Signatures of counter ion association and hydrogen bonding in vibrational circular dichroism spectra

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Supplementary Material for PCCP

Table 1: Frequencies (Freq.), dipole strengths (Dip. Str.), rotational strengths (Rot. Str.), angle ξ (Xi), and normal mode overlaps for the modes indicated by arrows in Fig. 4 in the manuscript. The label of the normal modes (NM) are the same as in Fig. 4. The differences (Diff.) between the values taken in the free molecule (FM) and in the molecular complexes are also given for all listed physical quantities.

Molecular labels:
FM = $\Lambda-\delta\delta\delta$; 2Cl = $\Lambda-\delta\delta\delta\cdots 2Cl^-$; 3Cl = $\Lambda-\delta\delta\delta\cdots 3Cl^-$; 5Cl = $\Lambda-\delta\delta\delta\cdots 5Cl^-$

Units: Freq. (cm^{-1}), R(10^{-44} $esu^2{\cdot}cm^2$), D(10^{-40} $esu^2{\cdot}cm^2$), ξ (degree).

Molec.	NM	Freq.	Diff.	Dip. Str.	Diff.	Rot. Str.	Diff.	Xi	Diff.	Overlap
FM	52	1069.2	---	7.0	---	113.1	---	0.4	---	---
2Cl	58	1074.1	5.0	38.3	31.4	234.8	121.7	0.3	-0.1	-0.99
5Cl	67	1126.4	57.3	1.8	-5.2	31.5	-81.5	3.4	3.0	0.96

Molec.	NM	Freq.	Diff.	Dip. Str.	Diff.	Rot. Str.	Diff.	Xi	Diff.	Overlap
FM	55	1121.7	---	138.8	---	-97.9	---	179.7	---	---
2Cl	61	1152.8	31.1	254.5	115.7	75.6	173.4	0.5	-179.2	0.94

Molec.	NM	Freq.	Diff.	Dip. Str.	Diff.	Rot. Str.	Diff.	Xi	Diff.	Overlap
FM	56	1122.2	---	139.1	---	-91.7	---	179.8	---	---
2Cl	62	1153.4	31.2	252.7	113.6	84.5	176.2	0.9	-178.9	0.94

Molec.	NM	Freq.	Diff.	Dip. Str.	Diff.	Rot. Str.	Diff.	Xi	Diff.	Overlap
FM	58	1175.8	---	0.5	---	19.4	---	3.2	---	---
5Cl	73	1212.1	36.2	4.8	4.4	-74.5	-93.9	179.0	175.7	0.98

Molec.	NM	Freq.	Diff.	Dip. Str.	Diff.	Rot. Str.	Diff.	Xi	Diff.	Overlap
FM	59	1176.1	---	0.6	---	22.8	---	3.1	---	---
5Cl	74	1212.5	36.3	4.6	4.0	-73.3	-96.1	179.0	175.8	0.98

Molec.	NM	Freq.	Diff.	Dip. Str.	Diff.	Rot. Str.	Diff.	Xi	Diff.	Overlap
1FM	60	1205.7	---	76.9	---	195.5	---	0.6	---	---
22Cl	68	1261.2	55.6	325.4	248.6	-410.0	-605.4	178.8	178.2	0.93
33Cl	69	1210.1	4.4	56.3	-20.6	151.4	-44.1	1.5	0.9	-0.91
45Cl	75	1244.9	39.2	124.4	47.6	-171.5	-367.0	179.2	178.7	-0.98

Molec.	NM	Freq.	Diff.	Dip. Str.	Diff.	Rot. Str.	Diff.	Xi	Diff.	Overlap
1FM	82	1591.9	---	161.8	---	-356.9	---	179.8	---	---
22Cl	88	1586.5	-5.4	46.8	-115.0	-189.7	167.2	179.0	-0.9	0.98
33Cl	91	1568.5	-23.4	67.2	-94.5	47.3	404.1	0.3	-179.5	0.97
45Cl	97	1586.5	-5.4	12.2	-149.6	-26.9	330.0	179.5	-0.3	0.99

Molec.	NM	Freq.	Diff.	Dip. Str.	Diff.	Rot. Str.	Diff.	Xi	Diff.	Overlap
1FM	83	1612.0	---	76.4	---	62.3	---	0.7	---	---
22Cl	90	1613.6	1.6	9.6	-66.8	56.4	-6.0	1.3	0.5	0.98
33Cl	92	1579.1	-32.9	0.9	-75.5	8.2	-54.2	2.5	1.8	0.97
45Cl	99	1604.7	-7.3	0.6	-75.8	-9.2	-71.5	175.1	174.4	-0.97

Molec.	NM	Freq.	Diff.	Dip. Str.	Diff.	Rot. Str.	Diff.	Xi	Diff.	Overlap
1FM	84	1612.1	---	76.1	---	61.9	---	0.6	---	---
22Cl	91	1614.1	2.1	9.8	-66.3	56.6	-5.3	3.1	2.4	0.98
33Cl	93	1579.1	-33.0	1.0	-75.1	8.4	-53.5	1.2	0.6	-0.97
45Cl	100	1604.8	-7.3	0.6	-75.4	-9.7	-71.6	171.9	171.3	0.97

Molec.	NM	Freq.	Diff.	Dip. Str.	Diff.	Rot. Str.	Diff.	Xi	Diff.	Overlap
1FM	86	1626.4	---	55.0	---	131.6	---	0.3	---	---
22Cl	92	1624.9	-1.5	5.1	-49.9	-0.8	-132.4	160.7	160.4	-0.98
33Cl	95	1594.4	-32.1	58.1	3.1	-104.4	-236.0	179.8	179.5	-0.97
45Cl	101	1615.7	-10.7	41.4	-13.6	-21.0	-152.7	177.5	177.2	-0.99

Molec.	NM	Freq.	Diff.	Dip. Str.	Diff.	Rot. Str.	Diff.	Xi	Diff.	Overlap
FM	87	1626.5	---	54.8	---	131.5	---	0.2	---	---
2Cl	93	1625.5	-1.0	5.4	-49.3	-0.1	-131.6	94.9	94.6	-0.98
3Cl	96	1594.4	-32.1	58.3	3.5	-104.1	-235.6	179.7	179.4	0.97
5Cl	102	1615.9	-10.6	41.5	-13.2	-21.6	-153.1	176.3	176.1	0.99

Table 2: Comparison of the Cartesian components of the electronic (el) and nuclear (nuc) components of the EDTM and MDTM of the modes: 60 of $\Lambda - \delta\delta\delta$ (1), 68 of $\Lambda - \delta\delta\delta\cdots 2\mathrm{Cl}^-$ (2), 69 of $\Lambda - \delta\delta\delta\cdots 3\mathrm{Cl}^-$ (3) and 75 of $\Lambda - \delta\delta\delta\cdots 5\mathrm{Cl}^-$ (4). Since the two modes have A_2 symmetry only the non-zero Z Cartesian components are shown. Units: EDTM (10^{-22} esu·cm), MDTM (10^{-24} esu·cm).

E & M DTMs of Molecule 1 for NM 60

Frag.	E_nuc_X	E_el_X	E_nuc_Y	E_el_Y	E_nuc_Z	E_el_Z	M_nuc_X	M_el_X	M_nuc_Y	M_el_Y	M_nuc_Z	M_el_Z
All Axial:	-0.7	0.5	-0.0	-0.1	127.7	-82.1	-2.3	0.8	-3.6	1.4	275.2	-311.5
All Equat:	-0.2	0.2	-0.0	0.1	220.7	-198.9	0.3	-0.0	0.5	-0.2	252.4	-59.2
REST:	0.7	-0.7	-0.0	0.2	-8.9	29.2	1.9	-1.8	3.2	-3.1	-276.2	342.3
TOTAL:	-0.2	0.1	-0.1	0.2	339.5	-251.8	-0.1	-1.0	0.1	-1.9	251.4	-28.4

E & M DTMs of Molecule 2 for NM 68

Frag.	E_nuc_X	E_el_X	E_nuc_Y	E_el_Y	E_nuc_Z	E_el_Z	M_nuc_X	M_el_X	M_nuc_Y	M_el_Y	M_nuc_Z	M_el_Z
All Axial:	2.4	-1.9	9.9	-8.1	285.1	-481.6	-2.3	0.9	-2.2	3.9	121.7	-181.1
All Equat:	-1.1	1.1	-7.9	7.4	172.7	-155.7	-0.3	0.3	-0.9	0.9	328.8	-112.3
REST:	-0.4	0.6	-2.1	2.9	-72.4	71.6	2.5	-2.4	4.3	-3.7	-215.2	285.4
TOTAL:	0.8	-0.3	-0.2	2.1	385.3	-565.7	0.0	-1.2	1.2	1.1	235.3	-8.0

E & M DTMs of Molecule 3 for NM 69

Frag.	E_nuc_X	E_el_X	E_nuc_Y	E_el_Y	E_nuc_Z	E_el_Z	M_nuc_X	M_el_X	M_nuc_Y	M_el_Y	M_nuc_Z	M_el_Z
All Axial:	-2.4	2.2	-3.2	2.9	100.6	-57.7	-5.3	2.1	-9.2	3.8	300.1	-312.4
All Equat:	-0.1	0.6	-0.5	1.2	305.9	-308.5	0.9	-0.4	1.7	-0.7	281.4	-153.5
REST:	1.8	-2.2	2.5	-3.0	-45.9	80.7	4.3	-4.4	7.6	-7.9	-378.5	464.6
TOTAL:	-0.7	0.6	-1.3	1.2	360.6	-285.5	-0.1	-2.7	0.1	-4.8	203.1	-1.3

E & M DTMs of Molecule 4 for NM 75

Frag.	E_nuc_X	E_el_X	E_nuc_Y	E_el_Y	E_nuc_Z	E_el_Z	M_nuc_X	M_el_X	M_nuc_Y	M_el_Y	M_nuc_Z	M_el_Z
All Axial:	0.2	-0.1	0.5	-0.3	227.9	-378.9	-2.1	0.6	-3.5	1.2	211.6	-248.7
All Equat:	-0.3	0.2	-1.7	1.8	313.9	-299.1	0.3	-0.1	0.6	-0.1	257.6	-107.9
REST:	0.4	-0.4	0.8	-0.7	-45.5	70.2	1.9	-1.9	3.0	-3.4	-279.2	320.3
TOTAL:	0.3	-0.2	-0.4	0.8	496.3	-607.8	0.1	-1.4	0.1	-2.3	190.0	-36.3

Table 3: Comparison of the Cartesian components of the electronic (el) and nuclear (nuc) components of the EDTM and MDTM of the modes: 82 of $\Lambda - \delta\delta\delta$ (1), 88 of $\Lambda - \delta\delta\delta\cdots 2\mathrm{Cl}^-$ (2), 91 of $\Lambda - \delta\delta\delta\cdots 3\mathrm{Cl}^-$ (3) and 97 of $\Lambda - \delta\delta\delta\cdots 5\mathrm{Cl}^-$ (4). Since the two modes have A_2 symmetry only the non-zero Z Cartesian components are shown. Units: EDTM (10^{-22} esu·cm), MDTM (10^{-24} esu·cm).

E & M DTMs of Molecule 1 for NM 82

Frag.	E_nuc_X	E_el_X	E_nuc_Y	E_el_Y	E_nuc_Z	E_el_Z	M_nuc_X	M_el_X	M_nuc_Y	M_el_Y	M_nuc_Z	M_el_Z
All Axial:	-1.0	0.9	-0.2	0.2	-74.6	64.7	0.6	-0.3	0.7	-0.5	567.7	-470.8
All Equat:	-0.3	0.2	0.0	-0.1	-772.3	667.5	-1.5	1.0	-0.9	0.6	351.6	-248.2
REST:	0.7	-0.7	0.0	-0.0	440.6	-453.0	0.5	-0.6	0.1	-0.1	-440.8	521.1
TOTAL:	-0.6	0.4	-0.2	0.1	-406.3	279.1	-0.5	0.2	-0.1	-0.0	478.5	-197.9

E & M DTMs of Molecule 2 for NM 88

Frag.	E_nuc_X	E_el_X	E_nuc_Y	E_el_Y	E_nuc_Z	E_el_Z	M_nuc_X	M_el_X	M_nuc_Y	M_el_Y	M_nuc_Z	M_el_Z
All Axial:	0.9	-0.9	7.2	-7.0	-123.7	155.8	-2.3	2.4	-5.3	4.1	574.9	-493.6
All Equat:	0.9	-0.9	3.3	-3.1	-635.9	565.7	1.4	-0.6	7.7	-4.8	331.0	-218.1
REST:	-1.0	1.0	-5.7	5.7	388.7	-419.1	0.5	-0.4	-1.1	2.1	-437.3	520.3
TOTAL:	0.8	-0.8	4.9	-4.3	-370.8	302.4	-0.4	1.4	1.3	1.4	468.7	-191.4

E & M DTMs of Molecule 3 for NM 91

Frag.	E_nuc_X	E_el_X	E_nuc_Y	E_el_Y	E_nuc_Z	E_el_Z	M_nuc_X	M_el_X	M_nuc_Y	M_el_Y	M_nuc_Z	M_el_Z
All Axial:	0.0	-0.0	-1.7	1.6	-3.1	6.3	-0.5	0.3	-0.7	0.5	435.3	-392.4
All Equat:	-0.5	0.4	-1.3	1.5	-852.4	768.1	0.6	-0.2	-1.3	1.3	519.9	-681.3
REST:	0.2	-0.2	1.6	-1.8	466.1	-466.9	-0.0	0.0	0.9	-1.2	-459.9	520.8
TOTAL:	-0.2	0.1	-1.4	1.3	-389.5	307.5	0.0	0.1	-1.0	0.7	495.3	-552.9

E & M DTMs of Molecule 4 for NM 97

Frag.	E_nuc_X	E_el_X	E_nuc_Y	E_el_Y	E_nuc_Z	E_el_Z	M_nuc_X	M_el_X	M_nuc_Y	M_el_Y	M_nuc_Z	M_el_Z
All Axial:	1.0	-1.0	2.9	-2.8	-48.8	110.7	-1.6	1.1	-0.2	-0.4	506.7	-456.9
All Equat:	0.6	-0.6	1.7	-2.0	-739.6	664.5	1.9	-0.9	3.2	-2.2	476.6	-527.0
REST:	-0.9	0.9	-2.5	2.6	418.9	-440.5	-0.1	0.1	-1.4	1.8	-473.8	551.5
TOTAL:	0.7	-0.6	2.1	-2.2	-369.6	334.7	0.1	0.3	1.6	-0.9	509.6	-432.4

Table 4: Comparison of the Cartesian components of the electronic (el) and nuclear (nuc) components of the EDTM and MDTM of the modes: 109 of $\Lambda - \delta\delta\delta$ (1) and 123 of $\Lambda - \delta\delta\delta \cdots 5Cl^-$ (4). Since the two modes have A_2 symmetry only the non-zero Z Cartesian components are shown. Units: EDTM (10^{-22} esu·cm), MDTM (10^{-24} esu·cm).

E & M DTMs of Molecule 1 for NM 107

Frag.	E_nuc_X	E_el_X	E_nuc_Y	E_el_Y	E_nuc_Z	E_el_Z	M_nuc_X	M_el_X	M_nuc_Y	M_el_Y	M_nuc_Z	M_el_Z
All Axial:	7.4	-11.8	-72.6	79.8	6.8	-5.5	204.2	-186.2	476.9	-360.4	0.6	-0.1
All Equat:	-40.8	38.9	-306.9	255.6	0.4	-0.5	123.0	-114.6	-110.8	97.3	6.2	-4.6
REST:	16.3	-16.6	186.1	-184.1	-3.6	3.6	-162.2	200.5	-180.3	200.4	-3.2	3.5
TOTAL:	-17.1	10.4	-193.4	151.4	3.6	-2.3	165.0	-100.3	185.8	-62.7	3.6	-1.2

E & M DTMs of Molecule 4 for NM 124

Frag.	E_nuc_X	E_el_X	E_nuc_Y	E_el_Y	E_nuc_Z	E_el_Z	M_nuc_X	M_el_X	M_nuc_Y	M_el_Y	M_nuc_Z	M_el_Z
All Axial:	-21.9	2.8	-113.9	15.5	2.4	-0.9	71.1	39.8	407.8	214.3	0.1	-0.2
All Equat:	-49.0	7.1	-258.7	39.3	-0.8	-0.1	-18.8	4.4	-87.4	28.1	-7.2	0.6
REST:	34.5	-37.7	181.4	-198.1	-0.9	0.9	-25.5	33.1	-156.7	203.8	2.8	-3.6
TOTAL:	-36.4	-27.8	-191.2	-143.3	0.7	-0.0	26.8	77.3	163.8	446.2	-4.2	-3.2