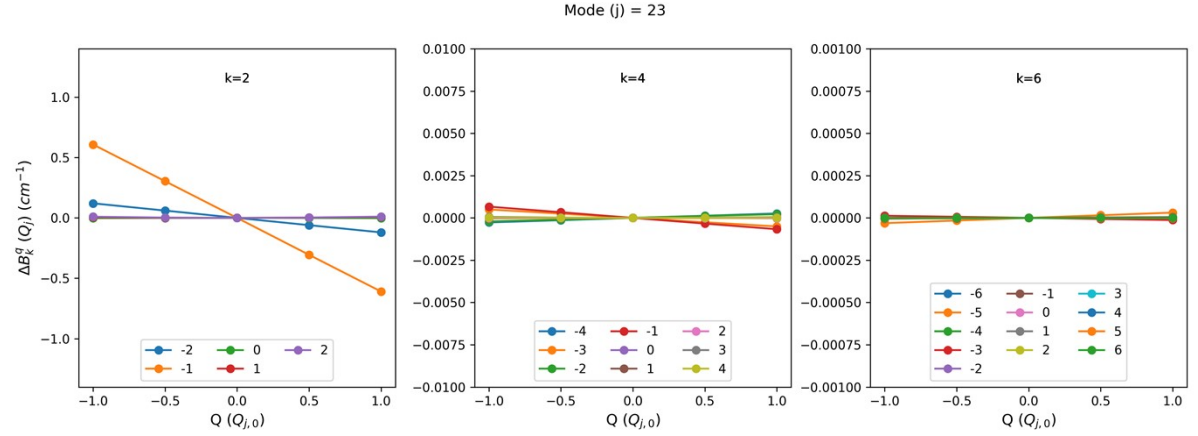
k=2
k=4
k=6
$\Delta B_k^q\ (Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)


Mode (j) = 23
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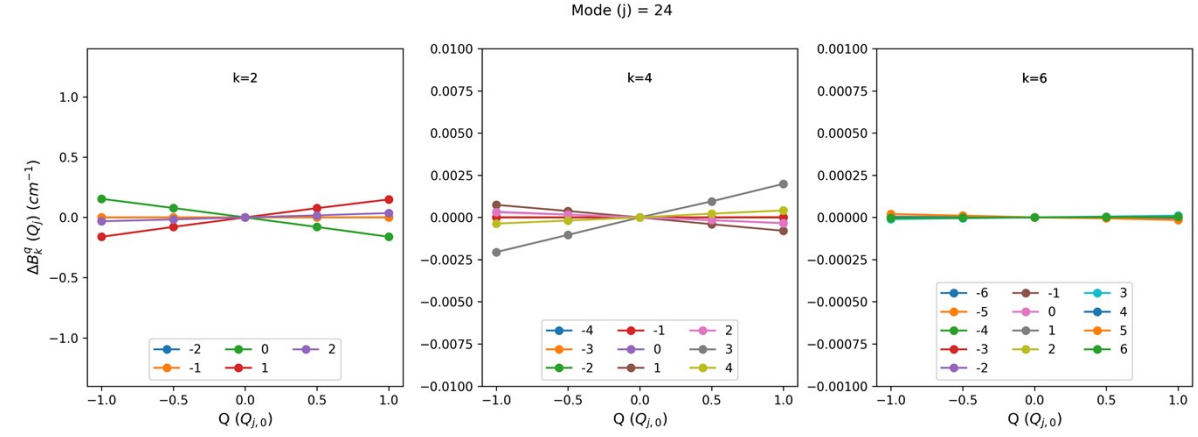
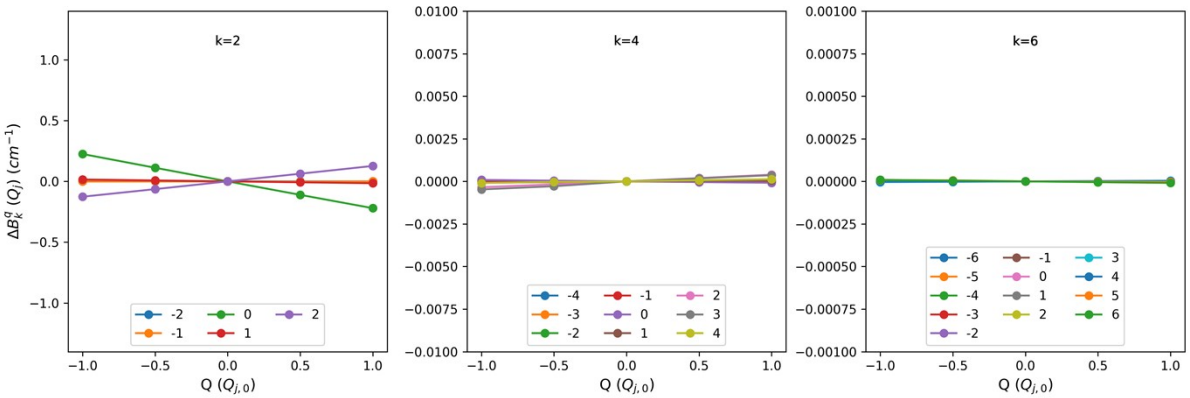
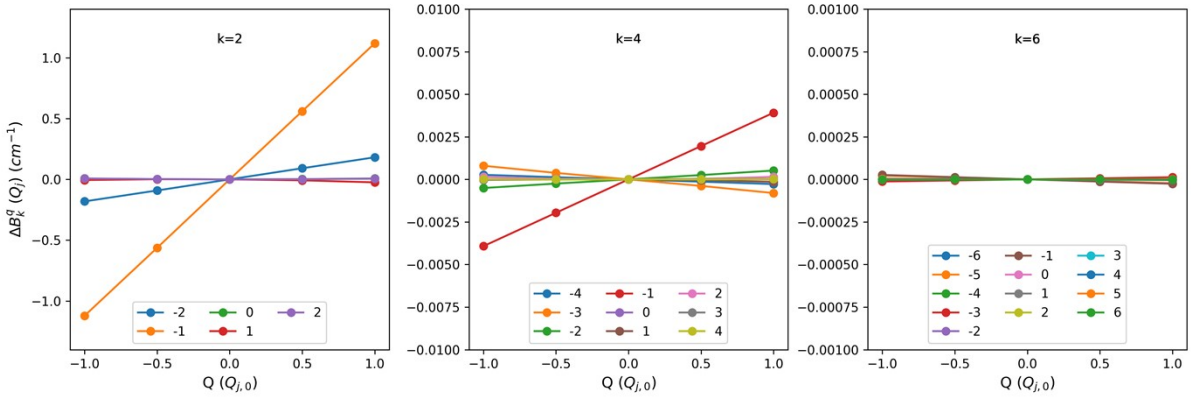
k=4
k=6
$\Delta B_k^q\ (Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)


Mode (j) = 24
k=2
k=4
k=6
$\Delta B_k^q\ (Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)

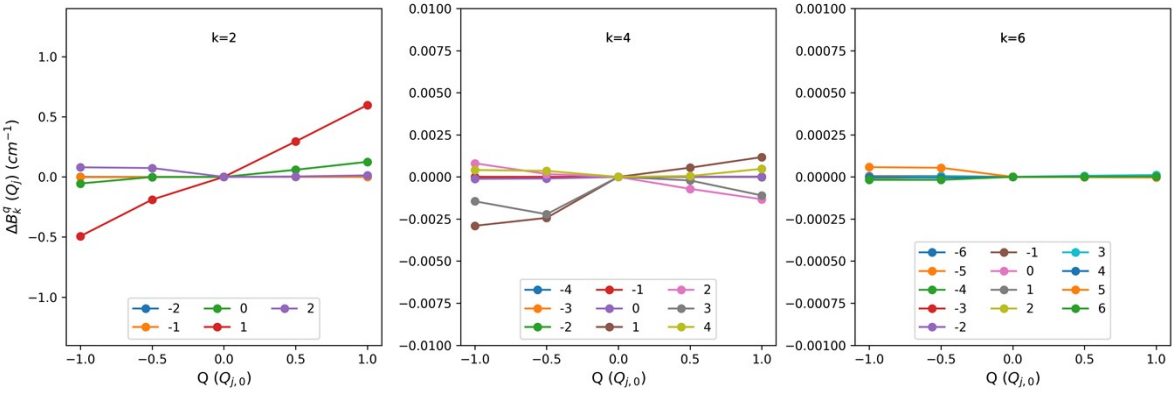
Mode (j) = 25



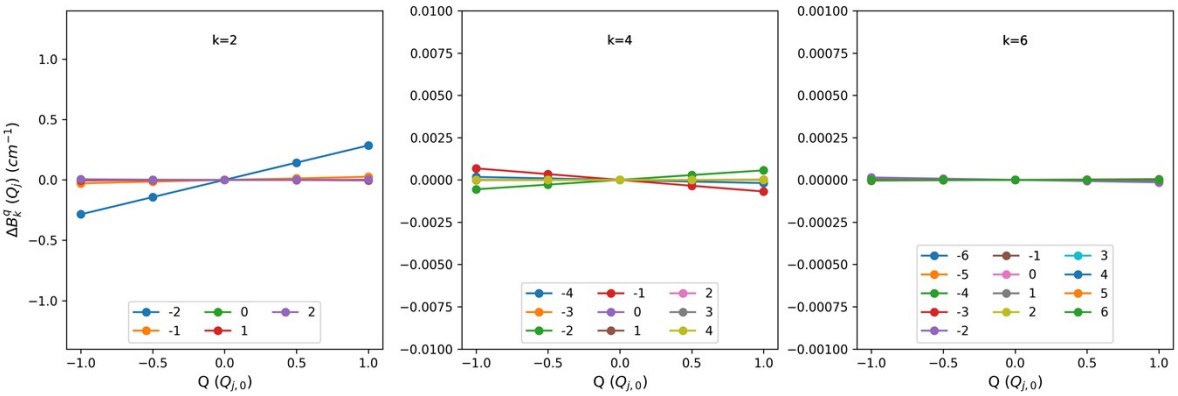
Mode (j) = 26

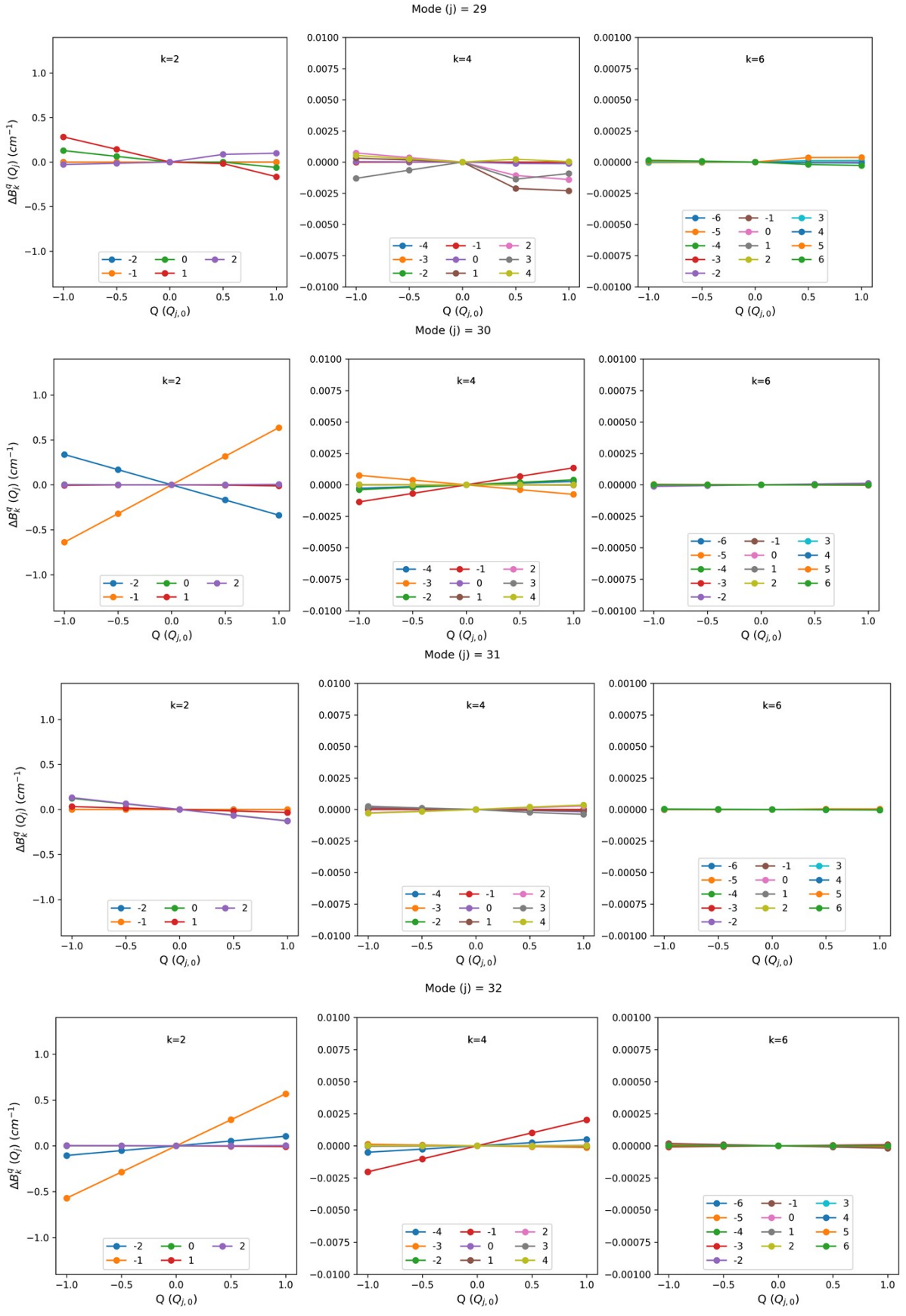


Mode (j) = 27



Mode (j) = 28




Mode (j) = 29
k=2
k=4
k=6
Mode (j) = 30
k=2
k=4
k=6
Mode (j) = 31
k=2
k=4
k=6
Mode (j) = 32
k=2
k=4
k=6
$\Delta B_k^q(Q_j)\ (cm^{-1})$
Q $(Q_{j,0})$

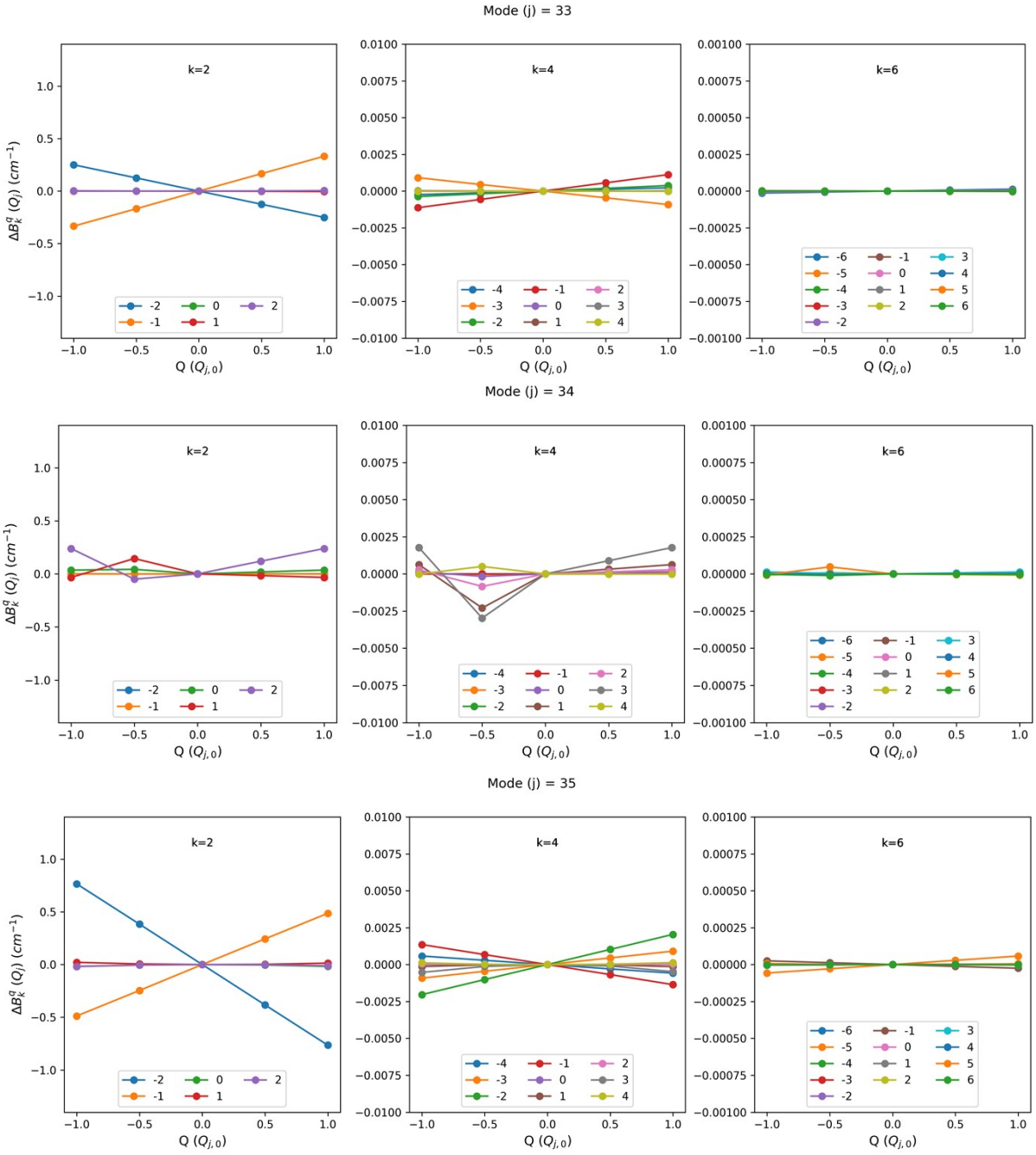


Figure S14. The variation of CFPs as a function of displacement for vibrational modes 1-35 of complex **1**.

Table S6. The computed energies (cm^{-1}) along with g tensor of eight $^6H_{15/2}$ KDs of the optimized geometry of **1-F**.

Energy	g_x	g_y	g_z	Angle of g_{zz} between ground and higher excited KDs (°)
0.0	0.001	0.001	19.972	
395.9	0.060	0.079	17.007	0.986
645.2	0.983	1.557	13.602	1.101
763.3	7.948	6.838	5.271	104.617
840.4	0.396	1.879	10.537	80.041
878.3	0.259	0.563	14.504	94.719
888.9	0.103	0.134	16.878	74.652
939.3	0.054	0.101	18.630	105.384

Table S7. The vibrational mode numbers (j), energy (cm^{-1}), oscilator strength (km mol^{-1}), population (at 100 K) of the first 35 normal modes of **1-F**, **1-pCH$_3$, 1-pCH$_3$F** and **1-CH$_3$**.

	1-F		**1-pCH$_3$**		**1-pCH$_3$F**		**1-CH$_3$**	
Mode number (j)	Energy	oscilator strength	Energy	oscilator strength	Energy	oscilator strength	Energy	oscilator strength
1	14.7	1.449	11.9	0.216	15.5	1.430	19.7	2.267
2	29.2	0.031	18.9	2.560	26.2	0.041	38.5	0.062
3	43.5	0.341	30.6	0.025	35.4	0.061	46.5	1.172
4	46.3	0.451	41.0	0.287	38.8	0.153	53.3	0.051
5	47.7	0.159	44.3	0.464	39.5	0.057	58.0	0.583
6	59.0	0.480	45.1	0.071	44.5	0.489	65.6	0.856
7	69.7	0.218	59.1	0.481	54.9	0.465	69.1	0.107
8	73.9	0.086	62.4	0.251	60.6	0.248	71.6	1.888
9	74.1	1.638	70.0	0.731	68.6	1.110	77.2	1.123
10	82.0	0.022	77.7	0.121	71.5	0.661	90.9	0.001
11	93.3	0.487	79.1	0.249	73.1	0.657	93.8	0.453
12	109.1	4.018	92.7	0.642	78.0	0.022	106.1	0.084
13	110.4	0.030	95.3	1.890	89.4	0.359	106.3	34.035
14	119.8	10.225	103.3	3.379	99.6	5.110	118.1	0.091
15	129.5	0.492	110.6	0.110	105.2	0.316	124.3	1.989
16	144.7	30.115	129.7	0.164	117.1	3.642	132.1	0.591
17	146.2	0.304	134.7	18.921	123.4	0.057	132.9	2.449
18	159.2	0.035	139.7	1.976	134.8	1.209	140.2	0.176
19	166.2	0.626	145.5	5.621	142.6	24.699	144.7	7.360
20	169.2	6.357	152.7	17.994	147.7	11.710	150.8	9.135
21	174.4	10.068	173.1	29.692	159.8	0.396	153.8	0.801
22	180.4	31.544	180.5	2.943	160.7	0.873	170.0	30.313
23	186.8	5.150	185.1	0.744	171.6	12.784	218.8	7.152
24	212.2	3.213	187.7	13.034	172.9	5.388	220.1	0.269
25	256.9	0.008	202.0	11.430	180.0	16.561	222.8	3.028
26	267.6	44.424	209.5	2.354	186.6	14.555	223.3	0.169
27	278.7	0.570	227.2	2.380	222.8	3.738	226.9	14.970
28	293.1	0.256	231.0	0.844	224.3	4.695	235.7	2.605
29	296.6	10.549	259.3	2.696	254.5	22.436	266.2	3.036
30	309.6	17.005	266.1	32.267	257.9	5.236	266.3	11.328
31	310.4	0.200	284.7	0.829	266.8	0.427	282.4	1.679
32	317.3	10.805	292.4	11.114	288.1	19.822	284.9	0.940
33	327.3	6.094	319.4	0.156	306.8	0.776	289.2	0.616
34	348.3	12.884	330.1	37.721	310.4	20.930	292.9	1.950
35	348.4	1.265	332.8	2.484	321.1	1.582	294.3	35.593

Table S8. The computed energies (cm^{-1}) along with g tensor of eight $^6H_{15/2}$ KDs of the optimized geometry of **1-pCH$_3$**.

Energy	g_x	g_y	g_z	Angle of g_{zz} between ground and higher excited KDs (°)
0.0	0.000	0.001	20.002	
393.7	0.054	0.066	17.075	0.984
641.4	0.729	1.055	13.923	1.215
764.2	8.159	6.540	4.861	84.765
831.7	1.783	3.045	11.863	79.573
855.1	0.122	0.367	17.404	85.429
873.5	0.038	0.193	13.110	95.825
902.3	0.007	0.318	16.403	74.008

Table S9. The computed energies (cm^{-1}) along with g tensor of eight $^6H_{15/2}$ KDs of the optimized geometry of **1-pCH$_3$F**.

Energy	g_x	g_y	g_z	Angle of g_{zz} between ground and higher excited KDs (°)
0.0	0.001	0.001	19.970	
402.9	0.052	0.066	17.011	0.001
658.1	0.830	1.263	13.754	1.305
782.3	7.551	7.358	5.010	98.394
857.5	1.038	2.430	10.575	79.558
899.9	0.101	0.185	14.450	94.462
907.9	0.092	0.352	16.787	105.274
951.2	0.036	0.114	18.449	74.774

Table S10. The CASSCF+RASSI-SO/SINGLE_ANISO computed relative energies of the eight-low lying KDs along with g tensors and deviations from the principal magnetization axis with respect to the first KD for complex **1-CH$_3$**.

Energy (cm^{-1})	g_x	g_y	g_z	Angle of g_{zz} between ground and higher excited KDs (°)
0.0	0.000	0.000	19.996	
443.1	0.005	0.006	17.094	3.759
799.5	0.154	0.154	14.389	10.414
1039.5	0.215	0.334	12.812	34.867
1126.6	0.400	0.765	12.933	33.014
1198.7	8.654	8.052	3.147	18.069
1274.1	1.702	3.386	10.484	73.381
1315.8	0.341	0.992	14.769	66.294

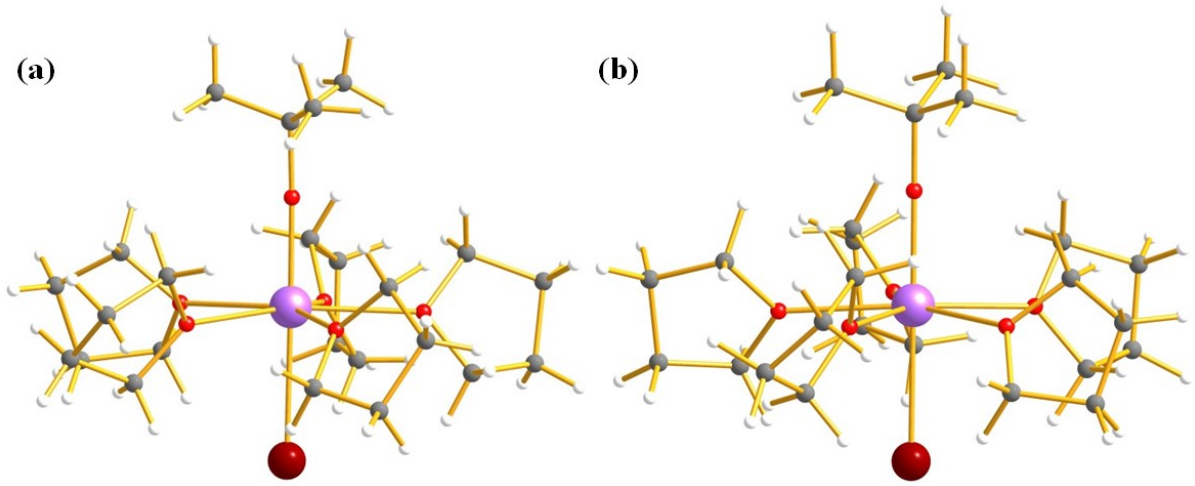


Figure S15. (a) The crystal structure and (b) DFT optimized structure of **2**. Colour code: Dy-blue violet, Br-brown, O-red, N-blue, C-grey and H-white.

Table S11. A comparison of selected structural parameters (bond lengths are shown in Å and bond angles are shown in degree) between optimized and X-ray crystal structures of **2**.

Structural parameter	Crystal structure	DFT optimized geometry	
		2	**2-crown**
Dy-O1 (CMe_3)	2.024	2.060	2.043
Dy-O2 (THF/crown)	2.449	2.447	2.444
Dy-O3 (THF/crown)	2.418	2.418	2.399
Dy-O4 (THF/crown)	2.444	2.424	2.422
Dy-O5 (THF/crown)	2.424	2.442	2.427
Dy-O6 (THF/crown)	2.417	2.419	2.399
Dy-Br	2.829	2.810	2.826
O1-Dy-Br	177.9	179.5	176.9

Table S12. A comparison of selected structural parameters (bond lengths are shown in Å and bond angles are shown in degree) between optimized and X-ray crystal structures of **3**.

Structural parameter	Crystal structure	DFT optimized geometry	
		3	**3-crown**
Dy-O1 ($SiMe_3$)	2.092	2.093	2.064
Dy-O2 (THF/crown)	2.416	2.470	2.399
Dy-O3 (THF/crown)	2.418	2.473	2.433
Dy-O4 (THF/crown)	2.402	2.462	2.398
Dy-O5 (THF/crown)	2.408	2.486	2.417
Dy-O6 (THF/crown)	2.410	2.465	2.420
Dy-Br	2.797	2.805	2.818
O1-Dy-Br	178.9	178.3	176.7

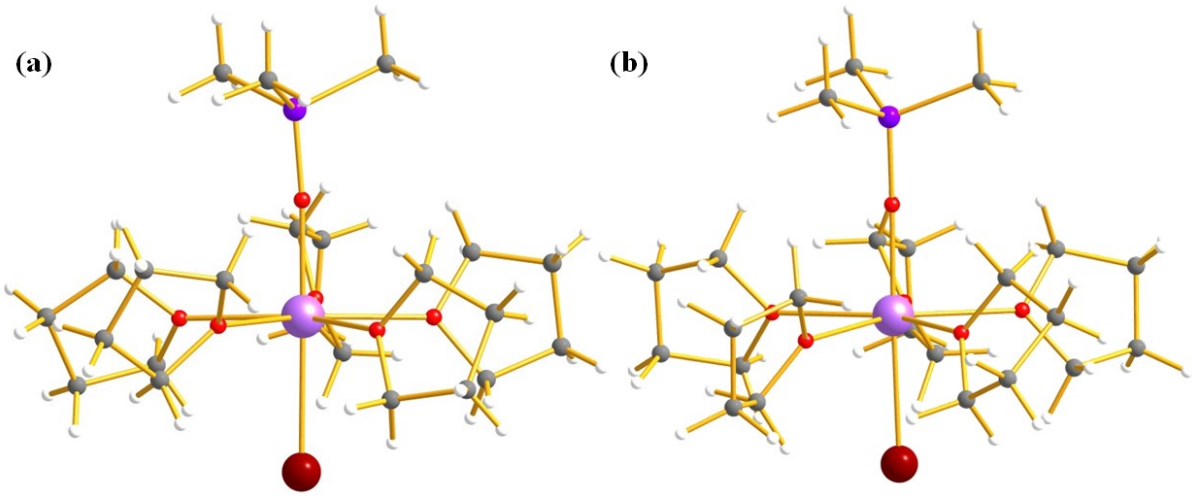


Figure S16. (a) The crystal structure and (b) DFT optimized structure of **3**. Colour code: Dy-blue violet, Br-brown, O-red, N-blue, C-grey and H-white.

Table S13. The computed energies (cm^{-1}) along with g tensor of eight $^6H_{15/2}$ KDs of optimized geometry of **2**. The values in parenthesis correspond to the calculations on the X-ray crystal structure.

Complex **2**			
Energy	g_x	g_y	g_z
0.0 (0)	0.000 (0.000)	0.000 (0.000)	19.987 (19.987)
361.3 (386.0)	0.027 (0.018)	0.032 (0.019)	17.008 (17.035)
492.9 (561.4)	1.649 (2.512)	4.659 (4.043)	15.386 (14.741)
533.7 (603.1)	3.146	4.227	5.772
564.3 (613.9)	0.266	1.242	13.077
576.7 (648.7)	0.253	2.180	6.884
619.2 (687.2)	0.421	1.095	11.366
633.3 (693.7)	0.013	0.813	13.989
Complex **2-caspt2**			
0.0	0.000	0.000	19.985
352.3	0.027	0.031	17.005
488.7	1.650	4.662	15.378
524.4	3.149	4.245	5.789
560.2	0.266	1.241	13.078
567.6	0.259	2.195	6.885
605.4	0.421	1.095	11.369
610.9	0.012	0.811	13.990

Table S14. The computed energies (cm^{-1}) along with g tensor of eight $^6H_{15/2}$ KDs of optimized geometry of **3**. The values in parenthesis correspond to the calculations on the X-ray crystal structure.

Complex **3**			
Energy	g_x	g_y	g_z
0.0 (0.0)	0.000 (0.000)	0.000 (0.000)	19.992 (19.985)
360.1 (359.2)	0.002 (0.022)	0.003 (0.030)	17.104 (17.026)
570.2 (477.9)	4.483 (1.380)	6.781 (6.642)	10.290 (14.079)
600.2 (520.8)	0.071	3.459	10.845
614.5 (568.9)	2.893	3.588	4.390
666.6 (588.6)	0.177	0.703	6.954
699.7 (636.0)	0.021	0.425	13.479
716.1 (667.8)	0.162	0.336	14.284

Complex **3-caspt2**			
0.0	0.000	0.000	19.992
354.3	0.003	0.003	17.105
552.8	11.6	7.452	3.086
589.5	1.141	2.517	11.439
596.8	5.365	3.842	2.224
651.6	0.151	0.658	6.926
689.5	0.027	0.369	13.702
704.9	0.152	0.289	14.720

Table S15. The computed CF parameters of X-ray structure and optimized geometry of **2** and **3**. The computed CF parameters of **2-crown** and **3-crown** are also shown. Here, the CF parameters have been computed according to Stevens Hamiltonian:

$$H_{CF} = \sum_{k=2,4,6} \sum_{q=-k}^{q=+k} B_k^q \tilde{O}_k^q$$

where B_k^q is the CF parameter and $\tilde{O}_k^q$ is the Stevens operator.

k	q	B_k^q					
		2 (X-ray)	**2** (opt)	**2-crown**	**3** (X-ray)	**3** (opt)	**3-crown**
2	-2	-3.35E-01	6.00E-02	-1.54E-01	-2.41E-02	1.40E-01	-1.22E-01
	-1	-1.99E-01	7.09E-02	1.98E-01	2.50E-03	2.62E-01	3.57E-01
	0	-3.10E+00	-2.67E+00	-5.18E+00	-2.62E+00	-3.27E+00	-5.35E+00
	1	-4.05E-02	-2.11E-01	-1.41E-01	6.38E-01	1.44E-01	-2.24E-01
	2	-2.24E-01	3.04E-01	-1.13E+00	2.48E-01	9.87E-02	-1.02E+00
4	-4	1.61E-03	-1.04E-03	1.98E-03	3.35E-03	2.55E-05	1.54E-03
	-3	-5.71E-03	5.17E-04	1.46E-03	8.83E-03	5.33E-03	1.22E-03
	-2	7.75E-04	-3.32E-04	3.71E-04	9.02E-04	2.40E-04	4.51E-04
	-1	4.02E-04	3.44E-04	-3.59E-04	-2.19E-04	-1.38E-03	-9.74E-04
	0	-1.23E-02	-1.19E-02	-1.07E-02	-1.30E-02	-1.22E-02	-1.15E-02
	1	2.13E-04	3.62E-04	4.10E-04	-3.34E-03	-1.11E-03	8.30E-04
	2	1.31E-03	-1.48E-03	2.54E-03	3.25E-04	-8.33E-04	2.58E-03
	3	-9.08E-04	-2.56E-03	7.47E-04	-4.91E-03	8.27E-05	6.56E-04
	4	2.95E-04	2.88E-04	1.28E-02	-1.57E-03	8.33E-04	1.30E-02
6	-6	-2.07E-05	1.33E-05	-6.21E-05	-2.01E-05	-2.02E-06	-4.55E-05
	-5	-1.39E-04	5.61E-04	5.87E-04	2.13E-04	-1.49E-04	4.82E-04
	-4	1.17E-05	-7.13E-06	7.31E-06	1.43E-05	1.46E-06	6.81E-06
	-3	-3.44E-05	2.43E-05	1.64E-05	5.30E-05	3.49E-05	2.18E-05
	-2	-1.10E-06	3.86E-06	-1.72E-06	1.85E-05	-8.62E-06	-1.66E-06
	-1	8.37E-06	-2.24E-05	-1.52E-05	6.24E-06	-3.93E-06	-2.44E-05
	0	3.41E-06	2.44E-06	1.36E-05	1.26E-05	1.68E-05	2.55E-05
	1	1.18E-05	1.03E-05	-2.78E-06	-1.75E-05	1.71E-06	2.19E-06
	2	7.25E-06	-1.16E-05	1.71E-05	3.09E-06	-8.91E-06	1.77E-05
	3	1.35E-05	-1.75E-05	-5.72E-07	-1.83E-05	-9.27E-06	6.42E-06
	4	3.46E-06	3.16E-06	5.43E-05	-6.74E-06	1.03E-05	5.83E-05
	5	-5.87E-04	1.85E-04	-7.03E-05	-4.45E-04	-4.12E-04	-5.33E-05
	6	-1.23E-05	-1.60E-06	-3.09E-04	2.20E-05	-8.49E-06	-3.13E-04

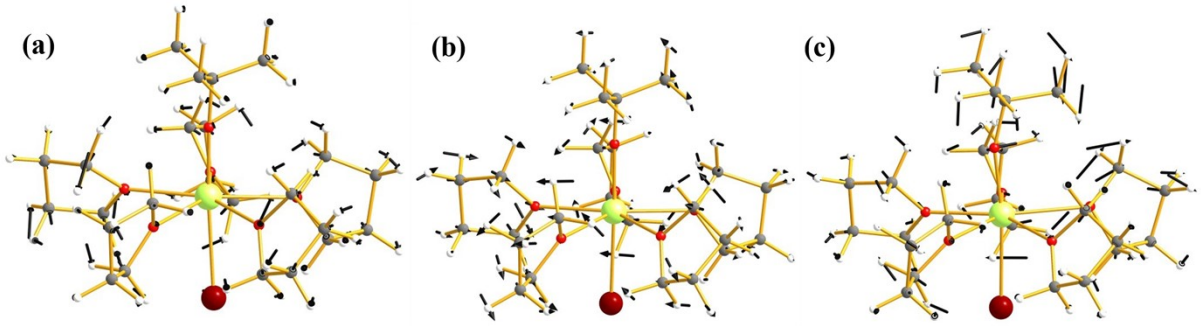


Figure S17. The molecular vibrations of **2** corresponds to (a) $^{\omega_1}$ (b) $^{\omega_2}$ and (c) $^{\omega_3}$ vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

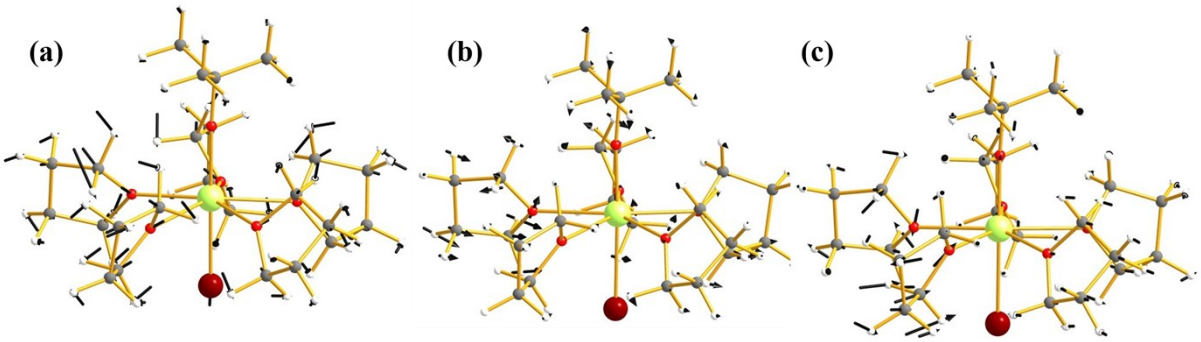


Figure S18. The molecular vibrations of **2** corresponds to (a) $^{\omega_4}$ (b) $^{\omega_5}$ and (c) $^{\omega_6}$ vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

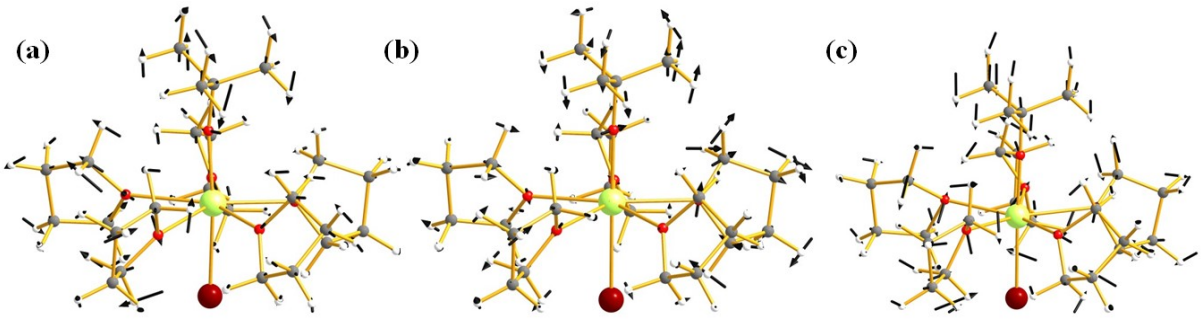


Figure S19. The molecular vibrations of **2** corresponds to (a) $^{\omega_7}$ (b) $^{\omega_8}$ and (c) $^{\omega_9}$ vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

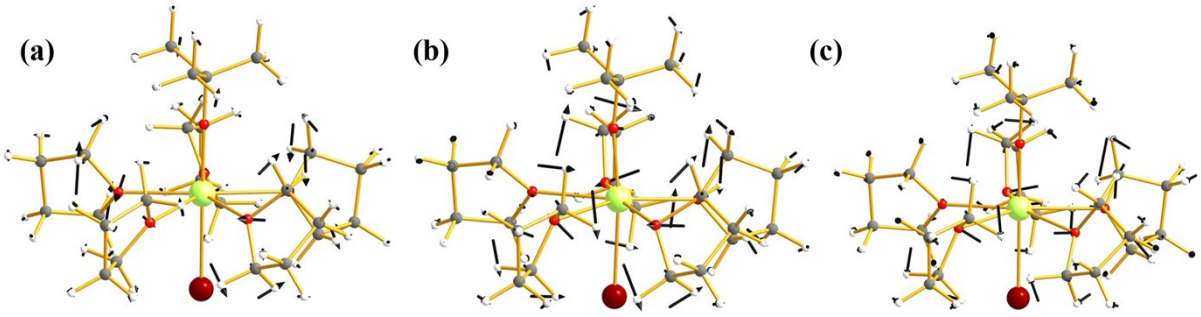


Figure S20. The molecular vibrations of **2** corresponds to (a) $^{\omega_{10}}$ (b) $^{\omega_{11}}$ and (c) $^{\omega_{12}}$ vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

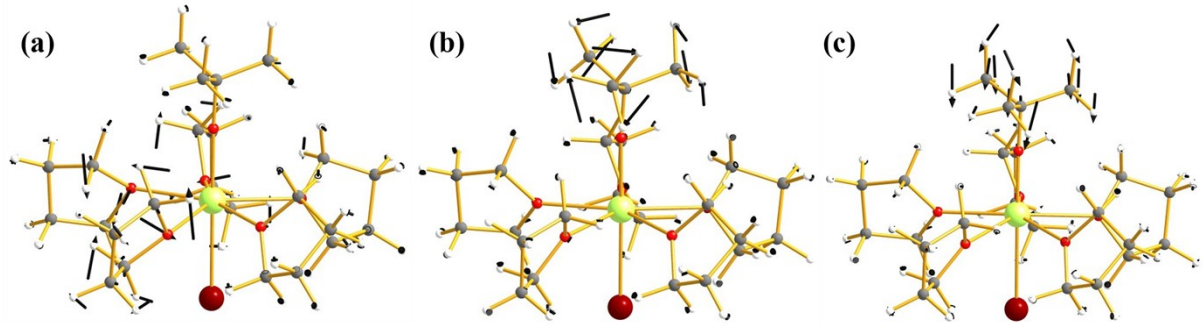


Figure S21. The molecular vibrations of **2** corresponds to (a) ω_{13} (b) ω_{14} and (c) ω_{15} vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

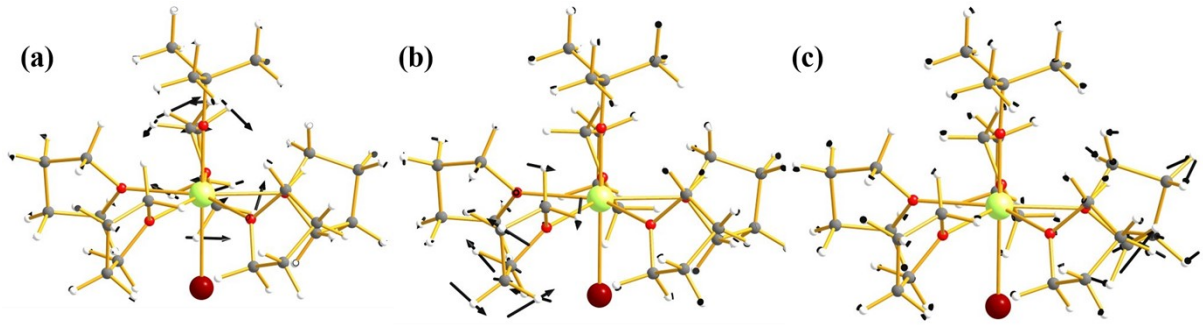


Figure S22. The molecular vibrations of **2** corresponds to (a) ω_{16} (b) ω_{17} and (c) ω_{18} vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

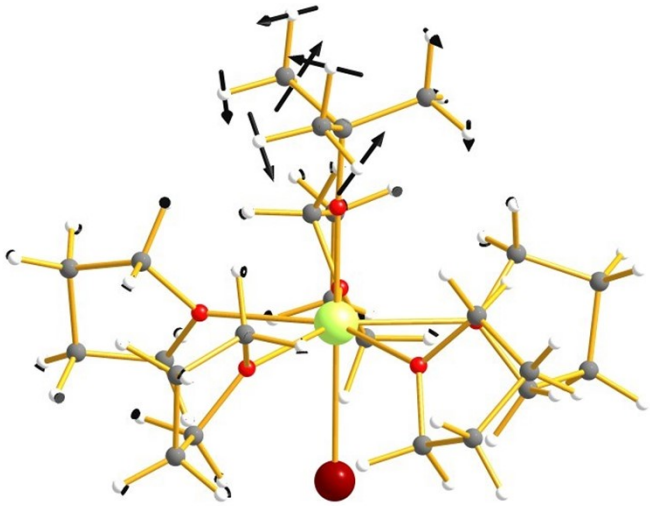
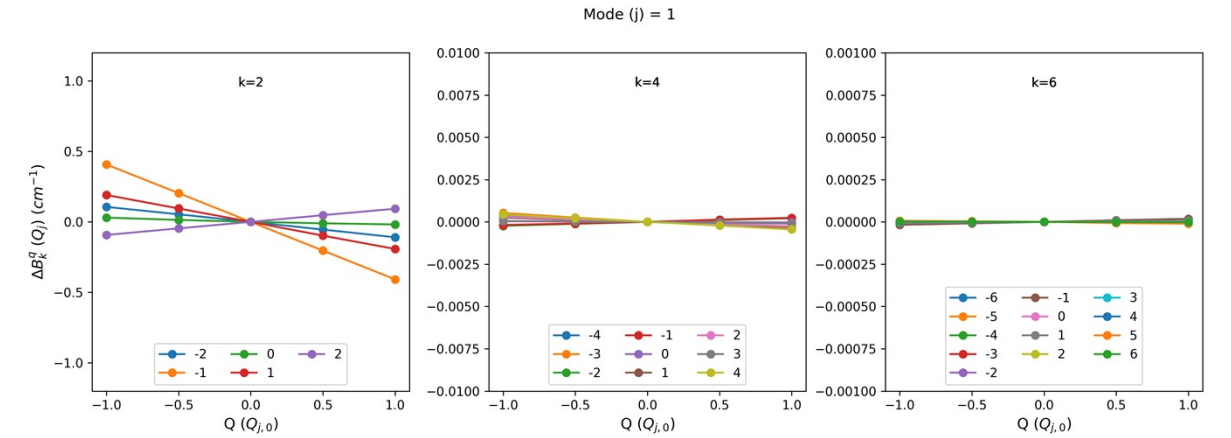
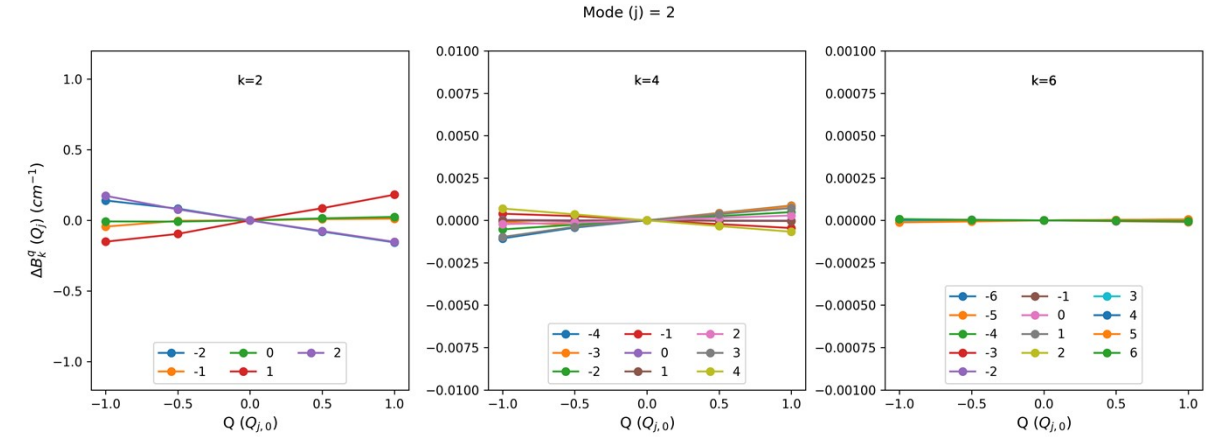
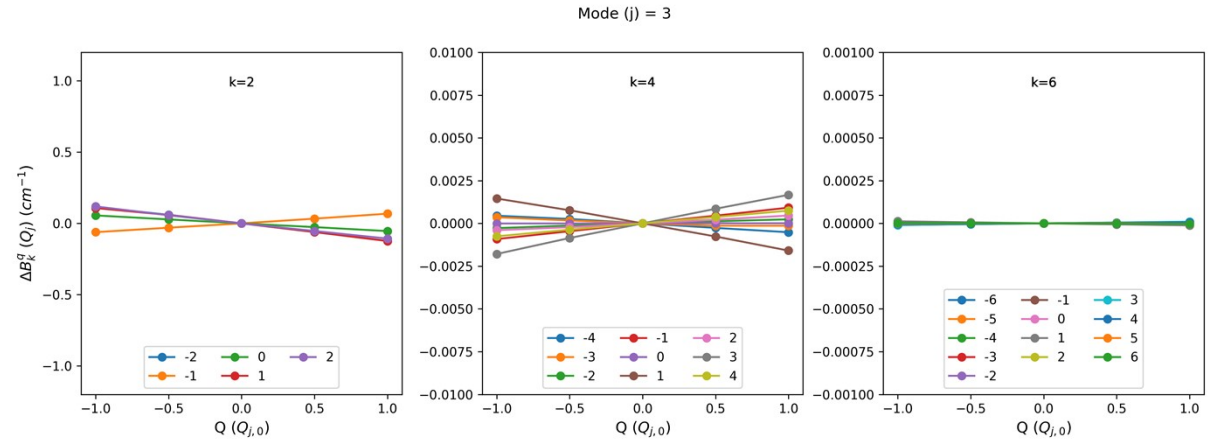
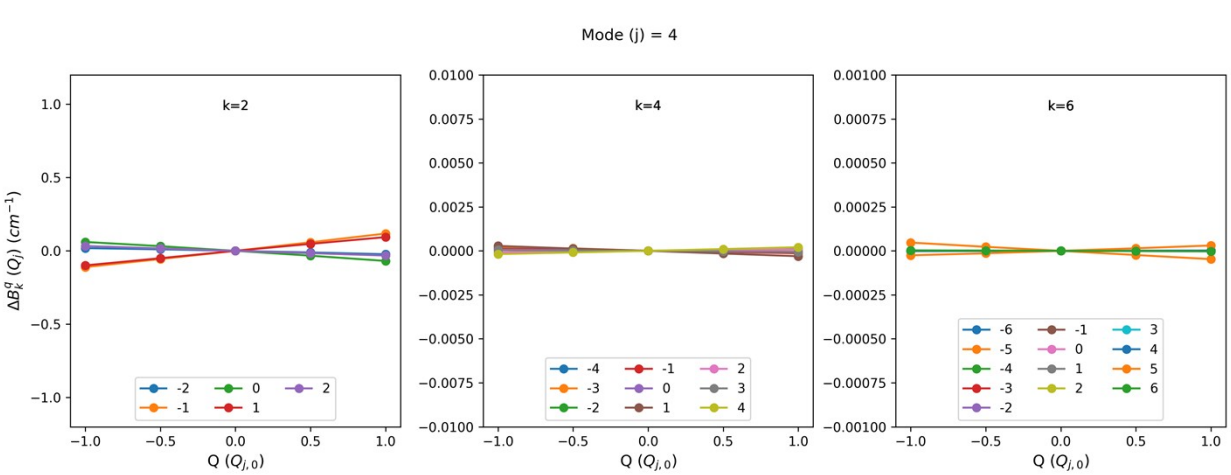


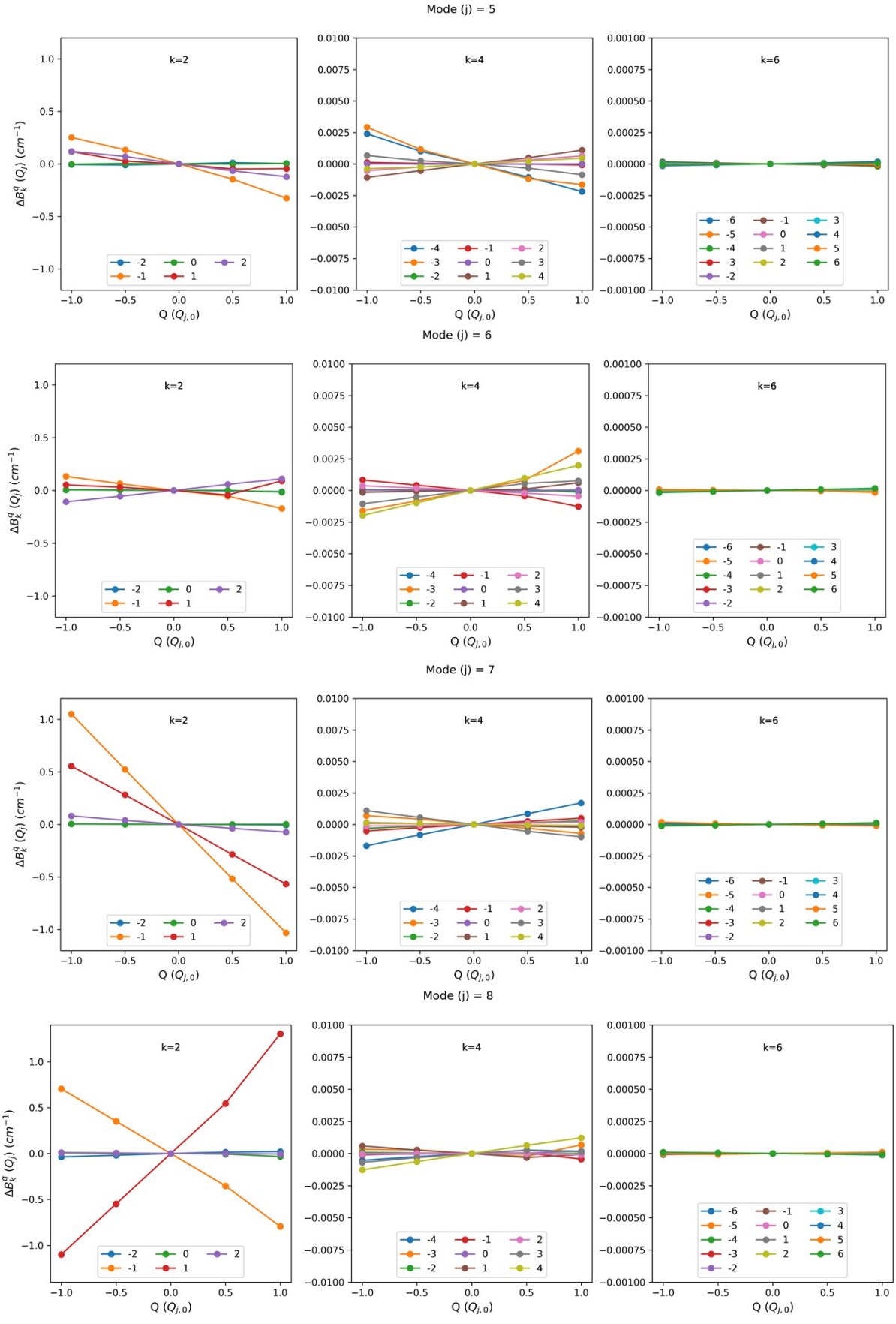
Figure S23. The molecular vibrations of **2** corresponds to ω_{19} vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

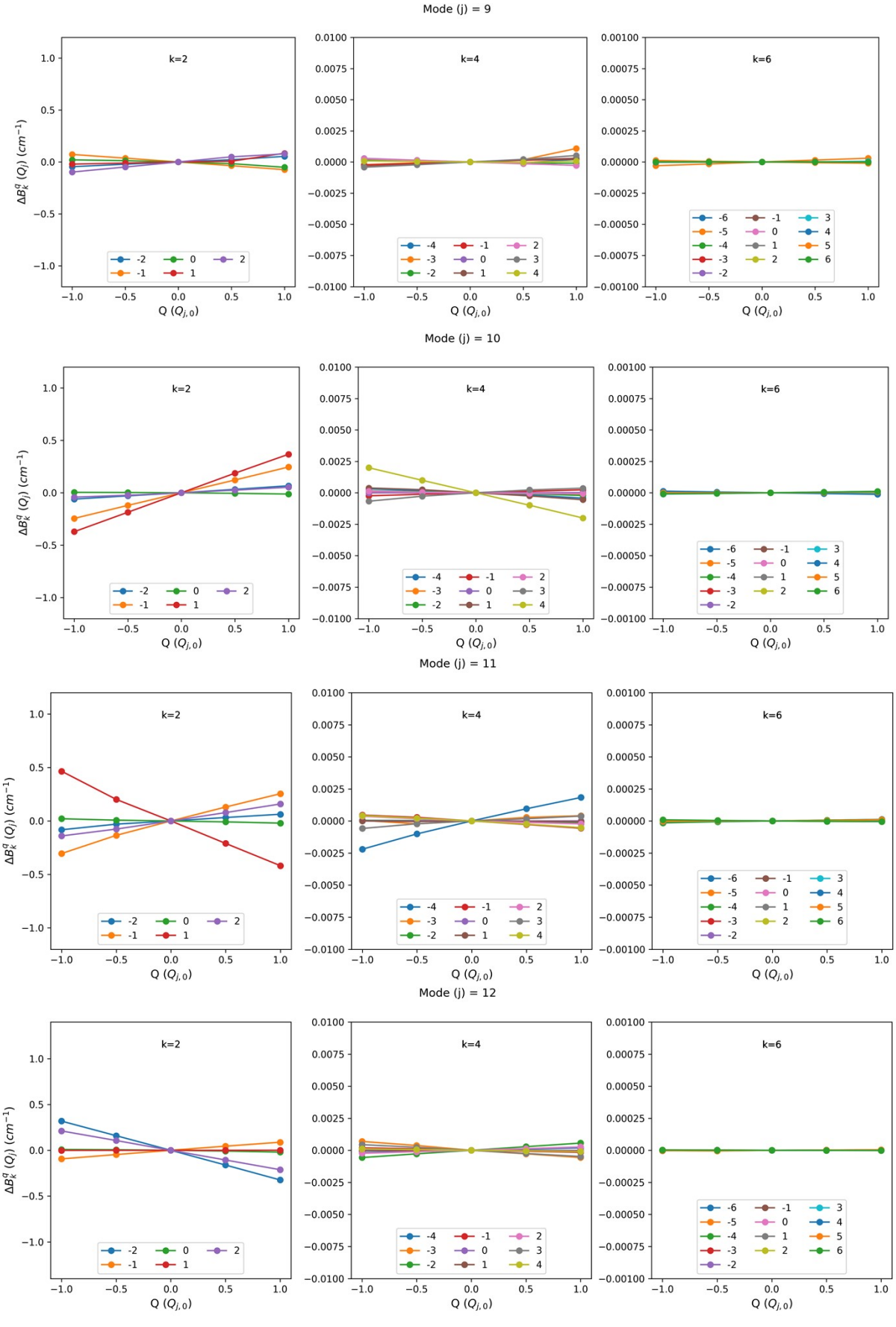

Mode (j) = 1
k=2
k=4
k=6
$\Delta B_k^q\ (Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)


Mode (j) = 2
k=2
k=4
k=6
$\Delta B_k^q\ (Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)

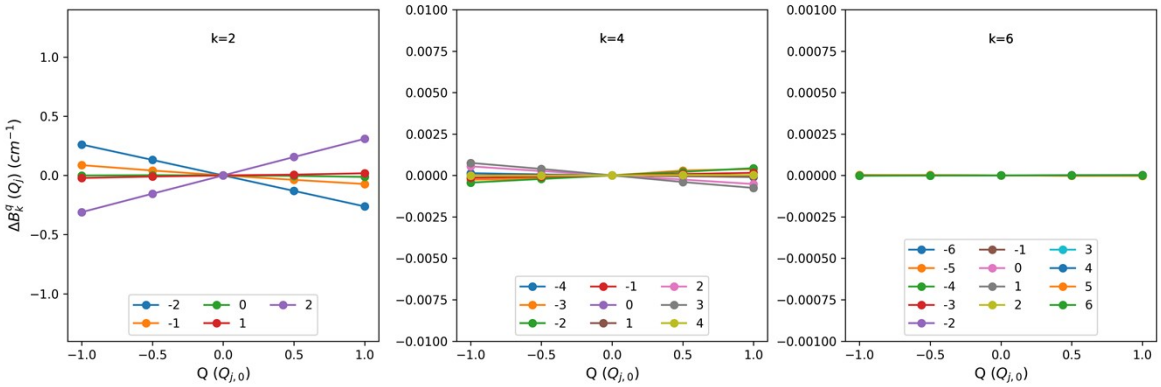

Mode (j) = 3
k=2
k=4
k=6
$\Delta B_k^q\ (Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)


Mode (j) = 4
k=2
k=4
k=6
$\Delta B_k^q\ (Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)

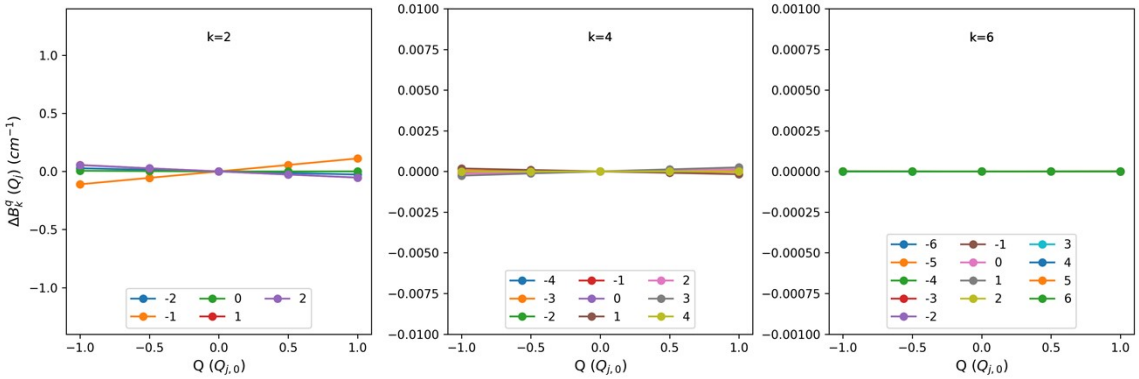

Mode (j) = 5
k=2
k=4
k=6
Mode (j) = 6
k=2
k=4
k=6
Mode (j) = 7
k=2
k=4
k=6
Mode (j) = 8
k=2
k=4
k=6
$\Delta B_k^q(Q_j)\ (cm^{-1})$
Q $(Q_{j,0})$


Mode (j) = 9
k=2
k=4
k=6
Mode (j) = 10
k=2
k=4
k=6
Mode (j) = 11
k=2
k=4
k=6
Mode (j) = 12
k=2
k=4
k=6
$\Delta B_k^q(Q_j)\ (cm^{-1})$
Q $(Q_{j,0})$

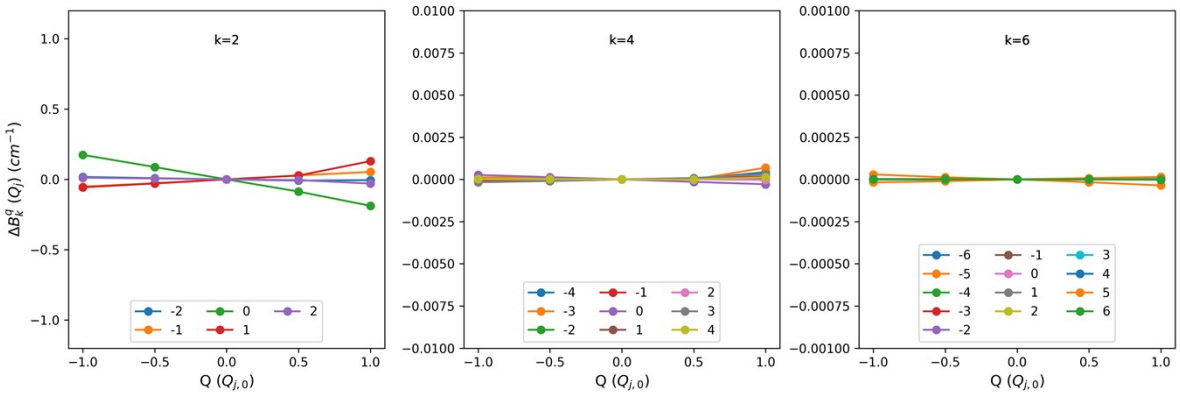
Mode (j) = 13



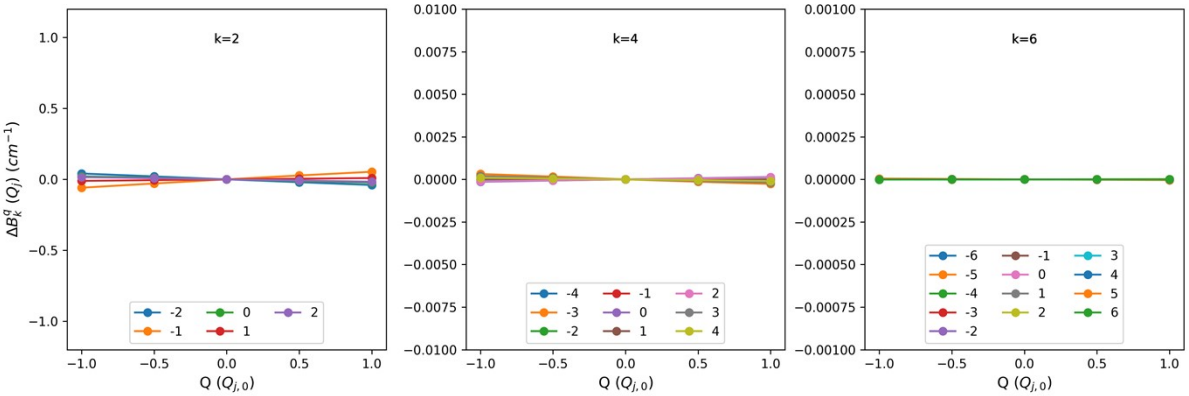
Mode (j) = 14

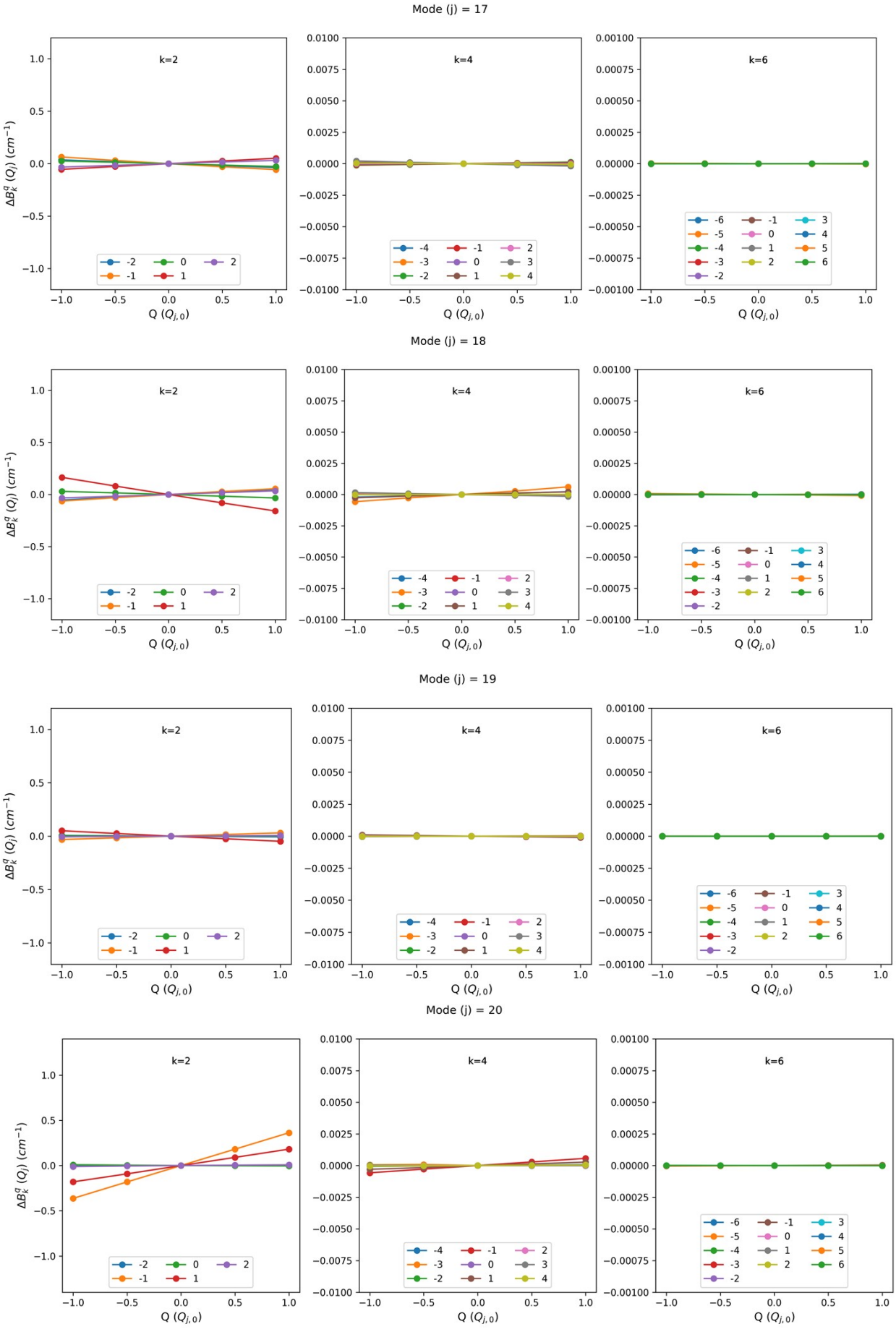


Mode (j) = 15



Mode (j) = 16




Mode (j) = 17
Mode (j) = 18
Mode (j) = 19
Mode (j) = 20
k=2
k=4
k=6
$\Delta B_k^q(Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)
-2 -1 0 1 2
-4 -3 -2 -1 0 1 2 3 4
-6 -5 -4 -3 -2 -1 0 1 2 3 4 5 6

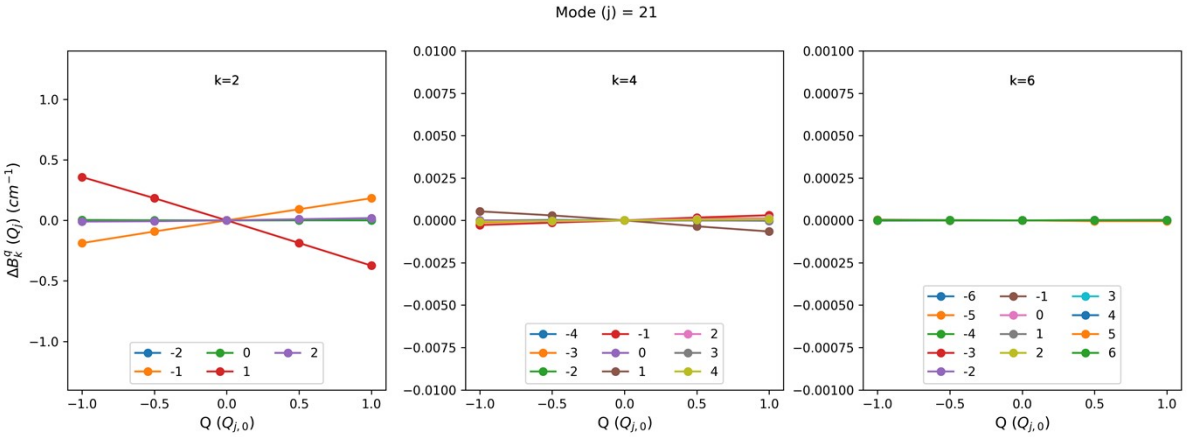


Figure S23. The variation of CFPs as a function of displacement for vibrational modes 1-21 of complex **2**.

Table S16. The vibrational mode numbers (ω), energy (cm^{-1}), oscilator strength (km mol^{-1}), population (at 100 K), maximum displacement (Q_k) and coupling strength (S_j in cm^{-1}) of the first 51 normal modes of **2**. The mode numbers corresponds to the one which has been taken into consideration in our study.

Mode number (j)	Energy	oscilator strength	population	Q_k	S_j
	22.7	0.032	0.065		
	33.5	0.753	0.056		
	38.4	0.938	0.052		
	41.0	0.128	0.050		
	45.9	0.355	0.047		
	46.2	0.043	0.046		
	49.1	0.748	0.045		
	55.2	1.016	0.041		
	58.4	0.614	0.039		
	59.8	0.588	0.038		
	62.8	0.951	0.037		
	65.4	1.283	0.035		
	73.6	1.074	0.031		
	74.9	0.152	0.031		
	80.4	0.808	0.028		
1	84.5	3.416	0.027	0.27	0.122
2	90.8	4.271	0.024	0.28	0.072
	93.4	0.998	0.024		
	97.3	0.222	0.022		
	98.2	0.287	0.022		
	103.3	1.021	0.020		
	106.9	1.422	0.019		
	116.3	0.569	0.017		
	119.8	0.155	0.016		
	123.0	0.491	0.015		
3	126.4	0.381	0.015	0.27	0.056
	130.1	1.877	0.014		
4	141.7	5.812	0.012	0.22	0.043
	145.1	0.583	0.011		
5	152.3	5.159	0.010	0.21	0.083
6	153.4	4.902	0.010	0.21	0.047
	156.8	1.068	0.009		
7	162.7	10.006	0.009	0.20	0.306
8	165.3	8.743	0.008	0.22	0.359

	166.2	2.453	0.008		
9	184.9	7.018	0.006	0.21	0.036
10	195.1	48.058	0.005	0.21	0.116
11	200.1	48.397	0.005	0.20	0.140
12	215.9	2.366	0.004	0.20	0.102
13	221.2	0.704	0.004	0.20	0.106
14	245.8	0.967	0.003	0.36	0.035
15	250.3	27.111	0.002	0.18	0.053
	253.1	0.345	0.002		
16	258.5	0.999	0.002	0.28	0.019
	266.6	0.515	0.002		
17	272.4	1.191	0.002	0.28	0.025
18	276.5	3.322	0.002	0.26	0.048
19	296.1	0.164	0.001	0.33	0.015
	311.0	0.190	0.001		
	351.2	6.178	0.001		0.104
	357.6	6.048	0.002		0.106
Total			1.00		

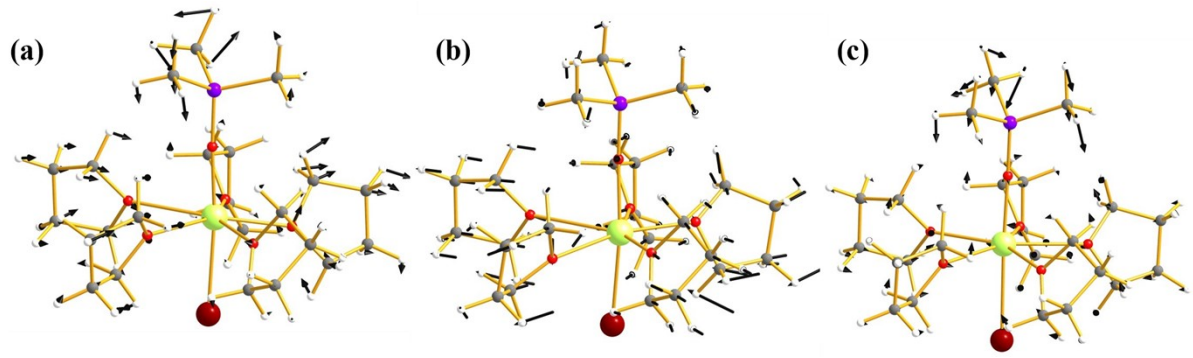


Figure S25. The molecular vibrations of **3** corresponds to (a) ω_1 (b) ω_2 and (c) ω_3 vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

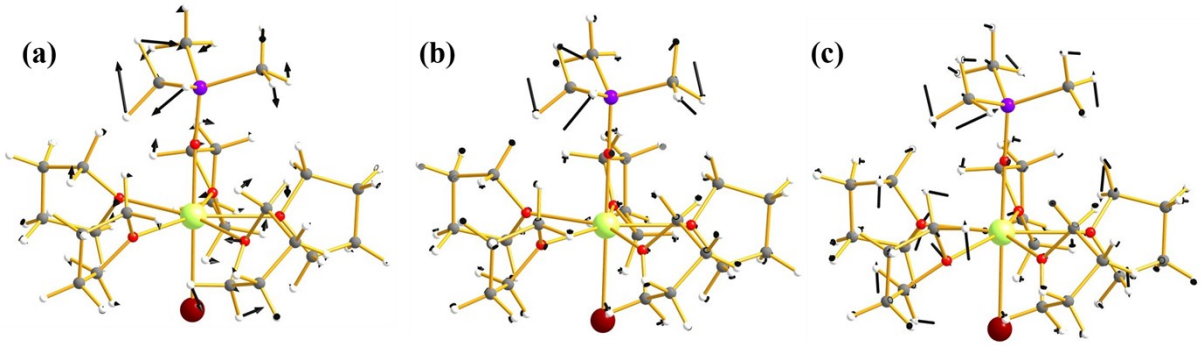


Figure S26. The molecular vibrations of **3** corresponds to (a) ω_4 (b) ω_5 and (c) ω_6 vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

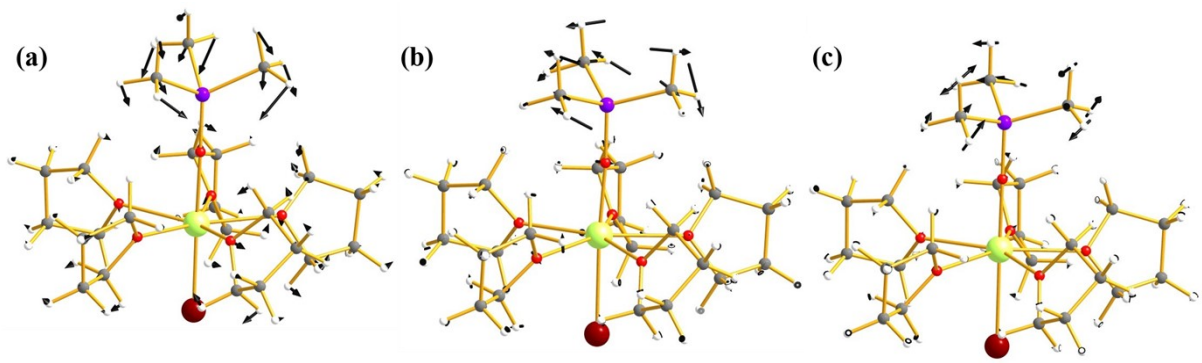


Figure S27. The molecular vibrations of **3** corresponds to (a) ω_7 (b) ω_8 and (c) ω_9 vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

Figure S28. The molecular vibrations of **3** corresponds to (a) ω_{10} (b) ω_{11} and (c) ω_{12} vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code

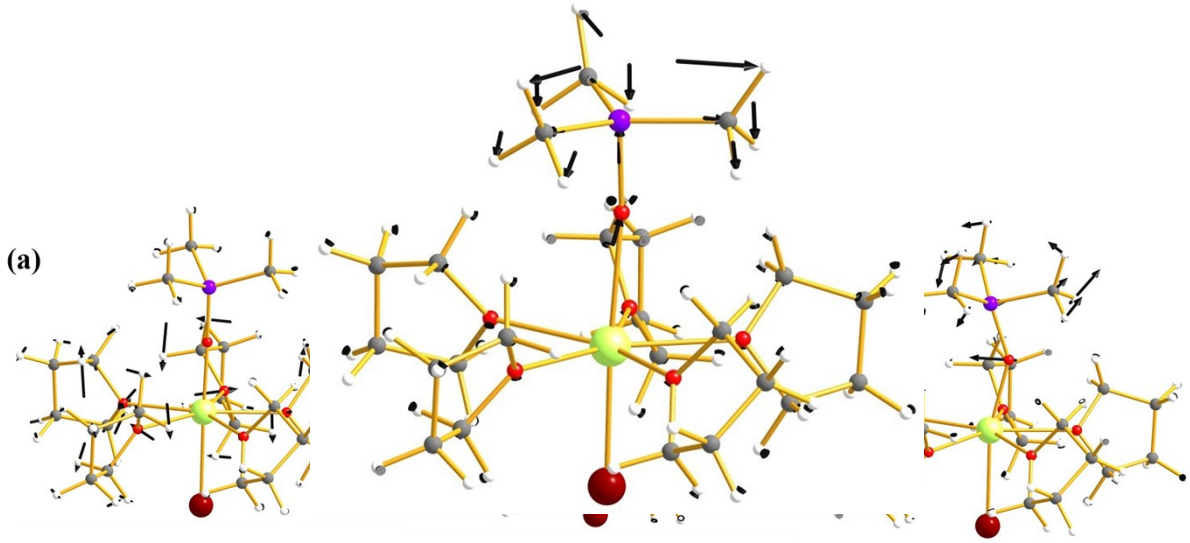
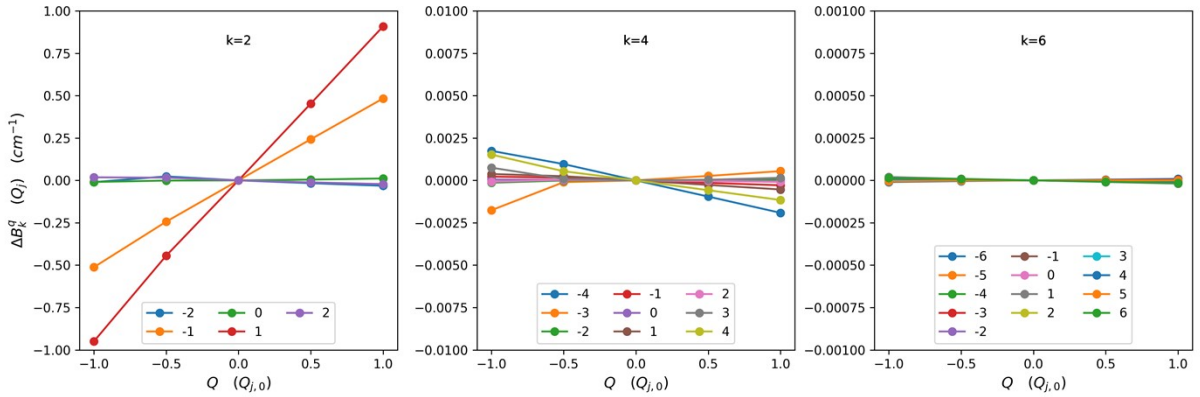
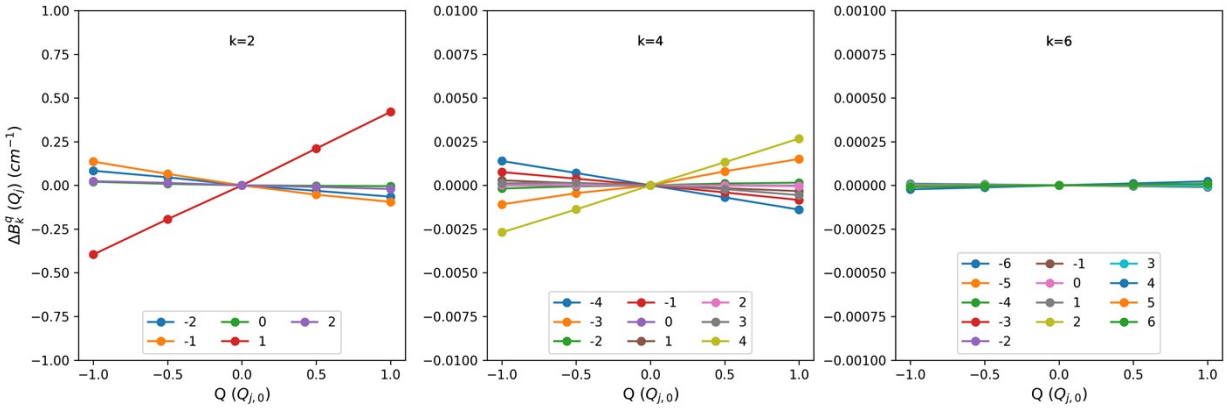


Figure S29. The molecular vibrations of **3** corresponds to ω_{13} vibrational mode. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

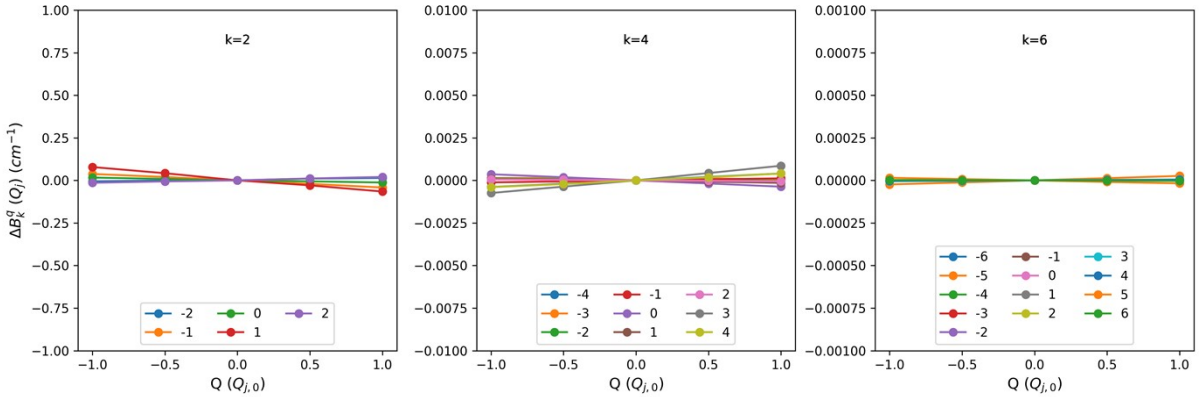
Mode (j) = 1



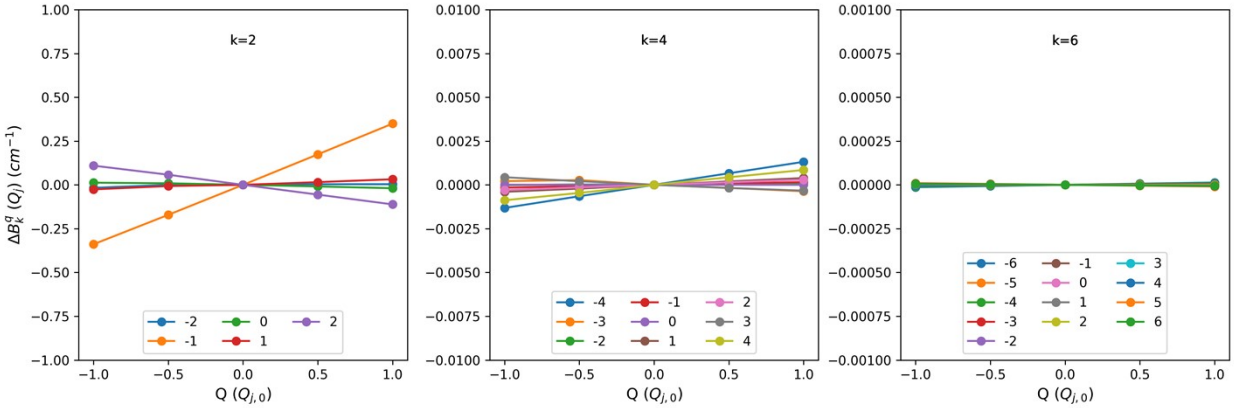
Mode (j) = 2



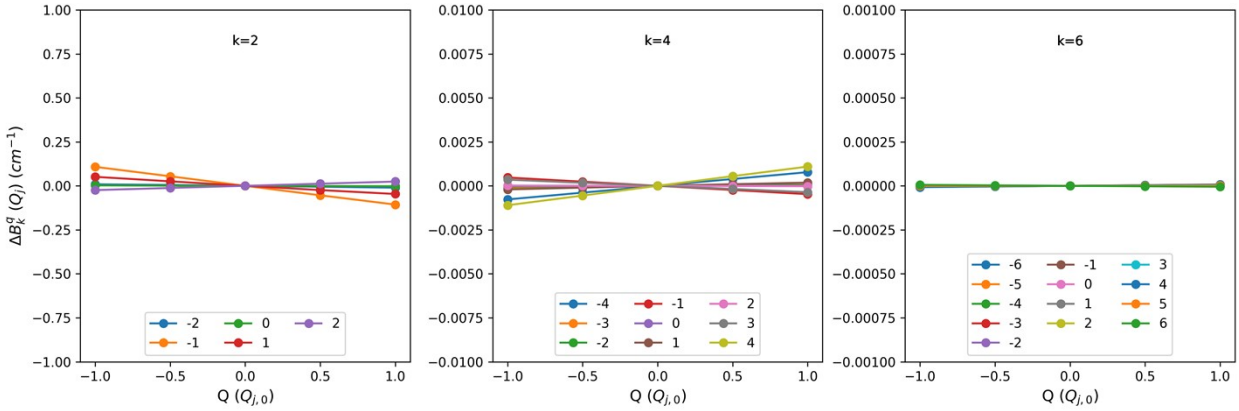
Mode (j) = 3



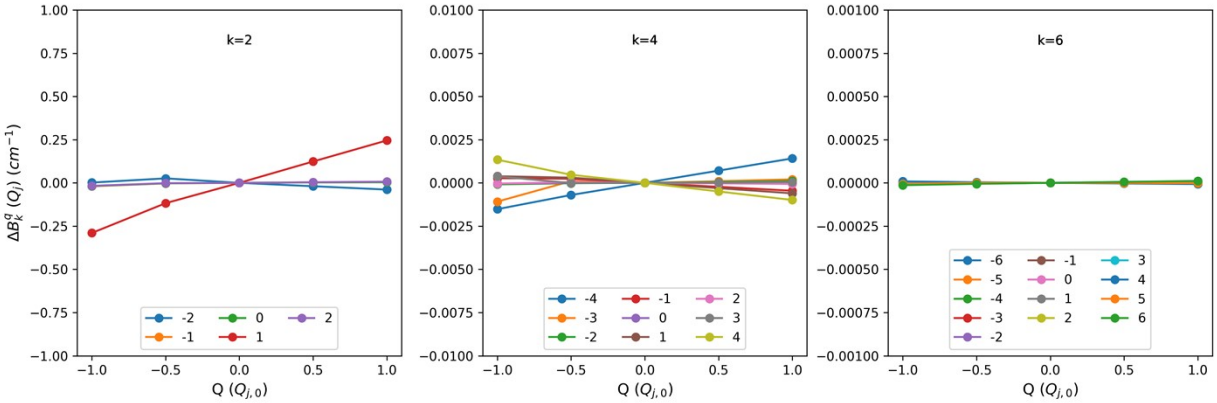
Mode (j) = 4



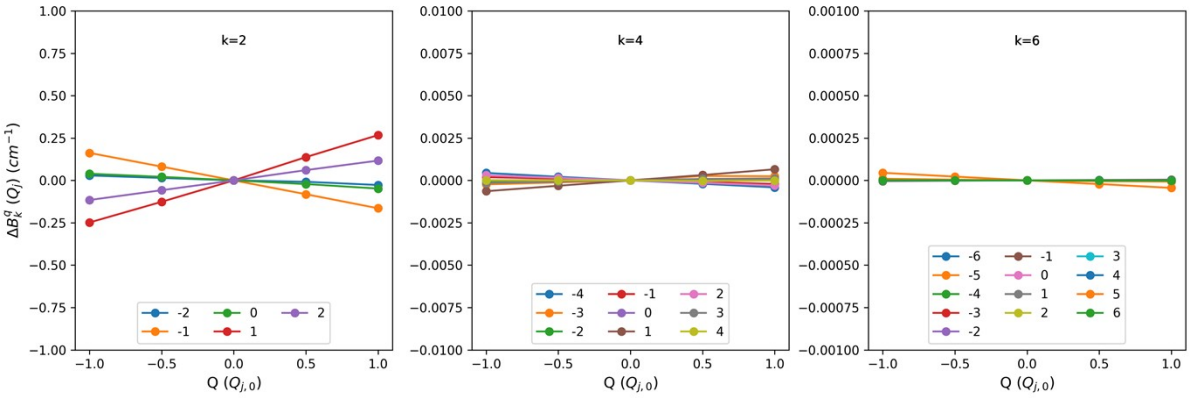
Mode (j) = 5



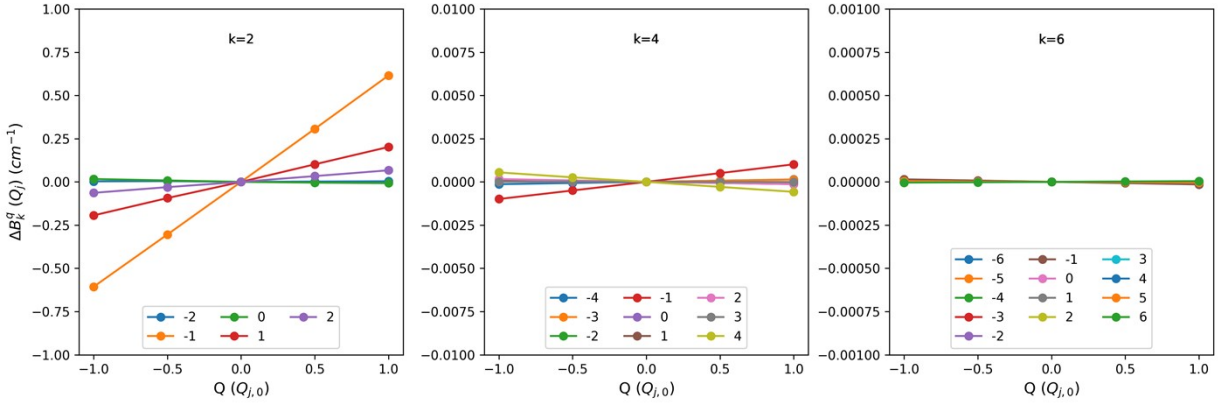
Mode (j) = 6



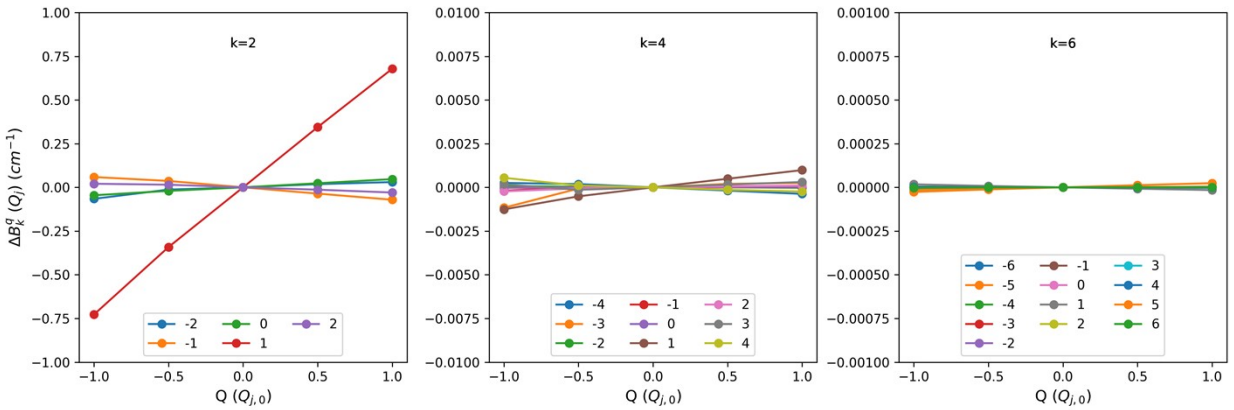
Mode (j) = 7



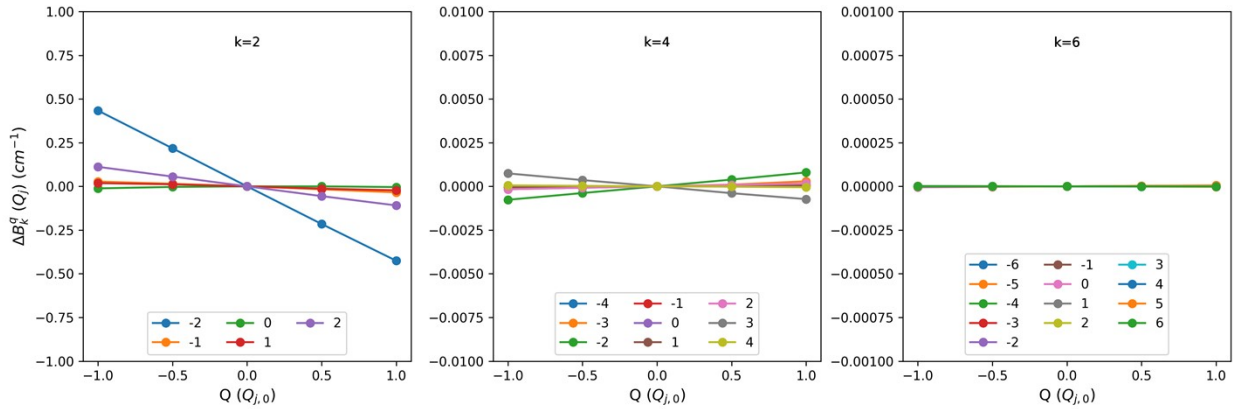
Mode (j) = 8



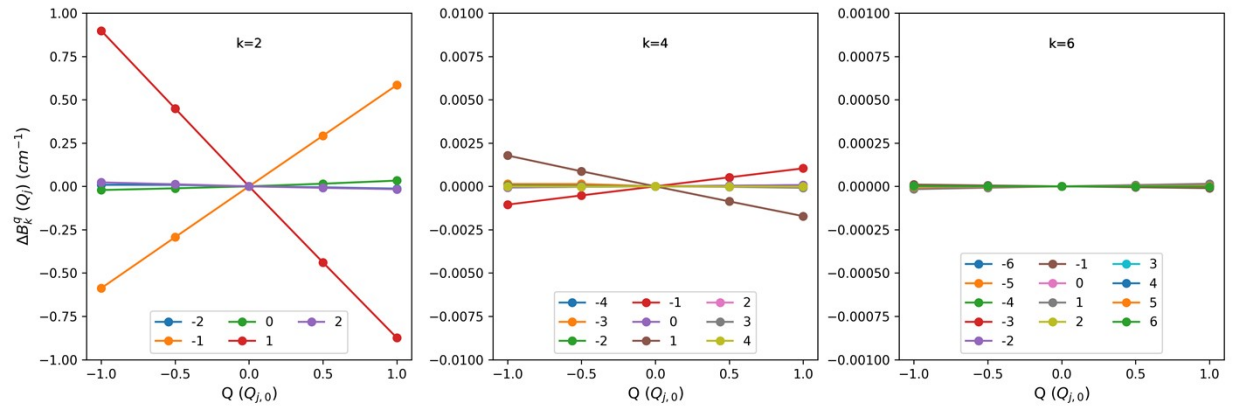
Mode (j) = 9



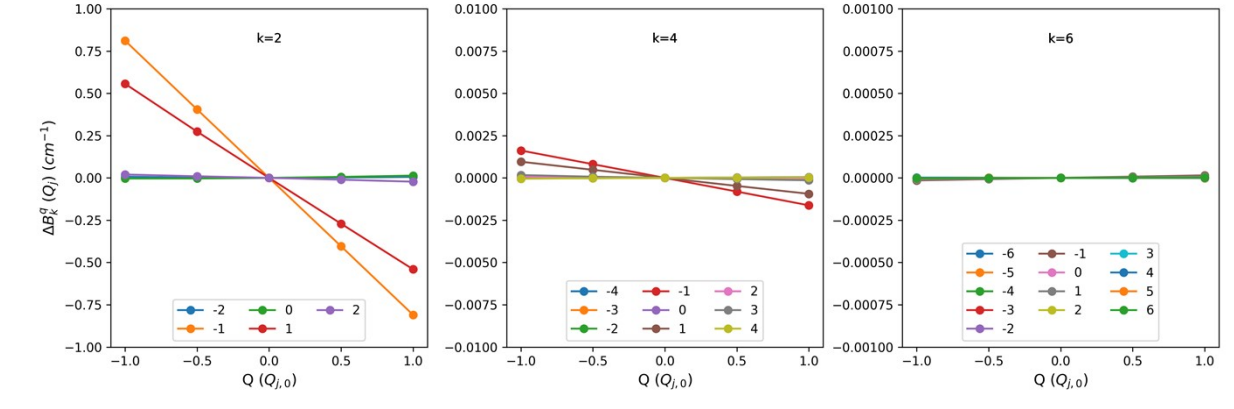
Mode (j) = 10



Mode (j) = 11



Mode (j) = 12



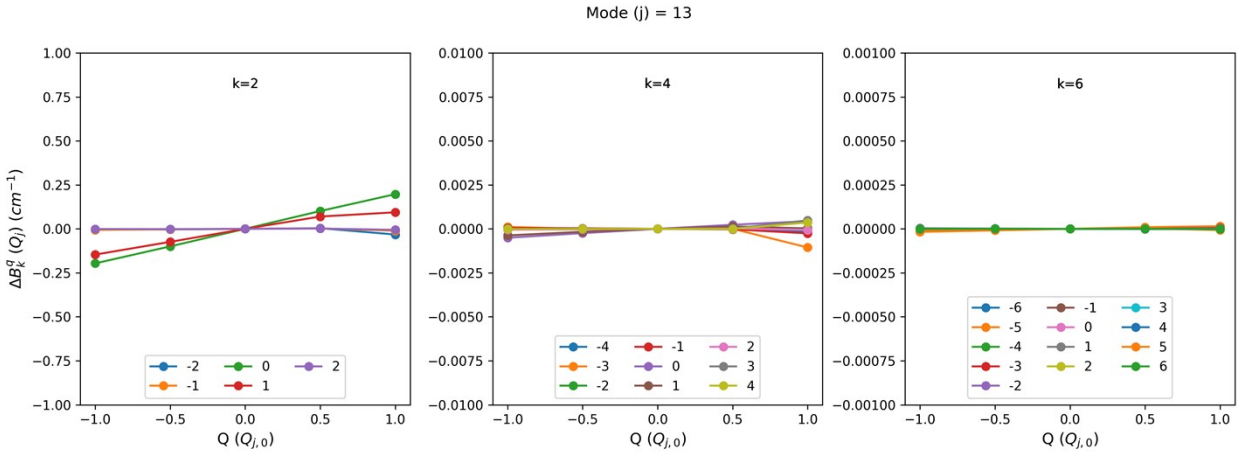


Figure S30. The variation of CFPs as a function of displacement for vibrational modes 1-13 of complex **3**.

Table S17. The vibrational mode numbers (ω), energy (cm^{-1}), oscilator strength ($km\ mol^{-1}$), population (at 100 K), maximum displacement (Q_k) and coupling strength (S_j in cm^{-1}) of the first 54 normal modes of **3**. The mode numbers corresponds to the one which has been taken into consideration in our study.

Mode number (j)	Energy	oscilator strength	population	Q_k	S_j
	15.2	0.029	0.066		
	29.4	0.286	0.054		
	33.8	0.764	0.051		
	36.5	0.640	0.049		
	40.1	0.989	0.046		
	41.4	0.068	0.045		
	44.9	0.832	0.043		
	47.5	0.540	0.042		
	52.7	0.682	0.038		
	53.9	1.354	0.038		
	59.3	0.942	0.035		
	61.7	0.155	0.034		
	67.4	0.777	0.031		
	69.2	1.307	0.030		
	75.0	1.042	0.028		
	77.7	2.212	0.027		
	84.5	3.904	0.024		
	88.1	0.300	0.023		
	95.0	0.378	0.021		
	95.7	0.261	0.021		
	102.6	0.131	0.019		
	102.8	0.140	0.019		
	109.8	3.296	0.017		
	113.4	3.018	0.016		
	119.2	0.134	0.015		
	121.1	0.141	0.014		
	132.9	0.943	0.012		
	137.8	2.986	0.011		
	143.2	2.052	0.010		
	146.5	0.740	0.010		
	151.9	3.318	0.009		
1	154.0	7.851	0.009	0.22	0.270

2	157.7	11.855	0.009	0.18	0.111
	158.8	1.515	0.008		
	160.9	0.068	0.008		
3	163.6	2.171	0.008	0.21	0.022
	168.8	0.701	0.007		
	184.8	1.527	0.006		
4	192.0	20.595	0.005	0.30	0.094
5	194.6	15.298	0.005	0.36	0.031
6	195.7	29.000	0.005	0.24	0.068
7	204.1	30.993	0.004	0.21	0.085
8	205.4	12.110	0.004	0.26	0.167
9	208.8	13.942	0.004	0.25	0.182
	218.1	2.271	0.004		
10	223.2	0.029	0.003	0.18	0.115
	259.6	0.632	0.002		
	260.2	0.118	0.002		
	262.4	0.410	0.002		
	265.8	0.394	0.002		
	269.8	0.243	0.002		
11	307.3	41.433	0.001	0.16	0.275
12	310.3	44.096	0.001	0.16	0.274
13	337.3	12.869	0.001	0.16	0.060
Total			1.00		

Table S18. The CASSCF+RASSI-SO/SINGLE_ANISO computed relative energies of the eight-low lying KDs along with g tensors and deviations from the principal magnetization axis with respect to the first KD for complex **2-crown**.

Energy (cm^{-1})	g_x	g_y	g_z	Angle of g_{zz} between ground and higher excited KDs (°)
0.0	0.001	0.001	19.984	
413.2	0.035	0.042	17.050	0.298
693.3	0.184	0.248	13.993	0.743
832.8	8.713	6.689	4.072	78.593
868.6	1.265	2.998	15.498	87.713
900.8	9.658	5.695	0.859	27.681
912.9	1.551	4.910	12.493	75.264
1027.4	0.168	0.238	19.319	92.873

Table S19. The CASSCF+RASSI-SO/SINGLE_ANISO computed relative energies of the eight-low lying KDs and g tensors and deviations from the principal magnetization axis regarding the first KD for complex **3-crown**.

Energy (cm^{-1})	g_x	g_y	g_z	Angle of g_{zz} between ground and higher excited KDs (°)
0.0	0.000	0.001	19.984	
411.6	0.033	0.038	17.058	0.726
713.7	0.321	0.402	13.983	1.011
869.1	2.468	4.459	11.183	88.233
891.1	3.434	4.108	12.750	85.384
934.1	2.070	5.248	11.492	89.941
950.6	0.671	2.277	10.650	72.912
1054.6	0.511	0.691	18.699	94.515

Table S20. The vibrational mode numbers (j), energy (cm^{-1}), oscilator strength (km mol^{-1}) of the first 54 normal modes of **2-crown** and **3-crown**.

Mode number (j)	**2-crown**		**3-crown**	
	Energy	oscilator strength	Energy	oscilator strength
1	15.4	0.006	17.4	0.021
2	32.5	2.001	21.4	1.290
3	36.7	2.225	25.4	2.203
4	54.8	3.563	51.8	3.949
5	61.3	2.812	56.0	6.068
6	63.8	4.636	60.1	2.554
7	66.0	5.764	62.2	2.605
8	70.6	0.034	65.9	3.066
9	107.4	6.161	78.1	7.121
10	108.5	1.736	94.6	3.478
11	119.3	3.254	113.3	0.031
12	144.9	3.664	140.1	0.792
13	154.2	4.640	149.3	0.126
14	162.6	3.382	150.6	2.609
15	166.6	7.581	158.1	0.145
16	175.5	2.429	162.4	0.776
17	183.4	3.895	167.3	0.285
18	188.5	4.253	170.2	1.100
19	196.3	10.020	174.1	5.364
20	203.3	5.635	175.6	1.682
21	210.2	4.454	182.3	4.364
22	223.5	0.103	188.4	5.703
23	251.0	60.209	192.0	3.973
24	273.9	4.106	195.6	1.503
25	277.1	0.133	205.0	7.391
26	281.6	9.120	207.2	5.337
27	284.6	0.428	215.9	58.037
28	291.6	13.688	275.7	3.227
29	296.9	3.322	283.2	10.072
30	301.1	9.685	290.0	21.693
31	316.2	2.784	294.4	2.536
32	345.5	1.644	302.7	5.348
33	347.4	3.248	307.3	33.079
34	349.7	5.596	309.1	18.046
35	351.9	2.694	317.5	3.386
36	364.2	8.334	345.6	9.720
37	366.0	13.031	345.8	6.423
38	436.2	0.418	350.1	13.226
39	485.0	12.201	364.8	14.202
40	487.9	0.751	366.7	9.199
41	488.8	13.119	435.9	0.584
42	507.6	28.320	489.7	0.179
43	542.0	0.086	542.2	0.087
44	543.5	0.136	543.1	0.045
45	546.1	0.106	545.5	0.073
46	562.9	0.008	563.0	0.004
47	780.2	25.768	610.0	1.045
48	783.5	14.549	684.3	9.112
49	835.8	10.956	684.8	8.798
50	839.0	11.593	693.2	0.031
51	869.6	12.444	777.8	20.555

52	881.3	49.390	779.2	17.679
53	890.7	7.949	780.7	27.837
54	915.7	0.030	835.4	9.430

Table S21. A comparison of selected structural parameters (bond lengths are shown in Å and bond angles are shown in degree) between optimized and X-ray crystal structures of **4**.

Structural parameter	Crystal structure	DFT optimized geometry
Dy-O1 ($SiPh_3$)	2.157	2.154
Dy-O2 ($SiPh_3$)	2.136	2.167
Dy-N1 (macrocycle)	2.571	2.545
Dy-N2H (macrocycle)	2.537	2.490
Dy-N3H (macrocycle)	2.507	2.576
Dy-N4 (macrocycle)	2.462	2.515
Dy-N5 (macrocycle)	2.399	2.613
O1-Dy-O2	176.5	174.0

Table S22. The computed energies (cm^{-1}) along with g tensor of eight $^6H_{15/2}$ KDs of optimized geometry of **4**. The values in parenthesis correspond to the previous calculations with the X-ray crystal structure (without counter anions).

Energy	g_x	g_y	g_z
0.0 (0.0)	0.000 (0.000)	0.000 (0.000)	19.989 (19.985)
503.1 (506.5)	0.015 (0.011)	0.018 (0.013)	17.023 (17.025)
887.6 (889.4)	0.314 (0.098)	0.500 (0.221)	14.037 (14.094)
1060.3	1.341	1.741	17.137
1114.0	2.515	5.624	11.319
1177.5	1.360	3.843	11.320
1266.5	0.925	1.888	17.891
1302.2	0.107	0.315	18.878

Table S23. The computed CF parameters of X-ray structure of **4**, optimized geometry of **4** and **4-N3O2**. Here, the CF parameters have been computed according to Stevens Hamiltonian:

$$H_{CF} = \sum_{k=2,4,6} \sum_{q=-k}^{q=+k} B_k^q \tilde{O}_k^q$$

where B_k^q is the CF parameter and $\tilde{O}_k^q$ is the Stevens operator.

k	q	B_k^q		
		4 (X-ray)	**4** (opt)	**4-N3O2**
2	-2	-1.62E+00	-1.62E+00	-6.64E-01
	-1	-6.98E-01	-9.29E-02	4.59E-01
	0	-6.48E+00	-6.80E+00	-8.07E+00
	1	1.32E+00	1.09E+00	2.72E-01
	2	3.83E-03	9.35E-01	9.85E-01
4	-4	1.54E-03	3.05E-03	-2.02E-03
	-3	1.19E-02	7.05E-03	-3.76E-03
	-2	5.45E-03	5.05E-03	2.73E-03
	-1	2.42E-03	4.71E-05	-2.51E-03
	0	-1.53E-02	-1.43E-02	-1.42E-02
	1	-5.13E-03	-5.35E-03	-2.66E-04

	2	-3.86E-04	-2.99E-03	-2.97E-03
	3	-7.73E-03	-4.69E-03	2.36E-02
	4	-7.41E-03	-9.27E-03	-5.97E-03
6	-6	-8.21E-05	-1.13E-04	-1.27E-04
	-5	2.68E-04	1.75E-04	-2.01E-04
	-4	1.50E-05	1.90E-05	3.02E-06
	-3	9.76E-05	3.11E-05	-2.30E-05
	-2	4.34E-05	2.65E-05	3.10E-06
	-1	4.97E-05	1.13E-05	-1.10E-05
	0	3.95E-05	3.77E-05	4.63E-05
	1	-7.00E-05	-3.78E-05	-3.31E-05
	2	2.53E-05	-1.65E-05	-2.66E-05
	3	-6.10E-05	-4.18E-05	1.19E-04
	4	-4.88E-05	-6.84E-05	-2.03E-05
	5	-4.47E-05	-6.64E-05	9.43E-05
	6	1.61E-04	1.50E-04	1.51E-04

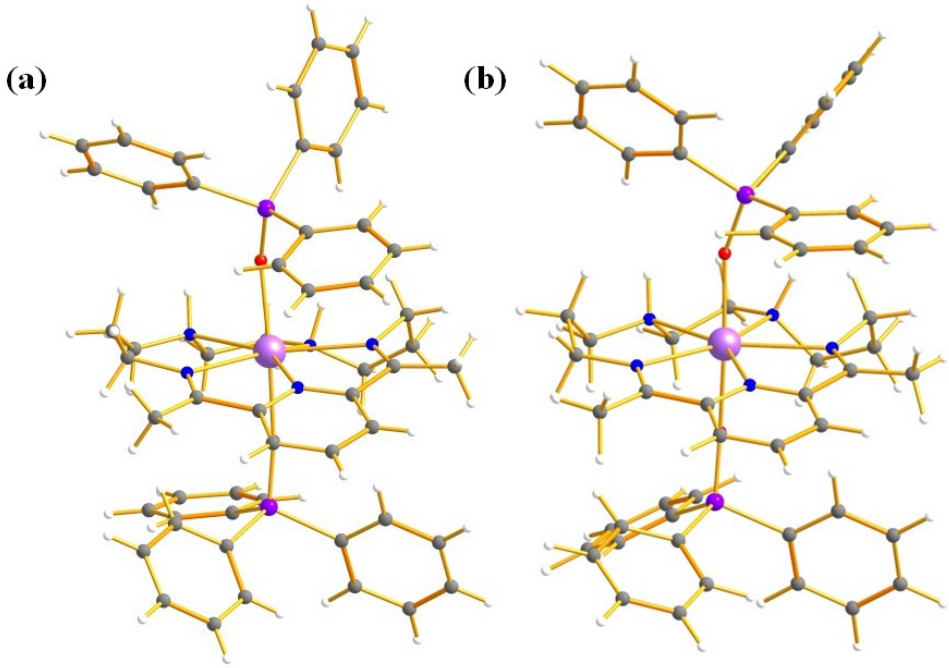


Figure S31. (a) The crystal structure and (b) DFT optimized structure of **4**. Colour code: Dy-blue violet, Si-purple, O-red, N-blue, C-grey and H-white.

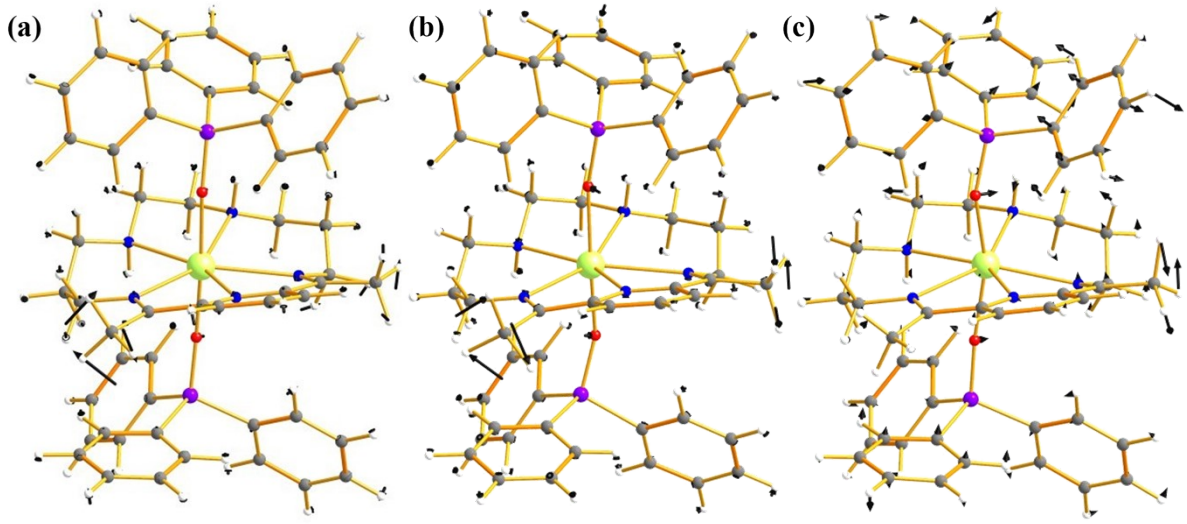


Figure S32. The molecular vibrations of **4** corresponds to (a) $^{\omega_1}$ (b) $^{\omega_2}$ and (c) $^{\omega_3}$ vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

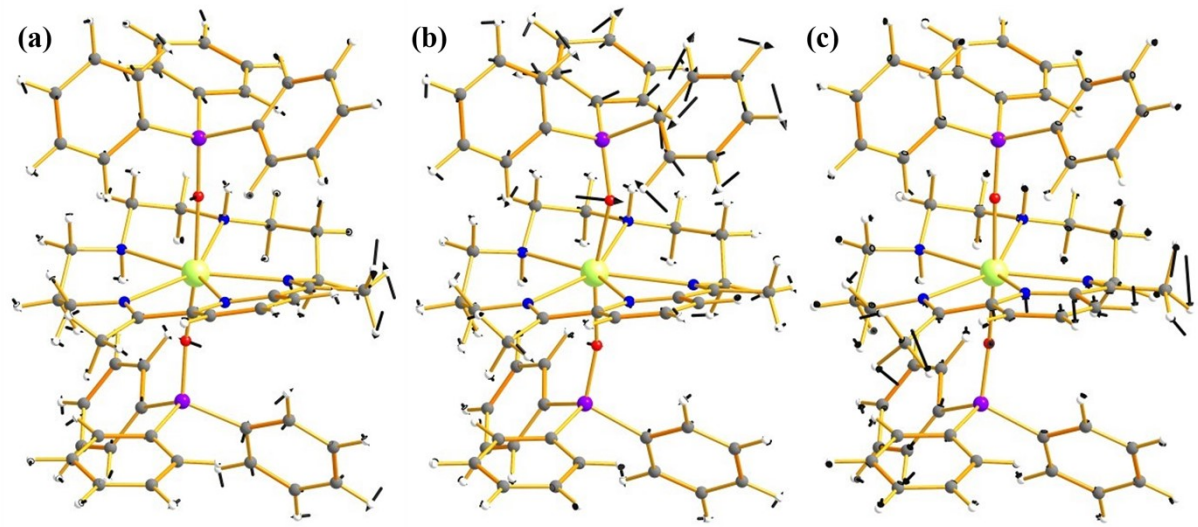


Figure S33. The molecular vibrations of **4** corresponds to (a) $^{\omega_4}$ (b) $^{\omega_5}$ and (c) $^{\omega_6}$ vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

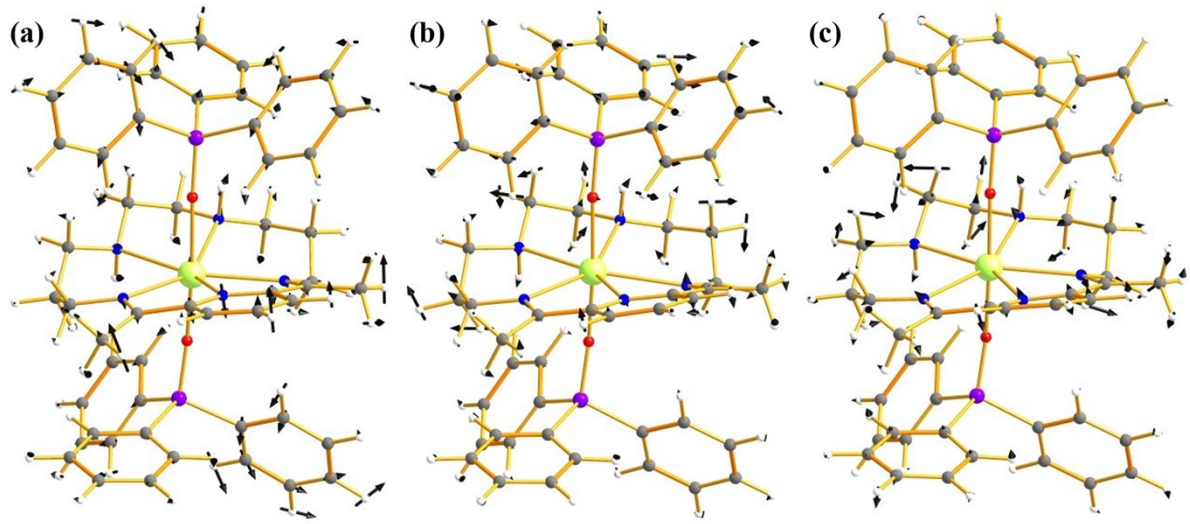


Figure S34. The molecular vibrations of **4** corresponds to (a) $^{\omega_7}$ (b) $^{\omega_8}$ and (c) $^{\omega_9}$ vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

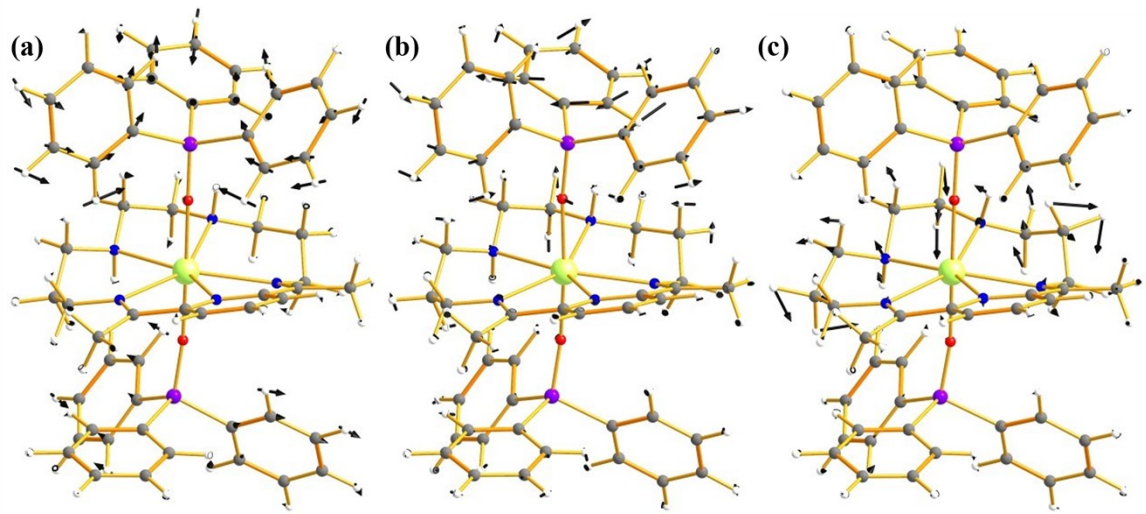


Figure S35. The molecular vibrations of **4** corresponds to (a) ω_{10} (b) ω_{11} and (c) ω_{12} vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code

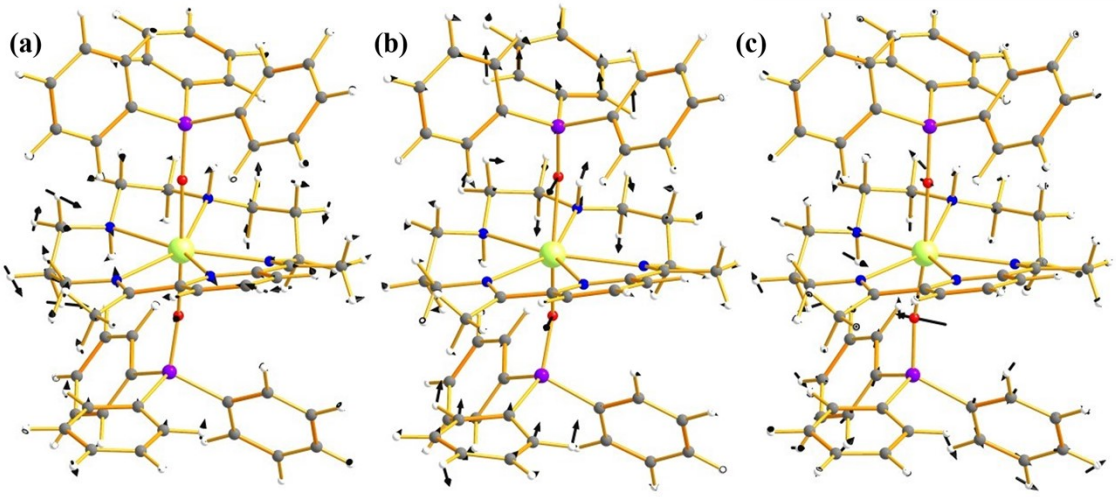


Figure S36. The molecular vibrations of **4** corresponds to (a) ω_{13} (b) ω_{14} and (c) ω_{15} vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

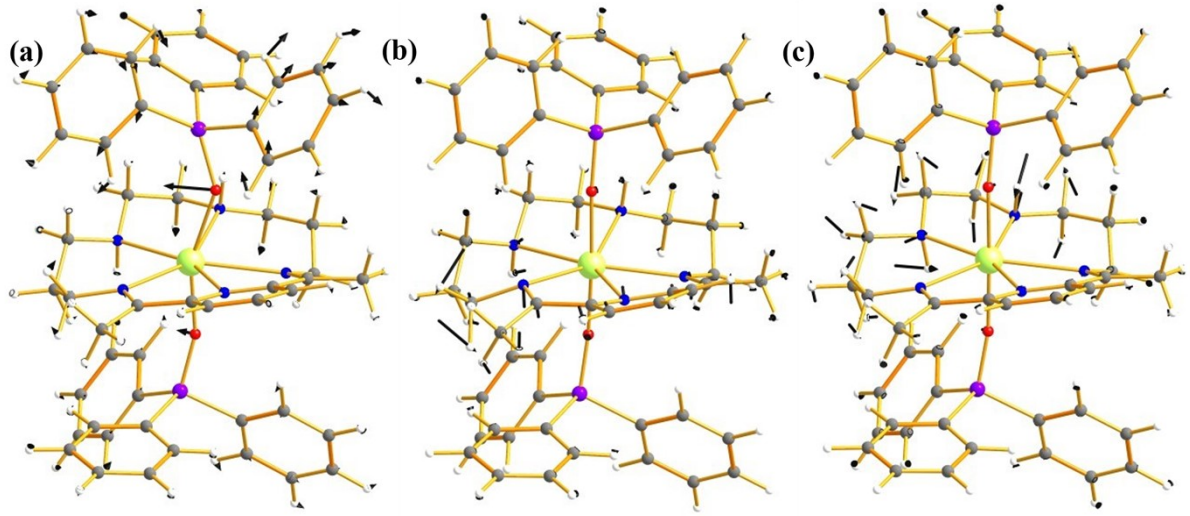


Figure S37. The molecular vibrations of **4** corresponds to (a) ω_{16} (b) ω_{17} and (c) ω_{18} vibrational modes. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

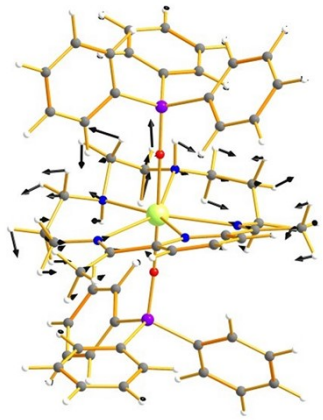
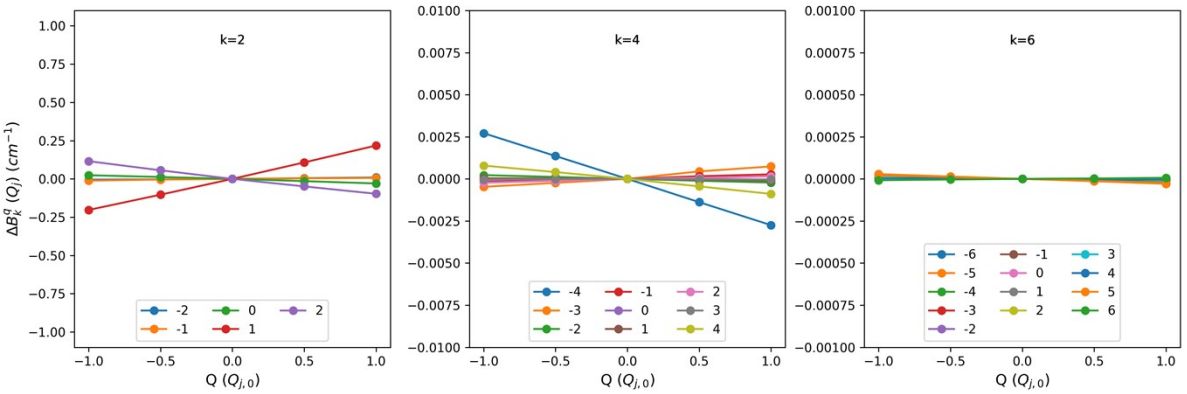
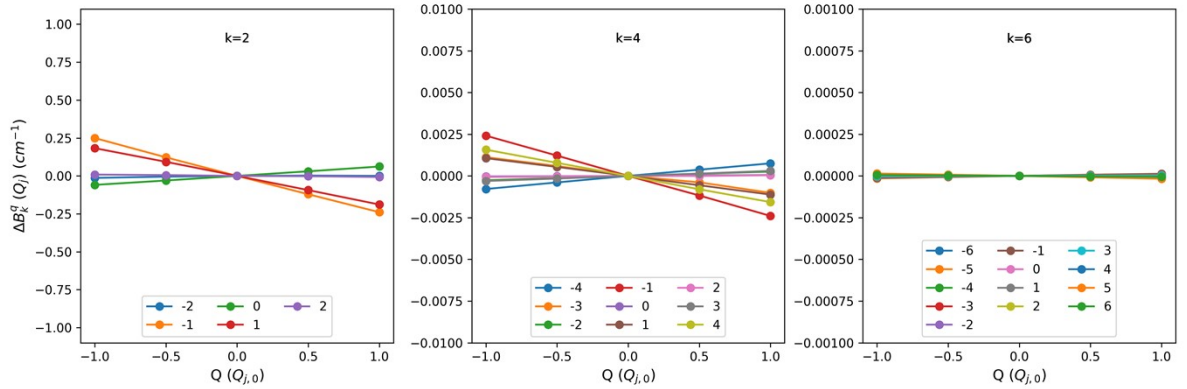


Figure S38. The molecular vibrations of **4** corresponds to ω_{19} vibrational mode. The black arrow corresponds to the scaled displacement vectors. See Figure S1 for colour code.

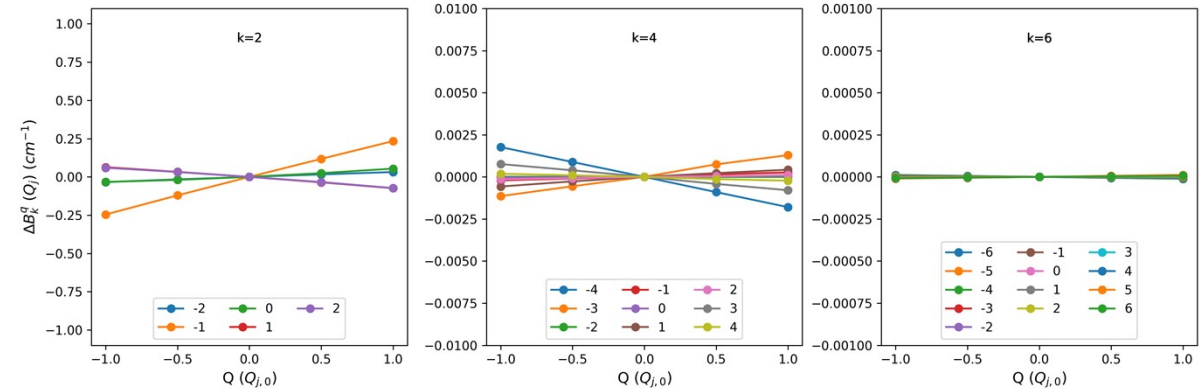
Mode (j) = 1



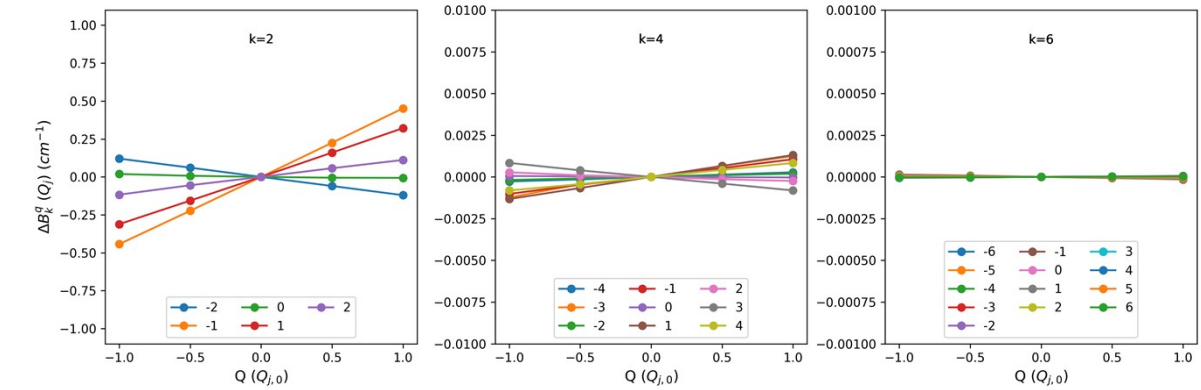
Mode (j) = 2

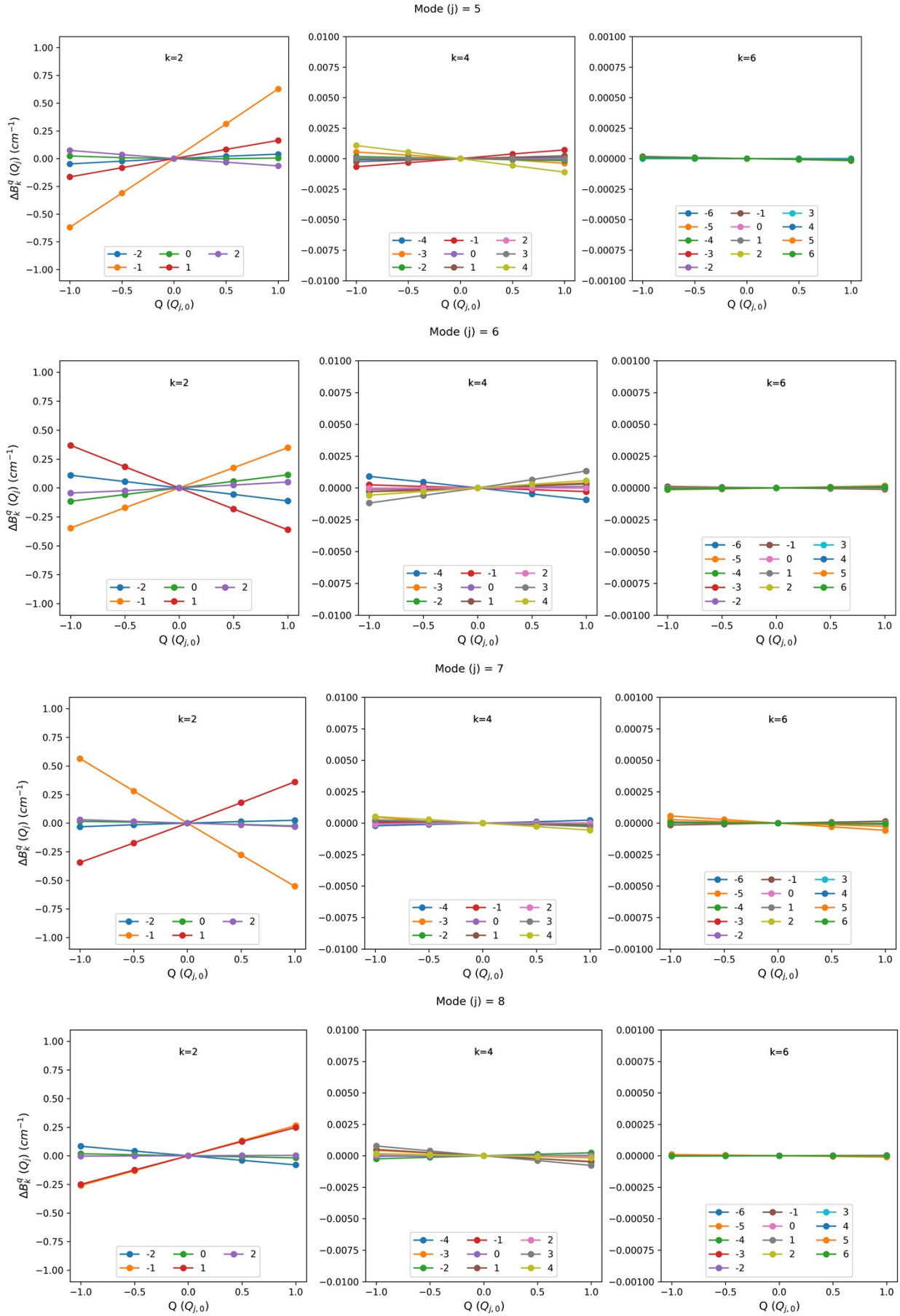


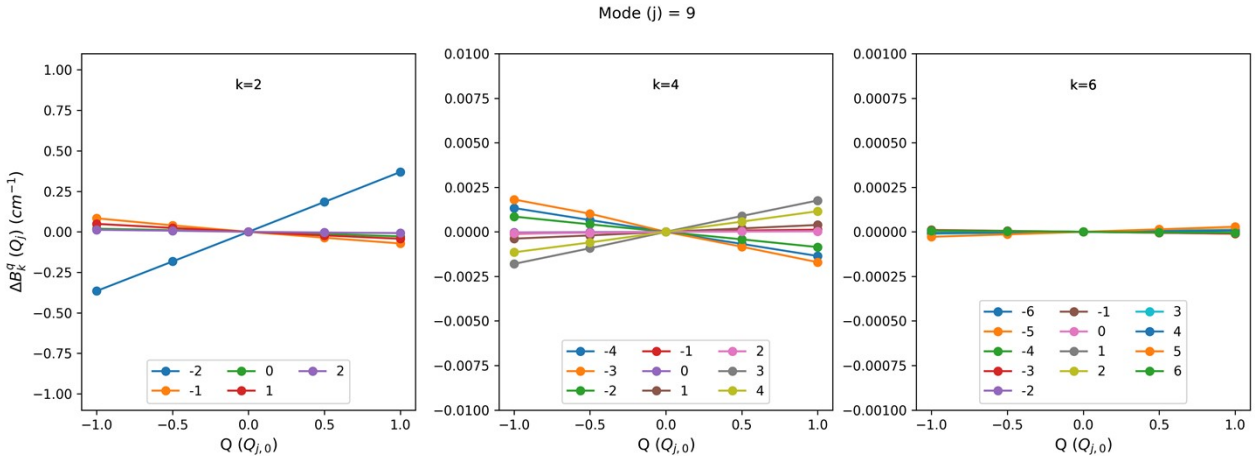
Mode (j) = 3

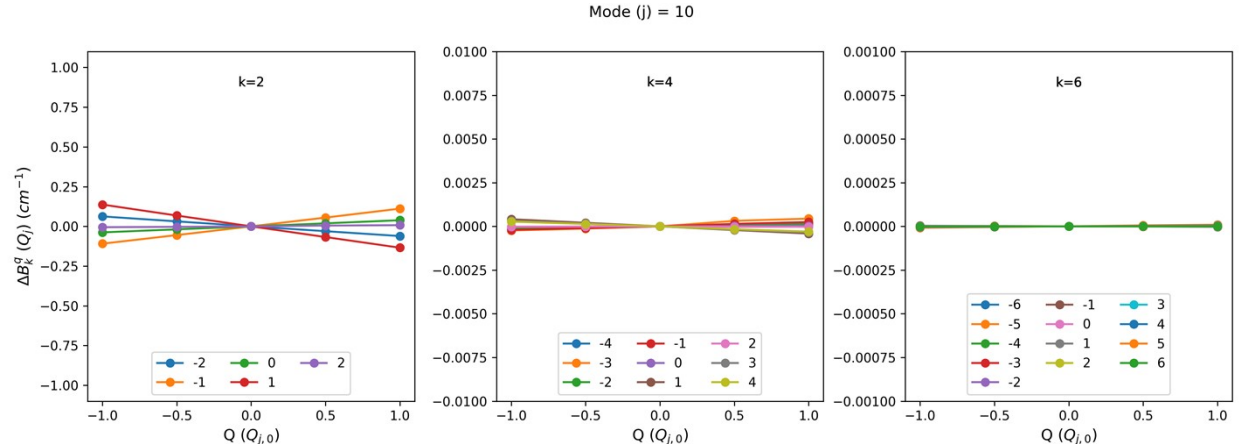


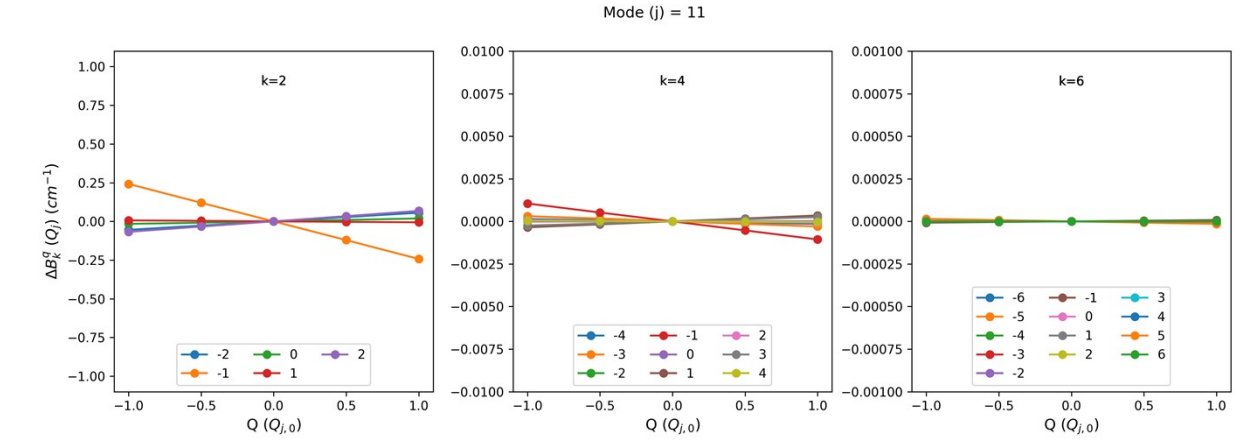
Mode (j) = 4

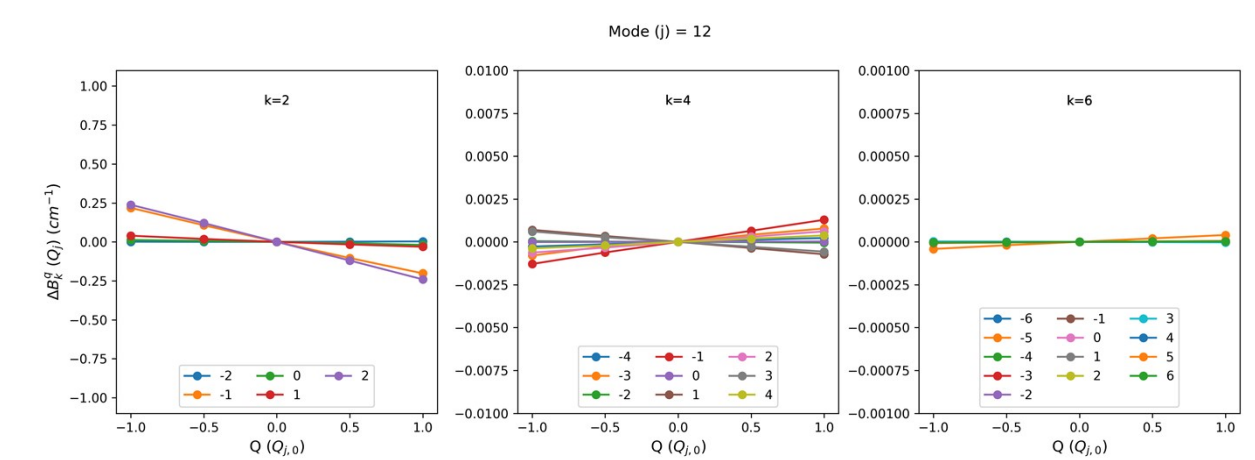


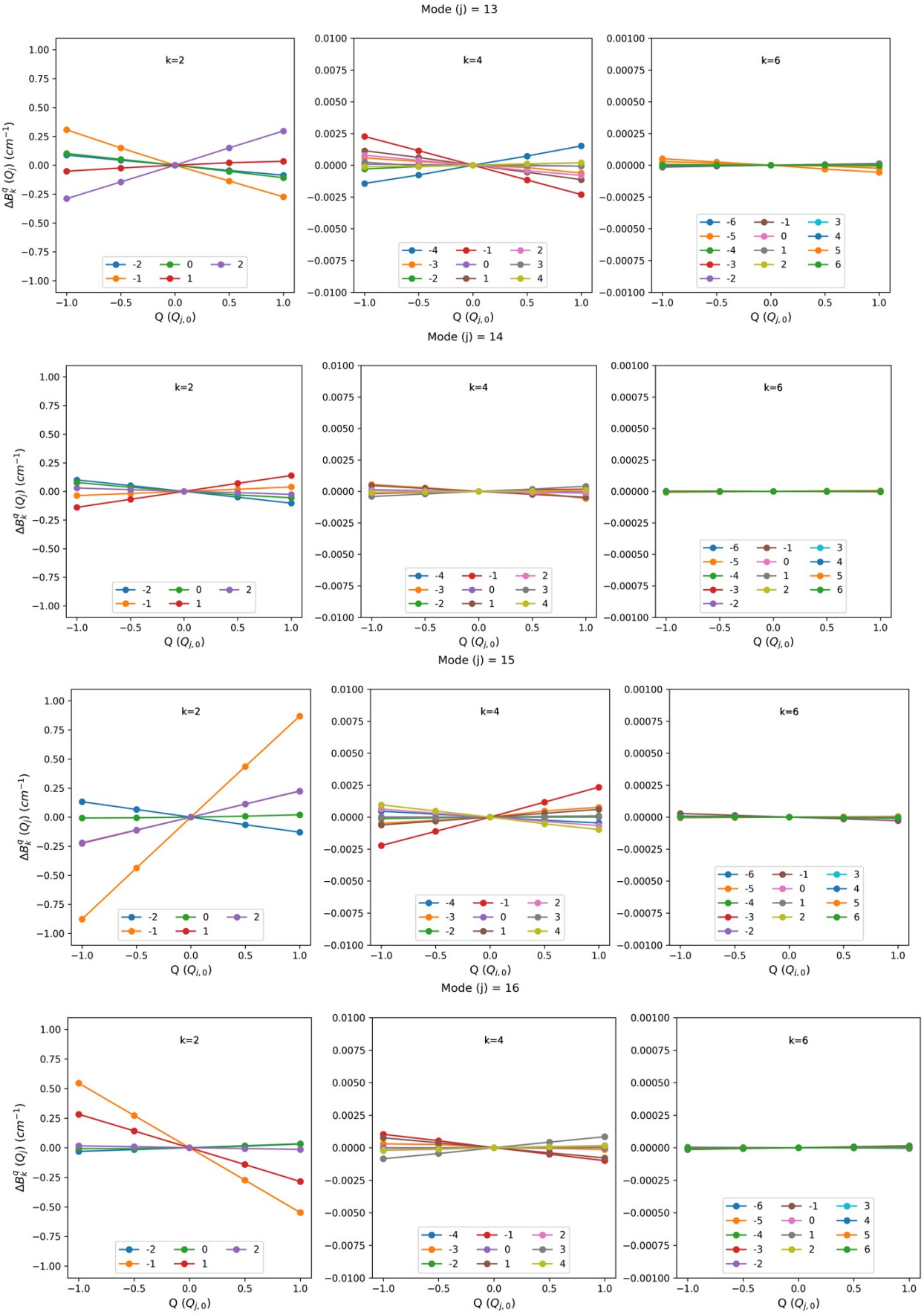

Mode (j) = 5
Mode (j) = 6
Mode (j) = 7
Mode (j) = 8
k=2
k=4
k=6
$\Delta B_k^q\ (Q_j)\ (cm^{-1})$
Q $(Q_{j,0})$


Mode (j) = 9
k=2
k=4
k=6
$\Delta B_k^q\ (Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)


Mode (j) = 10
k=2
k=4
k=6
$\Delta B_k^q\ (Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)


Mode (j) = 11
k=2
k=4
k=6
$\Delta B_k^q\ (Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)


Mode (j) = 12
k=2
k=4
k=6
$\Delta B_k^q\ (Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)


Mode (j) = 13
k=2
k=4
k=6
Mode (j) = 14
k=2
k=4
k=6
Mode (j) = 15
k=2
k=4
k=6
Mode (j) = 16
k=2
k=4
k=6
$\Delta B_k^q(Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)
Q ($Q_{i,0}$)

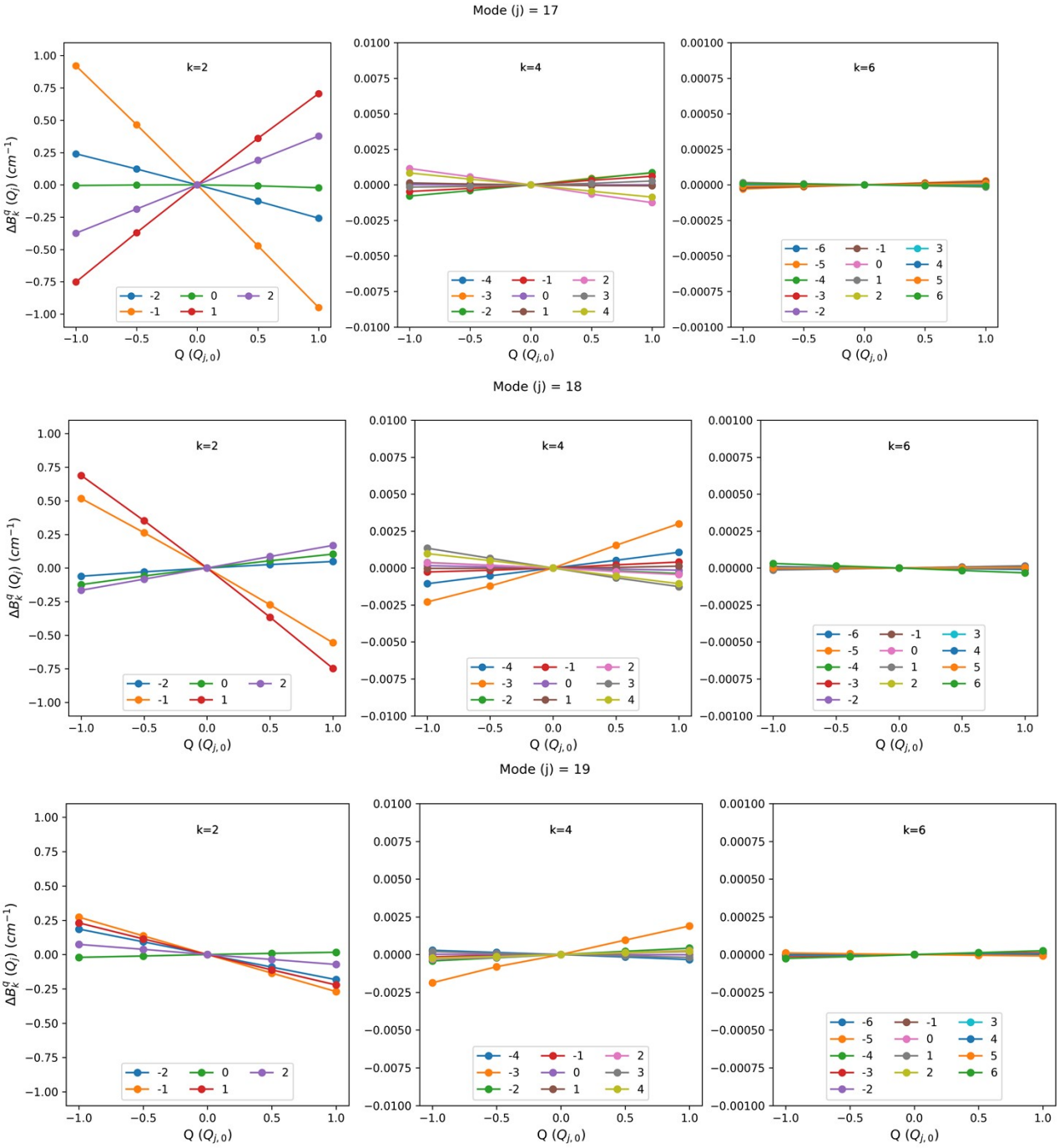


Figure S39. The variation of CFPs as a function of displacement for vibrational modes 1-19 of complex **4**.

Table S24. The vibrational mode numbers (ω), energy (cm^{-1}), oscilator strength (km mol^{-1}), population (at 100 K), maximum displacement (Q_k) and coupling strength (S_j in cm^{-1}) of the first 66 normal modes of **4**. The mode numbers corresponds to the one which has been taken into consideration in our study.

Mode number (j)	Energy	oscilator strength	population	Q_k	S_j
	8.4	0.013	0.053		
	12.1	0.254	0.050		
	15.1	0.207	0.048		
	18.3	0.389	0.046		
	22.9	0.284	0.043		

	28.4	0.759	0.040		
	29.2	0.356	0.039		
	32.3	0.299	0.037		
	35.1	0.708	0.036		
	36.6	0.745	0.035		
	39.6	1.154	0.034		
	41.2	0.972	0.033		
	43.5	0.164	0.032		
	45.3	1.185	0.031		
	47.3	0.050	0.030		
	50.6	2.118	0.029		
	52.4	1.981	0.028		
	55.8	0.136	0.027		
	57.1	0.424	0.026		
	59.0	1.184	0.026		
	60.8	0.441	0.025		
	61.2	0.374	0.025		
	70.9	0.781	0.022		
	78.5	0.594	0.019		
	81.0	0.942	0.019		
	86.9	2.094	0.017		
	93.7	0.298	0.015		
	122.9	0.513	0.010		
	127.4	1.620	0.010		
	136.2	0.378	0.008		
	139.6	0.247	0.008		
1	147.7	3.433	0.007	0.25	0.061
2	150.2	3.864	0.007	0.29	0.081
	153.4	2.126	0.007		
	156.6	2.123	0.006		
3	159.1	11.804	0.006	0.20	0.068
	166.0	2.147	0.005		
	167.3	1.676	0.005		
4	170.0	8.039	0.005	0.21	0.148
	172.8	0.910	0.005		
5	175.1	8.754	0.005	0.18	0.168
	176.9	0.718	0.005		
6	185.1	5.046	0.004	0.26	0.137
7	198.0	52.426	0.003	0.16	0.171
	223.4	0.434	0.002		
8	225.3	2.021	0.002	0.20	0.096
9	228.1	3.132	0.002	0.21	0.098
	229.7	0.733	0.002		
	232.0	1.597	0.002		
10	232.8	9.618	0.002	0.16	0.049
	246.6	0.354	0.002		
11	248.1	4.524	0.002	0.17	0.067
12	253.5	6.162	0.002	0.23	0.083
13	264.0	0.551	0.001	0.19	0.113
	266.6	1.318	0.001		
14	271.5	38.512	0.001	0.14	0.049
15	275.0	6.318	0.001	0.14	0.242
16	279.1	17.077	0.001	0.13	0.159
	286.6	1.184	0.001		
	304.4	1.937	0.001		
	307.0	1.520	0.001		
17	323.7	14.829	0.001	0.19	0.327
18	333.0	6.290	0.000	0.19	0.238

19	342.7	3.957	0.000	0.18	0.104
	346.8	1.945	0.000		
	380.9	0.295	0.000		
Total			1.00		

Table S25. The computed energies (cm^{-1}) along with g tensor of eight $^6H_{15/2}$ KDs of optimized geometry of **4-N3O2**.

Energy	g_x	g_y	g_z	Angle of g_{zz} between ground and higher excited KDs (°)
0.0	0.000	0.000	19.982	
457.0	0.028	0.032	17.047	0.813
826.7	0.454	0.672	13.986	1.731
998.7	0.769	2.648	15.603	88.928
1039.6	0.987	5.036	10.537	90.329
1098.5	0.922	4.264	8.190	92.051
1143.1	2.329	5.329	12.988	90.352
1246.6	0.666	0.996	18.022	89.709

Table S26. The computed energies (cm^{-1}) along with g tensor of eight $^6H_{15/2}$ KDs of optimized geometry of **4-N3O2**.

Table S27. The computed energies (cm^{-1}) along with g tensor of eight $^6H_{15/2}$ KDs of optimized geometry of **5**. The values in parenthesis correspond to the previous calculations with the X-ray crystal structure.

Energy	g_x	g_y	g_z
0.0 (0.0)	0.000 (0.000)	0.000 (0.000)	19.964 (19.979)
269.7 (316.8)	0.010 (0.012)	0.011 (0.014)	17.132 (17.160)
373.4 (471.3)	13.593 (0.707)	7.492 (2.930)	1.289 (17.120)
422.9	4.439	4.135	1.546
461.7	0.268	0.469	13.187
504.7	0.932	2.079	8.555
546.8	1.124	2.159	10.961
653.7	0.006	0.033	18.517

Table S28. A comparison of selected structural parameters (bond lengths are shown in Å and bond angles are shown in degree) between optimized and X-ray crystal structures of **5**.

Structural parameter	Crystal structure	DFT optimized geometry
Dy-O1 (P)	2.203	2.245
Dy-O2 (P)	2.207	2.245
Dy-O3 (OH_2)	2.363	2.347
Dy-O4 (OH_2)	2.365	2.347
Dy-O5 (OH_2)	2.356	2.369
Dy-O6 (OH_2)	2.375	2.363
Dy-O7 (OH_2)	2.363	2.372
O1-Dy-O2	175.2	176.1

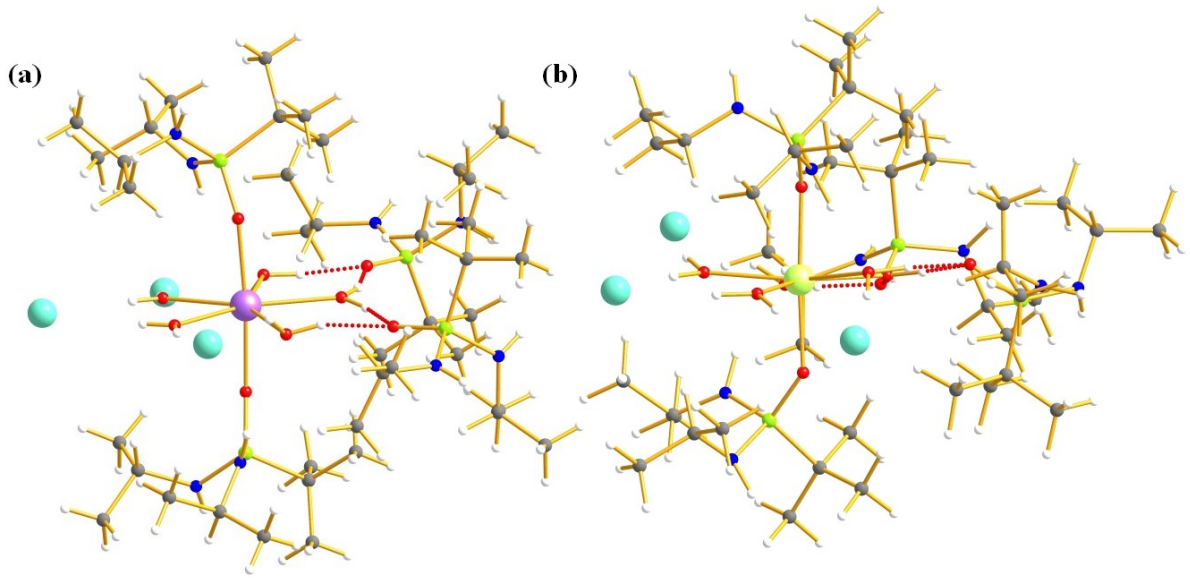


Figure S40. The crystal structure (left) and DFT optimized structure (right) of **5**. Colour code: Dy-blue violet, Y-yellow, P-green, I-aqua, O-red, N-blue, C-grey and H-white.

Table S29. The computed CF parameters of X-ray structure of **5**, H-optimized geometry of **5**. Here, the CF parameters have been computed according to Stevens Hamiltonian:

$$H_{CF} = \sum_{k=2,4,6} \sum_{q=-k}^{q=+k} B_k^q \tilde{O}_k^q$$

where B_k^q is the CF parameter and $\tilde{O}_k^q$ is the Stevens operator.

k	q	B_k^q	
		5 (X-ray)	**5** (opt)
2	-2	-2.49E-01	1.17E-01
	-1	9.19E-01	-2.07E+00
	0	-2.84E+00	-2.26E+00
	1	1.92E+00	-2.75E-01
	2	-3.51E-01	-3.79E-01
4	-4	2.88E-03	-2.68E-03
	-3	2.02E-02	3.30E-02
	-2	2.71E-03	9.64E-05
	-1	-4.17E-03	9.37E-03
	0	-1.25E-02	-1.17E-02
	1	-1.00E-02	1.18E-03
	2	1.86E-03	-4.27E-04
	3	-3.01E-03	1.51E-02
	4	-6.67E-04	4.28E-03
6	-6	-9.48E-06	-5.16E-05
	-5	7.42E-05	-3.63E-05
	-4	1.55E-05	-1.44E-05
	-3	1.01E-04	1.76E-04
	-2	-1.26E-05	-1.29E-05
	-1	-3.60E-05	7.84E-05
	0	2.92E-05	3.20E-05
	1	-4.80E-05	1.24E-05
	2	-2.81E-06	4.23E-05
	3	-2.52E-05	7.76E-05
	4	-4.62E-06	3.48E-05
	5	7.46E-05	-2.67E-05

	6	7.35E-05	2.58E-05

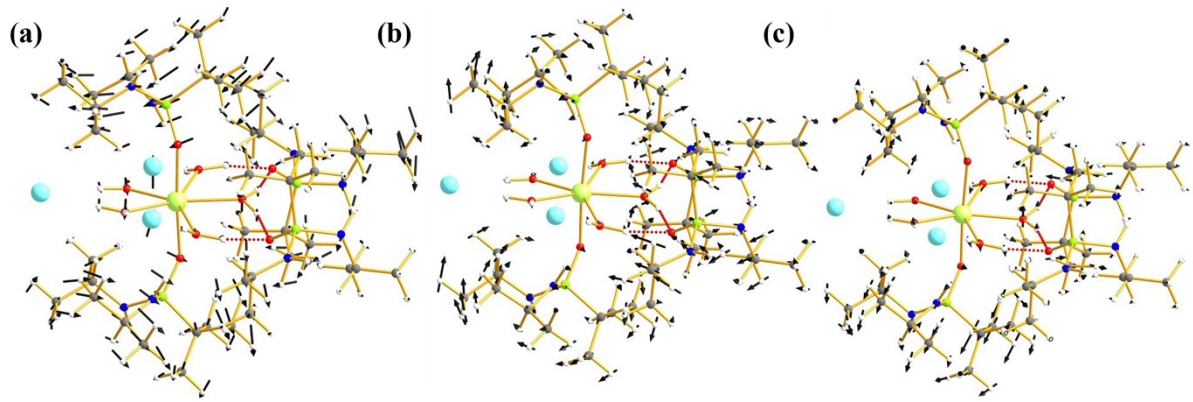


Figure S41. The molecular vibrations of **5** corresponds to (a) $^{\omega_1}$ (b) $^{\omega_2}$ and (c) $^{\omega_3}$ vibrational modes. The black arrow corresponds to the scaled displacement vectors. Colour code: Dy-blue violet, Y-yellow, P-green, I-aqua, O-red, N-blue, C-grey and H-white.

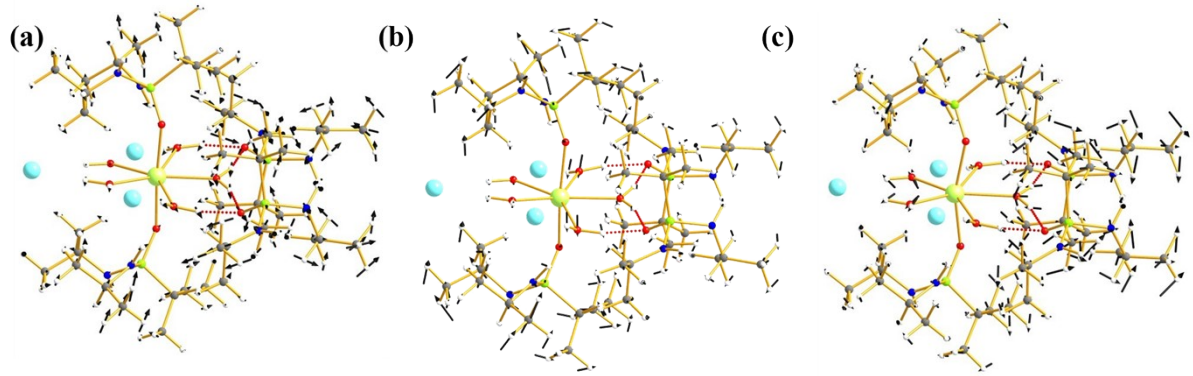


Figure S42. The molecular vibrations of **5** corresponds to (a) $^{\omega_4}$ (b) $^{\omega_5}$ and (c) $^{\omega_6}$ vibrational modes. The black arrow corresponds to the scaled displacement vectors. Colour code: Dy-blue violet, Y-yellow, P-green, I-aqua, O-red, N-blue, C-grey and H-white.

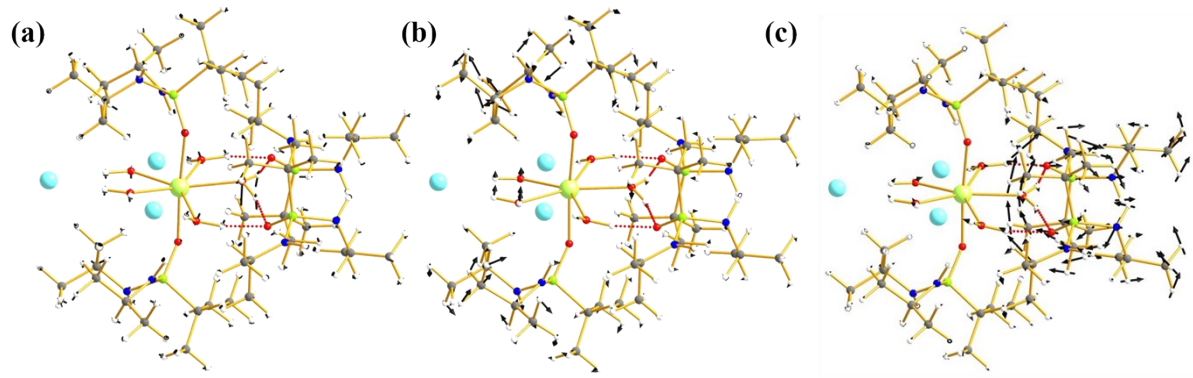
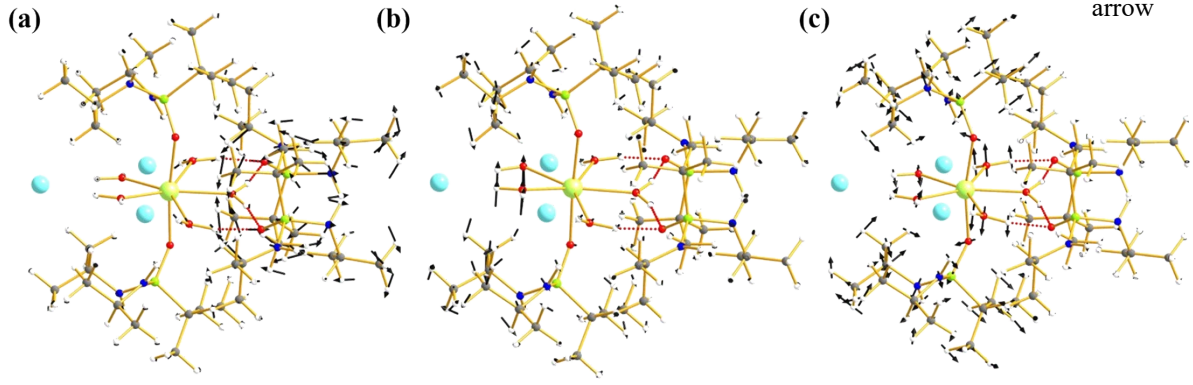


Figure S43. The molecular vibrations of **5** corresponds to (a) $^{\omega_7}$ (b) $^{\omega_8}$ and (c) $^{\omega_9}$ vibrational modes. The black arrow



corresponds to the scaled displacement vectors. Colour code: Dy-blue violet, Y-yellow, P-green, I-aqua, O-red, N-blue, C-grey and H-white.

Figure S44. The molecular vibrations of **5** corresponds to (a) ω_{10} (b) ω_{11} and (c) ω_{12} vibrational modes. The black arrow corresponds to the scaled displacement vectors. Colour code: Dy-blue violet, Y-yellow, P-green, I-aqua, O-red, N-blue, C-grey and H-white.

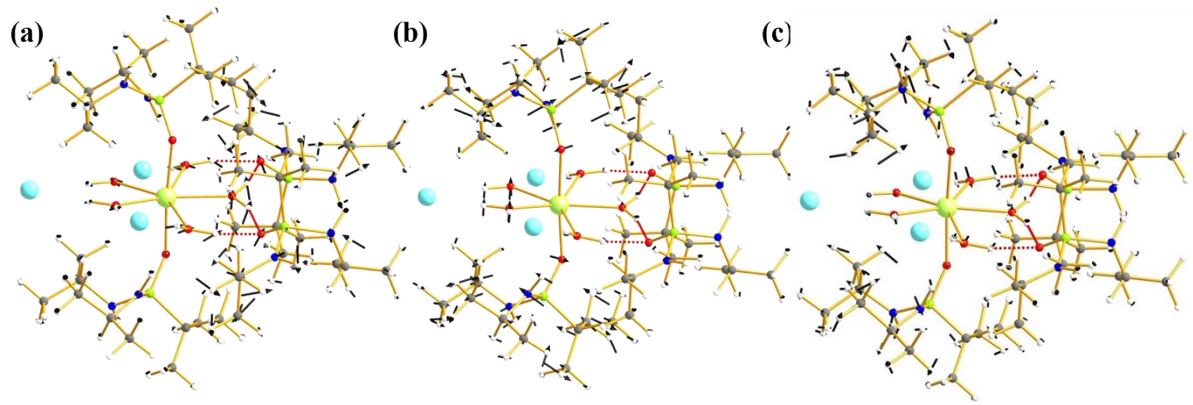


Figure S45. The molecular vibrations of **5** corresponds to (a) ω_{13} (b) ω_{14} and (c) ω_{15} vibrational modes. The black arrow corresponds to the scaled displacement vectors. Colour code: Dy-blue violet, Y-yellow, P-green, I-aqua, O-red, N-blue, C-grey and H-white.

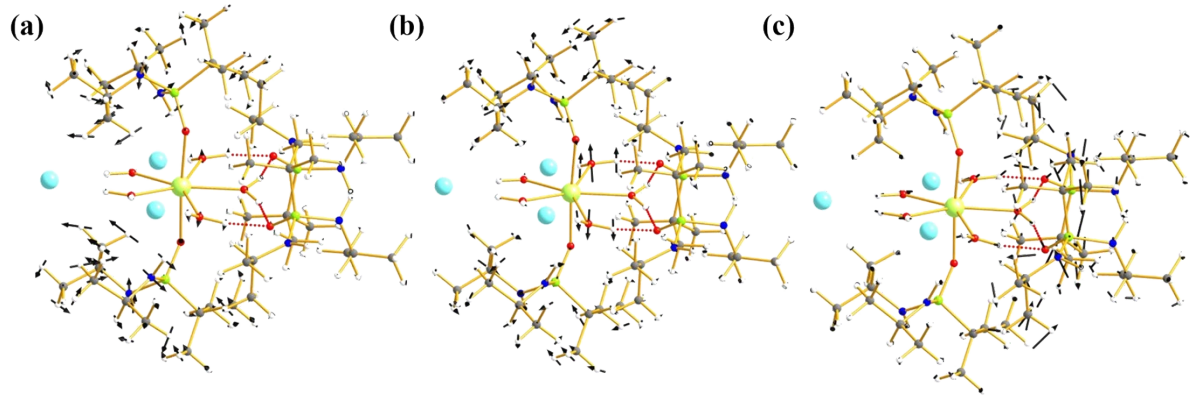


Figure S46. The molecular vibrations of **5** corresponds to (a) ω_{16} (b) ω_{17} and (c) ω_{18} vibrational modes. The black arrow corresponds to the scaled displacement vectors. Colour code: Dy-blue violet, Y-yellow, P-green, I-aqua, O-red, N-blue, C-grey and H-white.

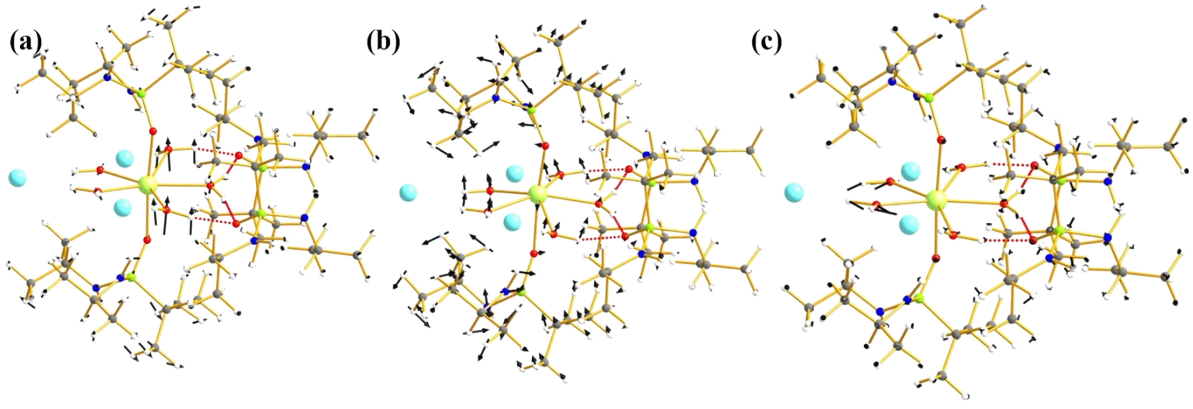


Figure S47. The molecular vibrations of **5** corresponds to (a) ω_{19} (b) ω_{20} and (c) ω_{21} vibrational modes. The black arrow corresponds to the scaled displacement vectors. Colour code: Dy-blue violet, Y-yellow, P-green, I-aqua, O-red, N-blue, C-grey and H-white.

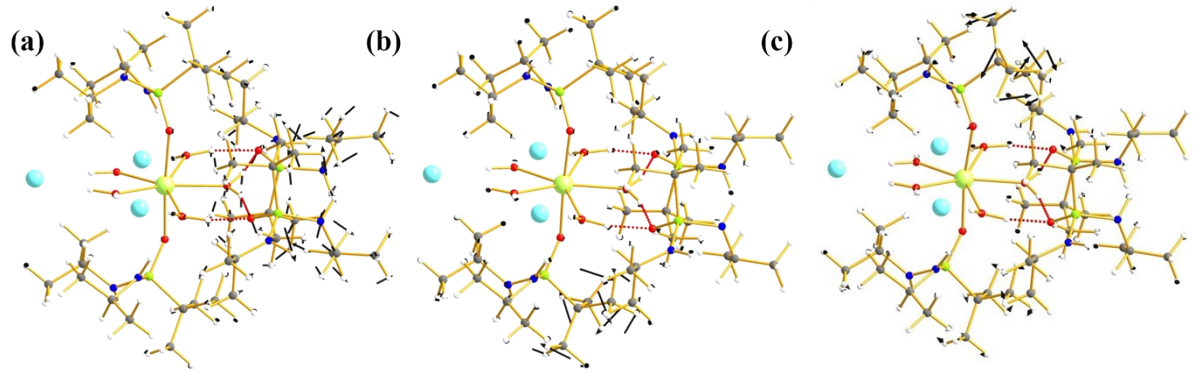


Figure S48. The molecular vibrations of **5** corresponds to (a) ω_{22} (b) ω_{23} and (c) ω_{24} vibrational modes. The black arrow corresponds to the scaled displacement vectors. Colour code: Dy-blue violet, Y-yellow, P-green, I-aqua, O-red, N-blue, C-grey and H-white.

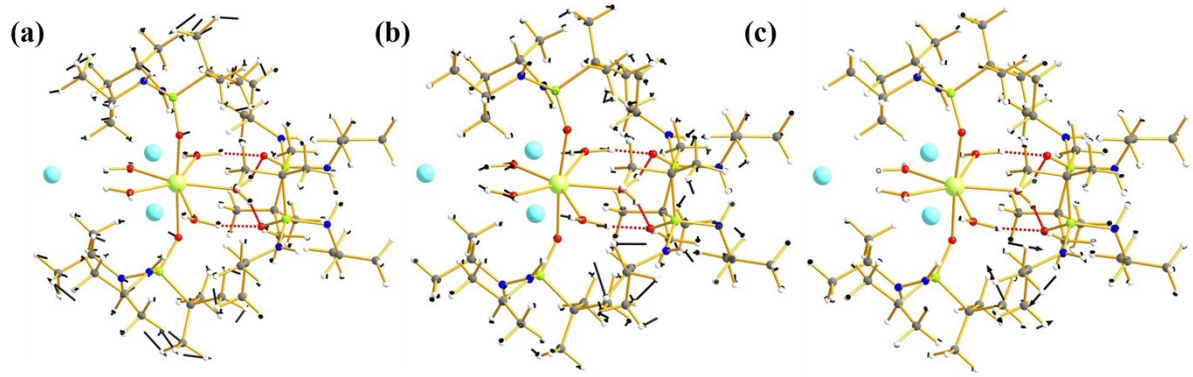


Figure S49. The molecular vibrations of **5** corresponds to (a) ω_{25} (b) ω_{26} and (c) ω_{27} vibrational modes. The black arrow corresponds to the scaled displacement vectors. Colour code: Dy-blue violet, Y-yellow, P-green, I-aqua, O-red, N-blue, C-grey and H-white.

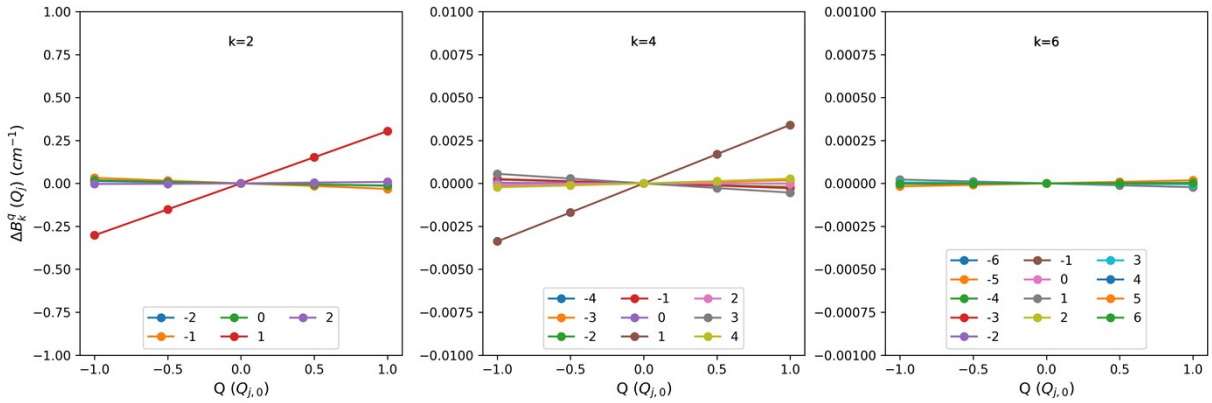
Table S30. The vibrational mode numbers (ω), energy (cm^{-1}), oscilator strength (km mol^{-1}), population (at 100 K), maximum displacement (Q_k) and coupling strength (S_j in cm^{-1}) of the first 66 normal modes of **5**. The mode numbers corresponds to the one which has been taken into consideration in our study.

Mode number (j)	Energy	oscilator strength	population	Q_k	S_j
	15.2	0.148	0.032		
	16.2	0.136	0.031		
1	18.8	2.634	0.030	0.48	0.079
	22.5	0.257	0.029		
	24.7	0.624	0.028		
	25.1	0.298	0.028		
	26.9	0.143	0.027		
	28.3	0.335	0.026		
	29.4	1.280	0.026		
	29.9	0.247	0.026		
	31.3	0.343	0.025		

	35.9	0.252	0.024		
	36.8	0.600	0.023		
	40.1	0.208	0.022		
	40.5	0.047	0.022		
	41.6	0.141	0.022		
	44.4	0.342	0.021		
	45.0	1.031	0.021		
	45.4	0.912	0.021		
	46.7	1.567	0.020		
	48.4	1.231	0.020		
	49.0	0.730	0.020		
	52.3	0.280	0.019		
	53.9	0.505	0.018		
2	54.8	2.274	0.018	0.38	0.022
	55.4	0.634	0.018		
	57.2	0.167	0.017		
	57.3	0.633	0.017		
	58.2	0.981	0.017		
	62.1	1.321	0.016		
	63.0	1.317	0.016		
	64.0	1.178	0.016		
	64.5	0.584	0.016		
	65.7	0.373	0.015		
	66.3	0.163	0.015		
	67.4	3.415	0.015		
	69.4	0.654	0.015		
	70.2	1.605	0.014		
	79.6	0.547	0.013		
3	80.3	3.812	0.012	0.30	0.052
4	82.4	2.827	0.012	0.31	0.084
	84.0	0.490	0.012		
	90.5	0.400	0.011		
	91.0	1.680	0.011		
	93.4	1.920	0.010		
	96.5	1.277	0.010		
5	99.6	5.416	0.009	0.27	0.087
6	100.6	7.860	0.009	0.32	0.057
7	114.6	6.297	0.008	0.22	0.139
8	117.3	4.533	0.007	0.29	0.149
	121.4	0.157	0.007		
	124.4	0.037	0.007		
9	129.3	9.377	0.006	0.24	0.129
10	132.4	6.856	0.006	0.24	0.047
11	134.6	0.632	0.006	0.24	0.104
12	143.5	10.821	0.005	0.23	0.079
13	149.0	9.222	0.005	0.23	0.015
14	158.9	6.201	0.004	0.22	0.191
	165.7	0.830	0.004		
15	167.0	3.992	0.004	0.22	0.078
	167.3	0.671	0.004		
16	168.3	1.678	0.004	0.22	0.101
17	172.3	6.489	0.003	0.22	0.100
18	173.6	3.411	0.003	0.22	0.085
19	178.5	7.717	0.003	0.18	0.132
20	183.6	29.181	0.003	0.22	0.116
	183.7	0.756	0.003		
21	191.4	5.648	0.003	0.20	0.060
22	211.0	14.923	0.002	0.22	0.005

23	214.6	13.093	0.002	0.22	0.031
	226.7	1.274	0.002	0.36	
24	229.0	3.156	0.001	0.34	0.038
	230.1	6.421	0.001		
25	233.4	3.955	0.001	0.23	0.123
26	234.2	5.340	0.001	0.24	0.039
27	236.6	7.354	0.001	0.35	0.016
	240.7	6.436	0.001		
	242.3	0.943	0.001		
	243.5	0.373	0.001		
	243.9	1.234	0.001		
	245.1	4.160	0.001		
	247.2	0.572	0.001		
	251.7	26.111	0.001		
	252.7	10.972	0.001		
	254.4	0.827	0.001		
	255.2	3.912	0.001		
	256.5	14.157	0.001		
	257.4	2.022	0.001		
Total			1.00		

Mode (j) = 1



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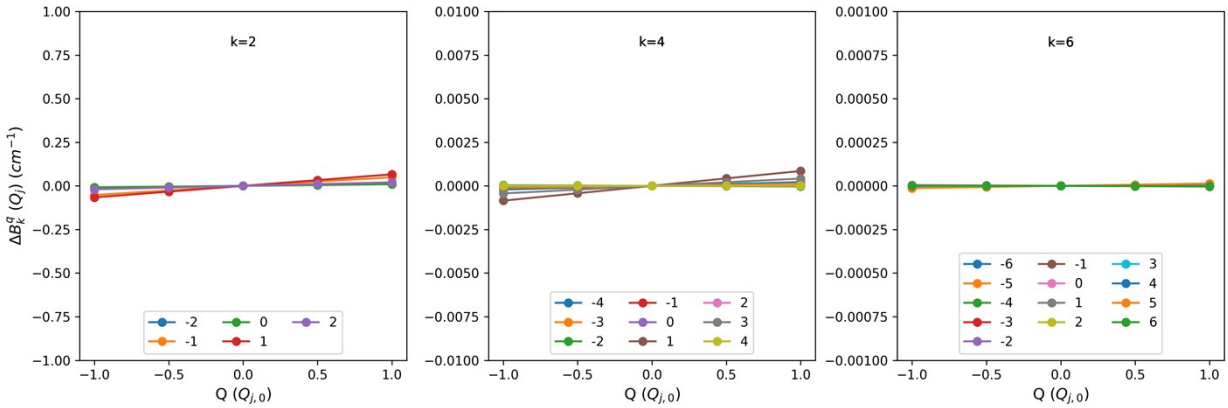

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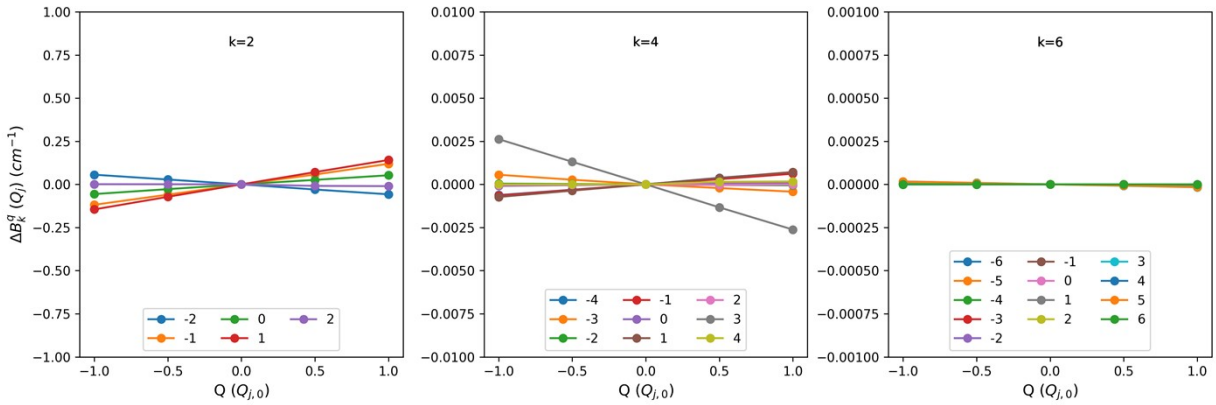

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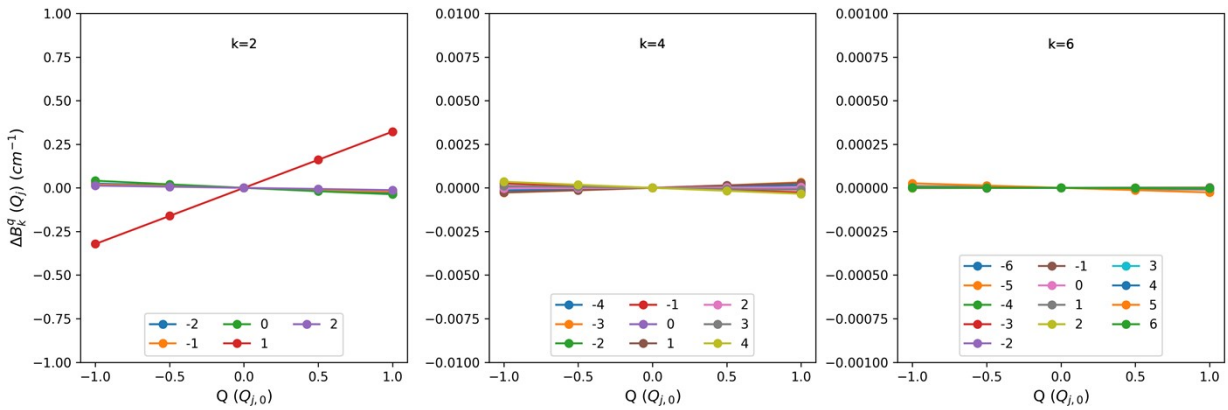

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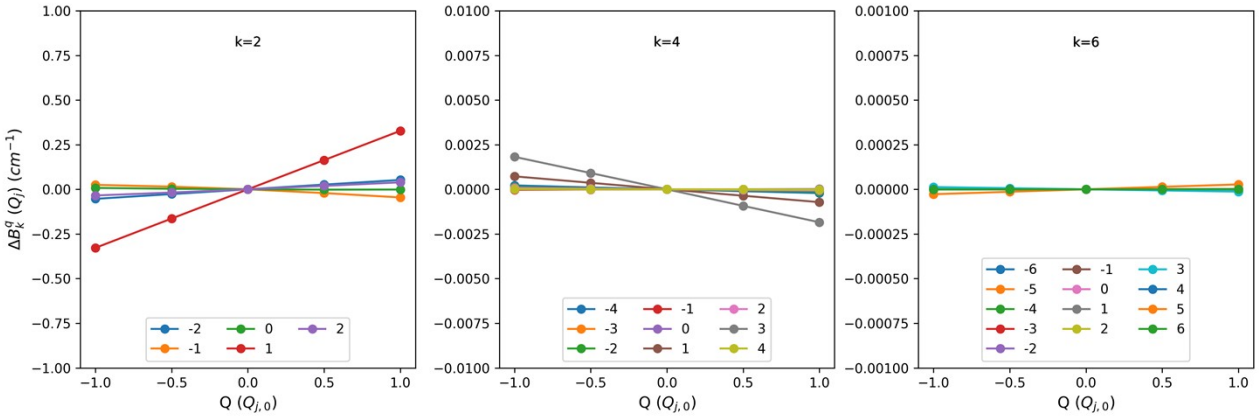

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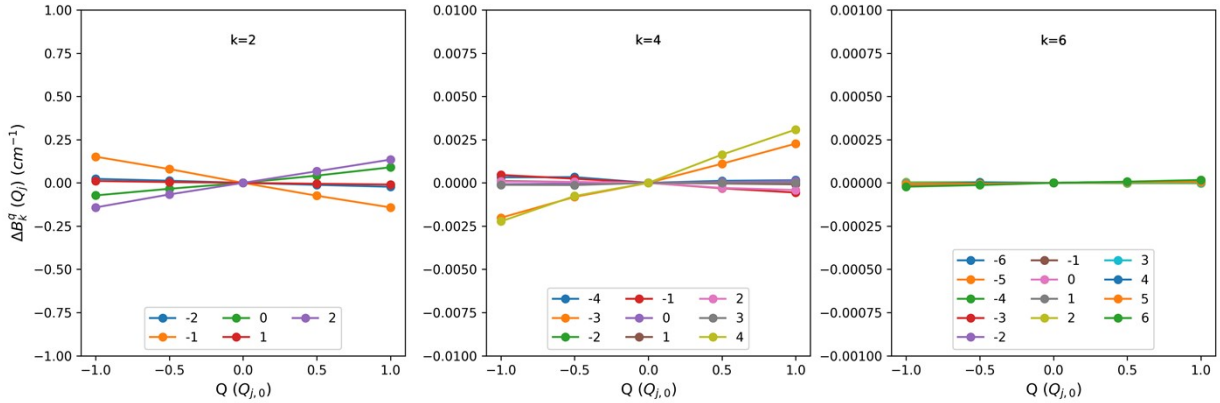

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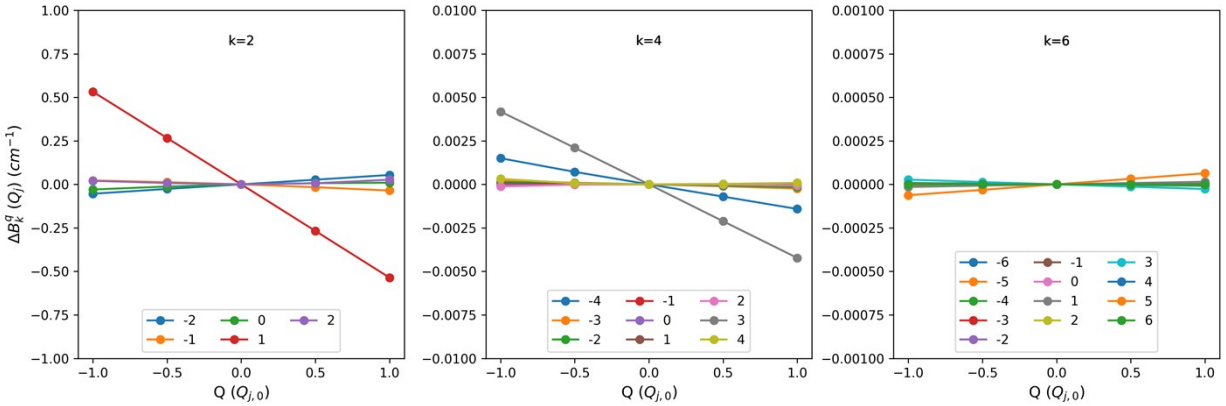

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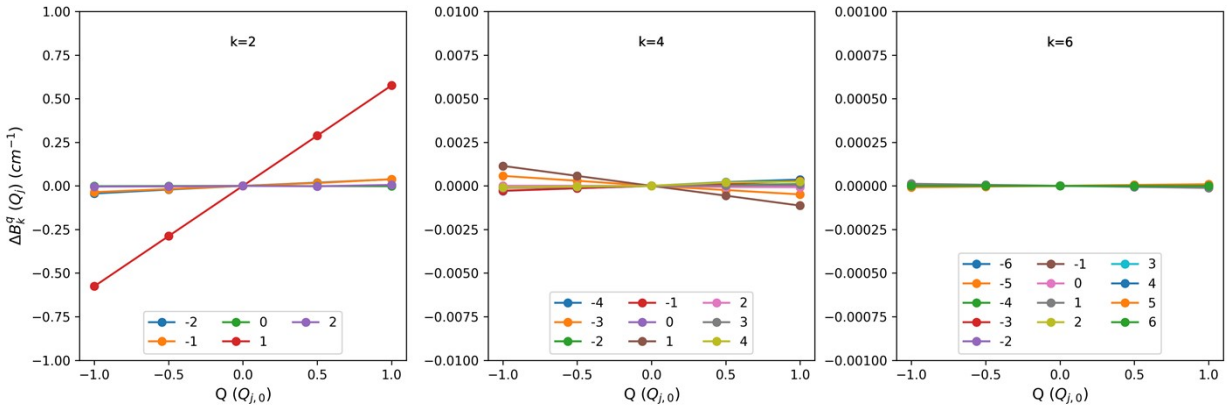

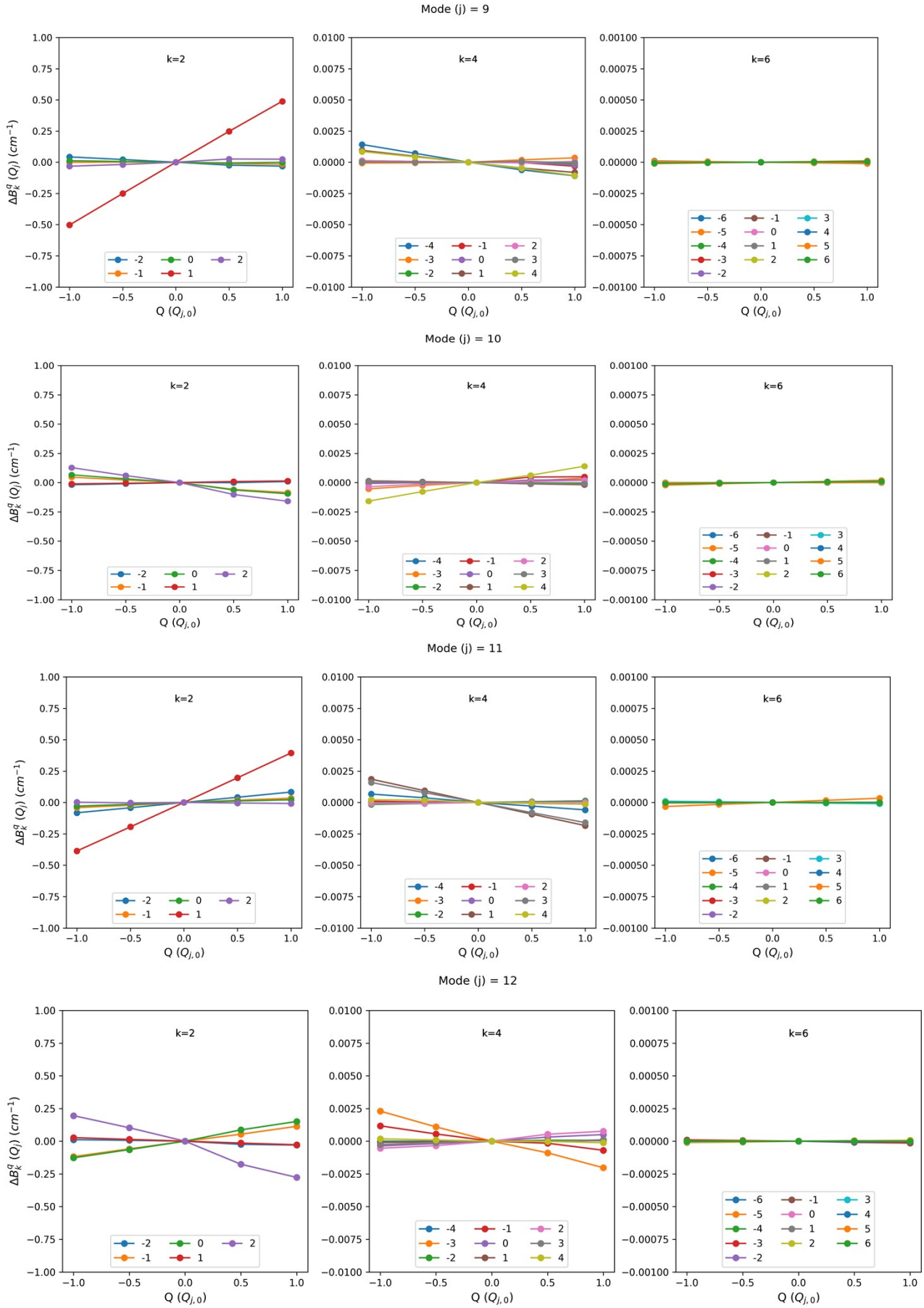
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k=6
Mode (j) = 10
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k=4
k=6
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k=2
k=4
k=6
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k=4
k=6
$\Delta B_k^q(Q_j)\ (cm^{-1})$
Q $(Q_{j,0})$

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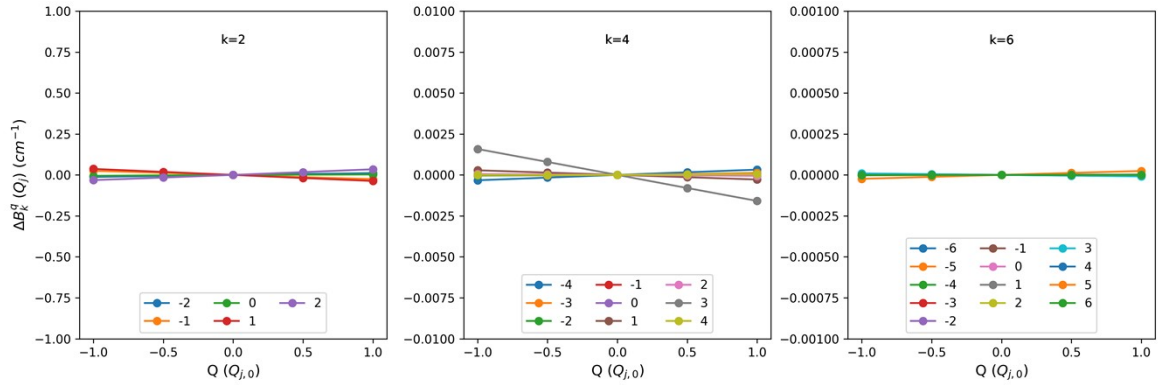

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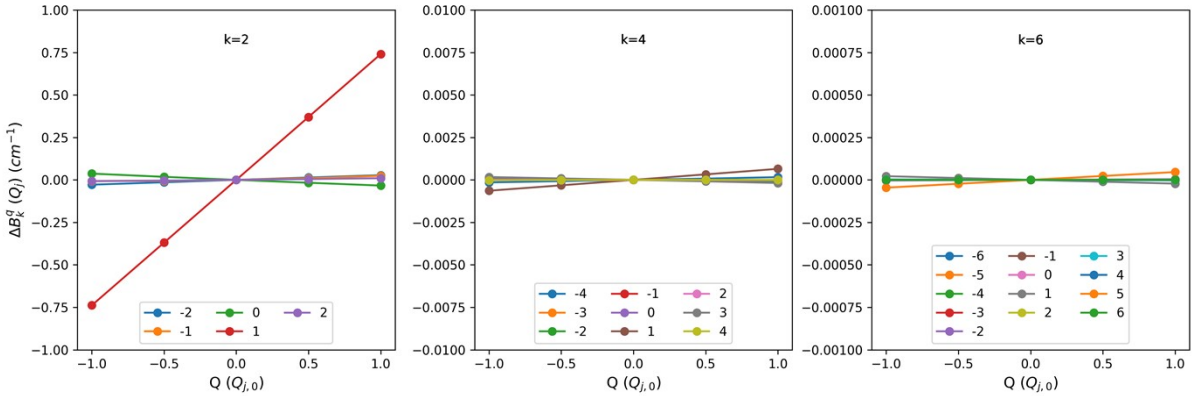
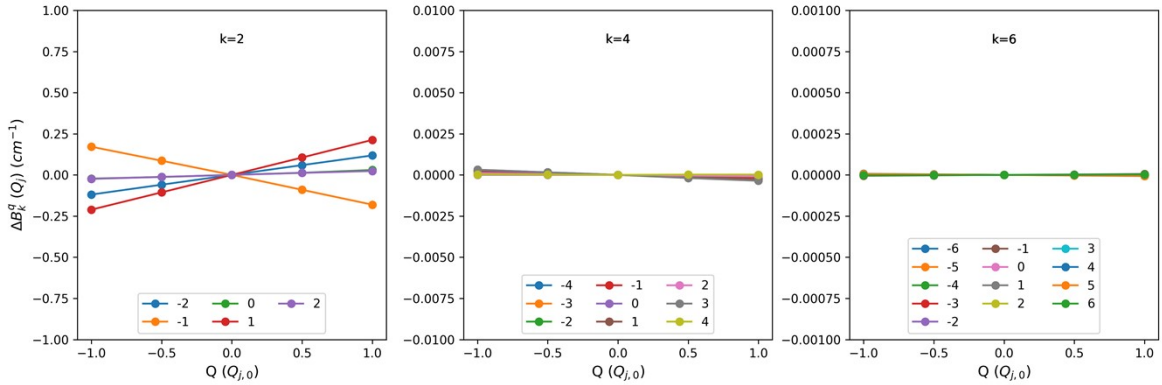
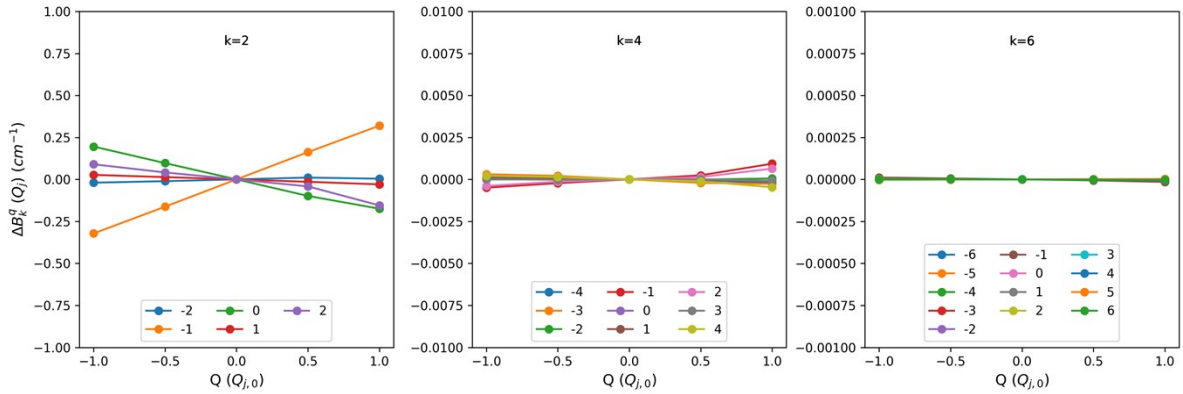
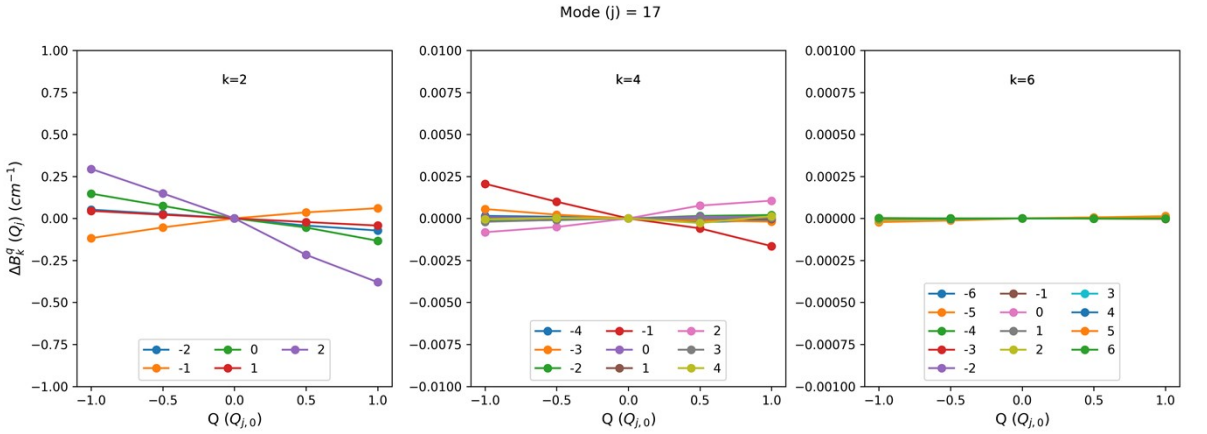


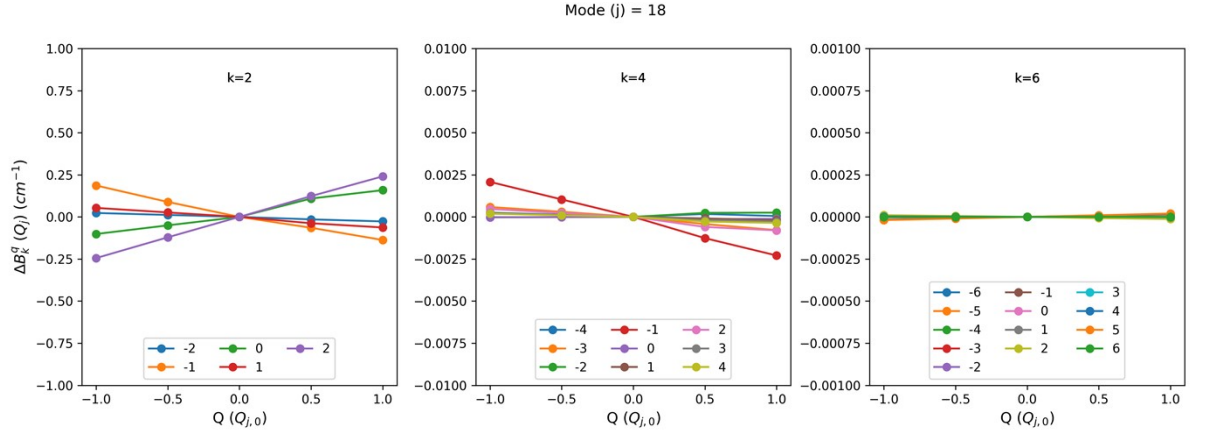
Mode (j) = 15

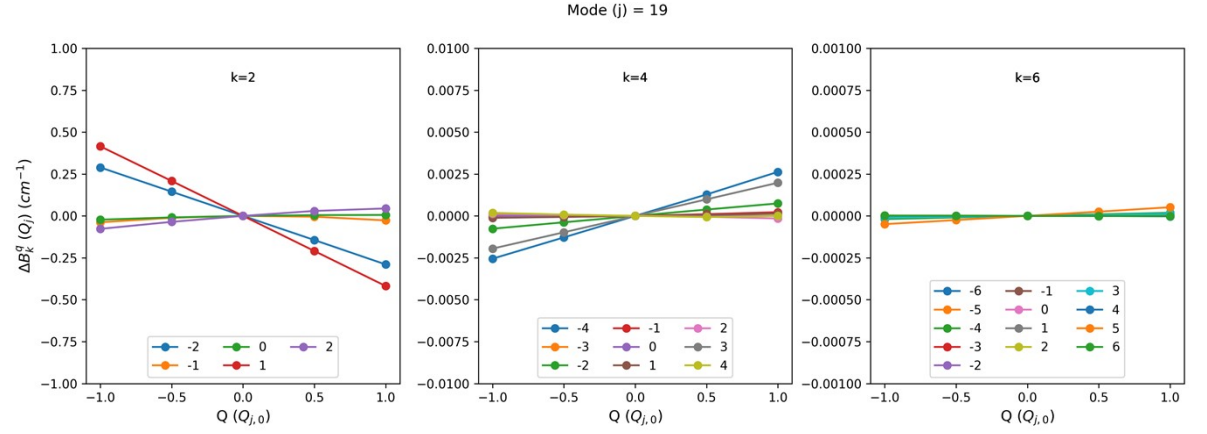


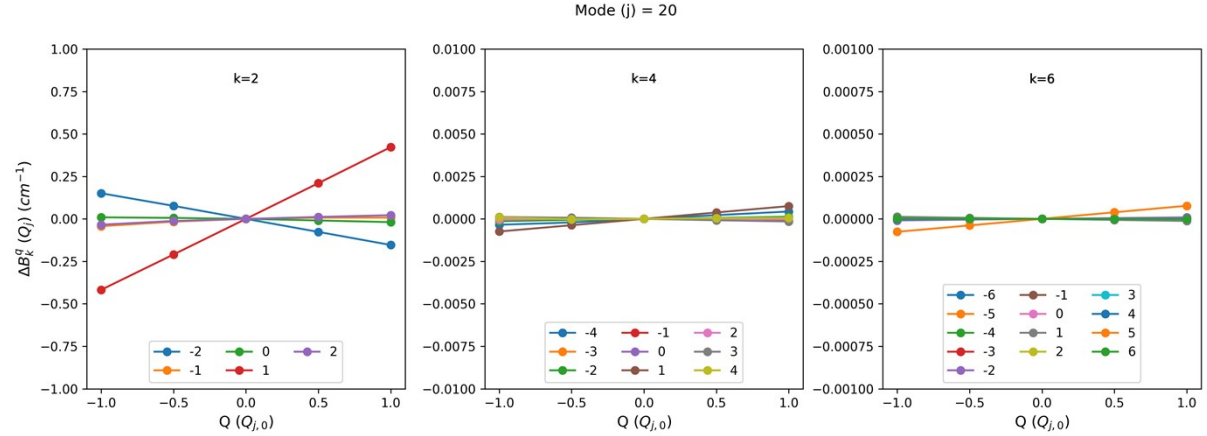
Mode (j) = 16

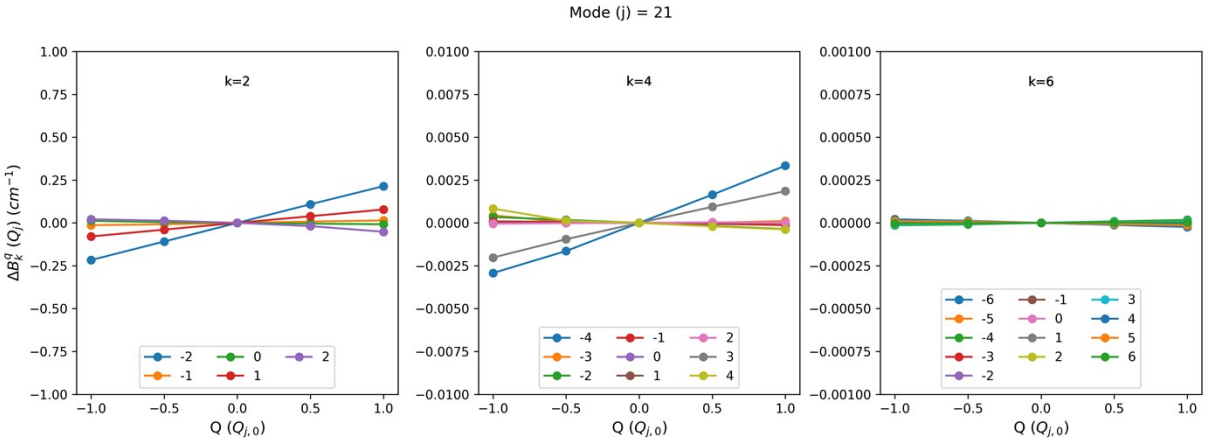


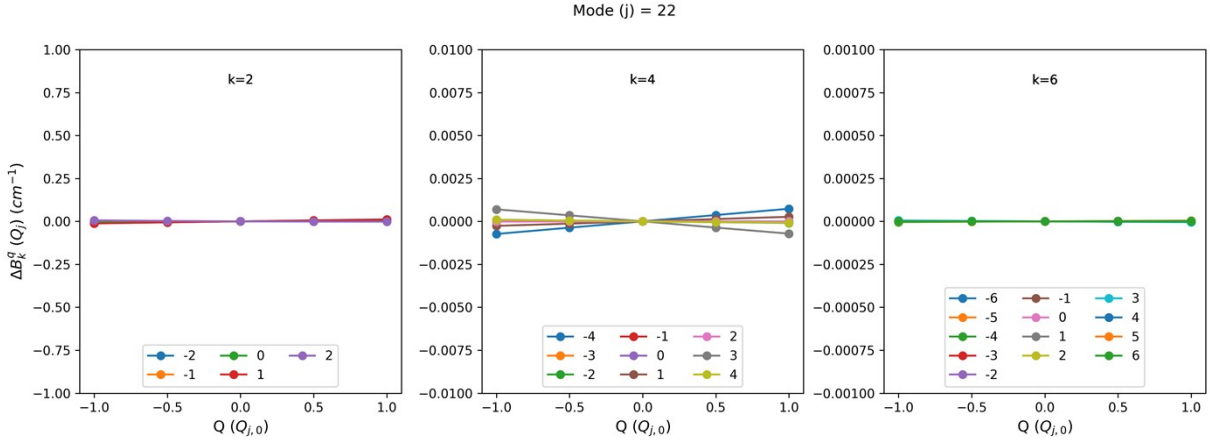

Mode (j) = 17
k=2
k=4
k=6
$\Delta B_k^q(Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)

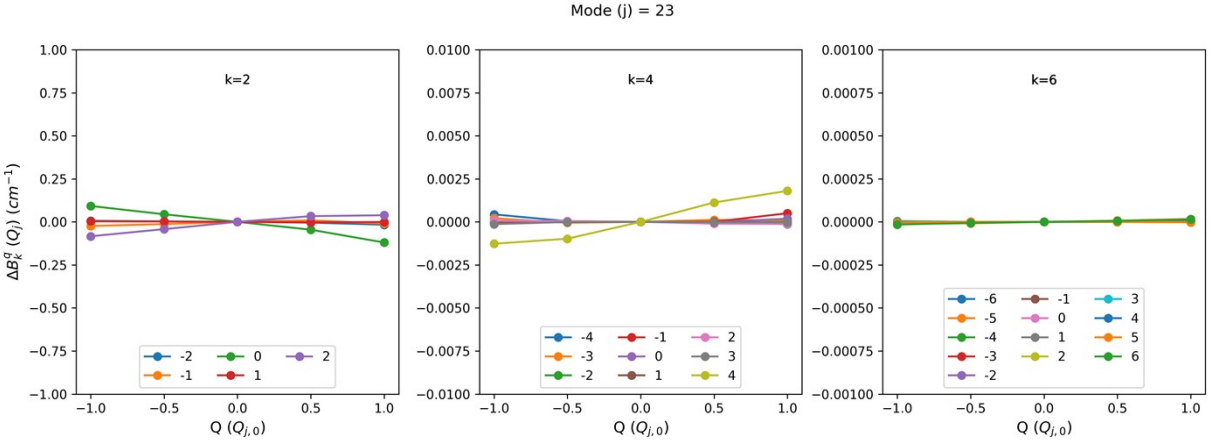

Mode (j) = 18
k=2
k=4
k=6
$\Delta B_k^q(Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)

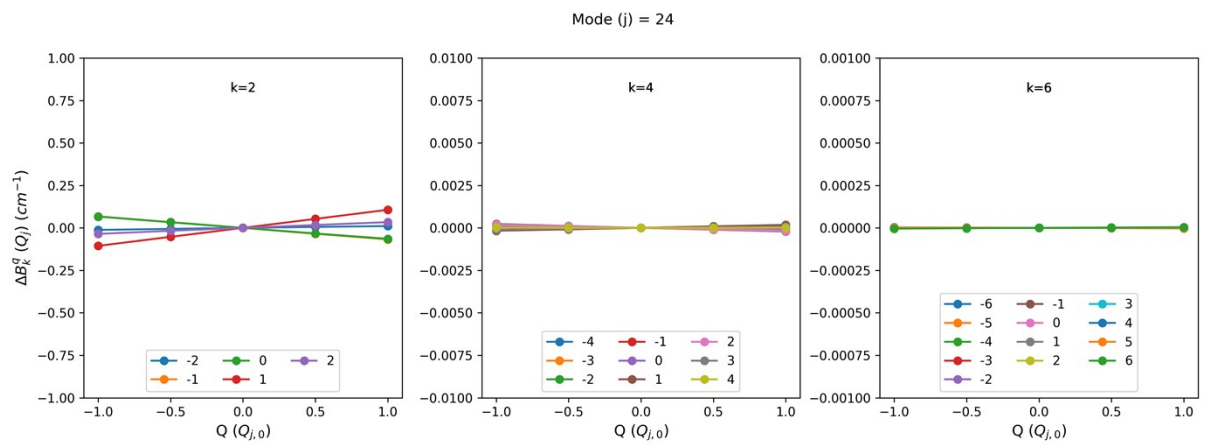

Mode (j) = 19
k=2
k=4
k=6
$\Delta B_k^q(Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)


Mode (j) = 20
k=2
k=4
k=6
$\Delta B_k^q(Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)


Mode (j) = 21
k=2
k=4
k=6
$\Delta B_k^q\ (Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)


Mode (j) = 22
k=2
k=4
k=6
$\Delta B_k^q\ (Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)


Mode (j) = 23
k=2
k=4
k=6
$\Delta B_k^q\ (Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)


Mode (j) = 24
k=2
k=4
k=6
$\Delta B_k^q\ (Q_j)\ (cm^{-1})$
Q ($Q_{j,0}$)

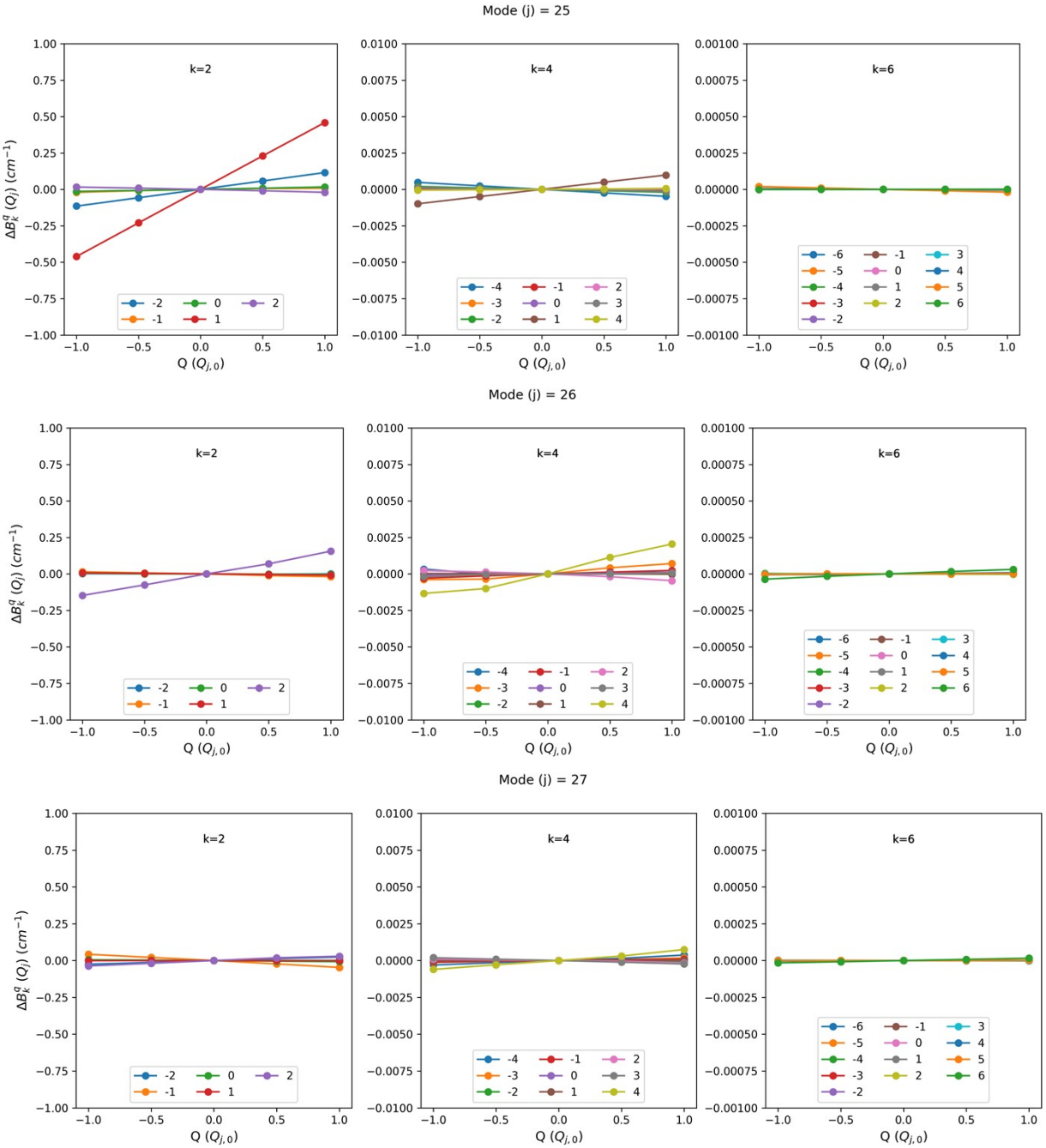


Figure S50. The variation of CFPs as a function of displacement for vibrational modes 1-27 of complex **5**.

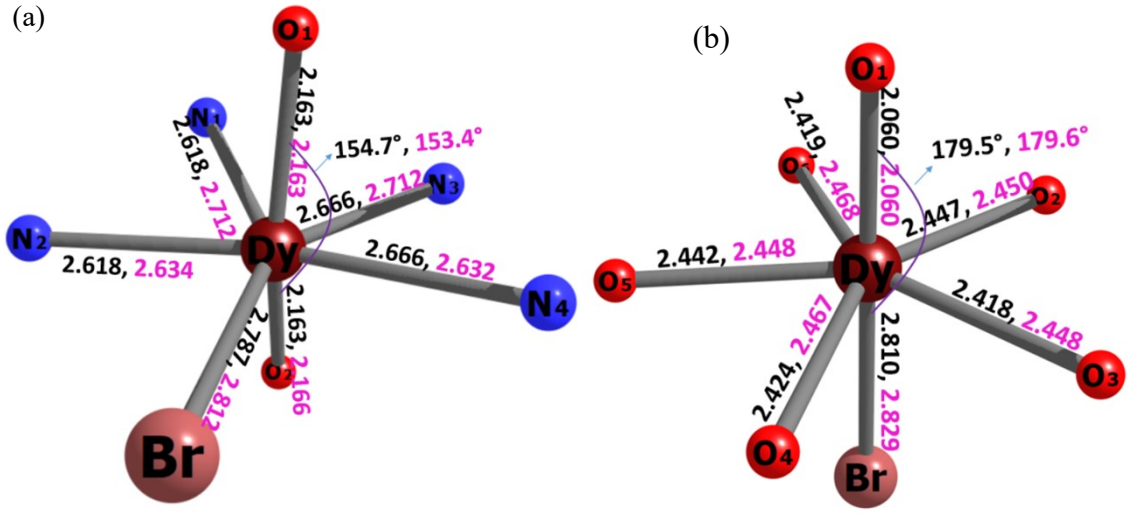


Figure S51: (a) optimized Structure **1** (b) **2**. The black colored font shows the structural parameters for the structures optimised with Y as the central ion, whereas magenta font shows the structural parameters for the structures optimised by taking Dy as the central ion. All the bond distances are in Å and bond angles in ◦.

Appendix S1. The optimized coordinates of complex **1**.

Dy	4.356800000	0.092324000	4.270750000
Br	4.356800000	-2.695193000	4.270750000
O	5.254645000	0.565808000	2.360212000
N	5.777436000	2.300230000	4.735625000
N	6.613197000	-0.270100000	5.548037000
C	7.260725000	-1.445861000	5.635593000
H	6.788269000	-2.275875000	5.122684000
C	8.447730000	-1.606495000	6.347918000
H	8.925498000	-2.579957000	6.383998000
C	8.991908000	-0.501277000	6.997412000
H	9.916841000	-0.585038000	7.561294000
C	8.331980000	0.722916000	6.900792000
H	8.729532000	1.612567000	7.379516000
C	7.145839000	0.802053000	6.170422000
C	6.380663000	2.098742000	6.071345000
H	5.571080000	2.078540000	6.807731000
H	7.044204000	2.939829000	6.334054000
C	4.928283000	3.517649000	4.779083000
H	5.542706000	4.415881000	4.603695000
H	4.512679000	3.600167000	5.782456000
C	6.881387000	2.424373000	3.726590000
H	7.543230000	3.251736000	4.033282000
H	7.460928000	1.498170000	3.791456000
C	6.449444000	2.626280000	2.299994000
C	6.821485000	3.764117000	1.580722000
H	7.409113000	4.533460000	2.079564000

C	6.455135000	3.930603000	0.242466000
H	6.754601000	4.821244000	-0.302077000
C	5.708383000	2.928379000	-0.384383000
H	5.422935000	3.037154000	-1.428279000
C	5.324315000	1.784725000	0.314987000
H	4.746038000	0.997345000	-0.161339000
C	5.674305000	1.614188000	1.671258000
O	3.458955000	0.565807000	6.181288000
N	2.936164000	2.300230000	3.805875000
N	2.100403000	-0.270100000	2.993463000
C	1.452875000	-1.445861000	2.905908000
H	1.925331000	-2.275875000	3.418816000
C	0.265870000	-1.606495000	2.193582000
H	-0.211898000	-2.579957000	2.157503000
C	-0.278308000	-0.501277000	1.544088000
H	-1.203241000	-0.585038000	0.980206000
C	0.381620000	0.722916000	1.640709000
H	-0.015932000	1.612567000	1.161984000
C	1.567761000	0.802053000	2.371078000
C	2.332938000	2.098742000	2.470155000
H	3.142520000	2.078540000	1.733769000
H	1.669396000	2.939829000	2.207446000
C	3.785317000	3.517649000	3.762417000
H	3.170894000	4.415882000	3.937805000
H	4.200921000	3.600167000	2.759044000
C	1.832214000	2.424373000	4.814909000
H	1.170370000	3.251736000	4.508218000
H	1.252672000	1.498170000	4.750044000
C	2.264156000	2.626280000	6.241506000
C	1.892115000	3.764117000	6.960778000
H	1.304487000	4.533460000	6.461936000
C	2.258465000	3.930603000	8.299034000
H	1.958999000	4.821244000	8.843577000
C	3.005217000	2.928379000	8.925883000
H	3.290665000	3.037154000	9.969779000
C	3.389285000	1.784725000	8.226513000
H	3.967562000	0.997345000	8.702839000
C	3.039295000	1.614188000	6.870242000

Appendix S2. The optimized coordinates of complex **1-F**.

Dy	8.672100000	8.744248000	12.804000000
Br	8.672100000	11.537646000	12.804000000
O	7.797423000	8.283927000	10.879709000
F	3.997709000	11.654764000	14.926988000
N	7.223988000	6.534459000	13.233779000
N	6.388992000	9.117763000	14.066268000

C	5.826591000	8.037937000	14.647658000
C	6.575510000	6.240208000	10.765072000
C	4.622265000	8.123175000	15.349594000
H	4.193950000	7.232675000	15.798849000
C	6.143678000	6.388918000	12.201548000
H	5.513612000	5.527406000	12.480826000
H	5.521198000	7.286040000	12.288347000
C	7.347219000	7.268621000	10.158423000
C	6.581472000	6.732441000	14.552938000
H	7.369415000	6.730863000	15.313786000
H	5.898258000	5.898500000	14.786988000
C	6.148600000	5.151529000	9.998656000
H	5.554603000	4.372800000	10.475209000
C	4.573789000	10.445522000	14.857408000
C	8.093881000	5.331803000	13.305006000
H	7.496825000	4.420292000	13.135278000
H	8.497974000	5.268901000	14.315453000
C	3.976421000	9.352371000	15.466538000
H	3.039530000	9.465139000	16.002457000
C	5.772112000	10.305281000	14.165404000
H	6.257082000	11.155455000	13.696340000
C	7.643552000	7.161154000	8.782573000
H	8.213522000	7.963101000	8.320582000
C	6.457617000	5.049794000	8.640213000
H	6.113598000	4.197649000	8.061466000
C	7.203673000	6.067271000	8.038490000
H	7.443161000	6.010905000	6.979003000
O	9.546777000	8.283927000	14.728291000
F	13.346491000	11.654764000	10.681013000
N	10.120212000	6.534459000	12.374221000
N	10.955208000	9.117763000	11.541732000
C	11.517609000	8.037937000	10.960342000
C	10.768690000	6.240208000	14.842928000
C	12.721935000	8.123175000	10.258407000
H	13.150250000	7.232675000	9.809151000
C	11.200522000	6.388918000	13.406452000
H	11.830588000	5.527406000	13.127174000
H	11.823002000	7.286040000	13.319653000
C	9.996981000	7.268621000	15.449577000
C	10.762728000	6.732441000	11.055062000
H	9.974785000	6.730863000	10.294214000
H	11.445942000	5.898500000	10.821012000
C	11.195600000	5.151529000	15.609344000
H	11.789597000	4.372800000	15.132791000
C	12.770411000	10.445522000	10.750592000
C	9.250319000	5.331803000	12.302994000

H	9.847375000	4.420292000	12.472722000
H	8.846226000	5.268901000	11.292547000
C	13.367779000	9.352371000	10.141463000
H	14.304670000	9.465139000	9.605544000
C	11.572088000	10.305281000	11.442596000
H	11.087118000	11.155455000	11.911660000
C	9.700648000	7.161154000	16.825427000
H	9.130678000	7.963101000	17.287418000
C	10.886583000	5.049794000	16.967787000
H	11.230602000	4.197649000	17.546534000
C	10.140527000	6.067272000	17.569510000
H	9.901039000	6.010905000	18.628997000

Appendix S3. The optimized coordinates of complex **1-pCH$_3$**.

Dy	3.619173000	4.277286000	8.301349000
Br	3.737816000	4.000032000	5.515869000
N	2.090165000	4.046706000	10.491401000
N	1.347548000	2.995027000	7.963926000
N	4.981943000	4.920034000	10.522387000
N	5.911274000	5.511038000	7.910972000
O	2.724208000	6.232271000	8.552602000
O	4.462112000	2.407558000	8.992176000
C	0.719255000	9.668859000	12.623726000
H	1.424576000	10.473601000	12.861781000
H	0.514700000	9.120589000	13.550405000
H	-0.221674000	10.147412000	12.317589000
C	1.262130000	8.756007000	11.547459000
C	2.051135000	9.250928000	10.499462000
H	2.296396000	10.311431000	10.472232000
C	2.529097000	8.418428000	9.489387000
H	3.133606000	8.815017000	8.677623000
C	2.236478000	7.038231000	9.484408000
C	1.429253000	6.527585000	10.535059000
C	0.967597000	7.386814000	11.536815000
H	0.348978000	6.974238000	12.334052000
C	1.004070000	5.081705000	10.506961000
H	0.346990000	4.879915000	11.370055000
H	0.411653000	4.909569000	9.601953000
C	1.457764000	2.712543000	10.385754000
H	0.746598000	2.546621000	11.212840000
H	2.247290000	1.958856000	10.478260000
C	0.749837000	2.501033000	9.067584000
C	-0.447696000	1.786264000	9.004738000
H	-0.900105000	1.411802000	9.917997000
C	-1.046863000	1.568264000	7.765188000
H	-1.978924000	1.014314000	7.694386000

C	-0.431991000	2.081630000	6.626267000
H	-0.859359000	1.944664000	5.638374000
C	0.760872000	2.787536000	6.771342000
H	1.289546000	3.195010000	5.916207000
C	2.916574000	4.083801000	11.725028000
H	3.323939000	3.085772000	11.885358000
H	2.286801000	4.324473000	12.598024000
C	4.067794000	5.090262000	11.680929000
H	3.656623000	6.098840000	11.638546000
H	4.630542000	5.006105000	12.625750000
C	6.063550000	3.917337000	10.796065000
H	6.666362000	4.281200000	11.645616000
H	6.711457000	3.926411000	9.912810000
C	5.637418000	2.496808000	11.065786000
C	6.041974000	1.841143000	12.232938000
H	6.612414000	2.400541000	12.974606000
C	5.751111000	0.493434000	12.477142000
C	5.024765000	-0.194867000	11.494485000
H	4.784403000	-1.245794000	11.647542000
C	4.604550000	0.432460000	10.323867000
H	4.050059000	-0.113863000	9.565073000
C	4.894723000	1.792180000	10.082576000
C	6.231538000	-0.201181000	13.731212000
H	5.472076000	-0.883122000	14.132279000
H	6.479553000	0.519702000	14.518281000
H	7.133537000	-0.801027000	13.545681000
C	5.619909000	6.222412000	10.228183000
H	6.270096000	6.539498000	11.061252000
H	4.826208000	6.971062000	10.130756000
C	6.420503000	6.209156000	8.946712000
C	7.611841000	6.929194000	8.841377000
H	7.990658000	7.472164000	9.701978000
C	8.299328000	6.936174000	7.628920000
H	9.227659000	7.491302000	7.525808000
C	7.777258000	6.210871000	6.561184000
H	8.275865000	6.177518000	5.598057000
C	6.584873000	5.513546000	6.746209000
H	6.129103000	4.943598000	5.943528000

Appendix S4. The optimized coordinates of complex **1-pCH_3F**.

Br	8.524154000	5.029296000	12.083029000
C	5.626322000	6.327577000	10.778234000
H	6.111311000	5.911716000	11.655638000
C	4.439751000	7.046305000	10.877483000
C	3.843941000	7.587640000	9.748382000
H	2.916293000	8.144935000	9.829706000

C	4.478752000	7.375687000	8.526181000
H	4.050643000	7.768812000	7.609404000
C	5.671418000	6.650212000	8.482258000
C	6.414583000	6.451031000	7.181759000
H	5.728906000	6.638115000	6.337939000
H	7.215800000	7.195427000	7.121569000
C	7.895406000	5.080792000	5.863984000
H	7.288798000	4.859207000	4.970014000
H	8.318255000	6.076205000	5.729476000
C	9.033539000	4.060225000	5.926309000
H	8.610337000	3.055848000	5.943089000
H	9.623049000	4.150966000	4.998638000
C	5.933723000	4.089838000	7.006268000
H	5.305812000	4.317172000	6.128087000
H	5.316407000	4.253169000	7.896210000
C	6.340484000	2.638999000	6.962680000
C	7.114044000	2.098510000	8.023161000
C	7.389084000	0.715146000	8.000646000
H	7.967132000	0.295812000	8.820196000
C	6.925346000	-0.092654000	6.964349000
H	7.155617000	-1.156710000	6.978655000
C	6.168700000	0.431481000	5.906557000
C	5.892336000	1.804120000	5.934318000
H	5.299038000	2.239014000	5.129788000
C	5.640265000	-0.455160000	4.801650000
H	6.348204000	-1.254696000	4.554021000
H	5.448450000	0.115253000	3.885768000
H	4.695269000	-0.939974000	5.084158000
C	11.014372000	5.202781000	6.882283000
H	11.642126000	5.171447000	7.779562000
H	11.633778000	4.849822000	6.040206000
C	10.606602000	6.631999000	6.630226000
C	9.846546000	7.324376000	7.608480000
C	9.574508000	8.691060000	7.387381000
H	9.007659000	9.228037000	8.143692000
C	10.028054000	9.336832000	6.239515000
H	9.801116000	10.392765000	6.101545000
C	10.771552000	8.660800000	5.261028000
C	11.044865000	7.306163000	5.485800000
H	11.627861000	6.755861000	4.747166000
C	11.287269000	9.375070000	4.032306000
H	10.539370000	10.063314000	3.620436000
H	11.558028000	8.666652000	3.241520000
H	12.183127000	9.971826000	4.253512000
C	10.538257000	2.891357000	7.401165000
H	9.736299000	2.147815000	7.461608000

H	11.210134000	2.584111000	6.581830000
C	11.302244000	2.877734000	8.704824000
C	12.492307000	2.158208000	8.833336000
H	12.903298000	1.635202000	7.975507000
C	13.146029000	2.118012000	10.063247000
H	14.072130000	1.571321000	10.208790000
C	12.571179000	2.819084000	11.112467000
C	11.386629000	3.524784000	10.929790000
H	10.919258000	4.065928000	11.746384000
F	3.873492000	7.209062000	12.082561000
F	13.155966000	2.826088000	12.319644000
N	6.232385000	6.136432000	9.596486000
N	7.032714000	5.109933000	7.073421000
N	9.918400000	4.203958000	7.111565000
N	10.761510000	3.549170000	9.742659000
O	7.588670000	2.881542000	8.981784000
O	9.381040000	6.691556000	8.675961000
Dy	8.494249000	4.819246000	9.296260000

Appendix S4. The optimized coordinates of complex **1-CH$_3$**.

Dy	4.356979000	0.064927000	4.271035000
Br	4.356860000	-2.745951000	4.271809000
O	5.711213000	0.383904000	2.643989000
N	5.981603000	2.477744000	4.747625000
N	6.650384000	-0.200259000	5.624984000
C	7.202265000	-1.424673000	5.695873000
H	6.601300000	-2.231168000	5.292059000
C	8.453947000	-1.674345000	6.250889000
H	8.839845000	-2.687987000	6.277520000
C	9.169815000	-0.598624000	6.764069000
H	10.149816000	-0.739044000	7.212308000
C	8.608207000	0.672729000	6.690465000
H	9.156653000	1.523060000	7.074948000
C	7.349694000	0.849914000	6.102583000
C	6.630410000	2.212433000	6.120726000
C	4.851116000	3.445635000	4.863826000
H	5.214591000	4.473664000	4.996177000
H	4.292885000	3.206272000	5.762668000
C	6.990249000	2.901967000	3.619515000
C	6.555300000	2.575257000	2.154803000
C	6.817186000	3.493080000	1.120187000
H	7.093415000	4.513294000	1.355697000
C	6.764210000	3.149413000	-0.232070000
H	6.977097000	3.900726000	-0.987458000
C	6.477382000	1.832044000	-0.592247000
H	6.468125000	1.533389000	-1.637919000

C	6.181530000	0.904536000	0.398563000
H	5.913630000	-0.120033000	0.154471000
C	6.166444000	1.261367000	1.764662000
O	3.002825000	0.383956000	5.898021000
N	2.731642000	2.477722000	3.794176000
N	2.064174000	-0.200698000	2.916369000
C	1.512574000	-1.425213000	2.844936000
H	2.113398000	-2.231582000	3.249186000
C	0.261364000	-1.675117000	2.288972000
H	-0.124252000	-2.688859000	2.261960000
C	-0.454408000	-0.599460000	1.775513000
H	-1.434074000	-0.739987000	1.326577000
C	0.106830000	0.672012000	1.849778000
H	-0.441620000	1.522242000	1.465122000
C	1.364967000	0.849398000	2.438429000
C	2.083608000	2.212228000	2.420898000
C	3.861938000	3.445787000	3.678656000
H	3.498304000	4.473819000	3.546558000
H	4.420495000	3.206943000	2.779894000
C	1.722475000	2.901284000	4.921905000
C	2.157203000	2.574927000	6.386714000
C	1.895287000	3.492779000	7.421224000
H	1.619404000	4.513087000	7.185703000
C	1.947995000	3.149149000	8.773526000
H	1.735167000	3.900538000	9.528852000
C	2.234655000	1.831801000	9.133821000
H	2.243530000	1.533194000	10.179515000
C	2.531006000	0.904319000	8.143123000
H	2.799014000	-0.120185000	8.387370000
C	2.546578000	1.261119000	6.776996000
C	0.386560000	2.116744000	4.824793000
H	-0.223706000	2.409345000	5.683885000
H	-0.194051000	2.334090000	3.927824000
H	0.554501000	1.041013000	4.894017000
C	3.136089000	1.994438000	1.300869000
H	3.660948000	2.908575000	1.014325000
H	3.859842000	1.230230000	1.562397000
H	2.605736000	1.636525000	0.412541000
C	8.326702000	2.118053000	3.715125000
H	8.936412000	2.412530000	2.856264000
H	8.907593000	2.334139000	4.612155000
H	8.159411000	1.042319000	3.644126000
C	5.578532000	1.993877000	7.241163000
H	5.052510000	2.907524000	7.527052000
H	4.855772000	1.228372000	6.980460000
H	6.109699000	1.637489000	8.129639000

C	7.520223000	3.353667000	6.679113000
H	7.786867000	3.132270000	7.717300000
H	8.447125000	3.530061000	6.132733000
H	6.948441000	4.285604000	6.701025000
C	7.317123000	4.417979000	3.717988000
H	6.508830000	5.048118000	3.335724000
H	7.524421000	4.733678000	4.736394000
H	8.210559000	4.641507000	3.129077000
C	1.193171000	3.353015000	1.862599000
H	0.928560000	3.132801000	0.823656000
H	0.265064000	3.527047000	2.407711000
H	1.763698000	4.285757000	1.843223000
C	1.394654000	4.417008000	4.823725000
H	2.202301000	5.047709000	5.206354000
H	1.186780000	4.732845000	3.805470000
H	0.501008000	4.639490000	5.412727000

Appendix S5. The optimized coordinates of complex **2**.

Dy	3.621347000	3.149400000	4.717732000
Br	4.244591000	1.825823000	7.116438000
O	3.178113000	4.112654000	2.951269000
O	5.945565000	2.946847000	4.084259000
O	4.795830000	5.068482000	5.618936000
O	2.009482000	4.457027000	6.003944000
O	1.510353000	1.968875000	4.765027000
O	3.937975000	0.968512000	3.653254000
C	1.563553000	5.668976000	2.079465000
H	0.750735000	5.079245000	2.518291000
H	1.183406000	6.161655000	1.177788000
H	1.855185000	6.445551000	2.794578000
C	2.765516000	4.763420000	1.764455000
C	3.919545000	5.615914000	1.209362000
H	4.232379000	6.366389000	1.942553000
H	3.620869000	6.139107000	0.294165000
H	4.783192000	4.986085000	0.970433000
C	2.363728000	3.707799000	0.721229000
H	3.224506000	3.077437000	0.469976000
H	2.004796000	4.173304000	-0.203325000
H	1.566509000	3.067299000	1.115232000
C	7.099930000	2.828334000	4.968230000
H	6.780736000	2.261800000	5.843718000
H	7.394908000	3.837788000	5.278509000
C	8.171616000	2.161498000	4.114434000
H	8.036306000	1.073916000	4.114135000
H	9.181562000	2.377578000	4.472826000
C	7.885208000	2.746643000	2.721594000

H	8.314486000	3.751575000	2.636445000
H	8.286913000	2.139081000	1.906245000
C	6.357127000	2.812586000	2.692192000
H	5.953936000	3.665842000	2.145648000
H	5.899578000	1.898014000	2.303410000
C	5.088974000	5.379708000	7.014647000
H	5.209724000	4.430761000	7.536467000
H	4.228809000	5.916656000	7.433056000
C	6.331145000	6.259043000	6.956320000
H	7.231036000	5.640082000	6.865918000
H	6.437867000	6.886423000	7.845205000
C	6.092304000	7.067521000	5.670833000
H	5.407037000	7.899546000	5.869219000
H	7.009046000	7.481981000	5.243001000
C	5.434947000	6.043311000	4.742102000
H	4.664579000	6.463031000	4.092574000
H	6.155817000	5.500254000	4.124058000
C	1.283064000	3.990820000	7.175636000
H	0.291941000	3.639658000	6.859178000
H	1.852762000	3.163627000	7.598242000
C	1.189448000	5.222846000	8.062704000
H	2.138905000	5.372389000	8.588450000
H	0.393441000	5.144749000	8.808019000
C	0.942334000	6.339970000	7.033798000
H	-0.124628000	6.404708000	6.795613000
H	1.265173000	7.323808000	7.384740000
C	1.738996000	5.875993000	5.802628000
H	1.187254000	5.989186000	4.867548000
H	2.707871000	6.369217000	5.702327000
C	1.246605000	0.723118000	5.478277000
H	1.250504000	0.938655000	6.550628000
H	2.072713000	0.045376000	5.259743000
C	-0.117051000	0.267448000	4.968996000
H	-0.635100000	-0.370396000	5.689899000
H	-0.012611000	-0.291953000	4.031603000
C	-0.833138000	1.604821000	4.718822000
H	-1.676628000	1.522249000	4.028306000
H	-1.205789000	2.017346000	5.663406000
C	0.289184000	2.477284000	4.158001000
H	0.392578000	2.381172000	3.072135000
H	0.208702000	3.535925000	4.412529000
C	4.821655000	-0.105195000	4.104758000
H	4.792843000	-0.114294000	5.194195000
H	5.838891000	0.132918000	3.773444000
C	4.284645000	-1.362316000	3.430638000
H	3.459632000	-1.786698000	4.015160000

H	5.052407000	-2.132420000	3.318383000
C	3.771103000	-0.813410000	2.090824000
H	3.044230000	-1.467296000	1.601491000
H	4.606600000	-0.655585000	1.398794000
C	3.158823000	0.523039000	2.503892000
H	3.217142000	1.300596000	1.742813000
H	2.118003000	0.420600000	2.826403000

Appendix S6. The optimized coordinates of complex **3**.

Dy	1.603909000	1.603840000	3.675011000
Br	0.080813000	1.957932000	1.345827000
Si	3.619958000	1.234324000	6.820192000
O	-0.450615000	2.023636000	4.985486000
O	0.434937000	-0.551868000	3.974056000
O	2.916702000	-0.156587000	2.554937000
O	3.475242000	2.687190000	2.447520000
O	1.445366000	4.031494000	4.053577000
O	2.698557000	1.373022000	5.443494000
C	3.850328000	-0.587514000	7.284805000
H	2.896504000	-1.072198000	7.529116000
H	4.494704000	-0.682883000	8.167750000
H	4.320463000	-1.163559000	6.477340000
C	5.329755000	2.004448000	6.553480000
H	5.868801000	1.527027000	5.725059000
H	5.951477000	1.892593000	7.450535000
H	5.264231000	3.078745000	6.339037000
C	2.794474000	2.121735000	8.276333000
H	2.612817000	3.181581000	8.058541000
H	3.434622000	2.079166000	9.166529000
H	1.834650000	1.665945000	8.551054000
C	-1.595105000	2.831872000	4.562612000
H	-1.750078000	2.645392000	3.499040000
H	-1.337417000	3.886873000	4.709925000
C	-2.740388000	2.401799000	5.472631000
H	-3.231552000	1.505552000	5.076030000
H	-3.498091000	3.182847000	5.579650000
C	-2.007206000	2.083746000	6.785484000
H	-1.784590000	3.007057000	7.332675000
H	-2.574753000	1.426969000	7.450522000
C	-0.720006000	1.425514000	6.290247000
H	0.150616000	1.601615000	6.924218000
H	-0.841426000	0.347109000	6.145581000
C	-0.880628000	-0.914053000	3.442098000
H	-0.935267000	-0.544643000	2.417392000
H	-1.638562000	-0.400279000	4.044050000
C	-0.967393000	-2.429807000	3.593479000

H	-0.514184000	-2.931368000	2.730425000
H	-2.001156000	-2.775725000	3.678599000
C	-0.138088000	-2.681395000	4.862716000
H	-0.730552000	-2.460358000	5.758288000
H	0.226529000	-3.708965000	4.945632000
C	1.003046000	-1.677500000	4.709327000
H	1.400597000	-1.293406000	5.650176000
H	1.829019000	-2.085693000	4.117099000
C	2.488812000	-0.950103000	1.402385000
H	1.945022000	-0.284601000	0.730384000
H	1.805766000	-1.727345000	1.763334000
C	3.772394000	-1.543648000	0.829896000
H	4.247074000	-0.840536000	0.135722000
H	3.589437000	-2.477024000	0.290611000
C	4.637199000	-1.730642000	2.086567000
H	4.346386000	-2.642728000	2.620544000
H	5.706964000	-1.795025000	1.869466000
C	4.292114000	-0.490868000	2.911179000
H	4.329060000	-0.643980000	3.991405000
H	4.923794000	0.365589000	2.652103000
C	3.678529000	2.649599000	0.998377000
H	2.696411000	2.729768000	0.530894000
H	4.121476000	1.679748000	0.744072000
C	4.635174000	3.799048000	0.701089000
H	5.208145000	3.631359000	-0.214970000
H	4.084930000	4.740447000	0.587746000
C	5.508531000	3.829066000	1.965098000
H	6.013578000	4.786290000	2.121140000
H	6.274858000	3.046671000	1.919159000
C	4.495839000	3.527039000	3.069198000
H	4.908704000	2.981595000	3.919121000
H	4.005873000	4.435972000	3.433641000
C	1.178395000	5.062630000	3.046773000
H	0.163546000	4.908041000	2.670401000
H	1.879814000	4.916256000	2.223532000
C	1.346205000	6.395194000	3.776204000
H	2.387928000	6.734123000	3.733959000
H	0.719952000	7.179336000	3.342213000
C	0.958120000	6.041170000	5.219817000
H	1.362207000	6.739155000	5.958264000
H	-0.132151000	6.024275000	5.331615000
C	1.538646000	4.637917000	5.376555000
H	2.594597000	4.660389000	5.668806000
H	0.993578000	3.998805000	6.072339000

Appendix S7. The optimized coordinates of model complex **2-crown**.

Dy	3.055208000	2.134600000	3.440677000
O	5.449464000	2.499812000	3.428494000
O	3.739504000	3.362101000	5.384435000
O	1.172558000	2.764247000	4.865663000
O	0.931760000	1.726171000	2.400603000
O	3.336499000	1.300393000	1.178548000
C	5.903897000	3.467640000	4.401547000
C	5.140624000	3.258090000	5.698899000
C	2.799929000	3.453736000	6.470021000
C	1.451778000	3.782740000	5.849723000
C	-0.103062000	2.874186000	4.198579000
C	-0.224983000	1.688703000	3.254812000
C	0.968364000	0.856431000	1.254076000
C	2.128020000	1.316943000	0.386774000
C	4.528485000	1.607117000	0.407407000
C	5.795189000	1.413783000	1.243039000
C	6.210848000	2.539036000	2.191625000
H	5.731196000	4.476661000	4.008089000
H	6.975519000	3.318618000	4.583965000
H	5.345542000	2.272865000	6.135914000
H	5.419270000	4.042940000	6.412470000
H	2.769898000	2.500739000	7.012846000
H	3.097794000	4.259006000	7.152286000
H	1.477322000	4.762301000	5.357060000
H	0.673345000	3.771541000	6.622365000
H	-0.910419000	2.845249000	4.940421000
H	-0.137444000	3.818715000	3.642347000
H	-1.135579000	1.790892000	2.652196000
H	-0.248862000	0.738403000	3.802513000
H	1.095987000	-0.181945000	1.584693000
H	0.033694000	0.950087000	0.688127000
H	1.956655000	2.335857000	0.019808000
H	2.243035000	0.629899000	-0.460901000
H	4.548645000	0.914137000	-0.442024000
H	4.444566000	2.634880000	0.032090000
H	5.747337000	0.461005000	1.784558000
H	6.616746000	1.314689000	0.522123000
H	7.266032000	2.411305000	2.460772000
H	6.074854000	3.524901000	1.728974000
C	3.368041000	-1.004912000	4.860730000
O	3.206891000	0.292464000	4.311188000
Br	2.968693000	4.647338000	2.151284000
C	2.025168000	-1.750971000	4.773402000
C	4.444819000	-1.755490000	4.057795000
C	3.800965000	-0.870383000	6.331104000
H	4.749819000	-0.324319000	6.399548000

H	3.041253000	-0.325111000	6.904183000
H	3.940952000	-1.850790000	6.800034000
H	2.098441000	-2.760621000	5.193117000
H	1.250300000	-1.207463000	5.327367000
H	1.707353000	-1.842621000	3.727478000
H	5.400017000	-1.219183000	4.106988000
H	4.602807000	-2.767470000	4.447605000
H	4.147041000	-1.837847000	3.005717000

Appendix S8. The optimized coordinates of model complex **3-crown**.

Dy	3.033893000	2.256239000	3.376954000
O	5.433621000	2.539427000	3.330143000
O	3.784974000	3.436235000	5.324323000
O	1.202438000	2.875656000	4.854367000
O	0.882534000	1.851337000	2.396212000
O	3.260723000	1.380230000	1.132833000
C	5.930953000	3.492110000	4.297547000
C	5.189583000	3.292171000	5.608678000
C	2.871735000	3.514937000	6.434409000
C	1.512915000	3.870768000	5.853386000
C	-0.097458000	2.984741000	4.235817000
C	-0.245700000	1.805020000	3.288550000
C	0.889516000	0.966420000	1.259506000
C	2.036502000	1.404961000	0.364728000
C	4.445013000	1.647843000	0.334656000
C	5.721891000	1.430219000	1.148047000
C	6.179748000	2.550414000	2.082857000
H	5.772736000	4.506588000	3.912052000
H	7.002284000	3.317490000	4.456761000
H	5.376930000	2.297994000	6.033190000
H	5.503124000	4.063218000	6.322781000
H	2.844353000	2.550851000	6.957209000
H	3.195017000	4.302603000	7.125576000
H	1.535459000	4.860434000	5.381225000
H	0.752678000	3.849297000	6.643536000
H	-0.876700000	2.944109000	5.006452000
H	-0.158744000	3.934230000	3.690312000
H	-1.175900000	1.906757000	2.716650000
H	-0.247011000	0.851327000	3.830855000
H	1.013376000	-0.068701000	1.601455000
H	-0.055038000	1.062657000	0.710617000
H	1.871003000	2.422670000	-0.008368000
H	2.126037000	0.708850000	-0.478448000
H	4.430403000	0.945141000	-0.506733000
H	4.379934000	2.673208000	-0.051076000
H	5.663071000	0.481231000	1.695132000

H	6.527702000	1.309804000	0.412645000
H	7.234442000	2.396186000	2.339161000
H	6.063902000	3.536740000	1.615650000
Si	3.387825000	-1.107892000	4.929038000
O	3.172368000	0.395734000	4.261469000
Br	2.978747000	4.760823000	2.087151000
C	1.857190000	-2.167123000	4.590901000
C	4.913054000	-1.921467000	4.161912000
C	3.633545000	-0.926195000	6.797115000
H	4.520067000	-0.320207000	7.026973000
H	2.765331000	-0.446830000	7.268136000
H	3.772452000	-1.899578000	7.283453000
H	1.962338000	-3.173933000	5.013487000
H	0.956900000	-1.720422000	5.032805000
H	1.682743000	-2.283793000	3.513188000
H	5.812426000	-1.314233000	4.327919000
H	5.103153000	-2.912896000	4.591219000
H	4.791695000	-2.052306000	3.078745000

Appendix S9. The optimized coordinates of complex **4**.

Dy	-9.436944000	3.934521000	5.008065000
Si	-6.652781000	3.042493000	7.427033000
Si	-12.427916000	4.820130000	2.986950000
O	-7.763511000	3.533646000	6.325458000
O	-10.949846000	4.380079000	3.540178000
N	-10.910099000	2.968708000	6.767900000
N	-9.814826000	1.395171000	4.800859000
N	-8.278624000	6.186172000	4.361390000
H	-8.968878000	6.809842000	3.945591000
N	-10.506729000	5.636352000	6.568943000
C	-4.925406000	2.948485000	6.643305000
C	-4.215289000	1.748853000	6.451971000
H	-4.637691000	0.810416000	6.800581000
C	-2.958911000	1.732711000	5.838310000
H	-2.432038000	0.790670000	5.709171000
C	-2.375357000	2.923738000	5.404917000
H	-1.396014000	2.913611000	4.933996000
C	-3.049755000	4.132535000	5.598203000
H	-2.591702000	5.067358000	5.284200000
C	-4.304445000	4.138949000	6.209688000
H	-4.800497000	5.094515000	6.373589000
C	-6.552580000	4.283771000	8.857966000
C	-5.369806000	4.461539000	9.600362000
H	-4.479119000	3.895785000	9.337587000
C	-5.306251000	5.360386000	10.667994000
H	-4.378947000	5.478224000	11.222464000

C	-6.430369000	6.109637000	11.020323000
H	-6.382301000	6.810596000	11.849393000
C	-7.617203000	5.952006000	10.300817000
H	-8.496465000	6.532040000	10.573971000
C	-7.671825000	5.049848000	9.235337000
H	-8.599678000	4.939737000	8.679454000
C	-7.119236000	1.338758000	8.131530000
C	-7.377792000	1.151123000	9.502327000
H	-7.301264000	1.996592000	10.181048000
C	-7.718295000	-0.102468000	10.019746000
H	-7.904846000	-0.215974000	11.084699000
C	-7.797345000	-1.211199000	9.175439000
H	-8.040430000	-2.190952000	9.578407000
C	-7.540412000	-1.055893000	7.809789000
H	-7.574073000	-1.919637000	7.149090000
C	-7.216172000	0.204241000	7.300097000
H	-7.011221000	0.299843000	6.235082000
C	-12.312660000	6.584104000	2.294374000
C	-11.060445000	7.110552000	1.923053000
H	-10.173883000	6.491302000	2.048245000
C	-10.932872000	8.386373000	1.367420000
H	-9.954271000	8.763029000	1.077801000
C	-12.068860000	9.174085000	1.169445000
H	-11.977435000	10.166827000	0.737231000
C	-13.324789000	8.672252000	1.517476000
H	-14.214296000	9.275460000	1.355544000
C	-13.441501000	7.393880000	2.068165000
H	-14.432007000	7.024390000	2.324339000
C	-12.990938000	3.642444000	1.617508000
C	-12.036442000	3.052837000	0.766996000
H	-10.980537000	3.260008000	0.929437000
C	-12.410653000	2.219388000	-0.288432000
H	-11.652683000	1.781644000	-0.933802000
C	-13.762639000	1.954452000	-0.520016000
H	-14.059779000	1.307469000	-1.341060000
C	-14.729928000	2.531577000	0.304446000
H	-15.783933000	2.333921000	0.126907000
C	-14.345797000	3.365575000	1.357397000
H	-15.117631000	3.802288000	1.986938000
C	-13.721897000	4.785800000	4.383539000
C	-14.296354000	3.564430000	4.791552000
H	-14.047722000	2.650720000	4.255523000
C	-15.208097000	3.497905000	5.847970000
H	-15.650337000	2.543853000	6.125059000
C	-15.574244000	4.661773000	6.529941000
H	-16.300656000	4.617527000	7.337487000

C	-15.021910000	5.886175000	6.146215000
H	-15.321762000	6.800895000	6.652720000
C	-14.106297000	5.941505000	5.090115000
H	-13.706185000	6.908753000	4.795192000
C	-11.049593000	1.634469000	6.849320000
C	-12.232744000	1.852497000	8.934025000
H	-12.744956000	1.414380000	9.784908000
C	-12.095079000	3.232537000	8.830370000
H	-12.507539000	3.875588000	9.596422000
C	-11.417763000	3.765531000	7.726167000
C	-11.252612000	5.247364000	7.542669000
C	-11.999303000	6.128815000	8.515619000
H	-11.708404000	5.886529000	9.543493000
H	-13.077830000	5.959928000	8.419958000
H	-11.807251000	7.189038000	8.365763000
C	-10.364244000	7.043493000	6.192713000
H	-10.686525000	7.099448000	5.145635000
H	-11.035236000	7.704094000	6.747062000
C	-8.930116000	7.589086000	6.333901000
H	-8.957821000	8.609848000	5.930969000
H	-8.671960000	7.676778000	7.395332000
C	-7.222476000	5.972657000	3.337055000
H	-6.378090000	6.656992000	3.493943000
H	-7.657067000	6.221583000	2.360588000
C	-7.422580000	2.216067000	2.821674000
H	-6.857833000	1.863886000	3.692383000
H	-6.735297000	2.193825000	1.962803000
C	-9.232844000	0.561344000	3.729188000
H	-8.452734000	-0.071172000	4.174887000
H	-10.002788000	-0.108243000	3.329543000
C	-10.473704000	0.804603000	5.739412000
C	-10.708791000	-0.685117000	5.840623000
H	-10.344529000	-1.234234000	4.975815000
H	-11.776670000	-0.901503000	5.950839000
H	-10.189878000	-1.075709000	6.724116000
C	-11.710048000	1.040056000	7.934436000
H	-11.809896000	-0.034389000	8.007372000
N	-7.843764000	3.607527000	3.090061000
H	-8.378355000	3.927466000	2.278680000
C	-7.813357000	6.789080000	5.639461000
H	-6.964461000	7.464459000	5.459835000
H	-7.458939000	5.982071000	6.284991000
C	-6.709447000	4.535393000	3.294027000
H	-5.969970000	4.445892000	2.482818000
H	-6.214286000	4.261092000	4.228924000
C	-8.636826000	1.317295000	2.539458000

H	-8.333920000	0.543967000	1.823408000
H	-9.424422000	1.896675000	2.041191000

Appendix S10. The optimized coordinates of complex **4-N3O2**.

Dy	0.000000000	0.000000000	0.000000000
Si	0.680020000	-0.769210000	-3.746280000
Si	-0.292170000	0.148310000	3.849880000
O	0.284820000	-0.524540000	-2.141090000
O	0.000000000	0.000000000	2.210950000
N	-1.494950000	1.847310000	-0.488900000
N	-2.443720000	-0.675510000	-0.095000000
N	1.136590000	2.256150000	-0.038530000
C	-2.138840000	0.517090000	4.206820000
C	-3.084830000	-0.524890000	4.254310000
H	-2.752470000	-1.562810000	4.153830000
C	-4.446390000	-0.269590000	4.445770000
H	-5.157750000	-1.099770000	4.485880000
C	-4.896470000	1.046200000	4.595040000
H	-5.959820000	1.250540000	4.748760000
C	-3.976060000	2.097170000	4.554590000
H	-4.317360000	3.129150000	4.675740000
C	-2.615850000	1.831150000	4.363340000
H	-1.912190000	2.667960000	4.342240000
C	0.751110000	1.579910000	4.572600000
C	0.923780000	2.756410000	3.817400000
H	0.475630000	2.821530000	2.821500000
C	1.661130000	3.837370000	4.311630000
H	1.776650000	4.742510000	3.708140000
C	2.253800000	3.761480000	5.576470000
H	2.831880000	4.604340000	5.965330000
C	2.103500000	2.599390000	6.338610000
H	2.569930000	2.527530000	7.325120000
C	1.359570000	1.524070000	5.839050000
H	1.261680000	0.622070000	6.449300000
C	0.130890000	-1.482750000	4.756020000
C	0.846550000	-2.491820000	4.088850000
H	1.134940000	-2.325710000	3.047780000
C	1.173920000	-3.694710000	4.725190000
H	1.728730000	-4.466020000	4.182730000
C	0.789190000	-3.912800000	6.051790000
H	1.040360000	-4.852320000	6.552280000
C	0.072220000	-2.923910000	6.733280000
H	-0.239110000	-3.088910000	7.768650000
C	-0.254860000	-1.726720000	6.087850000
H	-0.834890000	-0.975410000	6.633090000
C	2.577080000	-0.860560000	-4.023410000

C	3.314620000	0.284040000	-4.380610000
H	2.789290000	1.224270000	-4.572300000
C	4.707750000	0.247280000	-4.508700000
H	5.253120000	1.151380000	-4.793920000
C	5.401450000	-0.944610000	-4.277620000
H	6.489230000	-0.979090000	-4.383970000
C	4.692160000	-2.096320000	-3.919980000
H	5.222120000	-3.035130000	-3.736970000
C	3.299360000	-2.048170000	-3.797120000
H	2.765350000	-2.966300000	-3.531660000
C	-0.003480000	0.642330000	-4.834790000
C	-0.804420000	1.649950000	-4.270980000
H	-1.013220000	1.625220000	-3.198840000
C	-1.337470000	2.676130000	-5.059890000
H	-1.959000000	3.448080000	-4.597370000
C	-1.077800000	2.712030000	-6.432700000
H	-1.493730000	3.512320000	-7.051420000
C	-0.283200000	1.717040000	-7.012810000
H	-0.076100000	1.737750000	-8.086620000
C	0.244940000	0.694950000	-6.219000000
H	0.863800000	-0.073610000	-6.693170000
C	-0.082710000	-2.418900000	-4.352650000
C	-1.241150000	-2.911080000	-3.723610000
H	-1.655650000	-2.354540000	-2.877960000
C	-1.867300000	-4.082830000	-4.161690000
H	-2.770630000	-4.442200000	-3.659570000
C	-1.342660000	-4.792780000	-5.246780000
H	-1.829850000	-5.708450000	-5.593510000
C	-0.194050000	-4.320460000	-5.888550000
H	0.221260000	-4.867600000	-6.739800000
C	0.424650000	-3.146190000	-5.444480000
H	1.324620000	-2.797030000	-5.959830000
C	-1.000380000	3.133160000	-0.614710000
C	-1.846830000	4.185300000	-0.977080000
H	-1.465380000	5.199570000	-1.078170000
C	-3.205380000	3.945420000	-1.216320000
H	-3.871470000	4.762690000	-1.498290000
C	-3.696590000	2.643280000	-1.079580000
H	-4.754770000	2.457680000	-1.253820000
C	-2.838660000	1.601430000	-0.710000000
C	-3.305680000	0.231880000	-0.509400000
C	-4.755210000	-0.126970000	-0.747440000
H	-4.833500000	-1.012800000	-1.397590000
H	-5.329380000	0.674940000	-1.219700000
H	-5.257380000	-0.382110000	0.201660000
C	-2.936540000	-2.026980000	0.183810000

H	-3.190630000	-2.542950000	-0.765330000
H	-3.879010000	-1.974550000	0.757040000
C	-1.986950000	-2.918000000	0.990280000
H	-1.652490000	-2.394080000	1.899540000
H	-2.581670000	-3.783780000	1.327640000
C	-0.769480000	-3.488010000	0.277720000
H	-0.408620000	-4.384270000	0.815220000
H	-1.004780000	-3.784790000	-0.761720000
C	2.676470000	-2.173300000	0.311900000
H	2.743480000	-2.334200000	1.403150000
H	3.622130000	-2.505950000	-0.147420000
C	3.663470000	0.026520000	0.184950000
H	3.933420000	0.084060000	1.255810000
H	4.483550000	-0.488020000	-0.345220000
C	0.426730000	3.319590000	-0.343180000
O	0.302960000	-2.525490000	0.269650000
O	2.472940000	-0.779330000	0.041160000
C	1.548120000	-2.981800000	-0.284210000
H	1.520510000	-2.870170000	-1.379360000
H	1.705900000	-4.044890000	-0.030780000
C	3.482220000	1.412430000	-0.403850000
H	3.181420000	1.329200000	-1.460440000
H	4.490510000	1.860340000	-0.398660000
C	2.544490000	2.372200000	0.348490000
H	2.925910000	3.393430000	0.204180000
H	2.614580000	2.169600000	1.433900000
C	1.037000000	4.706000000	-0.390350000
H	1.396970000	5.015750000	0.604800000
H	0.334250000	5.469440000	-0.734160000
H	1.903980000	4.732510000	-1.069450000
Cl	5.913210000	-7.735160000	-0.925550000
Cl	4.306710000	-5.317320000	-1.638710000
C	4.506990000	-7.086600000	-1.812070000
H	4.645510000	-7.304230000	-2.876330000
H	3.603670000	-7.568860000	-1.424020000
C	9.012260000	-2.634660000	3.983310000
C	9.948370000	-3.510130000	3.371700000
H	9.882310000	-3.701310000	2.299410000
C	10.983380000	-4.082330000	4.106030000
H	11.719420000	-4.717250000	3.606160000
C	11.076170000	-3.852080000	5.485970000
H	11.880330000	-4.312900000	6.065550000
C	10.122820000	-3.045010000	6.125130000
H	10.191450000	-2.865720000	7.201260000
C	9.087050000	-2.473440000	5.392720000
H	8.353860000	-1.843260000	5.899060000

C	7.347040000	-0.420250000	3.792980000
C	8.229410000	0.557460000	4.297540000
H	9.307630000	0.370950000	4.269840000
C	7.772930000	1.764840000	4.834230000
H	8.491060000	2.494330000	5.220320000
C	6.402330000	2.040930000	4.878780000
H	6.037990000	2.981480000	5.300480000
C	5.500770000	1.098030000	4.378460000
H	4.425940000	1.297990000	4.411260000
C	5.973550000	-0.107240000	3.844310000
H	5.243250000	-0.824670000	3.458050000
C	8.402410000	-1.426950000	1.567450000
C	9.719530000	-1.016930000	1.278230000
H	10.465650000	-1.003590000	2.078610000
C	10.109670000	-0.615690000	-0.004390000
H	11.142780000	-0.304940000	-0.185950000
C	9.183990000	-0.610480000	-1.050920000
H	9.484660000	-0.299150000	-2.055070000
C	7.867480000	-1.008060000	-0.796600000
H	7.130070000	-1.010210000	-1.604730000
C	7.492110000	-1.403440000	0.491270000
H	6.454210000	-1.703860000	0.665050000
C	6.969310000	-3.116890000	3.252870000
C	6.933990000	-4.119230000	2.245800000
H	7.617950000	-4.053550000	1.398100000
C	5.988290000	-5.140020000	2.280270000
H	5.937060000	-5.860530000	1.460360000
C	5.101050000	-5.237350000	3.363520000
H	4.372000000	-6.051360000	3.401600000
C	5.165570000	-4.304660000	4.408770000
H	4.477900000	-4.379140000	5.254590000
C	6.107470000	-3.280460000	4.370350000
H	6.151310000	-2.564440000	5.192080000
B	7.919070000	-1.759930000	3.079150000

Appendix S11. The optimized coordinates of complex **5**.

C	12.610037000	5.722004000	9.354144000
C	12.119993000	6.582519000	10.533101000
H	11.341715000	6.079523000	11.116549000
H	11.717636000	7.541106000	10.189993000
H	12.960345000	6.793434000	11.206353000
C	13.156630000	4.369775000	9.852512000
H	14.035283000	4.539519000	10.488221000
H	13.450464000	3.735000000	9.013121000
H	12.423502000	3.818360000	10.453508000
C	13.713240000	6.473960000	8.577819000
H	13.351042000	7.439541000	8.210817000

H	14.067838000	5.896239000	7.719188000
H	14.564423000	6.660843000	9.244731000
C	8.826424000	4.146039000	8.329448000
H	8.811214000	4.547083000	7.311426000
C	8.983914000	2.626890000	8.250156000
H	9.926641000	2.347535000	7.772642000
H	8.162064000	2.194727000	7.670445000
H	8.962712000	2.181221000	9.254297000
C	7.532175000	4.559116000	9.028469000
H	7.497256000	4.158338000	10.050146000
H	6.673890000	4.170107000	8.471334000
H	7.445101000	5.648461000	9.082178000
C	9.633491000	7.737171000	7.967623000
H	9.356867000	7.391174000	8.969097000
C	10.205097000	9.158573000	8.053637000
H	11.081240000	9.198223000	8.711077000
H	9.451137000	9.856125000	8.435204000
H	10.504117000	9.502411000	7.055395000
C	8.399628000	7.693193000	7.057615000
H	8.653097000	8.054235000	6.054693000
H	7.609436000	8.339841000	7.456772000
H	8.002630000	6.679114000	6.965382000
C	12.729543000	3.277609000	0.149661000
C	13.989308000	2.766176000	0.882196000
H	13.845695000	1.745968000	1.251929000
H	14.246977000	3.402531000	1.734038000
H	14.837414000	2.759471000	0.185895000
C	12.972020000	4.712556000	-0.357953000
H	13.841252000	4.723931000	-1.028218000
H	13.164541000	5.393108000	0.474894000
H	12.119763000	5.105027000	-0.925699000
C	12.383272000	2.334917000	-1.017416000
H	11.500503000	2.670273000	-1.571909000
H	12.193615000	1.315446000	-0.666420000
H	13.225674000	2.296653000	-1.719432000
C	10.279977000	0.695784000	1.625869000
H	9.901456000	0.977058000	0.637577000
C	9.097923000	0.485211000	2.580218000
H	9.457018000	0.183458000	3.570403000
H	8.443083000	-0.309822000	2.204708000
H	8.504766000	1.395963000	2.694897000
C	11.127595000	-0.577910000	1.508752000
H	11.968579000	-0.437039000	0.820050000
H	10.519335000	-1.415432000	1.149326000
H	11.527140000	-0.853159000	2.492992000
C	8.739873000	4.041554000	1.311470000

H	8.844650000	3.651561000	2.328625000
C	7.536604000	3.363861000	0.657838000
H	7.382932000	3.743444000	-0.360956000
H	6.636339000	3.567850000	1.246262000
H	7.676924000	2.280103000	0.604589000
C	8.579379000	5.560556000	1.387424000
H	9.459424000	6.033735000	1.830538000
H	7.706633000	5.815624000	1.996938000
H	8.429540000	5.985517000	0.385256000
N	9.996478000	4.764496000	9.018279000
N	10.674949000	6.814237000	7.479713000
N	11.126983000	1.813334000	2.082426000
N	9.988546000	3.677785000	0.580473000
O	11.831248000	4.560260000	7.006538000
O	11.810075000	4.257633000	2.530361000
O	12.234371000	6.713428000	4.907976000
H	11.725853000	7.412844000	4.399659000
H	13.173681000	7.022696000	4.969087000
O	14.084539000	4.645438000	4.749828000
O	12.703578000	2.235507000	4.606193000
H	12.367513000	1.448916000	5.130279000
H	13.685069000	2.130733000	4.520727000
O	10.042848000	2.799382000	5.058872000
O	9.738802000	5.608518000	4.538683000
P	11.242897000	5.418831000	8.144041000
P	11.372240000	3.295313000	1.407764000
H	10.268905000	4.268888000	9.861356000
H	11.061629000	7.023187000	6.561904000
H	11.582431000	1.688311000	2.983935000
H	10.123443000	4.216388000	-0.269370000
H	14.725718000	3.895346000	4.667365000
H	14.555675000	5.514387000	4.806743000
H	10.167811000	1.892567000	5.424708000
H	9.061301000	2.976357000	5.035287000
H	8.816474000	5.232086000	4.593599000
H	9.660993000	6.521218000	4.174647000
C	15.419276000	7.645671000	2.253757000
C	16.201846000	8.628127000	1.361024000
H	15.997469000	8.401868000	0.307761000
H	17.284289000	8.563434000	1.516453000
H	15.890594000	9.662349000	1.544147000
C	15.853586000	6.190827000	1.977832000
H	15.626467000	5.937339000	0.935870000
H	15.311703000	5.484854000	2.614046000
H	16.929944000	6.032493000	2.120313000
C	13.905824000	7.786836000	1.982207000

H	13.521771000	8.778514000	2.238848000
H	13.318395000	7.046294000	2.530639000
H	13.717415000	7.634283000	0.913459000
C	13.986745000	10.077823000	4.898647000
H	13.239498000	9.343462000	4.586101000
C	13.612934000	11.407416000	4.246342000
H	14.325208000	12.196625000	4.524742000
H	12.613908000	11.713071000	4.569413000
H	13.594881000	11.315012000	3.155544000
C	13.988261000	10.146912000	6.428141000
H	14.266707000	9.174921000	6.847207000
H	12.992367000	10.413926000	6.799696000
H	14.704700000	10.897983000	6.784345000
C	17.955478000	8.055823000	5.590480000
H	17.354049000	8.774100000	6.159458000
C	19.386052000	8.587822000	5.479384000
H	20.008150000	7.904225000	4.886162000
H	19.843683000	8.678346000	6.470476000
H	19.401012000	9.568643000	4.994292000
C	17.895924000	6.692369000	6.295035000
H	16.860134000	6.358494000	6.395360000
H	18.347485000	6.747594000	7.292423000
H	18.449715000	5.940088000	5.715406000
N	15.306009000	9.628001000	4.391280000
N	17.354880000	8.006373000	4.238197000
O	14.870275000	7.144785000	4.950517000
P	15.691492000	8.057851000	4.038152000
H	15.963704000	10.348719000	4.122420000
H	17.830204000	7.354012000	3.620973000
I	6.817415000	3.880556000	4.844195000
I	10.311136000	8.988497000	3.416111000
C	16.081799000	1.991101000	7.178063000
C	16.216848000	3.503626000	7.453242000
H	15.525057000	4.085028000	6.836807000
H	17.233759000	3.879534000	7.283904000
H	15.970810000	3.703103000	8.502615000
C	17.070779000	1.187803000	8.044847000
H	18.113117000	1.471046000	7.862168000
H	16.971281000	0.112010000	7.863916000
H	16.852427000	1.367550000	9.104247000
C	14.636441000	1.543432000	7.485725000
H	14.446666000	1.656601000	8.559115000
H	14.456953000	0.493615000	7.235964000
H	13.896608000	2.146581000	6.953614000
C	15.113722000	-0.681678000	4.552399000
H	14.238436000	-0.123458000	4.895399000

C	15.086159000	-0.735092000	3.022486000
H	15.143585000	0.277361000	2.610867000
H	14.157822000	-1.201092000	2.672880000
H	15.933156000	-1.316617000	2.636884000
C	15.045016000	-2.066094000	5.194062000
H	15.897227000	-2.686691000	4.883767000
H	14.122213000	-2.570267000	4.893783000
H	15.041199000	-1.989897000	6.286246000
C	18.560095000	2.119995000	3.777089000
H	18.098928000	1.300540000	3.213849000
C	18.209219000	3.449692000	3.093297000
H	17.125113000	3.570657000	3.027017000
H	18.632204000	3.493762000	2.082913000
H	18.619401000	4.292627000	3.667646000
C	20.070683000	1.884558000	3.844314000
H	20.559520000	2.673600000	4.431370000
H	20.509582000	1.896477000	2.840751000
H	20.295025000	0.922323000	4.314754000
N	16.323610000	0.029497000	5.032412000
N	17.998824000	2.037450000	5.144363000
O	15.372443000	2.370087000	4.498281000
P	16.387047000	1.645223000	5.384944000
H	17.123320000	-0.540206000	5.277627000
H	18.347489000	2.768807000	5.757487000
I	11.341847000	-0.376823000	6.165181000
Dy	11.737908000	4.397817000	4.770343000

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