Supporting information for

Proton Delocalization in Short Hydrogen Bonds Assembling $HSeO_4^-$ Anions into Supramolecular Adducts

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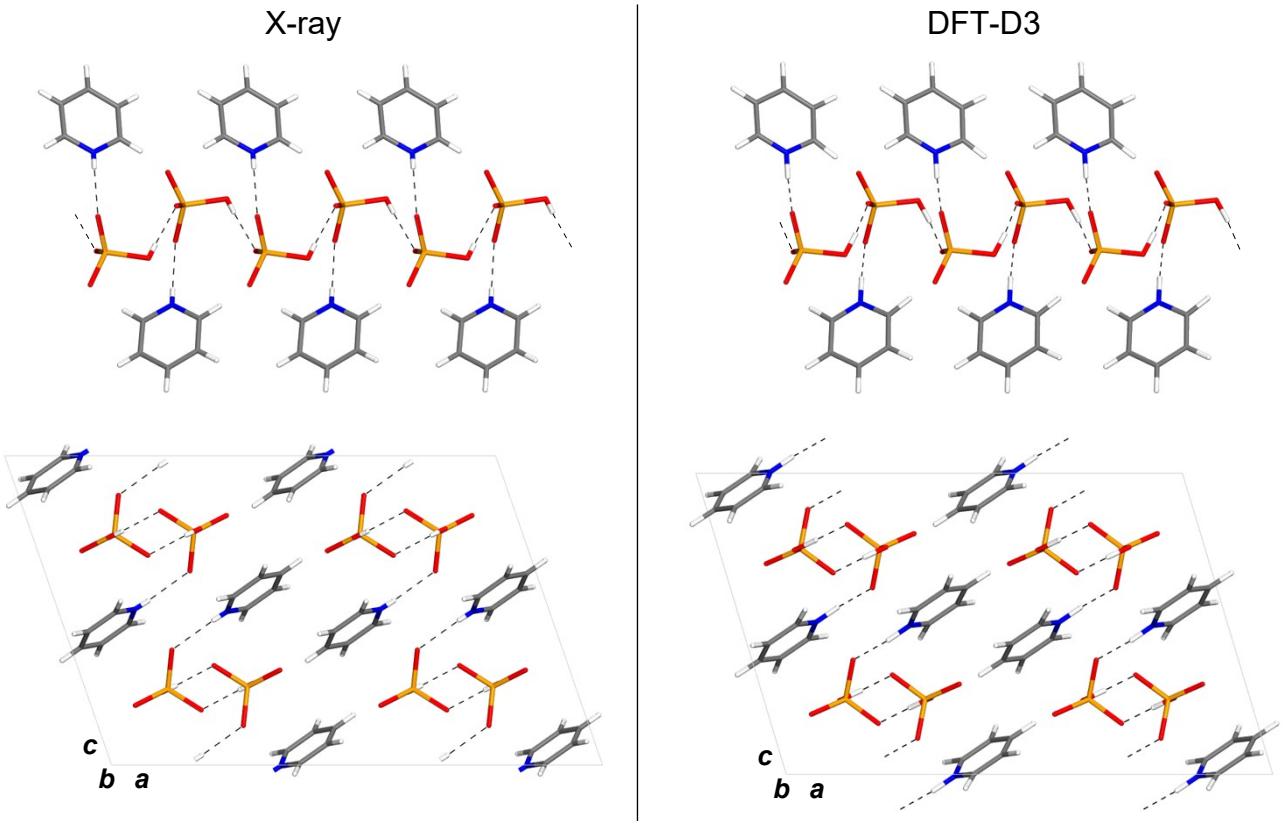


Figure S1. X-ray and DFT-D3 optimized crystal structures of **1a·2a** (chain fragments and crystallographic cells with labeled axes in a standard setting). The O–H···O and O···H–N bonds are shown as black dashed lines.

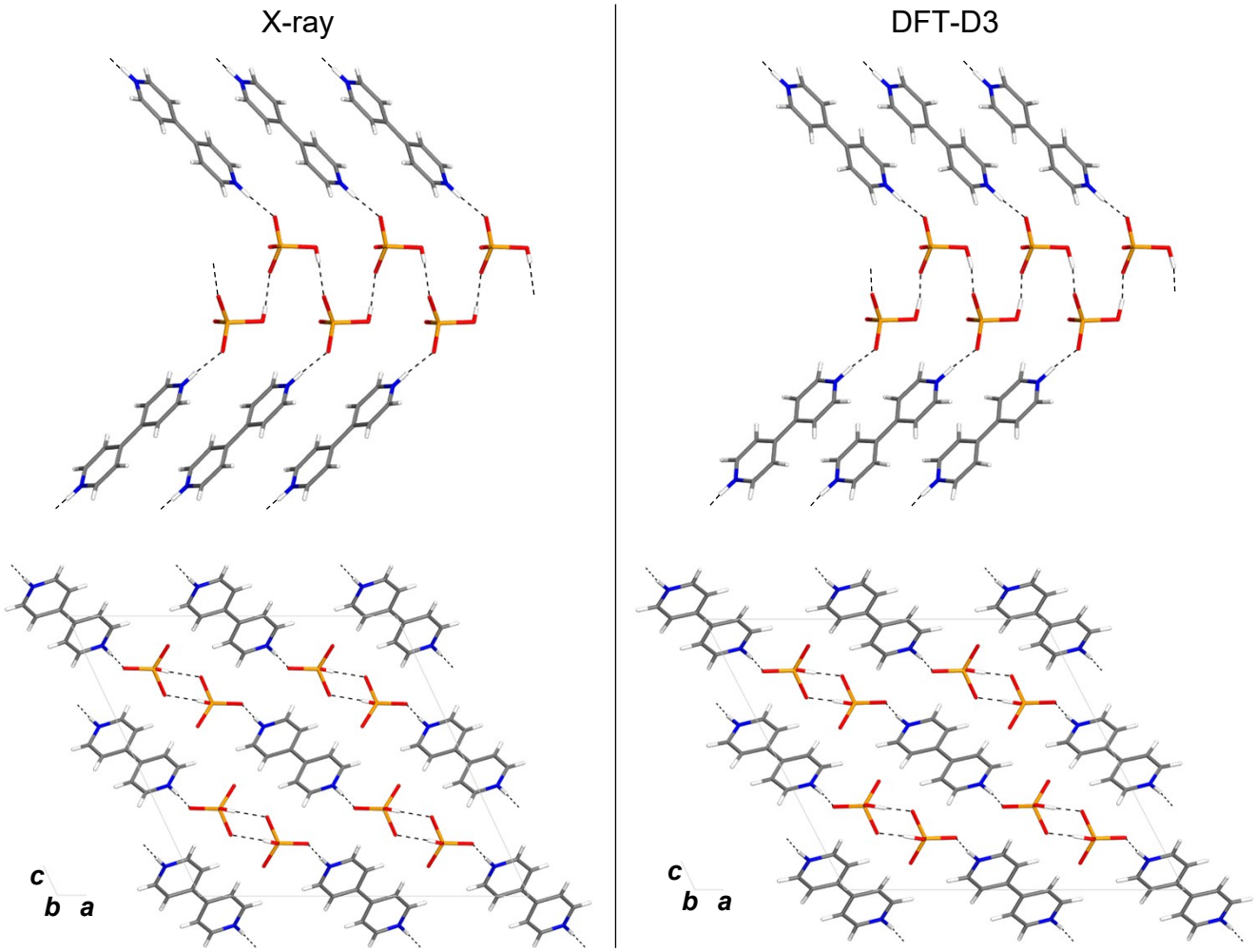


Figure S2. X-ray and DFT-D3 optimized crystal structures of **1a·2b** (chain fragments and crystallographic cells with labeled axes in a standard setting). The O–H···O and O···H–N bonds are shown as black dashed lines.

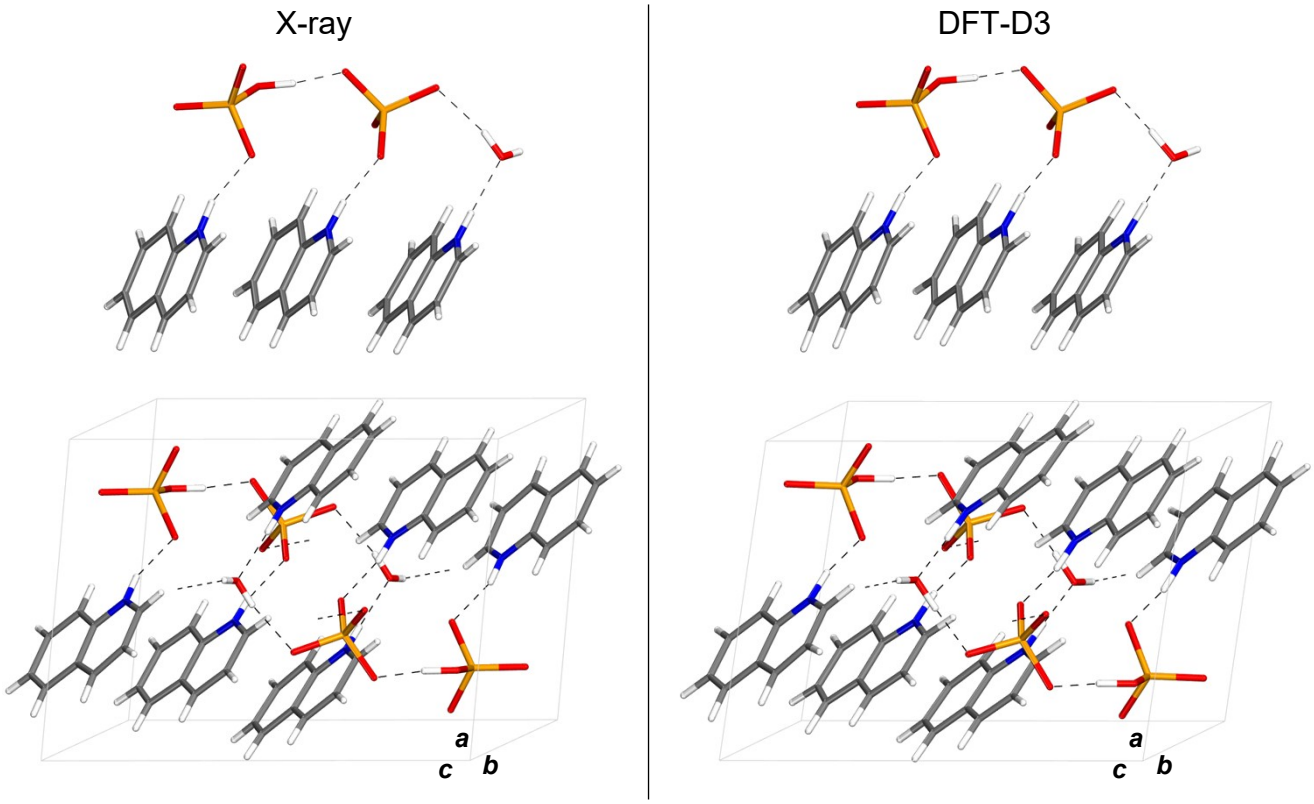


Figure S3. X-ray and DFT-D3 optimized crystal structures of **1a·1b·2c** (irreducible fragments and primitive cells with labeled axes). The O–H···O and O···H–N bonds are shown as black dashed lines.

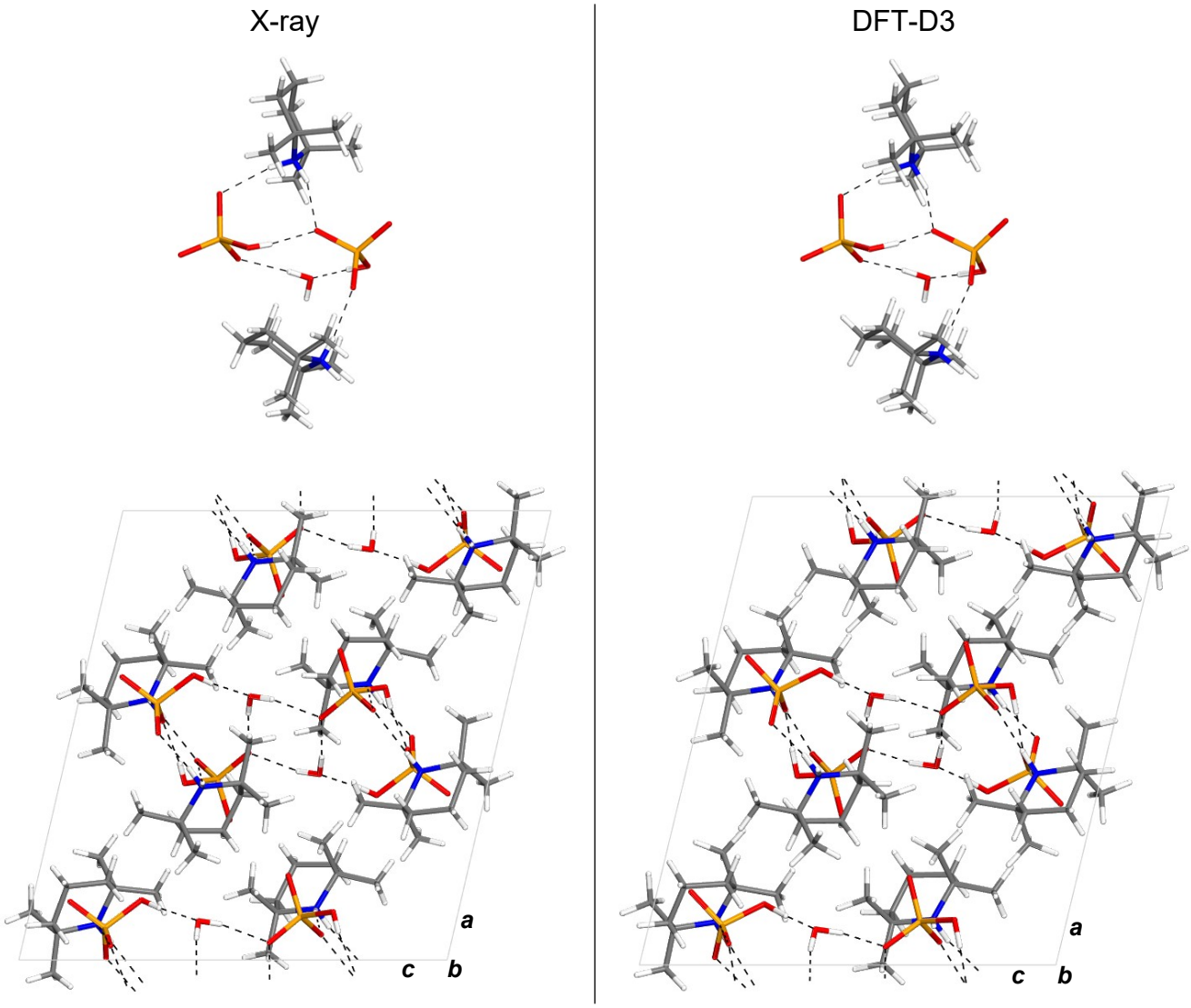


Figure S4. X-ray and DFT-D3 optimized crystal structures of **1a·2d** (irreducible fragments and primitive cells with labeled axes in a standard setting). The O–H···O and O···H–N bonds are shown as black dashed lines.

Table S1. Crystal data and structure refinement for **1a·2a** at 298 K.

Identification code	**1a·2a**
Empirical formula	$C_5H_7NO_4Se$
Formula weight	224.08
Temperature/K	298.01(10)
Crystal system	monoclinic
Space group	C2/c
a/Å	19.8196(2)
b/Å	6.26820(10)
c/Å	13.2167(2)
α/°	90
β/°	109.0590(10)
γ/°	90
Volume/Å^3	1551.95(4)
Z	8
ρ_{calc}/g·cm^{-3}	1.918
μ/mm^{-1}	6.363
F(000)	880.0
Crystal size/mm^3	0.2 × 0.1 × 0.05
Radiation	Cu Kα (λ = 1.54184 Å)
2Θ range for data collection/°	9.442 to 152.868
Index ranges	-24 ≤ h ≤ 24, -7 ≤ k ≤ 7, -16 ≤ l ≤ 16
Reflections collected	13252
Independent reflections	1547 [R_{int} = 0.0644, R_{sigma} = 0.0252]
Data/restraints/parameters	1547/0/109
Goodness-of-fit on F^2	1.124
Final R indexes [I>=2σ(I)]	R_1 = 0.0268, wR_2 = 0.0761
Final R indexes [all data]	R_1 = 0.0279, wR_2 = 0.0768
Largest diff. peak/hole/e·Å^{-3}	0.37/-0.40
CCDC Number	2417665

Table S2. Crystal data and structure refinement for **1a·2a** at 100 K.

Identification code	**1a·2a**
Empirical formula	$C_5H_7NO_4Se$
Formula weight	224.08
Temperature/K	100.01(11)
Crystal system	monoclinic
Space group	C2/c
a/Å	19.6801(4)
b/Å	6.20570(10)
c/Å	13.0059(2)
α/°	90
β/°	108.101(2)
γ/°	90
Volume/Å^3	1509.79(5)
Z	8
ρ_{calc}/g·cm^{-3}	1.972
μ/mm^{-1}	6.540
F(000)	880.0
Crystal size/mm^3	0.2 × 0.1 × 0.05
Radiation	Cu Kα (λ = 1.54184 Å)
2Θ range for data collection/°	9.456 to 153.35
Index ranges	-24 ≤ h ≤ 24, -7 ≤ k ≤ 7, -12 ≤ l ≤ 15
Reflections collected	12501
Independent reflections	1531 [R_{int} = 0.0540, R_{sigma} = 0.0261]
Data/restraints/parameters	1531/0/104
Goodness-of-fit on F^2	1.107
Final R indexes [I>=2σ(I)]	R_1 = 0.0282, wR_2 = 0.0793
Final R indexes [all data]	R_1 = 0.0295, wR_2 = 0.0806
Largest diff. peak/hole/e·Å^{-3}	0.69/-0.77
CCDC Number	2417668

Table S3. Crystal data and structure refinement for **1a·2b** at 298 K.

Identification code	**1a·2b**
Empirical formula	$C_5H_6NO_4Se$
Formula weight	223.07
Temperature/K	298.01(10)
Crystal system	monoclinic
Space group	C2/c
a/Å	18.0562(2)
b/Å	5.15783(5)
c/Å	16.9795(2)
α/°	90
β/°	115.2773(14)
γ/°	90
Volume/Å^3	1429.91(3)
Z	8
ρ_{calc}/g·cm^{-3}	2.072
μ/mm^{-1}	6.905
F(000)	872.0
Crystal size/mm^3	0.3 × 0.2 × 0.1
Radiation	Cu Kα (λ = 1.54184 Å)
2Θ range for data collection/°	10.838 to 150.78
Index ranges	-22 ≤ h ≤ 21, -6 ≤ k ≤ 6, -21 ≤ l ≤ 21
Reflections collected	12187
Independent reflections	1433 [R_{int} = 0.0360, R_{sigma} = 0.0170]
Data/restraints/parameters	1433/1/109
Goodness-of-fit on F^2	1.086
Final R indexes [I>=2σ(I)]	R_1 = 0.0211, wR_2 = 0.0580
Final R indexes [all data]	R_1 = 0.0218, wR_2 = 0.0585
Largest diff. peak/hole/e·Å^{-3}	0.35/-0.53
CCDC Number	2417669

Table S4. Crystal data and structure refinement for **1a·2b** at 100 K.

Identification code	**1a·2b**
Empirical formula	$C_5H_6NO_4Se$
Formula weight	223.07
Temperature/K	99.99(10)
Crystal system	monoclinic
Space group	I2/a
a/Å	16.7423(2)
b/Å	5.11409(7)
c/Å	18.4872(3)
α/°	90
β/°	118.2924(19)
γ/°	90
Volume/Å^3	1393.81(4)
Z	8
ρ_{calc}/g·cm^{-3}	2.126
μ/mm^{-1}	7.084
F(000)	872.0
Crystal size/mm^3	0.2 × 0.1 × 0.05
Radiation	Cu Kα (λ = 1.54184 Å)
2Θ range for data collection/°	10.87 to 153.098
Index ranges	-20 ≤ h ≤ 21, -5 ≤ k ≤ 6, -22 ≤ l ≤ 22
Reflections collected	11468
Independent reflections	1393 [R_{int} = 0.0321, R_{sigma} = 0.0150]
Data/restraints/parameters	1393/0/105
Goodness-of-fit on F^2	1.088
Final R indexes [I>=2σ(I)]	R_1 = 0.0190, wR_2 = 0.0514
Final R indexes [all data]	R_1 = 0.0193, wR_2 = 0.0516
Largest diff. peak/hole/e·Å^{-3}	0.41/-0.41
CCDC Number	2417697

Table S5. Crystal data and structure refinement for **1a·1b·2c** at 298 K.

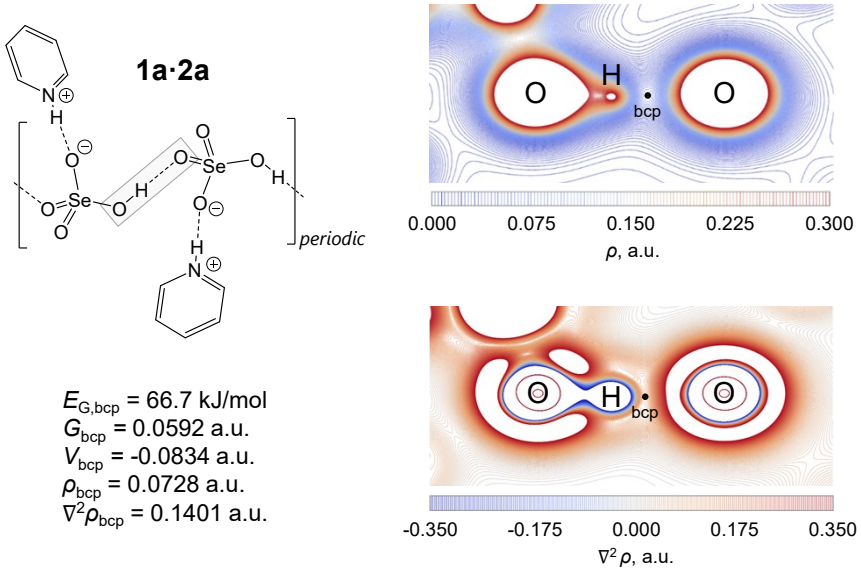
Identification code	**1a·1b·2c**
Empirical formula	$C_{27}H_{27}N_3O_9Se_2$
Formula weight	695.43
Temperature/K	298.4(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.91309(16)
b/Å	10.3638(2)
c/Å	14.6046(3)
α/°	76.9481(16)
β/°	89.2209(14)
γ/°	71.1833(16)
Volume/Å^3	1380.70(5)
Z	2
ρ_{calc}/g·cm^{-3}	1.673
μ/mm^{-1}	3.868
F(000)	700.0
Crystal size/mm^3	0.2 × 0.1 × 0.05
Radiation	Cu Kα (λ = 1.54184 Å)
2Θ range for data collection/°	6.226 to 152.074
Index ranges	-12 ≤ h ≤ 12, -11 ≤ k ≤ 12, -17 ≤ l ≤ 18
Reflections collected	47717
Independent reflections	5435 [R_{int} = 0.0384, R_{sigma} = 0.0179]
Data/restraints/parameters	5435/0/389
Goodness-of-fit on F^2	1.020
Final R indexes [I>=2σ(I)]	R_1 = 0.0288, wR_2 = 0.0745
Final R indexes [all data]	R_1 = 0.0363, wR_2 = 0.0811
Largest diff. peak/hole/e·Å^{-3}	0.53/-0.42
CCDC Number	2417671

Table S6. Crystal data and structure refinement for **1a·2d** at 298 K.

Identification code	**1a·2d**
Empirical formula	$C_{18}H_{44}N_2O_9Se_2$
Formula weight	590.47
Temperature/K	299.19(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	15.70227(9)
b/Å	10.12297(5)
c/Å	16.96831(9)
α/°	90
β/°	102.9938(6)
γ/°	90
Volume/Å^3	2628.11(3)
Z	4
ρ_{calc}/g·cm^{-3}	1.492
μ/mm^{-1}	3.916
F(000)	1224.0
Crystal size/mm^3	0.2 × 0.1 × 0.05
Radiation	Cu Kα (λ = 1.54184 Å)
2Θ range for data collection/°	6.934 to 152.74
Index ranges	-19 ≤ h ≤ 19, -12 ≤ k ≤ 12, -21 ≤ l ≤ 20
Reflections collected	47878
Independent reflections	5327 [R_{int} = 0.0417, R_{sigma} = 0.0220]
Data/restraints/parameters	5327/0/300
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ(I)]	R_1 = 0.0236, wR_2 = 0.0610
Final R indexes [all data]	R_1 = 0.0251, wR_2 = 0.0618
Largest diff. peak/hole/e·Å^{-3}	0.30/-0.57
CCDC Number	2417672

Table S7. Crystal data and structure refinement for **1a·2d** at 100 K.

Identification code	**1a·2d**
Empirical formula	$C_{18}H_{44}N_2O_9Se_2$
Formula weight	590.47
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	15.50150(10)
b/Å	10.08722(6)
c/Å	16.80632(11)
α/°	90
β/°	102.7673(6)
γ/°	90
Volume/Å^3	2562.98(3)
Z	4
ρ_{calc}/g·cm^{-3}	1.530
μ/mm^{-1}	4.015
F(000)	1224.0
Crystal size/mm^3	0.2 × 0.1 × 0.05
Radiation	Cu Kα (λ = 1.54184 Å)
2Θ range for data collection/°	7.024 to 153.42
Index ranges	-19 ≤ h ≤ 19, -12 ≤ k ≤ 12, -21 ≤ l ≤ 20
Reflections collected	46970
Independent reflections	5242 [R_{int} = 0.0500, R_{sigma} = 0.0249]
Data/restraints/parameters	5242/0/300
Goodness-of-fit on F^2	1.057
Final R indexes [I>=2σ(I)]	R_1 = 0.0225, wR_2 = 0.0567
Final R indexes [all data]	R_1 = 0.0247, wR_2 = 0.0579
Largest diff. peak/hole/e·Å^{-3}	0.35/-0.49
CCDC Number	2417674



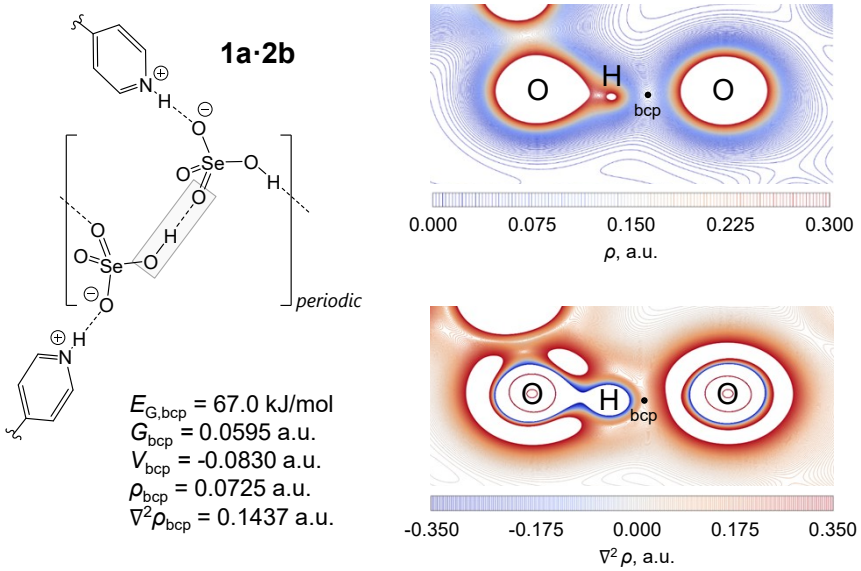
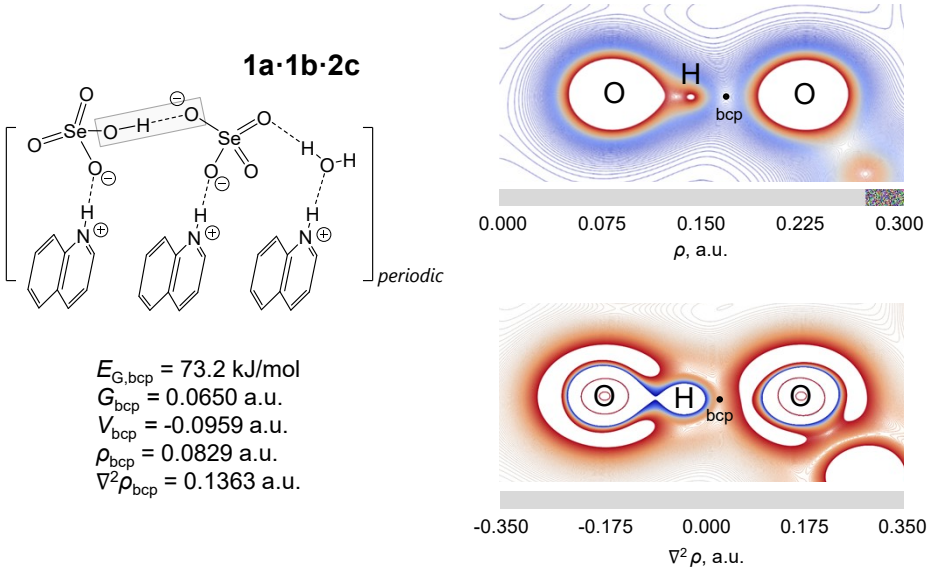


Figure S5. QTAIM analysis of 3D periodic electron density, ρ, and 2D distribution maps of ρ and the Laplacian of the electron density, $\nabla^2\rho$, around the SeO–H···OSe bonds in **1a·2a** and **1a·2b** in their equilibrium geometries.



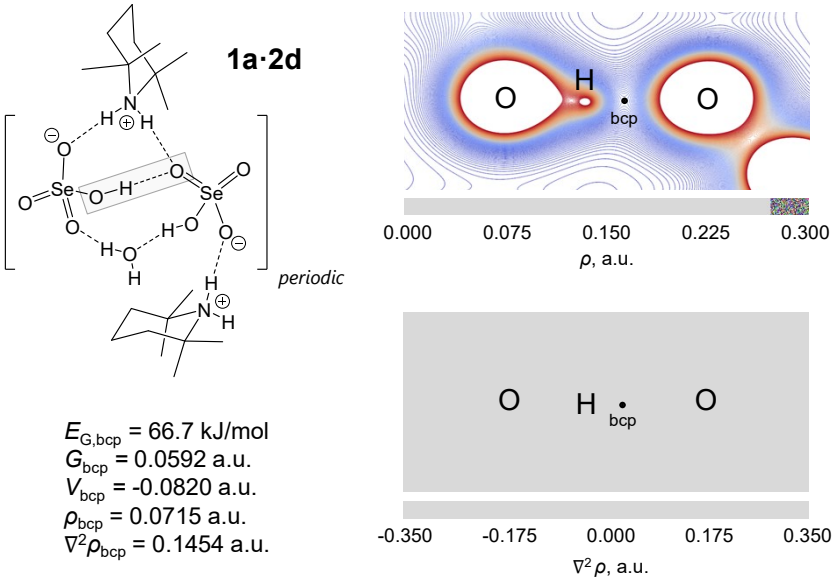


Figure S6. QTAIM analysis of 3D periodic electron density, ρ, and 2D distribution maps of ρ and the Laplacian of the electron density, $\nabla^2\rho$, around the SeO–H···OSe bonds in **1a·1b·2c** and **1a·2d** in their equilibrium geometries.

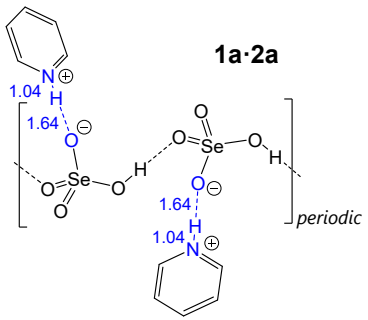
The values of the ρ, $\nabla^2\rho$ and the local electron potential and kinetic energy densities, V and G, at the bond critical points (BCPs) are given. The G_{bcp} values were converted into the values of the H-bond interaction energy, $E_{G,bcp} \equiv E_{OHO}$, according to the formula proposed in Refs. 1,2:

$$E_{G,bcp} = 0.429\ G_{bcp},$$

where G is in kJ/(mol·Å^3).

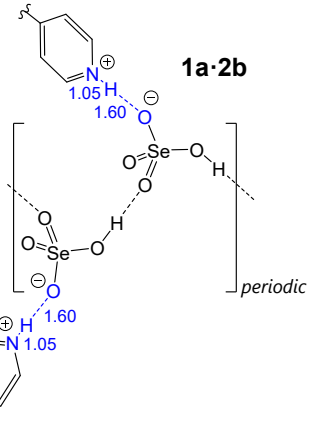
The exploration of the crystalline wave functions firmly places the studied crystals at an intermediate position between covalent and non-covalent bonds as the H-bonding is regarded with the non-spherical shape of the O–H groups, exhibiting high values of ρ_{bcp} but positive $\nabla^2\rho_{bcp}$ values and moderate positive net atomic charges of bridging hydrogen atoms (0.62–0.65 e), computed by integrating the ρ within the corresponding atomic basins.

1a·2a



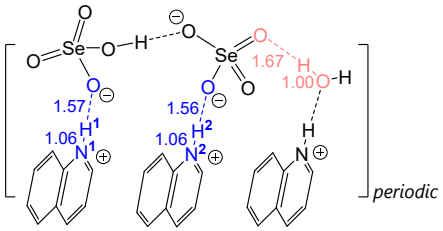
$E_{G,bcp}$ = 52.5 kJ/mol
G_{bcp} = 0.0466 a.u.
V_{bcp} = -0.0559 a.u.
$|V_{bcp}|/G_{bcp}$ = 1.2007
H_{bcp} = -0.0094 a.u.
ρ_{bcp} = 0.0517 a.u.
$\nabla^2\rho_{bcp}$ = 0.1489 a.u.
H_{bcp}/ρ_{bcp} = -0.1810 a.u.

1a·2b



$E_{G,bcp}$ = 57.6 kJ/mol
G_{bcp} = 0.0512 a.u.
V_{bcp} = -0.0645 a.u.
$|V_{bcp}|/G_{bcp}$ = 1.2614
H_{bcp} = -0.0134 a.u.
ρ_{bcp} = 0.0583 a.u.
$\nabla^2\rho_{bcp}$ = 0.1511 a.u.
H_{bcp}/ρ_{bcp} = -0.2294 a.u.

1a·1b·2c



OH^1N^1

$E_{G,bcp}$ = 61.9 kJ/mol
G_{bcp} = 0.0549 a.u.
V_{bcp} = -0.0710 a.u.
$|V_{bcp}|/G_{bcp}$ = 1.2934
H_{bcp} = -0.0161 a.u.
ρ_{bcp} = 0.0633 a.u.
$\nabla^2\rho_{bcp}$ = 0.1552 a.u.
H_{bcp}/ρ_{bcp} = -0.2546 a.u.

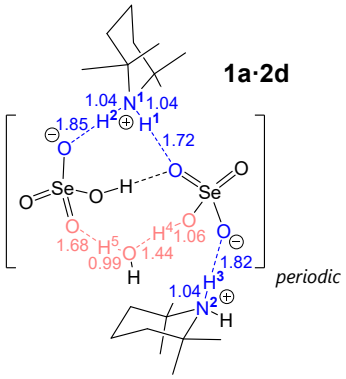
OH^2N^2

$E_{G,bcp}$ = 62.3 kJ/mol
G_{bcp} = 0.0553 a.u.
V_{bcp} = -0.0716 a.u.
$|V_{bcp}|/G_{bcp}$ = 1.2940
H_{bcp} = -0.0163 a.u.
ρ_{bcp} = 0.0636 a.u.
$\nabla^2\rho_{bcp}$ = 0.1562 a.u.
H_{bcp}/ρ_{bcp} = -0.2555 a.u.

OHO_{water}

$E_{G,bcp}$ = 48.9 kJ/mol
G_{bcp} = 0.0434 a.u.
V_{bcp} = -0.0536 a.u.
$|V_{bcp}|/G_{bcp}$ = 1.2337
H_{bcp} = -0.0101 a.u.
ρ_{bcp} = 0.0497 a.u.
$\nabla^2\rho_{bcp}$ = 0.1331 a.u.
H_{bcp}/ρ_{bcp} = -0.2041 a.u.

1a·2d



OH^1N^1

$E_{G,bcp}$ = 44.7 kJ/mol
G_{bcp} = 0.0397 a.u.
V_{bcp} = -0.0443 a.u.
$|V_{bcp}|/G_{bcp}$ = 1.1167
H_{bcp} = -0.0046 a.u.
ρ_{bcp} = 0.0437 a.u.
$\nabla^2\rho_{bcp}$ = 0.1402 a.u.
H_{bcp}/ρ_{bcp} = -0.1061 a.u.

OH^2N^1

$E_{G,bcp}$ = 32.0 kJ/mol
G_{bcp} = 0.0285 a.u.
V_{bcp} = -0.0288 a.u.
$|V_{bcp}|/G_{bcp}$ = 1.0120
H_{bcp} = -0.0003 a.u.
ρ_{bcp} = 0.0321 a.u.
$\nabla^2\rho_{bcp}$ = 0.1126 a.u.
H_{bcp}/ρ_{bcp} = -0.0106 a.u.

OH^3N^2

$E_{G,bcp}$ = 33.5 kJ/mol
G_{bcp} = 0.0297 a.u.
V_{bcp} = -0.0302 a.u.
$|V_{bcp}|/G_{bcp}$ = 1.0171
H_{bcp} = -0.0005 a.u.
ρ_{bcp} = 0.0330 a.u.
$\nabla^2\rho_{bcp}$ = 0.1168 a.u.
H_{bcp}/ρ_{bcp} = -0.0154 a.u.

OH^4O_{water}

$E_{G,bcp}$ = 75.0 kJ/mol
G_{bcp} = 0.0666 a.u.
V_{bcp} = -0.1017 a.u.
$|V_{bcp}|/G_{bcp}$ = 1.5275
H_{bcp} = -0.0351 a.u.
ρ_{bcp} = 0.0884 a.u.
$\nabla^2\rho_{bcp}$ = 0.1259 a.u.
H_{bcp}/ρ_{bcp} = -0.3976 a.u.

OH^5O_{water}

$E_{G,bcp}$ = 45.8 kJ/mol
G_{bcp} = 0.0407 a.u.
V_{bcp} = -0.0479 a.u.
$|V_{bcp}|/G_{bcp}$ = 1.1772
H_{bcp} = -0.0072 a.u.
ρ_{bcp} = 0.0451 a.u.
$\nabla^2\rho_{bcp}$ = 0.1339 a.u.
H_{bcp}/ρ_{bcp} = -0.1599 a.u.

Figure S7. QTAIM analysis of 3D periodic electron density around the SeO···H–N as well as SeO–H···O_{water} and SeO···H–O_{water} bonds in **1a·2a**, **1a·2b**, **1a·1b·2c** and **1a·2d** in their equilibrium geometries. The H-bond interatomic distances are given in Å. For each individual H-bond the values of the ρ, $\nabla^2\rho$, V, G, $|V|/G$, $H = (V + G)$ and H/ρ are given at the corresponding BCPs. The values of the H-bond interaction energy were estimated as $E_{G,bcp} = 0.429\ G_{bcp}$.[1,2]

Comments to **Figure S7**. Comparative analysis of the OHN and OHO_{water} H-bonds.

Let us introduce here the following notations for protonated N-heterocycles: pyridinium ≡ ①, 4,4'-bipyridilium ≡ ②, quinolinium ≡ ③, 2,2,6,6-tetramethylpyperidinium ≡ ④. According to pK_b values, the expected NH-acidity increases in the ① → ③ → ② → ④ sequence (considering the doubly protonated form ②). However, according to the geometric and QTAIM-parameters, the interaction energy of the SeO···H–N bonds does not follow this sequence: instead, $E_{G,bcp}$ values increase in the ④ → ① → ② → ③ sequence from ca. 30 kJ/mol to ca. 60 kJ/mol, in line with the calculated $\nu_{anharm\ av.}$(N–H) frequencies (see main text). The reasons for this are the following.

(i) Form ② simultaneously participates in two H-bonding interactions with selenate anions from neighbouring chains, which diminishes its effective NH-acidity making it intermediate between those of ① and ③.

(ii) The bulky structure of ④ precludes its approaching to the selenate anions on a sufficiently short distance within the dense crystal packing, thus making ④ effectively the weakest NH-donor in the series.

In turn, SeO···H–O_{water} bonds are similar in strength to SeO···H–N bonds, while the SeO–H···O_{water} bond in **1a·2d** is noticeably stronger, ca. 75 kJ/mol, which is likely to play an important role in the stabilization of the supramolecular assembly. It should be noted that other QTAIM parameters (ρ, $\nabla^2\rho$, V, G, $|V|/G$, $H = (V + G)$ and H/ρ) follow the same trend as $E_{G,bcp}$, so they are not discussed here separately. Formally, QTAIM parameters indicate that all H-bonds in the studied systems could be classified as moderate/moderately strong bonds.

Additionally, we investigated the π-stacking type dispersive interactions between aromatic cation units in **1a·2a**, **1a·2b**, and **1a·1b·2c**. QTAIM analysis indeed revealed the presence of BCPs of the (3, –1) type on the C···C bond pathways (two in **1a·2a**, one in **1a·2b**, and ten in **1a·1b·2c** per irreducible part of the unit cell) as well as on the C···N bond pathways (two in **1a·1b·2c** per irreducible part of the unit cell). All of these BCPs are characterized by narrow ranges of $0.009 > \rho_{bcp} > 0.005$ a.u. and $6.4 > E_{C\cdots C/C\cdots N} > 3.6$ kJ/mol, typical for π-stacking interactions. We suggest that the cumulative effect of such weak bonding interactions leads to a noticeable gain in the stabilization energy in these three crystalline systems (especially in case of **1a·1b·2c**), which potentially might be useful for future studies of their proton conductivity at elevated operating temperatures.

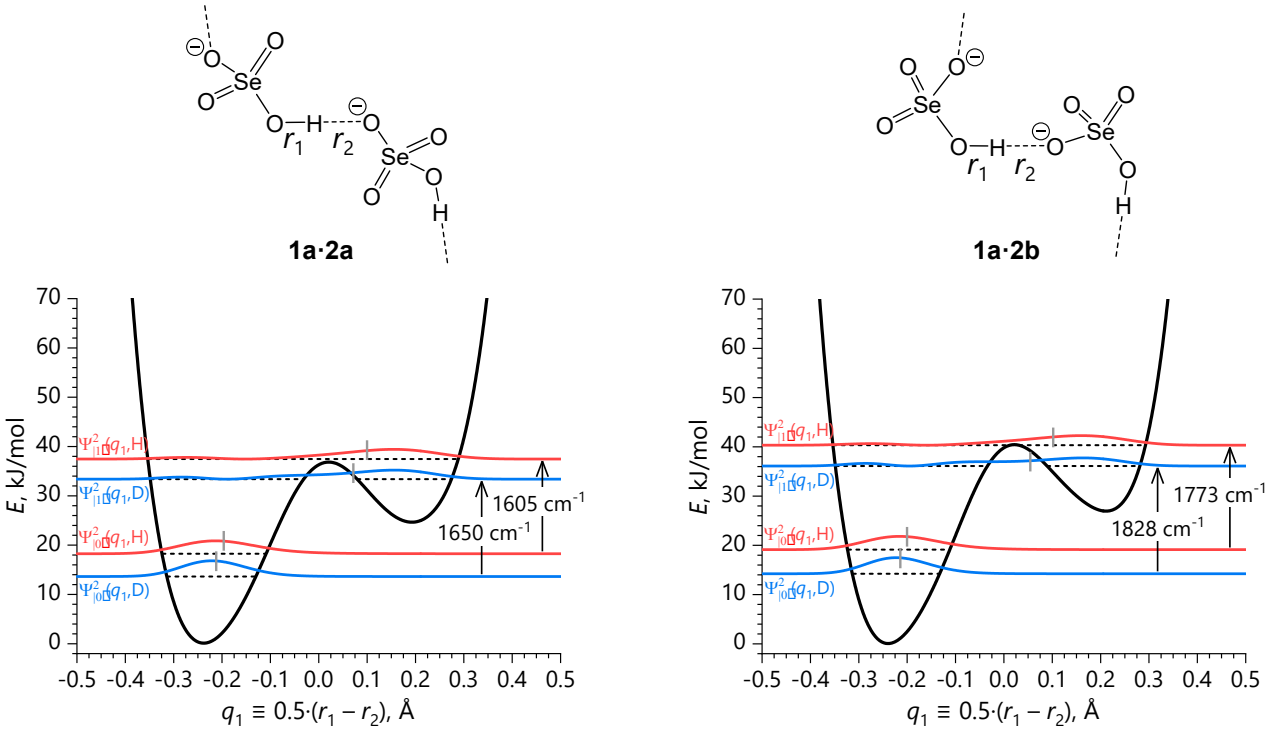
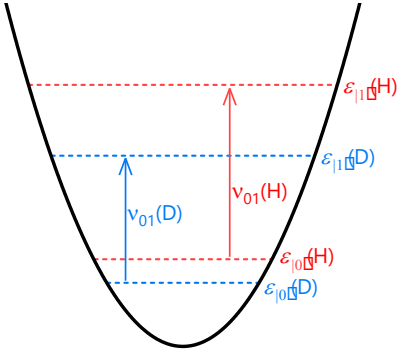


Figure S8. Asymmetric double-well 1D potentials of the coherent quasi-adiabatic transfer of the bridging hydrons along the SeO–L···OSe (L = H/D) bond q_1 coordinate with the corresponding $|0\rangle$ and $|1\rangle$ vibrational states and fundamental transition frequencies. Double-well potentials pertain to **1a·2a** and **1a·2b** featuring infinite SeO–L···OSe bond chains. Short grey vertical bars indicate the vibrationally-averaged positions of the hydron's q_1 coordinate:

$$\langle \Psi_{|n\rangle}(q_1,L) \,|\, q_1 \,|\, \Psi_{|n\rangle}(q_1,L) \rangle, \; n = 0,1.$$

Illustration to **Figure S8**. Comparative analysis of the H and D zero-point energy (ZPE) levels, $\varepsilon_{|0\rangle}$, and fundamental transition frequencies, $\nu_{01} = \varepsilon_{|1\rangle} - \varepsilon_{|0\rangle}$, corresponding to *ad hoc* harmonic, slightly anharmonic, and strongly anharmonic 1D oscillators (OH/OD stretching potentials).

Harmonic oscillator



$\varepsilon_{|0\rangle}(\mathrm{D}) < \varepsilon_{|0\rangle}(\mathrm{H})$

$\nu_{01}(\mathrm{D}) < \nu_{01}(\mathrm{H})$

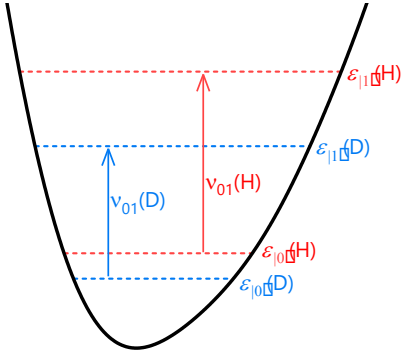
$$ZPE = \varepsilon_{|0\rangle} = \frac{1}{2}h\nu_{01}$$

$$\frac{\nu_{01}(\mathrm{H})}{\nu_{01}(\mathrm{D})} = \sqrt{2}$$

Exact equation for ZPE.

'Normal' isotope effect on vibrational frequency.

Anharmonic oscillator



$\varepsilon_{|0\rangle}(\mathrm{D}) < \varepsilon_{|0\rangle}(\mathrm{H})$

$\nu_{01}(\mathrm{D}) < \nu_{01}(\mathrm{H})$

$$ZPE = \varepsilon_{|0\rangle} \approx \frac{1}{2}h\nu_{01}$$

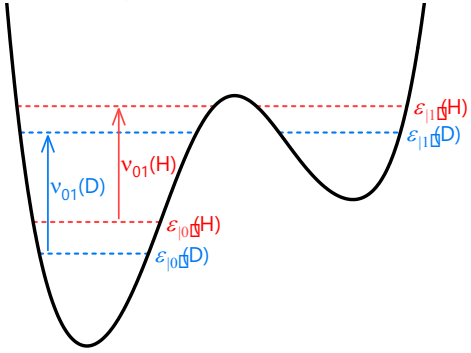
$$1 < \frac{\nu_{01}(\mathrm{H})}{\nu_{01}(\mathrm{D})} < \sqrt{2}$$

Approximate equation for ZPE.

'Normal' isotope effect on vibrational frequency.

Extremely anharmonic oscillator

(asymmetric double-well)



$\varepsilon_{|0\rangle}(\mathrm{D}) < \varepsilon_{|0\rangle}(\mathrm{H})$

$\nu_{01}(\mathrm{D}) > \nu_{01}(\mathrm{H})$

$$ZPE = \varepsilon_{|0\rangle} \neq \frac{1}{2}h\nu_{01}$$

$$\frac{\nu_{01}(\mathrm{H})}{\nu_{01}(\mathrm{D})} < 1$$

Equation for ZPE of a harmonic oscillator is inappropriate.

'Anomalous' isotope effect on vibrational frequency.

For most of the O–H(D)···O bonds, $\nu_{01}(D)$ frequencies of are lower than $\nu_{01}(H)$ ones ('normal' isotope effect). However, in some cases, depending on the shape of the stretching potential, the fundamental band of the O–D mode appears at higher frequency than that for the O–H one, *i.e.* $\nu_{01}(H) < \nu_{01}(D)$ ('anomalous' isotope effect). This happens when the anharmonically increased width of the potential makes the $\varepsilon_{|1\rangle}(H)$ and

$\varepsilon_{|1\rangle}(D)$ levels *closer* to each other in comparison to the $\varepsilon_{|0\rangle}(H)$ and $\varepsilon_{|0\rangle}(D)$ levels. Such peculiarity arises, in particular, in case of the low-barrier double-well potentials, and was experimentally demonstrated for very short H-bonds in Ref. 3.

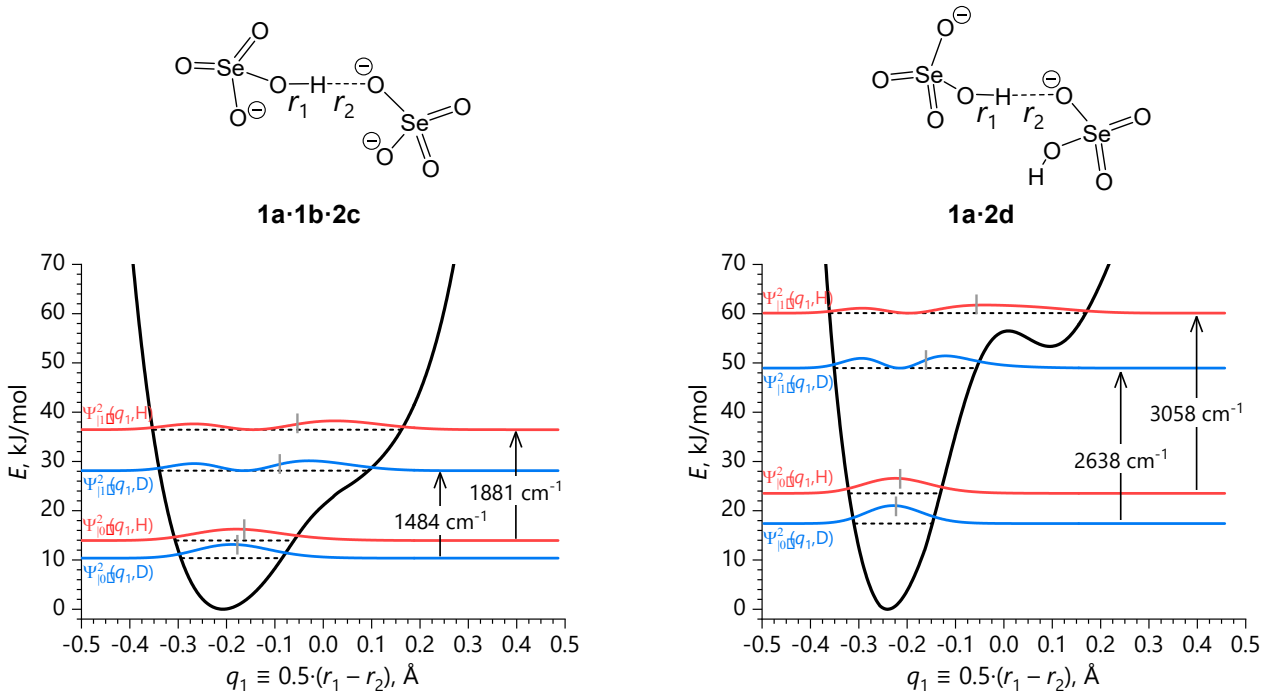


Figure S9. Asymmetric single-/double-well 1D potentials of the coherent quasi-adiabatic transfer of the bridging hydrons along the SeO–L···OSe (L = H/D) bond q_1 coordinate with the corresponding $|0\rangle$ and $|1\rangle$ vibrational states and fundamental transition frequencies. Single- and double-well potentials pertain to **1a·1b·2c** and **1a·2d**, respectively, featuring 'isolated' SeO–L···OSe bonds. Short grey vertical bars indicate the vibrationally-averaged positions of the hydron's q_1 coordinate:

$$\langle \Psi_{|n\rangle}(q_1,L) \,|\, q_1 \,|\, \Psi_{|n\rangle}(q_1,L) \rangle, \; n = 0,1.$$

The uncertainty of the bridging hydron position within the SeO–L···OSe bond should be regarded as a distribution of probability density of the significantly delocalized hydron. All symmetry-related hydrons participate in a collective (coherent) stretching mode. It means that an approximation to a single-particle hydron wave function in the ordered unperturbed vibrational state is consists of the ground state of the single-particle vibrational Hamiltonian, and a product of the hydrons' states, localized on single sites, is conceived to being tantamount to the vibrational state of the full crystal Hamiltonian.

Table S8. SeO–H···OSe and SeO···H–N interatomic distances, SeO···H–OSe bond angles, and relative total energies per unit cell calculated for **1a·2a**.

r(OHO), Å	*r*(OHO), Å	*r*(O…O), Å	*ϕ*(OHO), °	*r*(OHN), Å	*r*(OHN), Å	$E_{relative}$, Hartree
0.81407	1.85323	2.65312	167.2	1.63410	1.04469	0.166678010
0.83401	1.82549	2.64711	168.1	1.63295	1.04460	0.128152090
0.85398	1.79867	2.64159	168.8	1.63272	1.04452	0.096249110
0.87393	1.77111	2.63526	169.5	1.63276	1.04442	0.070429060
0.89391	1.74228	2.62765	170.3	1.63297	1.04436	0.049811140
0.91385	1.71267	2.61907	170.9	1.63308	1.04433	0.033764700
0.93381	1.68187	2.60928	171.6	1.63364	1.04420	0.021563940
0.95377	1.64998	2.59829	172.3	1.63410	1.04413	0.012649600
0.97375	1.61669	2.58584	173.0	1.63453	1.04406	0.006492120
0.99373	1.58222	2.57210	173.6	1.63483	1.04402	0.002623170
1.01371	1.54685	2.55744	174.2	1.63514	1.04393	0.000593240
1.03371	1.51044	2.54153	174.7	1.63582	1.04386	0.000000000
1.05371	1.47382	2.52533	175.2	1.63576	1.04384	0.000476900
1.07373	1.43747	2.50933	175.5	1.63601	1.04378	0.001707860
1.09374	1.40227	2.49436	175.8	1.63638	1.04371	0.003409430
1.11375	1.36935	2.48159	176.0	1.63677	1.04363	0.005358080
1.13376	1.33938	2.47171	176.1	1.63732	1.04351	0.007400990
1.15377	1.31167	2.46404	176.1	1.63789	1.04340	0.009430750
1.17378	1.28379	2.45617	176.1	1.63837	1.04332	0.011320770
1.19379	1.25195	2.44434	176.1	1.63910	1.04320	0.012854650
1.21380	1.21852	2.43091	176.1	1.63960	1.04313	0.013763850
1.23380	1.19098	2.42332	176.0	1.64019	1.04303	0.014031760
1.24381	1.17933	2.42165	176.0	1.64052	1.04298	0.013974810
1.28656	1.15942	2.44424	175.7	1.64259	1.04259	0.013277750
1.31471	1.13951	2.45229	175.4	1.64367	1.04239	0.012355240
1.34264	1.11955	2.46007	175.2	1.64467	1.04223	0.011368340
1.37241	1.09962	2.46966	174.9	1.64574	1.04206	0.010458620
1.40481	1.07967	2.48181	174.6	1.64709	1.04186	0.009751300
1.43962	1.05984	2.49646	174.3	1.64857	1.04163	0.009411870
1.47705	1.03984	2.51348	173.9	1.65011	1.04141	0.009650340
1.51587	1.01989	2.53184	173.5	1.65173	1.04117	0.010735850
1.55455	0.99999	2.55006	173.0	1.65337	1.04094	0.012995610
1.59195	0.98007	2.56696	172.6	1.65492	1.04071	0.016847680
1.62758	0.96015	2.58216	172.2	1.65604	1.04055	0.022750520
1.66151	0.94023	2.59571	171.9	1.65703	1.04041	0.031182820
1.69386	0.92032	2.60777	171.6	1.65778	1.04029	0.042653270
1.72469	0.90041	2.61842	171.4	1.65843	1.04018	0.057732300
1.75432	0.88049	2.62795	171.2	1.6589	1.04012	0.077063250
1.78271	0.86056	2.63631	171.1	1.65924	1.04003	0.101305890
1.80999	0.84065	2.64366	171.1	1.65964	1.03995	0.131137410
1.85677	0.81436	2.66131	169.3	1.66147	1.03979	0.178064400

Table S9. SeO–H···OSe and SeO···H–N interatomic distances, SeO···H–OSe bond angles, and relative total energies per unit cell calculated for **1a·2b**.

r(OHO), Å	*r*(OHO), Å	*r*(O…O), Å	*ϕ*(OHO), °	*r*(OHN), Å	*r*(OHN), Å	$E_{relative}$, Hartree
0.79205	1.84926	2.61783	163.3	1.59156	1.05423	0.2192363
0.81205	1.82848	2.61770	163.7	1.59151	1.05422	0.1711303
0.83335	1.80453	2.61594	164.1	1.59121	1.05428	0.1290837
0.85328	1.78072	2.61297	164.5	1.59164	1.05428	0.0971570
0.87322	1.75594	2.60916	165.0	1.59154	1.05432	0.0710962
0.89315	1.72984	2.60408	165.5	1.59184	1.05433	0.0503281
0.91315	1.70234	2.59776	166.0	1.59216	1.05433	0.0340569
0.93313	1.67355	2.59018	166.5	1.59286	1.05434	0.0217110
0.95242	1.64440	2.58153	167.1	1.59350	1.05428	0.0129556
0.97206	1.61308	2.57110	167.7	1.59443	1.05423	0.0067343
0.99217	1.57985	2.55923	168.3	1.59547	1.05424	0.0027079
1.01213	1.54592	2.54642	168.8	1.59688	1.05414	0.0006131
1.03205	1.51080	2.53232	169.4	1.59847	1.05403	0.0000000
1.05226	1.47482	2.51759	169.9	1.60012	1.05396	0.0005032
1.07248	1.43881	2.50272	170.4	1.60172	1.05387	0.0018129
1.09266	1.40402	2.48886	170.9	1.60340	1.05378	0.0036342
1.11257	1.37197	2.47726	171.2	1.60485	1.05369	0.0057082
1.13250	1.34278	2.46836	171.4	1.60590	1.05363	0.0079027
1.15244	1.31521	2.46101	171.6	1.60697	1.05356	0.0098830
1.17237	1.28842	2.45435	171.7	1.60802	1.05347	0.0121938
1.19234	1.25709	2.44326	171.9	1.60936	1.05342	0.0139461
1.25553	1.17810	2.42760	171.9	1.61130	1.05331	0.0149718
1.28797	1.15831	2.43984	171.7	1.60994	1.05336	0.0147628
1.31663	1.13853	2.44836	171.4	1.60874	1.05345	0.0138323
1.34547	1.11878	2.45704	171.2	1.60739	1.05354	0.0128081
1.37701	1.09901	2.46829	170.9	1.60588	1.05361	0.0118038
1.41152	1.07927	2.48237	170.5	1.60383	1.05372	0.0109313
1.44804	1.05952	2.49828	170.0	1.60131	1.05387	0.0103592
1.48483	1.03978	2.51437	169.5	1.59932	1.05393	0.0103386
1.52027	1.02006	2.52891	168.9	1.59697	1.05408	0.0111829
1.55380	1.00036	2.54154	168.3	1.59502	1.05418	0.0132552
1.58516	0.98065	2.55203	167.8	1.59333	1.05426	0.0169668
1.61463	0.96096	2.56070	167.3	1.59175	1.05433	0.0227486
1.64271	0.94128	2.56792	166.7	1.58993	1.05444	0.0310389
1.66961	0.92163	2.57426	166.3	1.58892	1.05450	0.0422975
1.69529	0.90222	2.57965	165.9	1.58793	1.05453	0.0568592
1.72034	0.88284	2.58437	165.4	1.58701	1.05458	0.0753737
1.74492	0.86347	2.58862	165.0	1.58606	1.05462	0.0984274
1.76881	0.84417	2.59238	164.6	1.58527	1.05466	0.1265922
1.79191	0.82488	2.59546	164.2	1.58458	1.05471	0.1605794
1.81428	0.80568	2.59820	164.0	1.58405	1.05469	0.2009184

Table S10. SeO–H···OSe and SeO···H–N interatomic distances, SeO···H–OSe bond angles, and relative total energies per unit cell calculated for **1a·1b·2c**. The atomic labels are indicated on the schematic structure provided below the table.

$r(\underline{O^1H^1}O^2)$, Å	$r(O^1\underline{H^1O^2})$, Å	$r(O^1\ldots O^2)$, Å	$\phi(O^1H^1O^2)$, °	$r(\underline{O^3H^2}N^1)$, Å	$r(O^3\underline{H^2N^1})$, Å	$r(\underline{O^4H^3}N^2)$, Å	$r(O^4\underline{H^3N^2})$, Å	$E_{relative.}$, Hartree
0.78000	1.82468	2.60283	175.3	1.53475	1.06628	1.59415	1.05233	0.132202750
0.82875	1.76972	2.59688	175.7	1.53799	1.06539	1.59148	1.05301	0.073866000
0.86875	1.72166	2.58895	175.9	1.54098	1.06460	1.58928	1.05365	0.042451010
0.90872	1.66940	2.57670	176.0	1.54500	1.06353	1.58674	1.05440	0.021941240
0.94872	1.61397	2.56122	176.0	1.54905	1.06244	1.58382	1.05528	0.009497840
0.96871	1.58501	2.55220	175.9	1.55146	1.06180	1.58211	1.05580	0.005577330
0.98871	1.55496	2.54217	176.0	1.55422	1.06109	1.58006	1.05641	0.002874390
1.00870	1.52478	2.53186	175.8	1.55698	1.06039	1.57867	1.05694	0.001168230
1.02870	1.49373	2.52079	175.8	1.56052	1.05951	1.57620	1.05770	0.000267340
1.04870	1.46307	2.51003	175.7	1.56386	1.05869	1.57411	1.05838	0.000000000
1.06870	1.43244	2.49933	175.6	1.56754	1.05780	1.57182	1.05915	0.000221390
1.08870	1.40284	2.48964	175.5	1.57155	1.05683	1.56941	1.05994	0.000806630
1.10870	1.37453	2.48130	175.5	1.57521	1.05597	1.56679	1.06080	0.001646390
1.12871	1.34823	2.47496	175.4	1.57907	1.05505	1.56446	1.06162	0.002665950
1.14871	1.32409	2.47072	175.3	1.58298	1.05418	1.56199	1.06242	0.003807110
1.16870	1.30056	2.46719	175.3	1.58710	1.05328	1.55904	1.06338	0.005009380
1.18871	1.27627	2.46283	175.2	1.59089	1.05242	1.55743	1.06409	0.006212670
1.20873	1.24811	2.45469	175.2	1.59574	1.05143	1.55364	1.06523	0.007308670
1.21547	1.23793	2.45128	175.2	1.59735	1.05109	1.55254	1.06560	0.007630920
1.24250	1.20194	2.44236	175.3	1.60356	1.04982	1.54815	1.06713	0.008685600
1.26951	1.17372	2.44114	175.3	1.60926	1.04869	1.54463	1.06836	0.009442400
1.29650	1.15100	2.44544	175.3	1.61427	1.04778	1.54170	1.06946	0.010076290
1.32335	1.10006	2.42148	175.4	1.62116	1.04646	1.53615	1.07133	0.011374280
1.34815	1.08000	2.42625	175.4	1.62631	1.04561	1.53351	1.07240	0.012340090
1.37385	1.06006	2.43208	175.5	1.63094	1.04484	1.53004	1.07357	0.013588230
1.40144	1.04001	2.43963	175.5	1.63553	1.04410	1.52799	1.07441	0.015223120
1.42975	1.02001	2.44798	175.6	1.63977	1.04339	1.52534	1.07552	0.017342850
1.45827	1.00001	2.45653	175.6	1.64405	1.04270	1.52273	1.07655	0.020095850
1.48649	0.98001	2.46476	175.6	1.64836	1.04208	1.52123	1.07729	0.023660780
1.51469	0.96000	2.47296	175.6	1.65239	1.04145	1.51876	1.07830	0.028240610
1.54187	0.94001	2.48021	175.7	1.65561	1.04097	1.51725	1.07905	0.034050120
1.59630	0.90001	2.49470	175.7	1.66290	1.03994	1.51416	1.08054	0.050378490
1.64922	0.86004	2.50776	175.8	1.66967	1.03905	1.51281	1.08151	0.075051530
1.70112	0.82005	2.51972	175.8	1.67544	1.03828	1.51121	1.08252	0.111111060
1.75107	0.78012	2.52972	175.8	1.67980	1.03768	1.50995	1.08343	0.162333500

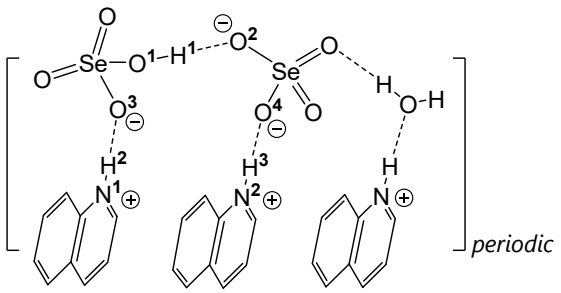


Table S11. SeO–H···OSe and SeO···H–N interatomic distances, SeO···H–OSe bond angles, and relative total energies per unit cell calculated for **1a·2d**. The atomic labels are indicated on the schematic structure provided below the table.

$r(\underline{O^1H^1}O^2)$, Å	$r(O^1\underline{H^1O^2})$, Å	$r(O^1\cdots O^2)$, Å	$\phi(O^1H^1O^2)$, °	$r(\underline{O^2H^2}N^1)$, Å	$r(O^2\underline{H^2N^1})$, Å	$r(\underline{O^3H^3}N^1)$, Å	$r(O^3\underline{H^3N^1})$, Å	$r(\underline{O^4H^4}N^2)$, Å	$r(O^4\underline{H^4N^2})$, Å	$r(O^5H^5)$, Å	$E_{relative,}$, Hartree
0.80893	1.80184	2.60360	170.8	1.70172	1.04442	1.87122	1.03590	1.79631	1.04275	1.04281	0.180030280
0.83879	1.76788	2.59998	171.2	1.70315	1.04406	1.86996	1.03610	1.79896	1.04250	1.04402	0.121210630
0.86872	1.73251	2.59500	171.6	1.70472	1.04366	1.86839	1.03632	1.80163	1.04223	1.04529	0.077438800
0.90821	1.68246	2.58501	172.1	1.70741	1.04306	1.86538	1.03669	1.80594	1.04182	1.04747	0.038094350
0.94819	1.62836	2.57135	172.4	1.71083	1.04234	1.86175	1.03712	1.81063	1.04137	1.05042	0.014635870
0.98816	1.57050	2.55379	172.7	1.71488	1.04150	1.85724	1.03765	1.81707	1.04079	1.05428	0.003141560
1.02815	1.50935	2.53291	173.0	1.71924	1.04055	1.85214	1.03830	1.82329	1.04021	1.05957	0.000000000
1.06817	1.44637	2.51004	173.1	1.72399	1.03951	1.84603	1.03902	1.83108	1.03953	1.06685	0.002238080
1.10819	1.38552	2.48909	173.0	1.72856	1.03844	1.83970	1.03981	1.83968	1.03887	1.07715	0.007514850
1.14823	1.33110	2.47436	172.7	1.73254	1.03744	1.83381	1.04059	1.84796	1.03830	1.09239	0.014153340
1.18817	1.27628	2.45901	172.4	1.73518	1.03672	1.82998	1.04115	1.85364	1.03811	1.12771	0.020888120
1.22822	1.19030	2.41252	171.9	1.72948	1.03801	1.84337	1.03970	1.83835	1.04085	1.36083	0.020527520
1.28170	1.14056	2.41546	171.4	1.73078	1.03683	1.83629	1.04055	1.84778	1.04003	1.38609	0.020842500
1.34837	1.09743	2.43737	170.4	1.73196	1.03561	1.82824	1.04147	1.85635	1.03921	1.40947	0.021021710
1.39014	1.05941	2.44037	170.0	1.73634	1.03476	1.82189	1.04215	1.85852	1.03874	1.42270	0.022355800
1.44628	1.02103	2.45649	169.1	1.74364	1.03384	1.81487	1.04297	1.85949	1.03826	1.43670	0.026373230
1.58458	0.94109	2.51434	168.8	1.79249	1.03203	1.79969	1.04468	1.84606	1.03776	1.48413	0.046607850
1.64448	0.89670	2.52746	167.5	1.80656	1.03138	1.79448	1.04545	1.84561	1.03737	1.49556	0.078432770
1.67508	0.87250	2.53237	166.8	1.81187	1.03111	1.79227	1.04581	1.84590	1.03716	1.50115	0.104358160
1.70714	0.84579	2.53604	166.0	1.81705	1.03083	1.79003	1.04615	1.84618	1.03697	1.50618	0.141870220
1.73443	0.82129	2.53759	165.4	1.82243	1.03062	1.78820	1.04642	1.84629	1.03681	1.51080	0.186406780

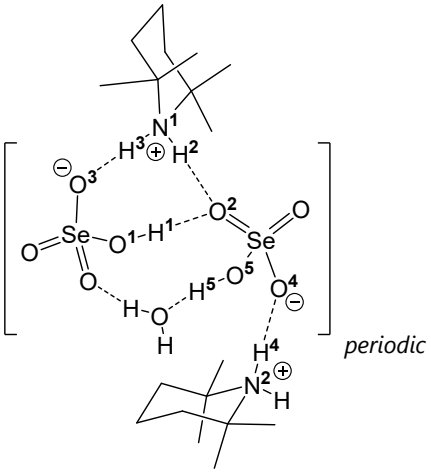


Table S12. Comparison of the SeO–L···OSe (L = H/D) bond interatomic distances in **1a·2a**, **1a·2b**, **1a·1b·2c** and **1a·2d** according to the single-crystal X-ray data and B3LYP-D3 computations.

	X-ray, Å	B3LYP-D3 (equilibrium distances), Å			B3LYP-D3 ($\|0\rangle$ vibrationally-averaged distances), Å							
	O…O	O…O	O–H	H···O	<O…O>$_H$	<O–H>	<H···O>	<O…O>$_D$	<O–D>	<D···O>	$\Delta\langle q_1\rangle_{[a]}$	$\Delta\langle q_2\rangle_{[b]}$
1a·2a	2.610	2.544	1.034	1.510	2.518	1.064	1.457	2.526	1.052	1.476	-0.016	0.007
1a·2b	2.605	2.543	1.032	1.511	2.512	1.059	1.461	2.519	1.050	1.478	-0.013	0.008
1a·1b·2c	2.538	2.512	1.049	1.463	2.492	1.084	1.411	2.497	1.072	1.427	-0.014	0.004
1a·2d	2.590	2.537	1.028	1.509	2.523	1.050	1.479	2.527	1.043	1.489	-0.009	0.003

[a] $\Delta\langle q_1\rangle = \langle q_1\rangle_D - \langle q_1\rangle_H$. [b] $\Delta\langle q_2\rangle = \langle q_2\rangle_D - \langle q_2\rangle_H$.

Table S13. (An)harmonic treatment of the O–L (L = H/D) stretching frequencies (in cm^{-1}) of A_g, A_u, B_g and B_u symmetries within the SeO–L···OSe bonds in **1a·2a**, **1a·2b**, **1a·1b·2c** and **1a·2d**.

O–H frequency	ω_h				ω_{01}	ω_{02}	$\omega_e x_e$	ω_h^e	ω_{01}^{e}[a]			ν_{01}	ν_{02}	$\Delta^{\nu_{01}}$[b]	$\Delta^{\nu_{02}}$[b]
Mode	A_g	A_u	B_g	B_u	A_g				A_u	B_g	B_u	A_g			
1a·2a	2581	2581	2680	2685	1806	3349	131	2068	2319	2418	2423	1605	2892	-201	-457
1a·2b	2616	2616	2712	2698	1863	3388	169	2199	2279	2375	2361	1773	3001	-90	-387
1a·1b·2c	2373	2358	–	–	1814	3505	61	1937	2235	–	–	1881	3620	67	115
1a·2d	2742	2748	2740	2736	2231	4076	193	2617	2362	2354	2350	3058	4461	828	385

O–D frequency	ω_h				ω_{01}	ω_{02}	$\omega_e x_e$	ω_h^e	ω_{01}^{e}[a]			ν_{01}	ν_{02}	$\Delta^{\nu_{01}}$[b]	$\Delta^{\nu_{02}}$[b]
Mode	A_g	A_u	B_g	B_u	A_g				A_u	B_g	B_u	A_g			
1a·2a	1894	1895	1963	1968	1454	2530	189	1831	1518	1586	1591	1650	2146	196	-384
1a·2b	1918	1918	1989	1982	1501	2601	201	1902	1517	1588	1581	1828	2254	327	-347
1a·1b·2c	1752	1742	–	–	1408	2585	116	1639	1511	–	–	1484	2660	76	75
1a·2d	2000	2009	2000	2001	1721	3173	134	1990	1874	1866	1867	2638	3877	917	703

[a] ω_{01}^{e} frequencies of A_u, B_g, and B_u symmetries were calculated correcting the corresponding ω_h frequencies with $\omega_e x_e$. [b] $\Delta^{\nu_{01(02)}} \equiv \nu_{01(02)} - \omega_{01(02)}$ (A_g only).

The corrected harmonic O–H(D) stretching frequencies, ω_h^e, were calculated by the following procedure implemented in Ugliengo's ANHARM code:[4]

(i) The O–H(D) distance was assumed as an independent mode (oscillator) and allowed to vary around the optimized equilibrium value (range: –0.20 ÷ +0.30 Å, step: 0.02 Å), and all the other optimized geometrical parameters being kept constant;
(ii) the potential energy was calculated for each value of the O–H(D) distance;
(iii) a polynomial curve of sixth degree was used to best fit the potential energy points, and the resulting root mean square error was securely below 10^{-6} Hartree;
(iv) the corresponding vibrational Schrödinger equation was solved numerically following the algorithm proposed by Lindberg[5] by means of the ANHARM code.

Afterwards, the Morse's[6,7] anharmonicity constant, $\omega_e x_e$, and the ω_h^e frequency were obtained from the fundamental transition frequency, ω_{01}, and the first overtone frequency, ω_{02}, as the following:

$$\omega_e x_e = (2\omega_{01} - \omega_{02})/2,$$

$$\omega_h^e = \omega_{01} + 2\omega_e x_e.$$

In our quasi-adiabatic approach (see main text) and in the non-adiabatic one described here, all equivalent O–H(D) bonds in the unit cell (two in **1a·1b·2c**, four in **1a·2a**, **1a·2b**, and **1a·2d**) were stretched simultaneously, *i.e.* the vibrational Schrödinger equation for each crystal

was solved for the in-phase (A_g) stretching modes, meeting the coherent displacement of the symmetry-related bridging hydrons. The calculated anharmonicity constants were also used for retrieving the ω_{01}^{e} frequencies of the remaining out-of-phase modes (A_u, B_g or B_u), see Table S13.

For **1a·2a** and **1a·2b**, the calculated ω_h frequencies are separated by ~100 cm^{-1} on two pairs of modes of quasi-degenerate A- and B-symmetry. Both unit cells contain four SeO–H(D) groups in the four hydrogen selenate chains and their vibrational analysis documents strong coupling of the stretching modes, where two pairs of bridging hydrons vibrate synchronously (A_g modes) or in antiphase (A_u, B_g, and B_u modes); for **1a·1b·2c**, the unit cell contains two 'isolated' hydrogen selenate SeO–H(D) groups with the coupled A_g and A_u modes; similarly, for **1a·2d**, the unit cell contains four SeO–H(D) groups with the four coupled A_g, A_u, B_g and B_u modes. We shall note that by coupling here we mean the kinematic coupling between the normal modes with close frequencies, which may be sufficient for resonance to arise thus leading to the mixing of modes and, consequently, to the change of their 'normal' frequency value by up to hundreds of cm^{-1}.

It is well known that the pronounced anharmonicity effects in the lattice vibrations are the case for the O–H stretching modes, where anharmonicity term is usually in a range of 50–250 cm^{-1}, indicating that the true potential energy surface (PES) is shallower than the harmonic potential and for a correct comparison with experimental values calculated harmonic frequencies ought to be corrected by this term. However, we point out that a non-adiabatic approach described here, being popular for treating the O–H stretching anharmonicity in layered materials and minerals featuring rather weak H-bonds with the strong covalent character of O–H bonds (see, *e.g.*, Refs. 8–16), is not valid here for O–H bonds engaged in the moderately strong H-bonding interactions with large deviation of the PES from the Morse-like behavior, as evidenced by the drastically red-shifted (for **1a·2a** and **1a·2b**) and blue-shifted (for **1a·1b·2c** and **1a·2d**) $\Delta^{\nu}_{01(02)} \equiv \nu_{01(02)} - \omega_{01(02)}$ differences of up to hundreds of cm^{-1}, see Table S13. Thus, an ordered H-bonding network in these crystals introduces significant anharmonic effects in the O–H and, apparently, in the N–H stretching regions of the IR and Raman spectra. Although treatment of efficient anharmonic corrections of simulated vibrational spectra for periodic systems is markedly demanding, it could provide insights in the spectra interpretation, as anharmonic effects have a significant impact on the one of the most specific and important bands of the studied systems (see Figs. S10–S13).

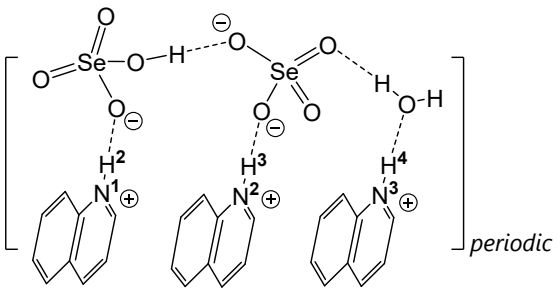
Note: in the main text, the ω_h and ω_{01} frequencies are re-identified as ν_{harm} and ν_{anharm}, respectively.

Table S14. (An)harmonic treatment of the N–H stretching frequencies (in cm^{-1}) of A_g, A_u, B_g and B_u symmetries within the CN–H···OSe bonds in **1a·2a**, **1a·2b**, **1a·1b·2c** and **1a·2d**. For the latter two structures, the H and N atomic labels are indicated on the schematic structures provided below the table.

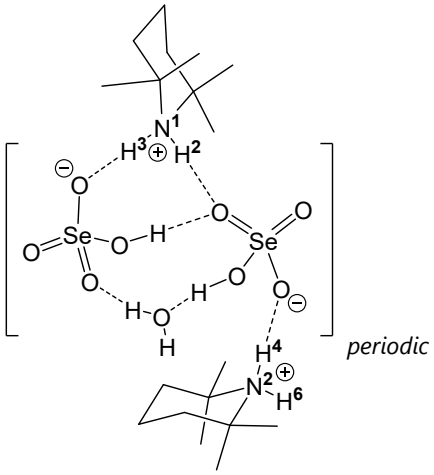
N–H frequency		ω_h				ω_{01}	ω_{02}	$\omega_e x_e$	ω_h^e	ω_{01}^{e}[a]			$\omega_{01\,av.}$	
Mode		A_g	A_u	B_g	B_u	A_g				A_u	B_g	B_u	*g*-modes	*u*-modes
1a·2a		3008	3036	3017	3029	2649	4887	206	3061	2624	2606	2618	2628	2621
1a·2b		2848	2847	2874	2858	2413	4396	215	2843	2417	2444	2428	2429	2422
1a·1b·2c	N^1–H^2	2785	2783	–	–	2299	4174	212	2723	2359	–	–	2296	2302
	N^2–H^3	2772	2789	–	–	2272	4093	225	2722	2339	–	–		
	N^3–H^4	2794	2776	–	–	2318	4069	283	2885	2209	–	–		
1a·2d	N^1–H^2	3093	3094	3093	3095	2871	5457	142	3155	2809	2809	2811	2872	2844
	N^1–H^3	3166	3167	3164	3162	2955	5653	129	3213	2909	2906	2904		
	N^2–H^4	3148	3150	3148	3149	2907	5532	141	3189	2868	2866	2867		
	N^2–H^6	3084	3086	3085	3085	2866	5440	146	3157	2795	2794	2793		

[a] ω_{01}^{e} frequencies of A_u, B_g, and B_u symmetries were calculated correcting the corresponding ω_h frequencies with $\omega_e x_e$.

1a·1b·2c



1a·2d



The ω_{01}, ω_{02}, and ω_h^e frequencies with the corresponding $\omega_e x_e$ constants were calculated using the ANHARM code (*vide supra*) with the only difference of 7 calculated points (instead of 26 ones) per each N–H bond with the following increments: –0.20, –0.16, –0.06, 0.16, 0.24, 0.30 Å.

Note: in the main text, the ω_h and ω_{01} frequencies are re-identified as ν_{harm} and ν_{anharm}, respectively.

Table S15. (An)harmonic treatment of the O–H stretching frequencies (in cm^{-1}) of A_g, A_u, B_g and B_u symmetries within the SeO–H···O_{water} bond in **1a·2d**.

O–H frequency	ω_h				ω_{01}	ω_{02}	$\omega_e x_e$	ω_h^e	ω_{01}^{e}[a]		
Mode	A_g	A_u	B_g	B_u	A_g				A_u	B_g	B_u
1a·2d	2248	2209	2243	2208	1720	3591	–76	1569	2360	2395	2359

[a] ω_{01}^{e} frequencies of A_u, B_g, and B_u symmetries were calculated correcting the corresponding ω_h frequencies with $\omega_e x_e$.

The ω_{01}, ω_{02}, and ω_h^e frequencies with the corresponding $\omega_e x_e$ constants were calculated using the ANHARM code (*vide supra*) with the only difference of 7 calculated points (instead of 26 ones) for the O–H bond with the following increments: –0.20, –0.16, –0.06, 0.16, 0.24, 0.30 Å.

Note: in the main text, the ω_h and ω_{01} frequencies are re-identified as ν_{harm} and ν_{anharm}, respectively.

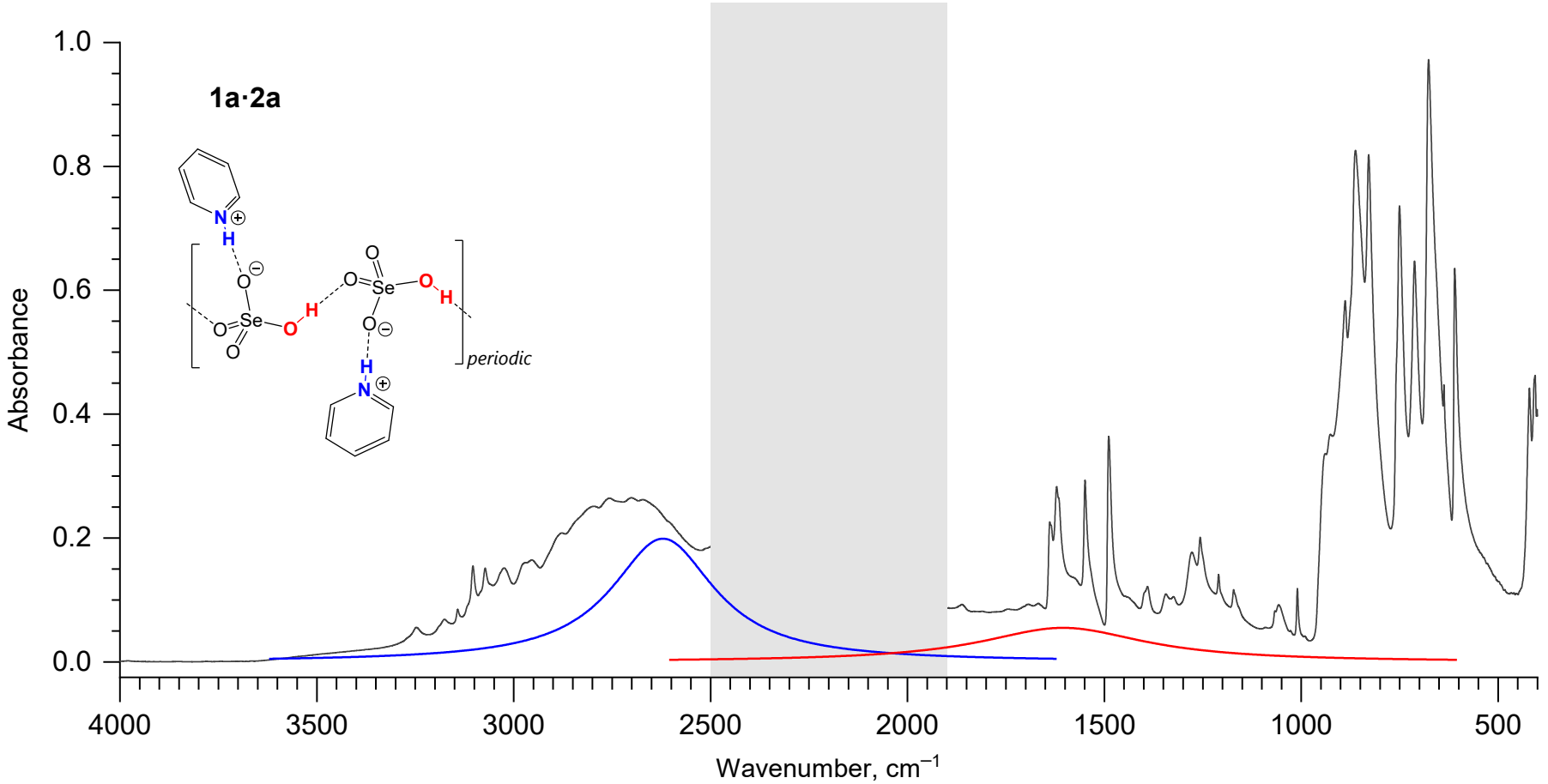


Figure S10. Experimental FT-IR spectrum of **1a·2a** at 298 K. Centers of the blue and red Lorentzian lineshapes pertain to the calculated $\omega_{01}(NH)$ and $\nu_{01}(OH)$ fundamental stretching frequencies, respectively (see main text for details). The opaque transmission window of the diamond cell in the gross frequency range of 1900–2500 cm^{-1} is highlighted by gray.

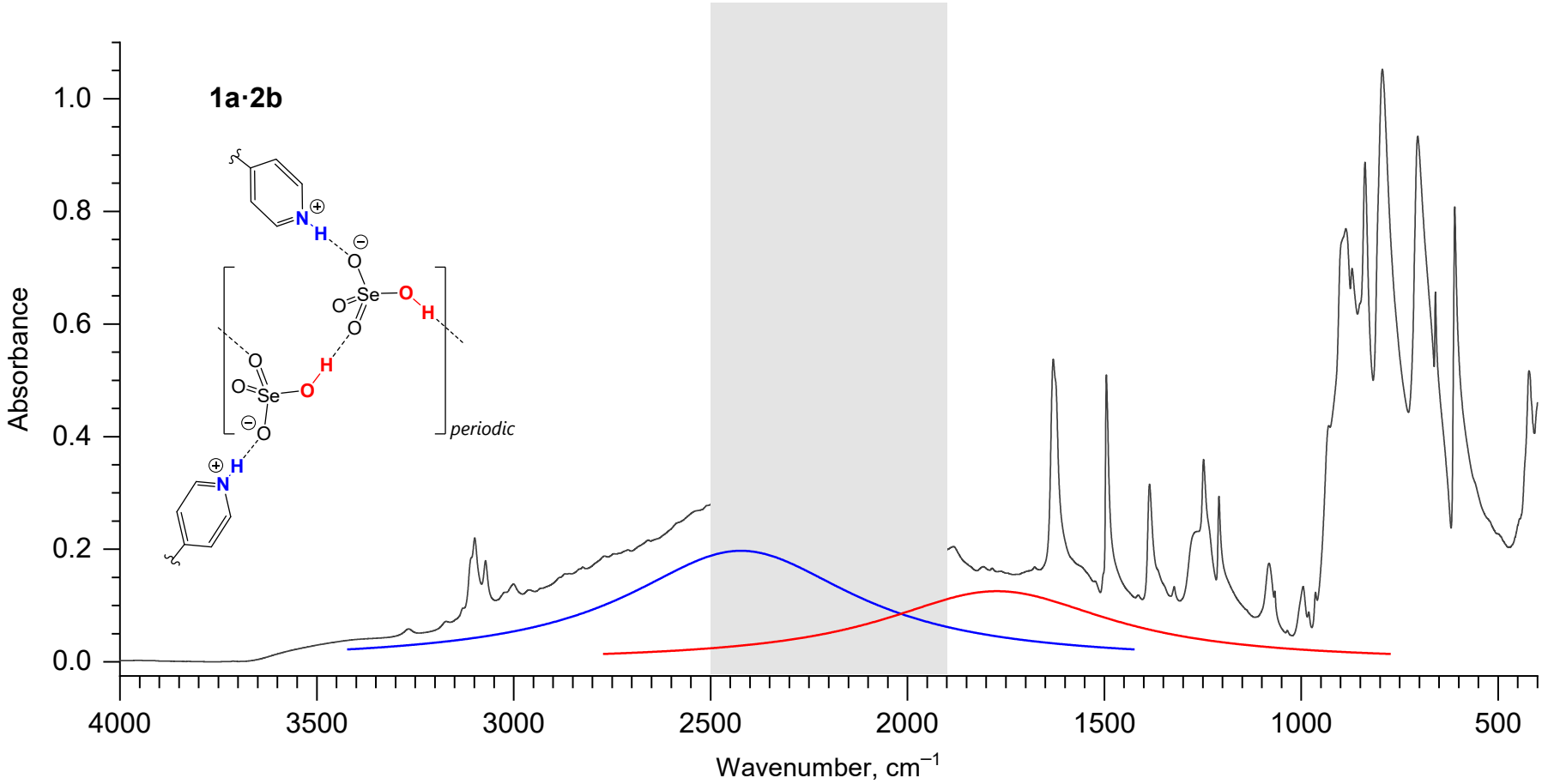


Figure S11. Experimental FT-IR spectrum of **1a·2b** at 298 K. Centers of the blue and red Lorentzian lineshapes pertain to the calculated $\omega_{01}(NH)$ and $\nu_{01}(OH)$ fundamental stretching frequencies, respectively (see main text for details). The opaque transmission window of the diamond cell in the gross frequency range of 1900–2500 cm^{-1} is highlighted by gray.

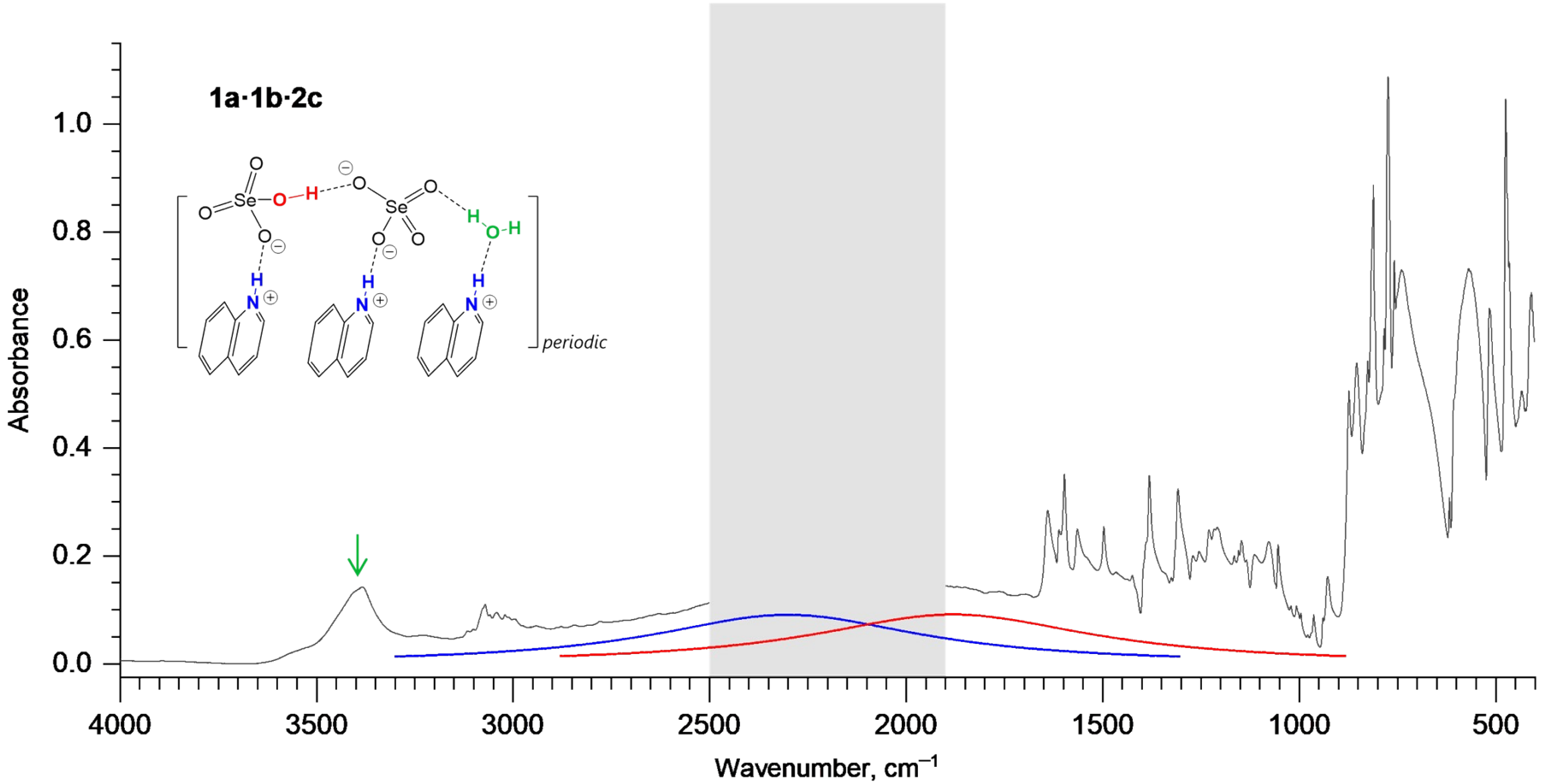


Figure S12. Experimental FT-IR spectrum of **1a·1b 2c** at 298 K. Centers of the blue and red Lorentzian lineshapes pertain to the calculated $\omega_{01}(NH)$ and $\nu_{01}(OH)$ fundamental stretching frequencies, respectively (see main text for details). The green arrow indicates the position of the OH stretching absorption band in structural water molecules. The opaque transmission window of the diamond cell in the gross frequency range of 1900–2500 cm^{-1} is highlighted by gray.

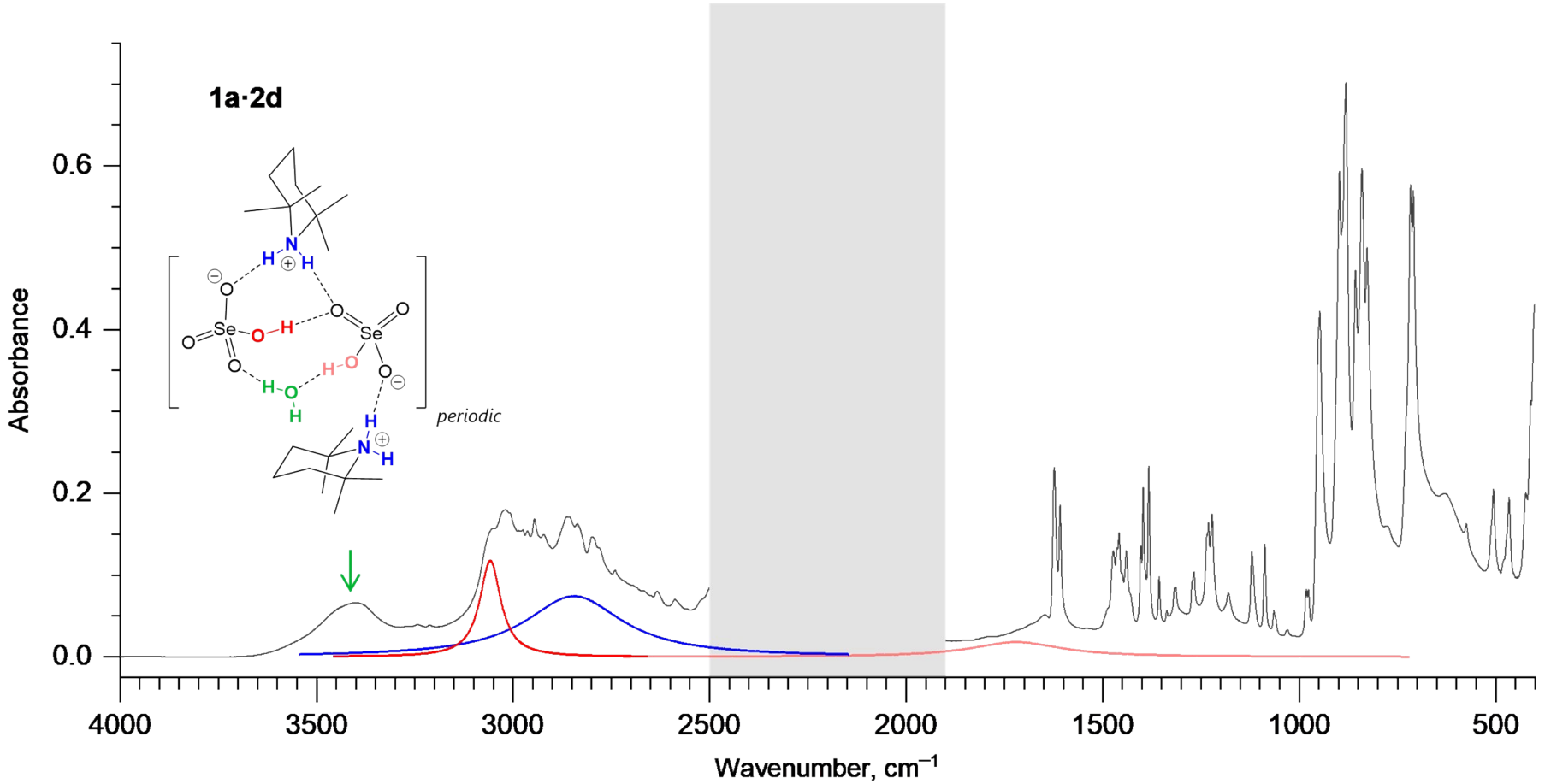


Figure S13. Experimental FT-IR spectrum of **1a·2d** at 298 K. Centers of the blue, red, and pale red Lorentzian lineshapes pertain to the calculated $\omega_{01}(NH)$, $\nu_{01}(OH)$, and $\omega_{01}(O\text{–}H\cdots O_{water})$ fundamental stretching frequencies, respectively (see main text for details). The green arrow indicates the position of the OH stretching absorption band in structural water molecules. The opaque transmission window of the diamond cell in the gross frequency range of 1900–2500 cm^{-1} is highlighted by gray.

Table S16. IR and Raman activity of **1a·2a**, **1a·2b**, **1a·1b·2c** and **1a·2d**.[a]

		1a·2a	**1a·2b**	**1a·1b·2c**	**1a·2d**
IR	Number of modes	105	99	201	447
	Irreducible representation of modes	A_u, B_u	A_u, B_u	A_u	A_u, B_u
Raman	Number of modes	108	102	204	450
	Irreducible representation of modes	A_g, B_g	A_g, B_g	A_g	A_g, B_g
	T[b]	$A_u \oplus 2B_u$	$A_u \oplus 2B_u$	$3A_u$	$A_u \oplus 2B_u$

[a] All structures possess a center of inversion, and the rule of mutual exclusion leads to equal numbers of the *g*- and *u*-modes. [b] *T* are pure translations, expected to be zero at the Γ point.

Symmetry analysis permits to classify the vibrational modes in terms of irreducible representations of the point group (C_{2h} for **1a·2a**, **1a·2b**, **1a·2d** and C_i for **1a·1b·2c**). The decomposition of the reducible phonon mode representation at the Γ point built on the basis of Cartesian coordinates of the unit cell atoms is the following:

$$\Gamma^{C_{2h}} = 54A_g \oplus 54A_u \oplus 54B_g \oplus 54B_u \text{ for } \mathbf{1a{\cdot}2a},$$

$$\Gamma^{C_{2h}} = 51A_g \oplus 51A_u \oplus 51B_g \oplus 51B_u \text{ for } \mathbf{1a{\cdot}2b},$$

$$\Gamma^{C_i} = 204A_g \oplus 204A_u \text{ for } \mathbf{1a{\cdot}1b{\cdot}2c},$$

$$\Gamma^{C_{2h}} = 225A_g \oplus 225A_u \oplus 225B_g \oplus 225B_u \text{ for } \mathbf{1a{\cdot}2d}.$$

In each case, there are no silent modes except three acoustic modes related to atom translations in the unit cell, other IR or Raman active optic modes are summarized in Table S16.

Table S17. Calculated wavenumbers v (cm^{-1}), IR intensities I ($km \cdot mol^{-1}$), Raman polycrystalline isotropic intensities I_tot, I_par, I_perp (arbitrary units) and single crystal directional intensities I_xx, I_xy, I_xz, I_yy, I_yz, I_zz (arbitrary units), and tentative interpretation of the bands in the IR and Raman spectra of **1a·2a**.

IR				Raman										
Mode	v	I	Interpretation	Mode	v	I_tot	I_par	I_perp	I_xx	I_xy	I_xz	I_yy	I_yz	I_zz	Interpretation
B_u	0.0	0.0		B_g	33.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	$\delta_{twist}(SeO_3)$; δ_{wagg}(ring); ν_β(NH)
B_u	0.0	0.0	acoustic modes	A_g	36.9	0.2	0.1	0.1	0.0	0.0	0.0	0.4	0.0	0.0	$\delta_{rock}(SeO_3)$; δ_{wagg}(ring)
A_u	0.0	0.0		A_g	42.4	0.3	0.2	0.1	0.5	0.0	0.0	0.1	0.0	0.1	$\delta_{twist}(SeO_3)$; δ_{wagg}(ring); ν_β(NH)
B_u	36.0	0.9	$\delta_{rock}(SeO_3)$; δ_{wagg}(ring); ν_β(NH)	B_g	51.0	0.1	0.1	0.1	0.0	0.2	0.0	0.0	0.0	0.0	
A_u	40.7	0.0	$\delta_{twist}(SeO_3)$; δ_{wagg}(ring); ν_β(NH)	B_g	59.0	0.5	0.3	0.2	0.0	0.1	0.0	0.0	0.6	0.0	$\delta_{rock}(SeO_3)$; δ_{wagg}(ring); ν_β(NH)
B_u	56.0	0.4	$\delta_{twist}(SeO_3)$; δ_{rock}(ring); δ_{wagg}(ring)	A_g	60.3	0.8	0.5	0.3	1.1	0.0	0.3	0.3	0.0	0.0	
A_u	66.7	5.1	$\delta_{rock}(SeO_3)$; δ_{wagg}(ring)	A_g	73.5	0.4	0.3	0.2	0.2	0.0	0.1	0.8	0.0	0.0	$\delta_{rock}(SeO_3)$; δ_{wagg}(ring)
B_u	67.5	7.9	$\delta_{twist}(SeO_3)$; δ_{rock}(ring)	A_g	76.2	0.3	0.2	0.1	0.0	0.0	0.2	0.2	0.0	0.1	$\delta_{twist}(SeO_3)$; δ_{wagg}(ring)
A_u	73.9	4.5	$\delta_{twist}(SeO_3)$; δ_{wagg}(ring); ν_β(NH)	B_g	81.5	0.1	0.1	0.1	0.0	0.2	0.0	0.0	0.0	0.0	
B_u	79.1	42.7	$\delta_{twist}(SeO_3)$; δ_{wagg}(ring)	A_g	94.6	0.7	0.4	0.3	0.4	0.0	0.2	1.3	0.0	0.0	δ_{wagg}(ring); $\delta_{twist}(SeO_3)$
A_u	82.8	18.6		B_g	94.6	0.8	0.5	0.3	0.0	0.6	0.0	0.0	0.5	0.0	$\delta_{rock}(SeO_3)$; δ_{wagg}(ring)
A_u	94.2	41.3	$\delta_{rock}(SeO_3)$; δ_{wagg}(ring)	B_g	104.5	1.2	0.7	0.5	0.0	1.4	0.0	0.0	0.2	0.0	
B_u	96.0	1.4	$\delta_{twist}(SeO_3)$; δ_{rock}(ring)	A_g	109.8	2.2	1.3	0.9	1.9	0.0	1.5	0.7	0.0	0.6	δ_{wagg}(ring); $\delta_{twist}(SeO_3)$
A_u	119.8	11.0	ν_β(OH); δ_{wagg}(ring)	B_g	115.8	1.4	0.8	0.6	0.0	0.6	0.0	0.0	1.3	0.0	
B_u	121.0	29.8		B_g	134.4	1.6	0.9	0.7	0.0	0.5	0.0	0.0	1.7	0.0	
A_u	131.6	0.6	δ_{wagg}(ring); $\delta_{twist}(SeO_3)$	B_g	146.0	4.1	2.3	1.7	0.0	5.0	0.0	0.0	0.6	0.0	δ_{rock}(ring); $\delta_{twist}(SeO_3)$
A_u	152.6	3.4	δ_{rock}(ring); δ_{wagg}(ring)	A_g	152.3	3.8	2.2	1.6	2.5	0.0	2.2	0.2	0.0	3.4	δ_{rock}(ring); ν_β(OH)
B_u	156.6	190.1	δ_{rock}(ring); δ_{wagg}(ring); $\delta_{rock}(SeO_3)$	B_g	157.9	10.8	6.2	4.6	0.0	6.0	0.0	0.0	8.9	0.0	ν_σ(OH); δ_{wagg}(ring)
A_u	165.6	1.1	ν_σ(NH); $\delta_{twist}(SeO_3)$; δ_{wagg}(ring)	A_g	158.1	12.6	7.4	5.2	0.3	0.0	2.5	22.5	0.0	6.9	δ_{wagg}(ring)
B_u	166.9	25.0	δ_{wagg}(ring)	B_g	167.3	2.0	1.1	0.9	0.0	0.4	0.0	0.0	2.3	0.0	ν_σ(NH); $\delta_{twist}(SeO_3)$; δ_{rock}(ring); δ_{wagg}(ring)
B_u	175.9	139.3	ν_σ(OH); ν_σ(NH); δ_{wagg}(ring)	A_g	171.9	6.3	3.8	2.5	10.7	0.0	2.1	0.0	0.0	2.3	ν_σ(NH); $\delta_{twist}(SeO_3)$; δ_{rock}(ring)
A_u	185.6	33.6	δ_{rock}(ring); δ_{wagg}(ring); ν_σ(OH)	B_g	189.3	5.1	2.9	2.2	0.0	0.2	0.0	0.0	6.9	0.0	$\delta_{twist}(SeO_3)$; ν_σ(OH); δ_{wagg}(ring)
B_u	192.2	45.6	$\delta_{twist}(SeO_3)$; ν_σ(OH); δ_{rock}(ring)	A_g	199.0	22.9	13.1	9.8	24.3	0.0	7.0	0.1	0.0	25.2	δ_{rock}(ring)
A_u	218.1	161.9	ν_σ(OH); δ_{rock}(ring)	A_g	216.6	0.7	0.5	0.1	0.7	0.0	0.3	0.0	0.0	0.3	ν_σ(OH)
A_u	300.0	0.5	$\delta_{scissor}$(OSeO)	A_g	299.7	1.6	0.9	0.7	1.8	0.0	0.1	0.0	0.0	2.3	$\delta_{scissor}$(OSeO)
B_u	300.4	1.4		B_g	300.9	10.6	6.1	4.6	0.0	3.2	0.0	0.0	11.5	0.0	
A_u	319.7	70.1	ν_σ(OH); $\delta_{umbrella}(SeO_3)$	A_g	318.8	5.4	3.2	2.2	4.9	0.0	1.4	6.3	0.0	0.7	ν_σ(OH); $\delta_{umbrella}(SeO_3)$
A_u	351.2	762.0	$\delta_{umbrella}(SeO_3)$	A_g	350.5	7.3	4.6	2.7	0.1	0.0	1.1	14.5	0.0	2.6	$\delta_{umbrella}(SeO_3)$
B_u	366.6	154.5	ν_σ(OH); $\delta_{umbrella}(SeO_3)$	B_g	365.9	3.9	2.2	1.7	0.0	4.8	0.0	0.0	0.5	0.0	ν_σ(OH); $\delta_{umbrella}(SeO_3)$
B_u	368.8	116.7	$\delta_{umbrella}(SeO_3)$	B_g	378.0	6.5	3.7	2.8	0.0	7.3	0.0	0.0	1.7	0.0	
B_u	392.4	548.8	$\delta_{scissor}$(OSeO)	B_g	388.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	$\delta_{scissor}$(OSeO)
A_u	396.6	1.1		A_g	390.0	19.8	11.3	8.5	3.1	0.0	24.5	2.5	0.0	0.1	
B_u	421.2	56.5	δ_{oop}(ring)	B_g	420.8	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.1	0.0	δ_{oop}(ring)
A_u	429.0	0.0	δ_{oop}(ring); ν_σ(OH)	A_g	427.0	15.3	8.8	6.5	15.5	0.0	6.4	0.2	0.0	13.9	δ_{oop}(ring); ν_σ(OH)
B_u	434.1	1.5	δ_{twist}(ring)	A_g	433.1	1.6	1.1	0.5	0.0	0.0	1.2	0.1	0.0	1.6	δ_{twist}(ring); ν_σ(OH)
A_u	434.3	32.1	δ_{twist}(ring); ν_σ(OH)	B_g	433.5	0.7	0.4	0.3	0.0	0.2	0.0	0.0	0.8	0.0	δ_{twist}(ring)
A_u	440.8	102.7		A_g	439.4	5.1	3.0	2.2	6.5	0.0	0.6	0.5	0.0	6.1	ν_σ(OH); δ_{twist}(ring)
B_u	449.4	200.3	ν_σ(OH)	B_g	450.3	8.0	4.6	3.4	0.0	10.7	0.0	0.0	0.3	0.0	ν_σ(OH)
B_u	632.3	90.6		B_g	630.0	1.0	0.6	0.4	0.0	0.0	0.0	0.0	1.4	0.0	
A_u	633.2	2.3	δ_{ip}(ring) [6-ring]	A_g	631.4	16.2	9.5	6.7	8.7	0.0	10.4	10.5	0.0	4.4	δ_{ip}(ring) [6-ring]
B_u	659.6	2.7		B_g	660.0	14.7	8.4	6.3	0.0	14.8	0.0	0.0	5.5	0.0	
A_u	660.1	8.7		A_g	660.4	1.8	1.0	0.8	2.1	0.0	0.4	0.0	0.0	2.0	

B_u	706.9	526.8	δ_{oop}(ring)	A_g	711.6	2.5	2.4	0.1	2.2	0.0	0.2	2.0	0.0	0.5	δ_{oop}(ring)
A_u	711.5	244.2	ν(SeO); δ_{oop}(ring)	B_g	711.8	1.4	0.8	0.6	0.0	2.0	0.0	0.0	0.0	0.0	δ_{oop}(ring); ν(SeO)
B_u	713.6	44.2	ν(SeO)	A_g	713.1	30.4	25.1	5.3	2.0	0.0	0.2	66.3	0.0	0.5	ν(SeO)
A_u	715.2	522.3	δ_{oop}(ring); ν(SeO)	B_g	714.7	0.5	0.3	0.2	0.0	0.6	0.0	0.0	0.0	0.0	δ_{oop}(ring); ν(SeO)
B_u	782.3	564.0	δ_{oop}(CH); δ_{oop}(NH) [γ(NH)]	A_g	789.3	0.8	0.7	0.1	1.1	0.0	0.1	0.1	0.0	0.4	δ_{oop}(CH); δ_{oop}(NH) [γ(NH)]
A_u	788.8	112.1		B_g	790.5	3.7	2.1	1.6	0.0	4.5	0.0	0.0	0.6	0.0	
A_u	825.0	226.2		A_g	823.6	165.4	161.6	3.8	196.0	0.0	0.3	55.9	0.0	75.1	ν(SeO); δ_{oop}(CH)
B_u	860.3	887.3	ν(SeO); δ_{oop}(CH)	B_g	863.2	2.8	1.6	1.2	0.0	3.8	0.0	0.0	0.0	0.0	
B_u	876.5	944.3		A_g	885.7	93.3	81.5	11.8	35.5	0.0	21.6	7.7	0.0	116.8	ν(SeO)
A_u	887.6	56.9	ν(SeO)	B_g	892.5	5.4	3.1	2.3	0.0	5.9	0.0	0.0	1.6	0.0	
B_u	928.0	764.5	δ_{oop}(CH); ν(SeO); δ_{ip}(OH)	A_g	930.0	2.7	2.2	0.5	1.8	0.0	0.5	3.6	0.0	0.0	δ_{oop}(CH)
A_u	928.8	7.2		B_g	930.5	1.3	0.8	0.6	0.0	1.6	0.0	0.0	0.3	0.0	
B_u	944.4	689.5	ν(SeO); δ_{oop}(CH)	B_g	943.3	8.6	4.9	3.7	0.0	8.0	0.0	0.0	3.9	0.0	
A_u	947.9	60.9	ν(SeO); δ_{oop}(CH); δ_{ip}(OH); δ_{oop}(NH) [γ(NH)]	A_g	948.5	27.7	21.6	6.1	51.2	0.0	5.9	2.4	0.0	0.0	ν(SeO); δ_{oop}(CH); δ_{ip}(OH); δ_{oop}(NH) [γ(NH)]
B_u	974.5	278.3	δ_{oop}(CH); δ_{oop}(NH) [γ(NH)];	A_g	975.9	7.4	4.7	2.8	0.7	0.0	6.5	5.4	0.0	0.7	δ_{oop}(CH); δ_{oop}(NH) [γ(NH)];
A_u	978.9	0.0	δ_{ip}(OH)	B_g	981.8	4.6	2.6	2.0	0.0	6.2	0.0	0.0	0.1	0.0	δ_{ip}(OH)
B_u	1012.0	566.2	δ_{ip}(OH); δ_{oop}(CH)	A_g	1010.4	1.3	1.1	0.2	0.1	0.0	0.0	2.9	0.0	0.0	δ_{ip}(OH); δ_{oop}(CH)
A_u	1014.4	10.1		B_g	1024.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{ip}(OH)
A_u	1034.2	0.0	δ_{oop}(CH)	A_g	1036.6	27.3	25.6	1.8	13.0	0.0	5.3	12.2	0.0	20.5	δ_{ip}(ring) [ν(CN)]; δ_{ip}(ring)
B_u	1035.7	15.8		B_g	1036.9	1.5	0.8	0.6	0.0	1.5	0.0	0.0	0.5	0.0	[ν(CC)]; δ_{oop}(CH); δ_{ip}(OH)
A_u	1041.0	0.5	δ_{ip}(ring) [ν(CN)]; δ_{ip}(ring) [ν(CC)]; δ_{ip}(OH)	A_g	1041.3	97.3	90.0	7.3	97.7	0.0	17.8	41.9	0.0	27.3	δ_{ip}(ring) [ν(CN)]; δ_{ip}(ring) [ν(CC)]; δ_{ip}(OH)
B_u	1042.1	37.5		B_g	1041.4	0.1	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	δ_{ip}(ring) [ν(CN)]; δ_{ip}(ring) [ν(CC)]; δ_{oop}(CH)
A_u	1060.7	0.1	δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]	B_g	1061.6	8.3	4.7	3.6	0.0	4.3	0.0	0.0	7.1	0.0	δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring)
B_u	1061.0	3.7		A_g	1062.4	203.2	197.8	5.5	120.2	0.0	14.1	169.5	0.0	86.0	[ν(CN)]
A_u	1076.7	0.7	δ_{oop}(CH); δ_{ip}(ring) [ν(CC)]	A_g	1078.9	10.3	9.9	0.4	8.8	0.0	0.0	10.3	0.0	1.4	δ_{oop}(CH); δ_{ip}(ring) [ν(CC)]
B_u	1081.6	0.6		B_g	1083.8	0.6	0.4	0.3	0.0	0.8	0.0	0.0	0.1	0.0	
B_u	1098.3	2.8	δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring)	B_g	1098.1	0.6	0.3	0.3	0.0	0.3	0.0	0.0	0.5	0.0	δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring)
A_u	1098.8	26.9	[ν(CN)]; δ_{ip}(CH); δ_{oop}(CH); δ_{ip}(NH)	A_g	1098.2	2.0	1.5	0.5	1.5	0.0	0.2	0.3	0.0	2.6	[ν(CN)]; δ_{ip}(CH); δ_{oop}(CH); δ_{ip}(NH)
B_u	1107.1	14.1	δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring)	B_g	1107.4	0.6	0.4	0.3	0.0	0.8	0.0	0.0	0.1	0.0	δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring)
A_u	1111.6	9.4	[ν(CN)]; δ_{ip}(CH); δ_{oop}(CH)	A_g	1111.6	6.6	4.9	1.7	3.2	0.0	4.3	0.0	0.0	4.1	[ν(CN)]; δ_{ip}(CH); δ_{oop}(CH)
A_u	1143.8	52.4	δ_{oop}(NH) [γ(NH)]; δ_{oop}(CH);	B_g	1148.2	0.5	0.3	0.2	0.0	0.7	0.0	0.0	0.0	0.0	δ_{oop}(NH) [γ(NH)]; δ_{oop}(CH);
B_u	1144.2	65.0	δ_{ip}(OH)	A_g	1150.7	1.8	1.1	0.7	0.0	0.0	0.0	1.2	0.0	3.7	δ_{ip}(OH)
B_u	1192.8	9.0	δ_{ip}(CH); δ_{ip}(ring) [ν(CC)]	B_g	1192.1	12.3	7.0	5.3	0.0	13.1	0.0	0.0	3.8	0.0	δ_{ip}(CH); δ_{ip}(ring) [ν(CC)]
A_u	1202.1	6.0		A_g	1200.5	5.2	3.0	2.2	6.9	0.0	1.0	2.5	0.0	2.9	
B_u	1237.8	11.4	δ_{ip}(CH); δ_{ip}(ring) [ν(CC)];	B_g	1236.0	8.3	4.8	3.6	0.0	5.0	0.0	0.0	6.6	0.0	δ_{ip}(CH); δ_{ip}(ring) [ν(CC)];
A_u	1239.1	11.7	δ_{ip}(ring) [ν(CN)]	A_g	1239.3	53.3	30.9	22.4	17.3	0.0	23.5	77.5	0.0	4.7	δ_{ip}(ring) [ν(CN)]
B_u	1309.5	5.1	δ_{ip}(ring) [ν(CN)]; δ_{ip}(ring) [ν(CC)]; δ_{ip}(NH)	B_g	1315.3	10.1	5.8	4.3	0.0	6.1	0.0	0.0	7.8	0.0	δ_{ip}(ring) [ν(CN)]; δ_{ip}(ring) [ν(CC)]; δ_{ip}(NH); δ_{oop}(OH) [γ(OH)]
A_u	1311.0	24.9		A_g	1317.2	1.2	0.8	0.4	2.4	0.0	0.0	0.1	0.0	0.3	δ_{ip}(ring) [ν(CN)]; δ_{ip}(ring) [ν(CC)]; δ_{ip}(NH)
B_u	1364.7	153.6	δ_{oop}(OH) [γ(OH)]; δ_{ip}(CH); δ_{ip}(NH); δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]	A_g	1365.5	0.8	0.5	0.3	0.7	0.0	0.0	1.3	0.0	0.1	δ_{oop}(OH) [γ(OH)]; δ_{ip}(CH); δ_{ip}(NH); δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]
A_u	1366.3	49.1	δ_{oop}(OH) [γ(OH)]; δ_{ip}(CH); δ_{ip}(NH)	B_g	1372.7	1.7	1.0	0.7	0.0	1.7	0.0	0.0	0.6	0.0	
A_u	1369.0	150.9	δ_{oop}(OH) [γ(OH)]; δ_{ip}(CH);	B_g	1374.1	0.8	0.4	0.3	0.0	0.7	0.0	0.0	0.4	0.0	δ_{oop}(OH) [γ(OH)]; δ_{ip}(CH); δ_{ip}(NH)
B_u	1377.1	148.3	δ_{ip}(NH); δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]	A_g	1374.6	1.3	0.9	0.5	2.4	0.0	0.0	0.2	0.0	0.8	δ_{oop}(OH) [γ(OH)]; δ_{ip}(CH); δ_{ip}(NH); δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]

B_u	1431.2	18.6	δ_{ip}(NH); δ_{ip}(CH); δ_{ip}(ring)
A_u	1432.7	136.7	[v(CC)]
B_u	1521.2	407.2	δ_{ip}(CH); δ_{ip}(ring) [v(CC)];
A_u	1523.6	0.2	δ_{ip}(ring) [v(CN)]
A_u	1597.7	139.0	δ_{ip}(NH); δ_{ip}(CH); δ_{ip}(ring)
B_u	1598.8	34.2	[v(CC)]
B_u	1670.9	58.3	
A_u	1671.8	304.3	δ_{ip}(NH); δ_{ip}(ring) [v(CC)];
A_u	1680.8	30.2	δ_{ip}(ring) [v(CN)]
B_u	1681.2	309.0	
A_u	2581.1	6049.9	v(OH)
B_u	2685.5	8440.4	
B_u	3029.5	17129.1	v(NH)
A_u	3035.5	16.8	
B_u	3220.1	31.8	
A_u	3221.6	28.0	
B_u	3233.2	9.4	
A_u	3238.2	0.9	
B_u	3245.5	139.3	v(CH)
A_u	3245.7	15.5	
B_u	3253.9	230.1	
A_u	3255.3	409.0	
B_u	3260.9	91.8	
A_u	3261.3	86.5	

B_g	1431.6	8.7	5.0	3.7	0.0	9.9	0.0	0.0	2.1	0.0	δ_{ip}(NH); δ_{ip}(CH); δ_{ip}(ring)
A_g	1432.9	1.2	1.0	0.2	2.5	0.0	0.0	0.0	0.0	0.3	[v(CC)]
B_g	1523.5	0.9	0.5	0.4	0.0	0.6	0.0	0.0	0.6	0.0	δ_{ip}(CH); δ_{ip}(ring) [v(CC)];
A_g	1523.8	5.4	3.3	2.1	6.6	0.0	1.6	3.7	0.0	1.0	δ_{ip}(ring) [v(CN)]
A_g	1597.0	3.9	2.3	1.6	6.8	0.0	0.9	1.7	0.0	0.4	δ_{ip}(NH); δ_{ip}(CH); δ_{ip}(ring)
B_g	1598.3	6.1	3.5	2.6	0.0	3.1	0.0	0.0	5.4	0.0	[v(CC)]
B_g	1672.4	25.4	14.5	10.9	0.0	32.5	0.0	0.0	2.5	0.0	
A_g	1672.5	26.8	16.1	10.7	0.1	0.0	16.5	32.1	0.0	7.4	δ_{ip}(NH); δ_{ip}(ring) [v(CC)];
B_g	1681.5	9.7	5.5	4.1	0.0	1.0	0.0	0.0	12.3	0.0	δ_{ip}(ring) [v(CN)]
A_g	1682.0	50.0	29.9	20.1	10.2	0.0	19.3	84.0	0.0	2.9	
A_g	2580.7	439.9	371.0	68.9	636.0	0.0	49.4	249.0	0.0	0.6	v(OH)
B_g	2680.4	170.6	97.5	73.1	0.0	222.8	0.0	0.0	13.0	0.0	
A_g	3008.5	1000.0	722.3	277.7	722.3	0.0	692.3	0.6	0.0	364.5	v(NH)
B_g	3017.1	14.4	8.3	6.2	0.0	14.8	0.0	0.0	5.1	0.0	
B_g	3220.0	18.0	10.3	7.7	0.0	9.9	0.0	0.0	15.1	0.0	
A_g	3221.6	252.2	173.3	79.0	305.9	0.0	118.3	32.8	0.0	65.6	
B_g	3232.9	73.4	42.0	31.5	0.0	38.9	0.0	0.0	62.6	0.0	
A_g	3238.0	44.6	37.5	7.1	0.5	0.0	3.4	59.2	0.0	33.7	
B_g	3243.8	117.0	66.8	50.1	0.0	142.5	0.0	0.0	19.2	0.0	v(CH)
A_g	3244.1	253.5	229.4	24.1	207.8	0.0	29.1	260.3	0.0	10.8	
A_g	3253.8	138.6	122.8	15.9	97.1	0.0	11.8	177.0	0.0	1.3	
B_g	3254.3	100.6	57.5	43.1	0.0	134.9	0.0	0.0	4.1	0.0	
B_g	3261.0	110.3	63.0	47.3	0.0	8.0	0.0	0.0	144.4	0.0	
A_g	3261.9	759.6	718.3	41.3	179.0	0.0	40.1	1000.0	0.0	290.4	

Table S18. Calculated wavenumbers v (cm^{-1}), IR intensities I ($km \cdot mol^{-1}$), Raman polycrystalline isotropic intensities I_tot, I_par, I_perp (arbitrary units) and single crystal directional intensities I_xx, I_xy, I_xz, I_yy, I_yz, I_zz (arbitrary units), and tentative interpretation of the bands in the IR and Raman spectra of **1a·2b**.

IR				Raman											
Mode	v	I	Interpretation	Mode	v	I_tot	I_par	I_perp	I_xx	I_xy	I_xz	I_yy	I_yz	I_zz	Interpretation
B_u	0.0	0.0	acoustic modes	B_g	41.5	0.2	0.1	0.1	0.0	0.2	0.0	0.0	0.0	0.0	δ_{rock}(ring); δ_{rock}(SeO_3)
B_u	0.0	0.0		A_g	59.7	1.3	0.9	0.4	0.8	0.0	0.0	0.7	0.0	0.3	
A_u	0.0	0.0		A_g	63.6	1.0	0.6	0.4	0.3	0.0	0.0	1.2	0.0	0.0	δ_{rock}(ring); δ_{rock}(SeO_3); ν_β(NH)
B_u	55.8	20.0	δ_{rock}(ring); δ_{rock}(SeO_3)	B_g	66.6	1.4	0.8	0.6	0.0	0.8	0.0	0.0	0.3	0.0	δ_{wagg}(ring); δ_{rock}(SeO_3)
A_u	57.5	0.4	δ_{wagg}(ring); δ_{rock}(SeO_3)	B_g	79.0	0.7	0.4	0.3	0.0	0.0	0.0	0.0	0.5	0.0	δ_{rock}(ring); δ_{rock}(SeO_3);
A_u	62.1	1.1	δ_{rock}(ring); δ_{rock}(SeO_3)	A_g	81.8	1.9	1.3	0.6	2.5	0.0	0.0	0.2	0.0	0.0	ν_β(NH)
B_u	63.2	3.4	δ_{wagg}(ring); δ_{rock}(SeO_3)	B_g	86.3	5.0	2.9	2.1	0.0	3.8	0.0	0.0	0.1	0.0	δ_{rock}(ring); δ_{twist}(SeO_3); ν_β(NH)
B_u	81.2	38.9	δ_{rock}(SeO_3)	A_g	101.0	4.2	2.5	1.8	1.4	0.0	0.9	2.4	0.0	1.0	δ_{wagg}(ring); δ_{rock}(SeO_3); ν_β(NH)
A_u	82.0	0.2	δ_{rock}(ring); δ_{rock}(SeO_3)	B_g	103.8	0.7	0.4	0.3	0.0	0.5	0.0	0.0	0.1	0.0	
A_u	96.4	21.1		A_g	104.3	6.3	3.9	2.5	0.6	0.0	1.9	5.2	0.0	0.0	
A_u	107.0	42.9	δ_{twist}(SeO_3)	B_g	117.6	0.2	0.1	0.1	0.0	0.2	0.0	0.0	0.0	0.0	δ_{wagg}(ring); δ_{rock}(SeO_3)
B_u	108.7	128.0	δ_{rock}(ring); ν_β(NH)	A_g	121.1	1.2	0.7	0.5	1.3	0.0	0.0	0.2	0.0	0.2	δ_{twist}(SeO_3)
A_u	118.0	0.4	δ_{twist}(SeO_3)	B_g	131.8	0.2	0.1	0.1	0.0	0.1	0.0	0.0	0.0	0.0	δ_{rock}(SeO_3)
B_u	119.6	1.7		A_g	134.4	24.9	14.2	10.7	1.9	0.0	0.5	13.5	0.0	22.2	δ_{rock}(ring); δ_{rock}(SeO_3)
A_u	127.1	84.6	δ_{rock}(ring); δ_{rock}(SeO_3); ν_β(OH)	A_g	145.9	30.4	17.4	13.0	8.1	0.0	16.6	0.0	0.0	5.9	δ_{rock}(ring); ν_β(OH);
A_u	140.9	19.1	δ_{rock}(ring); δ_{rock}(SeO_3)	B_g	158.9	32.4	18.5	13.9	0.0	19.5	0.0	0.0	5.6	0.0	δ_{rock}(SeO_3)
B_u	141.4	25.7		B_g	222.8	7.9	4.5	3.4	0.0	5.8	0.0	0.0	0.3	0.0	δ_{rock}(SeO_3)
B_u	154.7	137.6	δ_{wagg}(ring); δ_{rock}(SeO_3)	A_g	224.6	1.4	0.8	0.6	0.9	0.0	0.4	0.4	0.0	0.0	ν_σ(NH); ν_σ(OH); δ_{rock}(SeO_3)
B_u	172.7	74.7	δ_{wagg}(ring)	B_g	268.1	1.7	1.0	0.8	0.0	1.3	0.0	0.0	0.1	0.0	δ_{oop}(ring)
A_u	179.9	6.5		A_g	268.4	4.9	2.8	2.1	0.5	0.0	0.8	4.4	0.0	1.2	
A_u	193.3	0.0	δ_{rock}(ring); ν_β(NH)	A_g	300.3	11.4	7.1	4.3	0.9	0.0	7.8	0.2	0.0	0.5	δ_{twist}(SeO_3)
B_u	193.8	12.5		B_g	305.6	17.0	9.7	7.3	0.0	0.2	0.0	0.0	13.1	0.0	
B_u	226.0	25.7	ν_σ(NH); ν_σ(OH); δ_{rock}(SeO_3)	A_g	313.1	11.3	6.6	4.7	3.2	0.0	2.9	2.7	0.0	5.6	$\delta_{scissor}$(OSeO)
A_u	240.7	62.8		B_g	347.7	7.6	4.4	3.3	0.0	1.1	0.0	0.0	4.9	0.0	δ_{rock}(SeO_3); δ_{twist}(ring)
A_u	300.3	13.0	δ_{twist}(SeO_3)	A_g	351.6	13.1	8.0	5.2	0.2	0.0	0.0	3.2	0.0	16.5	$\delta_{umbrella}$(SeO_3); δ_{ip}(ring) [6-ring]
B_u	306.9	65.8		B_g	362.2	0.4	0.2	0.2	0.0	0.2	0.0	0.0	0.1	0.0	δ_{rock}(SeO_3)
A_u	316.1	8.2	$\delta_{scissor}$(OSeO)	B_g	364.3	10.6	6.1	4.5	0.0	5.7	0.0	0.0	2.6	0.0	$\delta_{umbrella}$(SeO_3)
B_u	350.8	571.7	$\delta_{umbrella}$(SeO_3)	A_g	366.1	20.9	12.4	8.5	18.3	0.0	4.6	0.1	0.0	4.3	$\delta_{umbrella}$(SeO_3); δ_{twist}(ring)
B_u	359.5	279.7	δ_{rock}(SeO_3)	A_g	388.1	18.2	10.7	7.5	3.4	0.0	5.1	14.1	0.0	0.2	ν_σ(NH); δ_{rock}(SeO_3); δ_{twist}(ring)
A_u	361.3	359.0	$\delta_{umbrella}$(SeO_3)	B_g	409.9	27.7	15.8	11.9	0.0	20.0	0.0	0.0	1.5	0.0	ν_σ(NH); ν_σ(OH); δ_{twist}(ring)
A_u	380.8	537.3	δ_{rock}(SeO_3); ν_σ(NH); δ_{twist}(ring)	A_g	426.7	4.1	2.5	1.7	0.8	0.0	2.0	0.4	0.0	1.1	
B_u	399.2	100.0	$\delta_{umbrella}$(SeO_3); ν_σ(NH); δ_{twist}(ring)	B_g	427.7	1.0	0.6	0.4	0.0	0.7	0.0	0.0	0.1	0.0	δ_{twist}(ring)
A_u	412.0	0.6	δ_{twist}(ring)	A_g	434.1	1.9	1.1	0.8	1.9	0.0	0.1	0.1	0.0	0.8	
B_u	413.9	2.3		B_g	434.3	0.6	0.3	0.3	0.0	0.3	0.0	0.0	0.1	0.0	
B_u	445.9	297.2	ν_σ(OH)	B_g	451.9	7.6	4.3	3.3	0.0	5.3	0.0	0.0	0.7	0.0	ν_σ(OH)
A_u	452.2	17.8	ν_σ(OH); ν_σ(NH)	A_g	455.3	46.2	27.3	19.0	14.2	0.0	18.2	7.1	0.0	13.1	ν_σ(OH); ν_σ(NH)
A_u	466.2	75.9	δ_{oop}(ring); ν_σ(OH)	A_g	578.1	12.4	7.1	5.3	1.4	0.0	7.0	3.5	0.0	0.3	δ_{oop}(ring)
B_u	466.4	61.4	δ_{oop}(ring)	B_g	579.4	6.6	3.8	2.8	0.0	5.0	0.0	0.0	0.1	0.0	
A_u	633.9	43.9	δ_{ip}(ring) [6-ring]	A_g	664.9	35.2	21.9	13.3	45.6	0.0	0.3	0.4	0.0	6.2	δ_{ip}(ring) [6-ring]
B_u	636.5	74.5		B_g	665.3	25.1	14.4	10.8	0.0	6.6	0.0	0.0	13.0	0.0	
B_u	683.3	9.1		B_g	708.8	0.4	0.2	0.2	0.0	0.2	0.0	0.0	0.1	0.0	
A_u	683.7	1.5	v(SeO)	A_g	709.5	116.3	93.5	22.8	3.1	0.0	0.2	147.7	0.0	0.2	v(SeO)
B_u	709.4	18.8		A_g	757.6	1.1	0.6	0.5	0.1	0.0	0.1	0.8	0.0	0.6	δ_{oop}(ring); δ_{ip}(OH)
A_u	709.4	941.1		B_g	758.5	1.0	0.6	0.4	0.0	0.1	0.0	0.0	0.7	0.0	δ_{oop}(ring)

B_u	742.4	58.5	δ_{oop}(ring)	A_g	776.4	47.3	34.9	12.4	11.3	0.0	17.9	0.0	0.0	17.8	δ_{ip}(ring) [6-ring]
A_u	742.4	10.2		B_g	778.8	12.4	7.1	5.3	0.0	9.2	0.0	0.0	0.5	0.0	
B_u	831.7	499.4	δ_{oop}(CH); δ_{oop}(NH) [γ(NH)]; δ_{ip}(OH)	A_g	838.6	404.4	397.0	7.3	201.9	0.0	1.9	63.8	0.0	178.0	ν(SeO)
A_u	838.6	342.1	ν(SeO)	B_g	869.5	8.4	4.8	3.6	0.0	4.2	0.0	0.0	2.3	0.0	δ_{oop}(CH); δ_{oop}(NH) [γ(NH)]; δ_{ip}(OH); ν(SeO)
A_u	843.5	418.3	δ_{oop}(CH); δ_{oop}(NH) [γ(NH)]	A_g	873.0	12.2	7.7	4.5	0.3	0.0	5.2	6.8	0.0	0.6	δ_{oop}(CH); δ_{oop}(NH) [γ(NH)]; δ_{ip}(OH)
B_u	867.1	766.8	δ_{oop}(CH); ν(SeO)	B_g	874.2	0.8	0.4	0.3	0.0	0.0	0.0	0.0	0.6	0.0	ν(SeO); δ_{oop}(CH); δ_{oop}(NH) [γ(NH)]
A_u	876.9	5.0	δ_{oop}(CH); δ_{ip}(OH)	B_g	884.7	27.1	15.5	11.6	0.0	17.1	0.0	0.0	3.9	0.0	δ_{oop}(CH); δ_{ip}(OH); ν(SeO)
B_u	877.5	876.9	ν(SeO); δ_{oop}(CH); δ_{ip}(OH)	A_g	898.6	130.7	108.6	22.2	115.1	0.0	9.8	0.1	0.0	31.4	δ_{oop}(CH); δ_{oop}(NH) [γ(NH)]; ν(SeO)
B_u	888.5	1218.5	δ_{oop}(CH); ν(SeO)	A_g	903.2	92.1	82.0	10.1	90.8	0.0	0.2	18.8	0.0	1.2	δ_{oop}(CH); ν(SeO); δ_{ip}(OH)
A_u	903.6	128.0	ν(SeO); δ_{oop}(CH); δ_{ip}(OH)	B_g	906.0	8.3	4.8	3.6	0.0	6.2	0.0	0.0	0.3	0.0	δ_{oop}(CH); ν(SeO)
B_u	924.3	1087.7	ν(SeO); δ_{ip}(OH)	B_g	933.3	0.3	0.2	0.1	0.0	0.2	0.0	0.0	0.0	0.0	ν(SeO); δ_{ip}(OH); δ_{oop}(CH)
A_u	934.4	25.6	ν(SeO); δ_{ip}(OH); δ_{oop}(CH)	A_g	934.9	110.2	70.2	40.0	0.9	0.0	60.3	5.5	0.0	36.4	
A_u	985.7	8.3	δ_{ip}(OH); δ_{oop}(CH)	A_g	982.9	5.2	3.2	2.0	2.8	0.0	2.5	0.0	0.0	0.2	δ_{ip}(OH); δ_{oop}(CH)
B_u	990.6	806.3	δ_{ip}(OH); δ_{oop}(CH); δ_{oop}(NH) [γ(NH)]	B_g	997.8	0.9	0.5	0.4	0.0	0.0	0.0	0.0	0.6	0.0	
A_u	1011.8	0.7		B_g	1008.1	4.0	2.3	1.7	0.0	1.3	0.0	0.0	1.8	0.0	δ_{oop}(CH); δ_{ip}(OH); δ_{oop}(NH) [γ(NH)]
B_u	1013.8	201.5	δ_{ip}(OH); δ_{oop}(CH)	A_g	1011.2	8.1	7.6	0.6	3.1	0.0	0.7	4.2	0.0	0.8	
B_u	1021.5	101.2	δ_{ip}(OH); δ_{oop}(CH); δ_{oop}(NH) [γ(NH)]	B_g	1030.1	25.0	14.3	10.7	0.0	5.5	0.0	0.0	13.8	0.0	
A_u	1027.5	7.6		A_g	1031.6	76.3	74.2	2.1	40.9	0.0	1.9	27.5	0.0	13.1	δ_{oop}(CH); δ_{ip}(OH)
B_u	1031.5	48.1	δ_{ip}(ring) [ν(CN)]; δ_{ip}(ring) [ν(CC)]	A_g	1042.8	307.2	303.8	3.5	155.0	0.0	2.3	106.4	0.0	71.7	δ_{ip}(ring) [ν(CN)]; δ_{oop}(CH)
A_u	1031.7	33.1	δ_{ip}(ring) [ν(CN)]; δ_{ip}(OH); δ_{oop}(CH)	B_g	1045.3	66.8	38.2	28.6	0.0	27.4	0.0	0.0	24.5	0.0	δ_{ip}(ring) [ν(CN)]; δ_{ip}(OH); δ_{oop}(CH)
A_u	1067.4	0.6	δ_{ip}(ring) [ν(CC)]	B_g	1118.5	4.5	2.6	2.0	0.0	2.4	0.0	0.0	1.2	0.0	
B_u	1068.9	5.3		A_g	1119.0	117.0	112.7	4.3	82.6	0.0	1.7	22.2	0.0	23.8	δ_{ip}(ring) [ν(CN)]
B_u	1098.5	0.2	δ_{ip}(ring) [ν(CN)]	B_g	1142.4	4.4	2.5	1.9	0.0	0.9	0.0	0.0	2.5	0.0	
A_u	1099.7	0.4	δ_{ip}(ring) [ν(CN)]; δ_{ip}(OH)	A_g	1143.2	8.0	4.8	3.2	8.3	0.0	1.1	0.0	0.0	1.7	δ_{ip}(CH)
A_u	1162.2	8.4	δ_{ip}(CH); δ_{ip}(NH)	A_g	1166.5	5.8	3.4	2.3	0.2	0.0	1.6	3.8	0.0	1.7	
B_u	1162.6	0.6		B_g	1175.7	0.4	0.2	0.2	0.0	0.0	0.0	0.0	0.3	0.0	δ_{oop}(NH) [γ(NH)]; δ_{oop}(CH)
A_u	1167.3	183.8	δ_{oop}(NH) [γ(NH)]; δ_{oop}(CH)	B_g	1269.4	13.7	7.8	5.9	0.0	7.5	0.0	0.0	3.1	0.0	
B_u	1174.5	111.1		A_g	1271.6	25.5	18.4	7.0	0.0	0.0	9.6	8.9	0.0	7.2	δ_{ip}(CH)
B_u	1238.1	81.0	δ_{ip}(CH)	B_g	1307.3	52.8	30.1	22.6	0.0	26.6	0.0	0.0	14.4	0.0	δ_{ip}(ring) [ν(CN)]; δ_{ip}(ring) [ν(CC)]
A_u	1239.8	5.1		A_g	1307.9	91.9	55.4	36.5	112.4	0.0	1.6	1.4	0.0	22.6	
B_u	1301.9	81.3	δ_{ip}(ring) [ν(CN)]; δ_{ip}(ring) [ν(CC)]	A_g	1319.7	979.0	957.1	21.9	393.1	0.0	30.0	417.0	0.0	218.2	δ_{ip}(ring) [ν(CC)]
A_u	1302.6	8.3		B_g	1320.0	360.1	205.8	154.3	0.0	133.2	0.0	0.0	146.4	0.0	
A_u	1354.3	143.1	δ_{oop}(OH) [γ(OH)]; δ_{ip}(CH); δ_{ip}(NH)	A_g	1355.8	4.6	2.7	2.0	4.4	0.0	0.7	1.2	0.0	0.3	δ_{oop}(OH) [γ(OH)]
B_u	1356.1	46.7	δ_{ip}(CH); δ_{ip}(NH)	B_g	1359.8	10.0	5.7	4.3	0.0	2.3	0.0	0.0	5.5	0.0	δ_{ip}(CH); δ_{ip}(NH)
A_u	1360.4	78.6	δ_{ip}(CH); δ_{ip}(NH); δ_{oop}(OH) [γ(OH)]	A_g	1361.6	7.6	4.6	3.0	3.2	0.0	1.7	3.7	0.0	1.3	δ_{ip}(CH); δ_{ip}(NH)
B_u	1382.4	421.1	δ_{oop}(OH) [γ(OH)]	B_g	1382.0	5.8	3.3	2.5	0.0	4.5	0.0	0.0	0.0	0.0	δ_{oop}(OH) [γ(OH)]
B_u	1428.4	314.6	δ_{ip}(NH); δ_{ip}(CH); δ_{ip}(ring)	B_g	1423.0	40.0	22.9	17.2	0.0	10.9	0.0	0.0	20.2	0.0	δ_{ip}(NH); δ_{ip}(CH); δ_{ip}(ring)
A_u	1430.6	0.7	[ν(CC)]; δ_{ip}(ring) [ν(CN)]	A_g	1423.5	48.7	29.6	19.0	63.1	0.0	0.0	1.5	0.0	8.9	[ν(CC)]
B_u	1529.5	165.1	δ_{ip}(CH); δ_{ip}(ring) [ν(CC)];	B_g	1571.7	113.0	64.6	48.4	0.0	51.0	0.0	0.0	36.7	0.0	δ_{ip}(CH); δ_{ip}(ring) [ν(CC)];
A_u	1530.3	87.7	δ_{ip}(ring) [ν(CN)]	A_g	1571.9	195.5	181.1	14.5	63.6	0.0	18.4	105.8	0.0	22.2	δ_{ip}(ring) [ν(CN)]
B_u	1543.4	22.5	δ_{ip}(NH); δ_{ip}(CH); δ_{ip}(ring)	B_g	1587.6	1.1	0.7	0.5	0.0	0.6	0.0	0.0	0.3	0.0	δ_{ip}(NH); δ_{ip}(CH); δ_{ip}(ring)
A_u	1543.7	19.6	[ν(CC)]; δ_{ip}(ring) [ν(CN)]	A_g	1587.7	13.5	10.1	3.4	14.7	0.0	1.3	0.8	0.0	0.2	[ν(CC)]; δ_{ip}(ring) [ν(CN)]
B_u	1681.4	367.2		B_g	1685.3	20.3	11.6	8.7	0.0	0.4	0.0	0.0	15.3	0.0	δ_{ip}(NH); δ_{ip}(ring) [ν(CC)];
A_u	1682.7	61.0	δ_{ip}(NH); δ_{ip}(ring) [ν(CC)];	A_g	1686.7	14.2	9.3	4.9	19.6	0.0	0.0	0.2	0.0	1.0	δ_{ip}(ring) [ν(CN)]
B_u	1685.6	265.2	δ_{ip}(ring) [ν(CN)]	B_g	1691.9	540.5	308.9	231.7	0.0	288.3	0.0	0.0	131.4	0.0	δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]
A_u	1688.2	211.4		A_g	1692.0	638.6	483.6	155.0	61.6	0.0	242.4	289.5	0.0	27.0	

A_u	2615.8	3275.3	v(OH)	A_g	2616.0	1000.0	807.8	192.2	1000.0	0.0	87.9	120.3	0.0	0.0	v(OH)
B_u	2697.5	20329.7	v(OH); v(NH)	B_g	2711.8	480.3	274.5	205.9	0.0	337.2	0.0	0.0	35.9	0.0	v(OH); v(NH)
A_u	2847.0	6758.9	v(NH)	A_g	2847.6	755.0	604.7	150.3	187.2	0.0	240.3	282.6	0.0	33.9	v(NH)
B_u	2858.0	4127.2	v(NH); v(OH)	B_g	2874.3	619.9	354.3	265.7	0.0	244.7	0.0	0.0	236.8	0.0	v(NH); v(OH)
B_u	3223.9	43.4		A_g	3224.0	97.1	55.5	41.6	95.7	0.0	0.8	17.1	0.0	36.4	
A_u	3224.0	50.8		B_g	3224.0	64.5	36.9	27.6	0.0	18.0	0.0	0.0	32.1	0.0	
B_u	3247.1	637.3		A_g	3246.9	672.1	552.1	119.9	410.8	0.0	154.6	20.4	0.0	120.6	
A_u	3247.3	49.9	v(CH)	B_g	3247.7	87.3	49.9	37.4	0.0	38.7	0.0	0.0	29.1	0.0	v(CH)
B_u	3283.5	317.9		B_g	3283.3	81.8	46.7	35.1	0.0	35.0	0.0	0.0	28.5	0.0	
A_u	3284.1	81.6		A_g	3283.8	322.8	222.3	100.5	449.4	0.0	0.7	2.5	0.0	6.9	
B_u	3285.3	94.2		A_g	3285.3	992.8	944.9	47.9	430.4	0.0	75.0	198.0	0.0	353.1	
A_u	3285.3	217.7		B_g	3286.0	226.0	129.1	96.8	0.0	16.8	0.0	0.0	158.7	0.0	

Table S19. Calculated wavenumbers v (cm^{-1}), IR intensities I ($km \cdot mol^{-1}$), Raman polycrystalline isotropic intensities I_tot, I_par, I_perp (arbitrary units) and single crystal directional intensities I_xx, I_xy, I_xz, I_yy, I_yz, I_zz (arbitrary units), and tentative interpretation of the bands in the IR and Raman spectra of **1a·1b·2c**.

IR				Raman										
Mode	v	I	Interpretation	Mode	v	I_tot	I_par	I_perp	I_xx	I_xy	I_xz	I_yy	I_yz	I_zz	Interpretation
A_u	0.0	0.0		A_g	22.4	1.8	1.1	0.8	1.8	0.1	0.4	2.1	0.0	0.7	δ_{rock}(ring)
A_u	0.0	0.0	acoustic modes	A_g	33.5	7.2	4.5	2.8	0.6	0.6	0.7	1.1	0.1	17.0	δ_{rock}(ring); δ_{rock}(SeO_3); ν_β(OH); δ_{twist}(SeO_3)
A_u	0.0	0.0		A_g	40.4	0.2	0.1	0.1	0.2	0.1	0.0	0.0	0.0	0.1	δ_{rock}(SeO_3); δ_{rock}(ring)
A_u	22.0	5.6	δ_{rock}(ring)	A_g	49.2	1.3	0.8	0.5	0.5	0.3	0.3	0.0	1.1	0.1	
A_u	43.8	6.1	δ_{rock}(SeO_3); δ_{rock}(ring)	A_g	54.3	1.6	1.1	0.5	1.7	0.1	0.1	0.6	0.9	0.1	δ_{rock}(SeO_3); ν_β(NH); δ_{rock}(ring)
A_u	52.2	6.9		A_g	56.6	0.6	0.4	0.2	0.1	0.0	0.1	1.0	0.1	0.4	δ_{rock}(ring); δ_{rock}(SeO_3)
A_u	57.3	35.4	δ_{rock}(SeO_3); ν_β(NH); δ_{rock}(ring)	A_g	58.1	1.2	0.7	0.5	0.3	0.0	0.0	1.0	0.7	1.0	δ_{rock}(SeO_3); ν_β(NH); δ_{rock}(ring)
A_u	58.9	7.3	δ_{rock}(SeO_3); ν_β(OH); δ_{rock}(ring)	A_g	61.1	0.3	0.2	0.1	0.5	0.0	0.2	0.0	0.0	0.1	δ_{twist}(SeO_3); δ_{rock}(SeO_3); δ_{rock}(ring)
A_u	59.9	18.7	δ_{twist}(SeO_3); δ_{rock}(SeO_3); δ_{rock}(ring); ν_β(NH)	A_g	70.8	1.1	0.7	0.4	0.1	0.0	0.5	0.7	0.8	0.0	ν_β(NH); δ_{twist}(SeO_3); δ_{rock}(SeO_3); δ_{rock}(ring)
A_u	70.4	1.0	δ_{twist}(SeO_3); δ_{rock}(SeO_3); δ_{rock}(ring)	A_g	73.7	6.6	3.8	2.8	0.0	0.3	0.7	9.5	0.4	8.0	δ_{rock}(ring); δ_{rock}(SeO_3)
A_u	76.2	8.4	δ_{twist}(SeO_3); δ_{rock}(ring); δ_{rock}(SeO_3); ν_β(OH)	A_g	79.3	2.0	1.3	0.7	0.2	0.3	0.0	4.0	0.2	1.0	δ_{twist}(SeO_3); δ_{rock}(SeO_3); δ_{rock}(ring)
A_u	80.0	0.4	δ_{twist}(SeO_3); δ_{rock}(SeO_3); δ_{rock}(ring)	A_g	83.7	3.2	1.9	1.4	0.8	0.6	0.7	3.6	0.9	1.2	δ_{rock}(ring); δ_{rock}(SeO_3)
A_u	81.8	14.0	ν_β(NH); δ_{twist}(SeO_3); δ_{rock}(SeO_3); δ_{rock}(ring)	A_g	88.5	1.5	0.9	0.5	1.1	0.1	0.1	2.1	0.2	0.6	δ_{twist}(SeO_3); δ_{rock}(SeO_3); δ_{rock}(ring)
A_u	85.5	24.7	δ_{rock}(ring); δ_{rock}(SeO_3)	A_g	88.8	6.8	3.9	2.9	3.3	1.4	0.3	1.7	0.0	12.5	δ_{rock}(ring); δ_{rock}(SeO_3)
A_u	89.4	6.6	ν_β(OH); δ_{rock}(SeO_3); δ_{rock}(ring)	A_g	93.9	0.3	0.2	0.1	0.1	0.0	0.1	0.0	0.0	0.6	δ_{twist}(SeO_3); ν_β(OH); δ_{rock}(ring)
A_u	96.7	27.6	δ_{rock}(ring); δ_{twist}(SeO_3); ν_β(OH)	A_g	97.3	0.7	0.4	0.3	0.7	0.0	0.2	0.0	0.1	0.7	δ_{rock}(ring); δ_{rock}(SeO_3); ν_α(OH)
A_u	99.5	15.8	δ_{rock}(ring); δ_{wagg}(ring);	A_g	103.0	11.0	6.5	4.5	1.7	7.5	1.9	0.0	1.3	10.3	
A_u	103.4	64.3	δ_{rock}(SeO_3)	A_g	104.4	10.5	6.0	4.5	6.1	8.1	2.8	0.3	0.4	3.5	δ_{rock}(ring); δ_{rock}(SeO_3)
A_u	107.0	45.1	δ_{rock}(ring); δ_{rock}(SeO_3)	A_g	110.1	16.0	9.1	6.8	20.3	2.6	1.4	0.2	1.0	18.9	δ_{rock}(ring); δ_{rock}(SeO_3); δ_{twist}(SeO_3)
A_u	111.9	22.1	δ_{twist}(SeO_3); δ_{rock}(ring)	A_g	112.4	10.5	6.0	4.5	0.1	5.5	3.9	5.2	3.0	2.5	δ_{rock}(ring); δ_{rock}(SeO_3)
A_u	122.4	46.8	δ_{rock}(ring); δ_{rock}(SeO_3); δ_{twist}(SeO_3)	A_g	116.2	14.5	8.3	6.2	0.0	5.8	5.3	5.6	4.8	7.7	δ_{rock}(ring); δ_{rock}(SeO_3); ν_β(OH)
A_u	130.3	39.5	δ_{twist}(SeO_3); ν_α(OH); ν_α(NH); δ_{rock}(ring); δ_{wagg}(ring)	A_g	119.0	3.3	1.9	1.4	3.1	1.2	1.4	0.2	0.1	1.8	δ_{rock}(ring); δ_{rock}(SeO_3); δ_{twist}(SeO_3); ν_α(OH)
A_u	131.8	5.3	δ_{rock}(ring); δ_{rock}(water); δ_{twist}(SeO_3)	A_g	125.8	5.7	3.3	2.4	9.7	0.0	0.3	4.5	1.0	0.8	δ_{rock}(ring); δ_{twist}(SeO_3)
A_u	150.3	14.5	δ_{rock}(ring); δ_{rock}(water); δ_{rock}(SeO_3)	A_g	127.2	9.0	5.2	3.8	1.6	3.8	2.9	2.2	5.2	0.3	δ_{twist}(SeO_3); ν_α(OH); ν_α(NH); δ_{rock}(ring)
A_u	151.9	17.7	δ_{rock}(ring); δ_{rock}(SeO_3)	A_g	146.0	17.2	9.9	7.3	10.2	3.7	2.1	11.5	9.7	0.7	δ_{rock}(ring); δ_{twist}(SeO_3); δ_{rock}(water)
A_u	165.6	14.0	δ_{wagg}(ring); δ_{rock}(SeO_3)	A_g	150.8	12.8	7.4	5.4	11.3	0.0	1.2	3.8	8.3	5.4	δ_{rock}(ring); δ_{twist}(SeO_3);
A_u	166.7	8.2	δ_{wagg}(ring); δ_{twist}(SeO_3)	A_g	160.4	1.4	0.9	0.5	0.1	0.4	0.2	1.6	0.6	0.0	δ_{rock}(SeO_3); δ_{twist}(SeO_3); δ_{rock}(water)
A_u	170.0	133.6	ν_β(NH); δ_{wagg}(ring); δ_{rock}(ring); δ_{twist}(SeO_3)	A_g	174.8	2.5	1.5	1.0	4.6	0.1	0.0	1.2	0.8	0.1	ν_β(NH); δ_{rock}(SeO_3); δ_{wagg}(ring)
A_u	175.9	10.7	δ_{rock}(water); δ_{wagg}(ring);	A_g	176.2	18.4	10.7	7.7	26.8	0.0	1.7	2.6	9.9	4.2	δ_{rock}(ring); δ_{rock}(water);

A_u	188.5	145.5	$\delta_{twist}(SeO_3)$ δ_{rock}(water); δ_{wagg}(ring); $\delta_{rock}(SeO_3)$	A_g	187.4	3.2	2.9	0.3	0.2	0.2	0.1	3.5	0.2	3.0	$\delta_{twist}(SeO_3)$ δ_{rock}(water); δ_{wagg}(ring); $\delta_{rock}(SeO_3)$; $\delta_{twist}(SeO_3)$
A_u	196.0	83.3	δ_{wagg}(ring); $\delta_{rock}(SeO_3)$	A_g	195.0	4.8	2.9	1.9	5.7	0.7	0.4	1.4	0.6	3.9	ν_σ(OH); ν_σ(NH); δ_{wagg}(ring); $\delta_{rock}(SeO_3)$
A_u	202.5	9.0	δ_{wagg}(ring); ν_σ(NH); $\delta_{rock}(SeO_3)$	A_g	204.1	1.0	0.8	0.2	0.7	0.1	0.3	0.3	0.4	0.2	δ_{wagg}(ring); $\delta_{rock}(SeO_3)$
A_u	219.5	5.0	δ_{wagg}(ring)	A_g	226.5	1.5	1.1	0.4	1.5	0.1	0.1	0.9	0.7	0.1	δ_{wagg}(ring)
A_u	222.2	15.1		A_g	227.7	0.8	0.5	0.3	0.0	0.8	0.0	0.9	0.0	0.0	δ_{twist}(ring)
A_u	228.0	20.3	δ_{twist}(ring); $\delta_{rock}(SeO_3)$	A_g	233.3	0.3	0.2	0.1	0.6	0.0	0.0	0.0	0.1	0.1	
A_u	236.7	26.1		A_g	242.2	1.9	1.1	0.8	1.5	0.0	0.0	0.1	0.5	3.3	δ_{twist}(ring); $\delta_{rock}(SeO_3)$
A_u	240.9	1.6	δ_{twist}(ring)	A_g	245.4	2.3	1.4	0.9	0.8	1.1	0.5	0.0	0.0	3.0	δ_{twist}(ring)
A_u	261.8	180.4	ν_σ(OH); ν_β(NH); $\delta_{twist}(SeO_3)$; $\delta_{scissor}$(OSeO)	A_g	258.6	2.1	1.2	0.9	0.0	0.0	0.0	0.1	2.7	0.8	ν_σ(OH); ν_β(NH); $\delta_{twist}(SeO_3)$; $\delta_{scissor}$(OSeO)
A_u	285.9	93.4	$\delta_{scissor}$(OSeO); ν_σ(NH); $\delta_{twist}(SeO_3)$	A_g	287.8	3.0	1.7	1.3	0.6	1.0	0.4	0.7	2.6	0.2	$\delta_{scissor}$(OSeO); ν_σ(NH); $\delta_{twist}(SeO_3)$
A_u	306.1	88.5	$\delta_{scissor}$(OSeO)	A_g	310.1	9.8	5.6	4.2	2.2	6.9	5.3	0.4	0.1	3.1	$\delta_{scissor}$(OSeO)
A_u	329.3	227.7		A_g	325.8	16.9	9.8	7.0	0.2	0.0	1.1	3.7	14.5	16.8	$\delta_{scissor}$(OSeO); ν_σ(OH)
A_u	334.5	55.2	$\delta_{scissor}$(OSeO); ν_σ(OH)	A_g	337.5	19.8	11.4	8.4	16.6	6.4	0.2	7.2	8.9	6.5	$\delta_{umbrella}(SeO_3)$; ν_σ(OH); δ_{rock}(ring)
A_u	353.3	449.9		A_g	352.2	9.3	5.3	4.0	14.9	0.0	1.1	7.3	1.0	2.4	
A_u	370.6	301.2		A_g	371.3	8.7	5.5	3.2	3.8	0.7	2.7	12.1	0.6	1.8	
A_u	376.3	370.9	δ_{rock}(ring); $\delta_{umbrella}(SeO_3)$	A_g	378.8	8.6	5.1	3.6	0.2	1.8	10.4	0.0	0.3	1.2	δ_{rock}(ring); $\delta_{umbrella}(SeO_3)$
A_u	382.7	73.5		A_g	383.0	3.3	1.9	1.4	2.8	0.1	0.9	0.3	0.0	5.0	
A_u	386.0	42.0		A_g	386.4	6.0	3.5	2.5	0.2	6.0	1.0	0.3	1.5	1.0	
A_u	390.3	40.6		A_g	387.5	0.8	0.5	0.3	0.3	0.0	0.4	0.3	0.0	0.9	
A_u	393.7	129.3	ν_σ(OH); $\delta_{umbrella}(SeO_3)$; δ_{rock}(ring); δ_{oop}(ring)	A_g	396.3	3.9	2.2	1.6	1.5	2.9	0.0	1.1	0.1	3.5	δ_{oop}(ring); $\delta_{umbrella}(SeO_3)$
A_u	404.6	60.7	δ_{oop}(ring); $\delta_{umbrella}(SeO_3)$	A_g	399.6	9.4	5.4	4.0	0.9	6.0	6.5	1.5	0.8	0.1	ν_σ(OH); $\delta_{umbrella}(SeO_3)$; δ_{oop}(ring); δ_{rock}(ring)
A_u	408.5	48.2	δ_{oop}(ring); $\delta_{scissor}$(OSeO)	A_g	406.5	17.3	10.1	7.2	2.3	3.7	0.2	7.2	0.3	35.2	δ_{oop}(ring); $\delta_{scissor}$(OSeO); ν_σ(OH)
A_u	414.6	23.3		A_g	414.0	1.4	0.8	0.5	0.0	0.2	0.2	0.5	0.0	2.8	δ_{oop}(ring); $\delta_{scissor}$(OSeO)
A_u	421.9	338.4	$\delta_{scissor}$(OSeO); ν_σ(NH); ν_σ(OH); δ_{oop}(ring)	A_g	426.0	10.3	5.9	4.4	0.4	9.9	1.4	0.6	2.1	4.1	$\delta_{scissor}$(OSeO); ν_σ(OH); δ_{rock}(ring)
A_u	427.2	350.7	$\delta_{scissor}$(OSeO); δ_{rock}(ring)	A_g	427.1	8.0	4.8	3.3	3.9	0.7	0.0	0.3	0.4	17.8	δ_{oop}(ring); ν_σ(NH); $\delta_{scissor}$(OSeO); $\delta_{umbrella}(SeO_3)$
A_u	467.2	286.8	$\delta_{scissor}$(OSeO)	A_g	467.2	22.4	13.9	8.5	8.8	0.1	2.6	15.7	14.6	7.8	$\delta_{scissor}$(OSeO)
A_u	485.0	17.0		A_g	481.6	0.5	0.3	0.2	0.0	0.4	0.0	0.5	0.1	0.0	
A_u	487.9	36.5	δ_{twist}(ring)	A_g	488.1	2.3	1.3	1.0	3.8	0.0	0.1	0.7	1.1	0.2	δ_{twist}(ring)
A_u	494.7	1.8		A_g	491.4	2.3	1.7	0.6	1.2	0.6	0.0	0.7	1.5	0.2	
A_u	497.1	203.6		A_g	500.2	6.4	3.7	2.7	4.9	0.1	1.3	1.2	3.8	3.5	
A_u	499.0	0.6	δ_{oop}(ring); δ_{oop}(NH) [γ(NH)]	A_g	502.5	0.6	0.4	0.2	0.2	0.2	0.1	0.1	0.4	0.1	δ_{oop}(ring); δ_{oop}(NH) [γ(NH)]
A_u	512.7	34.9		A_g	512.2	1.8	1.2	0.7	0.3	0.3	0.0	0.0	0.6	3.3	
A_u	532.9	12.7		A_g	534.2	60.1	45.7	14.4	5.8	10.6	11.6	8.4	20.8	61.8	
A_u	533.2	9.0		A_g	535.3	1.0	0.6	0.4	0.2	0.5	0.2	0.3	0.0	1.4	
A_u	537.2	24.7	δ_{ip}(ring) [6-ring]	A_g	537.1	55.7	41.8	13.8	3.7	8.7	9.2	11.3	25.1	49.8	δ_{ip}(ring) [6-ring]
A_u	540.0	3.5		A_g	539.5	3.0	1.8	1.2	0.8	0.6	3.0	0.2	0.0	0.6	
A_u	540.5	4.3		A_g	540.9	8.0	5.5	2.5	0.3	1.0	0.4	11.9	3.7	0.7	
A_u	542.6	31.2		A_g	543.2	68.0	44.9	23.1	5.9	0.6	14.3	93.1	31.6	5.7	
A_u	632.0	21.8	δ_{oop}(ring); δ_{ip}(ring) [6-ring]	A_g	634.1	1.0	0.6	0.4	0.6	0.0	0.3	0.0	0.9	0.0	δ_{oop}(ring); δ_{ip}(ring) [6-ring]
A_u	637.1	3.9		A_g	635.3	1.7	1.0	0.7	2.2	0.1	0.5	0.5	0.7	0.0	δ_{ip}(ring) [6-ring]
A_u	638.2	12.1	δ_{oop}(ring); δ_{ip}(ring) [6-ring]; δ_{oop}(NH) [γ(NH)]	A_g	637.1	1.1	0.6	0.5	0.8	0.4	0.2	0.2	0.5	0.2	δ_{oop}(ring); δ_{ip}(ring) [6-ring]
A_u	639.5	129.9		A_g	637.9	3.6	2.2	1.4	0.9	1.2	0.8	1.0	1.5	2.0	δ_{oop}(ring); δ_{ip}(ring) [6-ring]; δ_{oop}(NH) [γ(NH)]
A_u	643.2	16.3	δ_{oop}(ring); δ_{ip}(ring) [6-ring]	A_g	643.7	0.5	0.3	0.2	0.0	0.0	0.3	0.3	0.1	0.5	δ_{oop}(ring); δ_{ip}(ring) [6-ring]

A_u	644.0	18.8		A_g	645.0	0.7	0.4	0.3	0.2	0.3	0.0	0.0	0.2	0.9	
A_u	726.6	547.1	ν(SeO)	A_g	727.7	30.5	23.3	7.2	0.3	0.2	2.4	73.5	0.3	2.1	δ_{ip}(NH); δ_{oop}(OH) [γ(OH)]; ν(SeO); δ_{oop}(CH)
A_u	737.8	215.3	δ_{ip}(NH); δ_{oop}(OH) [γ(OH)]	A_g	734.5	1.5	1.2	0.3	0.3	0.0	0.0	2.7	0.4	0.1	δ_{ip}(NH); δ_{oop}(OH) [γ(OH)]; ν(SeO)
A_u	760.2	38.1	δ_{oop}(CH); δ_{oop}(ring); δ_{ip}(NH); δ_{oop}(OH) [γ(OH)]	A_g	758.1	5.1	3.2	1.9	0.9	1.0	0.1	3.8	3.7	1.0	δ_{oop}(CH); δ_{oop}(ring); δ_{ip}(NH); δ_{oop}(OH) [γ(OH)]
A_u	774.2	109.6	δ_{oop}(CH); δ_{oop}(ring)	A_g	770.7	3.2	1.9	1.2	0.0	0.2	2.9	2.8	0.3	0.1	δ_{oop}(CH); δ_{oop}(ring)
A_u	793.3	20.1	δ_{ip}(ring) [6-ring]	A_g	792.0	12.1	7.6	4.5	0.7	3.4	11.2	2.9	1.5	0.4	δ_{oop}(CH); ν(SeO)
A_u	794.0	44.1	δ_{ip}(ring) [6-ring]; δ_{oop}(CH); δ_{ip}(OH); ν(SeO)	A_g	796.4	2.3	1.4	1.0	0.1	0.5	1.7	2.3	0.0	0.2	δ_{ip}(ring) [6-ring]; δ_{oop}(CH); δ_{oop}(ring)
A_u	795.9	53.6	δ_{ip}(ring) [6-ring]; δ_{oop}(CH);	A_g	797.4	13.1	11.1	2.0	6.8	2.2	3.0	11.9	1.0	1.8	δ_{ip}(ring) [6-ring]
A_u	796.9	73.6	δ_{oop}(ring)	A_g	798.2	121.9	111.8	10.1	51.0	13.6	11.5	125.4	5.7	48.6	δ_{ip}(ring) [6-ring]; δ_{ip}(OH); ν(SeO)
A_u	804.8	424.5	δ_{oop}(CH); δ_{oop}(ring); ν(SeO)	A_g	805.1	3.5	2.0	1.5	2.9	2.0	0.8	2.0	0.2	0.0	δ_{oop}(CH); δ_{oop}(ring); ν(SeO)
A_u	807.3	10.4	δ_{oop}(CH); δ_{ip}(OH); δ_{ip}(ring) [6-ring]; ν(SeO); δ_{ip}(NH)	A_g	806.4	37.1	36.7	0.4	24.5	0.1	0.0	36.0	0.5	19.5	δ_{oop}(CH); δ_{oop}(ring); δ_{ip}(OH); δ_{oop}(NH) [γ(NH)]; ν(SeO)
A_u	811.4	477.5	δ_{oop}(CH); ν(SeO); δ_{oop}(ring); δ_{ip}(OH); δ_{oop}(NH) [γ(NH)]	A_g	815.6	91.8	90.1	1.7	80.7	0.0	0.7	71.2	3.7	42.2	δ_{oop}(CH); δ_{ip}(OH); δ_{oop}(NH) [γ(NH)]; ν(SeO); δ_{ip}(ring) [6-ring]
A_u	820.4	262.7	δ_{oop}(CH); δ_{ip}(OH); δ_{oop}(ring);	A_g	816.7	103.9	100.4	3.6	115.8	0.8	1.3	38.2	5.5	64.2	δ_{oop}(CH); ν(SeO); δ_{oop}(ring);
A_u	823.4	155.8	ν(SeO); δ_{ip}(ring) [6-ring]	A_g	818.9	48.5	47.3	1.2	43.4	3.1	0.4	24.4	0.1	32.8	δ_{ip}(OH); δ_{ip}(NH)
A_u	828.9	127.4	δ_{ip}(ring) [6-ring]; ν(SeO)	A_g	829.6	16.9	15.8	1.2	9.4	0.1	1.8	6.3	1.8	16.4	δ_{ip}(ring) [6-ring]; ν(SeO)
A_u	830.2	114.1		A_g	830.8	3.3	2.5	0.8	0.2	0.5	0.9	1.4	1.1	2.1	δ_{ip}(ring) [6-ring]
A_u	832.5	79.0	δ_{ip}(OH); δ_{ip}(NH); ν(SeO);	A_g	832.6	19.5	18.2	1.3	4.8	1.6	1.2	20.7	0.5	13.1	δ_{ip}(ring) [6-ring]; δ_{ip}(OH); ν(SeO); δ_{ip}(NH)
A_u	843.8	107.1	δ_{ip}(ring) [6-ring]	A_g	839.2	73.5	69.4	4.1	21.8	2.8	6.6	85.0	0.1	42.7	ν(SeO); δ_{ip}(NH); δ_{ip}(ring) [6-ring]
A_u	847.5	877.1	δ_{oop}(CH); ν(SeO); δ_{ip}(NH); δ_{oop}(NH) [γ(NH)]	A_g	850.8	77.9	71.6	6.3	93.3	11.7	4.8	29.7	0.0	26.9	δ_{oop}(CH); ν(SeO)
A_u	850.3	314.5	δ_{oop}(CH); ν(SeO); δ_{ip}(OH)	A_g	854.8	50.4	43.6	6.8	65.1	12.2	2.7	21.7	1.1	5.2	δ_{oop}(CH); ν(SeO); δ_{oop}(NH) [γ(NH)]
A_u	853.9	1585.6		A_g	859.4	22.8	19.6	3.3	8.5	0.0	4.3	2.6	3.7	29.5	δ_{oop}(CH); ν(SeO)
A_u	861.0	129.0	δ_{oop}(CH); δ_{ip}(NH); δ_{oop}(NH); ν(SeO)	A_g	871.0	14.1	8.3	5.9	4.6	11.8	1.2	0.7	5.2	1.7	δ_{oop}(CH); δ_{oop}(ring); δ_{ip}(NH); δ_{oop}(NH); ν(SeO)
A_u	877.8	108.5	δ_{oop}(CH); δ_{oop}(ring); δ_{ip}(OH); δ_{ip}(NH); ν(SeO)	A_g	882.1	5.6	3.2	2.4	0.2	2.0	0.8	1.7	4.9	0.0	δ_{oop}(CH); δ_{oop}(ring); δ_{ip}(OH); δ_{ip}(NH)
A_u	889.1	91.8	δ_{oop}(CH); δ_{oop}(ring); δ_{ip}(OH); δ_{oop}(NH) [γ(NH)]; ν(SeO)	A_g	888.4	9.9	5.7	4.2	0.8	7.7	1.2	0.5	5.6	0.3	δ_{oop}(CH); δ_{oop}(ring); δ_{ip}(OH); δ_{oop}(NH) [γ(NH)]; ν(SeO)
A_u	901.7	285.8	δ_{oop}(CH); δ_{oop}(ring); δ_{ip}(OH); δ_{oop}(NH) [γ(NH)]	A_g	902.5	7.1	5.2	1.9	4.9	0.2	0.3	0.1	5.5	2.5	δ_{oop}(CH); δ_{oop}(ring); δ_{ip}(OH); δ_{oop}(NH) [γ(NH)]
A_u	904.9	280.3		A_g	905.7	54.9	52.4	2.5	30.3	3.2	3.1	25.0	1.1	54.5	δ_{oop}(CH); δ_{oop}(ring); δ_{ip}(OH); δ_{ip}(NH); ν(SeO)
A_u	907.1	1208.4	δ_{oop}(CH); δ_{oop}(ring); δ_{ip}(OH); δ_{ip}(NH); ν(SeO)	A_g	908.3	57.2	51.2	6.1	22.5	0.6	13.1	11.2	0.6	75.0	ν(SeO); δ_{oop}(CH); δ_{oop}(ring); δ_{ip}(OH)
A_u	910.5	617.5		A_g	921.5	2.6	1.6	1.0	1.0	1.0	0.1	0.1	0.2	4.2	δ_{oop}(CH); δ_{oop}(ring); δ_{ip}(OH);
A_u	931.2	9.8		A_g	929.0	4.9	3.9	1.0	2.0	0.2	1.8	2.6	1.5	1.2	δ_{ip}(NH); ν(SeO)
A_u	948.7	653.8	ν(SeO); δ_{oop}(CH); δ_{ip}(OH)	A_g	949.3	28.1	16.9	11.3	15.5	1.8	0.2	3.6	15.9	30.7	ν(SeO); δ_{oop}(CH); δ_{ip}(OH)
A_u	964.2	11.5		A_g	962.8	2.9	1.8	1.1	0.5	1.1	0.2	0.0	0.2	5.3	
A_u	966.8	15.2	δ_{ip}(ring) [6-ring]	A_g	964.6	1.6	1.4	0.2	1.7	0.6	0.0	0.4	0.0	0.7	δ_{ip}(ring) [6-ring]
A_u	968.6	83.5		A_g	967.2	1.5	1.1	0.4	0.0	0.0	1.0	0.6	0.0	1.5	
A_u	991.6	27.9		A_g	990.4	3.1	2.0	1.0	5.5	0.0	1.1	0.3	0.1	0.7	
A_u	999.7	15.1	δ_{oop}(CH); δ_{oop}(ring); δ_{oop}(NH) [γ(NH)]	A_g	996.9	6.1	3.6	2.4	0.3	0.0	5.4	0.3	3.3	0.4	δ_{oop}(CH); δ_{oop}(ring);
A_u	1005.8	36.7		A_g	1006.8	1.8	1.1	0.7	0.5	0.1	0.5	2.3	0.1	1.3	δ_{oop}(NH) [γ(NH)]
A_u	1009.6	2.9		A_g	1011.1	2.7	1.9	0.9	0.0	0.3	0.1	0.2	0.0	6.9	

A_u	1020.0	14.0		A_g	1018.6	4.3	2.5	1.8	0.0	0.5	3.6	0.3	2.4	0.0	
A_u	1027.5	8.7		A_g	1029.5	2.8	2.3	0.5	0.0	0.2	0.1	4.4	0.4	1.4	
A_u	1029.8	25.9	δ_{oop}(CH); δ_{oop}(ring)	A_g	1031.4	3.5	2.5	1.0	0.6	1.1	0.6	2.9	1.4	0.0	δ_{oop}(CH); δ_{oop}(ring)
A_u	1036.2	11.3		A_g	1034.3	4.1	3.2	0.9	5.3	0.3	0.1	0.8	1.9	0.2	
A_u	1044.0	15.4	δ_{oop}(CH)	A_g	1043.1	3.0	1.8	1.2	3.8	0.6	1.5	0.0	0.2	0.6	δ_{oop}(CH)
A_u	1049.9	12.9	δ_{ip}(ring) [ν(CC)]; δ_{ip}(CH);	A_g	1049.3	15.3	13.2	2.1	24.7	1.2	1.6	0.7	0.5	5.8	
A_u	1055.0	8.1	δ_{oop}(CH)	A_g	1055.7	45.2	41.7	3.5	15.8	0.2	6.5	40.1	4.6	27.3	δ_{ip}(ring) [ν(CC)]; δ_{ip}(CH);
A_u	1056.8	4.9	δ_{oop}(CH)	A_g	1057.5	33.8	31.4	2.3	14.4	2.2	0.1	41.7	3.4	11.0	δ_{oop}(CH)
A_u	1058.3	8.9	δ_{ip}(ring) [ν(CC)]; δ_{ip}(CH);	A_g	1060.7	3.7	2.5	1.2	1.3	0.1	0.7	4.1	0.6	2.6	δ_{oop}(CH); δ_{ip}(CH)
A_u	1067.5	1.5	δ_{oop}(CH)	A_g	1068.5	8.1	7.5	0.7	10.9	0.6	0.1	4.5	0.5	1.3	δ_{ip}(ring) [ν(CC)]; δ_{ip}(CH);
A_u	1073.6	146.9	δ_{oop}(CH); δ_{oop}(OH) [γ(OH)]	A_g	1073.9	6.4	5.1	1.3	11.0	0.4	0.2	2.2	1.1	0.0	δ_{oop}(CH) δ_{oop}(CH); δ_{oop}(OH) [γ(OH)]
A_u	1094.1	21.4	δ_{ip}(ring) [ν(CC)]; δ_{oop}(OH) [γ(OH)]; δ_{ip}(CH)	A_g	1095.0	33.2	32.9	0.3	21.5	0.4	0.1	23.7	0.7	25.3	δ_{ip}(ring) [ν(CC)]; δ_{oop}(OH) [γ(OH)]; δ_{ip}(CH)
A_u	1096.9	7.6	δ_{ip}(ring) [ν(CC)]; δ_{ip}(NH);	A_g	1097.6	105.0	98.1	7.0	58.1	0.1	13.4	55.0	11.0	81.2	δ_{ip}(ring) [ν(CC)]; δ_{ip}(NH);
A_u	1101.4	6.3	δ_{ip}(CH)	A_g	1102.2	96.2	93.6	2.6	53.0	0.4	4.6	81.8	3.5	62.7	δ_{ip}(CH)
A_u	1112.9	298.7	δ_{oop}(OH) [γ(OH)]; δ_{oop}(CH); δ_{ip}(CH)	A_g	1112.3	17.1	16.3	0.8	8.2	0.0	2.5	11.5	0.2	13.6	δ_{oop}(OH) [γ(OH)]; δ_{oop}(CH); δ_{ip}(CH)
A_u	1141.0	172.8	δ_{oop}(NH) [γ(NH)]; δ_{oop}(CH); δ_{ip}(CH)	A_g	1139.4	7.5	4.4	3.1	5.2	1.7	1.1	3.2	2.6	3.8	δ_{oop}(NH) [γ(NH)]; δ_{oop}(CH); δ_{ip}(CH)
A_u	1155.2	22.7		A_g	1156.4	1.6	0.9	0.7	0.4	0.3	1.6	0.0	0.4	0.2	
A_u	1160.2	8.3	δ_{oop}(NH) [γ(NH)]; δ_{ip}(CH)	A_g	1160.1	9.1	5.2	3.9	4.0	0.2	3.2	11.9	1.7	2.3	δ_{oop}(NH) [γ(NH)]; δ_{ip}(CH)
A_u	1165.9	77.8		A_g	1165.2	1.4	0.8	0.6	0.4	0.1	1.0	1.0	0.5	0.2	
A_u	1169.7	44.8		A_g	1169.4	13.1	7.6	5.5	0.3	2.8	13.4	2.3	0.2	4.9	
A_u	1177.0	38.3		A_g	1177.1	6.1	3.8	2.4	0.5	1.3	0.8	0.2	1.9	9.8	
A_u	1178.7	28.9		A_g	1179.5	31.4	17.9	13.4	7.3	14.9	16.6	21.1	0.1	5.7	
A_u	1179.8	46.5	δ_{ip}(CH)	A_g	1181.9	31.2	18.0	13.2	7.5	2.7	14.8	37.3	6.7	3.2	δ_{ip}(CH)
A_u	1185.6	3.2		A_g	1188.6	22.3	13.0	9.4	2.9	10.5	12.9	11.4	3.9	0.0	
A_u	1186.9	2.7		A_g	1190.6	15.6	8.9	6.7	4.3	10.8	6.5	8.4	0.1	0.9	
A_u	1188.4	2.9		A_g	1195.2	19.0	11.0	8.0	0.8	11.9	8.6	9.7	0.2	6.7	
A_u	1223.9	150.1	δ_{oop}(NH) [γ(NH)]; δ_{oop}(CH)	A_g	1224.6	1.6	0.9	0.7	2.3	0.0	0.2	1.9	0.2	0.1	δ_{oop}(NH) [γ(NH)]; δ_{oop}(CH)
A_u	1257.6	320.8		A_g	1255.4	1.3	0.9	0.3	0.6	0.8	0.1	0.9	0.0	0.0	δ_{ip}(CH); δ_{ip}(ring) [ν(CC)];
A_u	1260.0	22.4		A_g	1258.6	1.0	0.6	0.4	0.0	0.1	0.2	0.2	1.2	0.0	δ_{ip}(ring) [ν(CN)]
A_u	1262.2	9.9		A_g	1261.2	8.1	4.6	3.4	3.4	3.9	0.1	0.0	6.1	1.3	
A_u	1267.6	8.0	δ_{ip}(CH); δ_{ip}(ring) [ν(CC)];	A_g	1269.5	1.5	0.9	0.6	0.1	0.5	1.0	0.1	0.6	0.0	
A_u	1269.6	34.7	δ_{ip}(ring) [ν(CN)]; δ_{ip}(NH)	A_g	1271.1	2.8	1.7	1.1	2.2	1.4	0.1	0.1	1.6	0.2	δ_{ip}(CH); δ_{ip}(ring) [ν(CC)];
A_u	1275.2	9.8		A_g	1275.8	4.8	3.4	1.4	4.1	1.3	0.2	4.1	0.7	0.7	δ_{ip}(ring) [ν(CN)]; δ_{ip}(NH)
A_u	1305.3	11.2		A_g	1306.1	15.5	9.1	6.4	3.7	0.7	8.3	17.1	4.4	0.1	
A_u	1311.2	4.9	δ_{ip}(CH); δ_{ip}(ring) [ν(CC)]; δ_{ip}(NH)	A_g	1311.5	7.8	4.7	3.0	0.0	1.2	1.2	15.5	0.1	2.9	δ_{ip}(CH); δ_{ip}(ring) [ν(CC)]; δ_{ip}(NH)
A_u	1314.9	3.2	δ_{ip}(CH); δ_{ip}(ring) [ν(CC)]	A_g	1315.4	10.5	6.0	4.5	0.9	4.8	5.6	7.4	0.8	2.2	δ_{ip}(CH); δ_{ip}(ring) [ν(CC)]
A_u	1351.7	141.3	δ_{ip}(CH); δ_{ip}(NH); δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]	A_g	1353.0	3.8	3.1	0.7	0.2	0.6	1.1	1.5	0.2	4.1	
A_u	1353.5	25.5		A_g	1353.4	13.4	10.0	3.3	0.1	1.7	1.1	13.1	5.2	7.0	δ_{ip}(CH); δ_{ip}(NH); δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]
A_u	1355.9	418.8		A_g	1356.8	20.2	14.3	5.9	0.3	0.2	0.3	22.1	13.9	5.4	
A_u	1369.6	220.3	δ_{ip}(OH)	A_g	1369.2	0.8	0.5	0.3	0.1	0.1	0.3	0.9	0.3	0.1	δ_{ip}(OH)
A_u	1412.4	80.3	δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]	A_g	1412.3	212.3	179.7	32.6	37.8	0.0	19.4	161.5	87.1	119.5	
A_u	1415.1	172.7		A_g	1415.2	327.0	278.2	48.7	33.4	1.3	26.6	360.9	104.8	156.0	δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]; δ_{ip}(NH)
A_u	1416.0	8.7		A_g	1416.3	13.5	10.6	2.9	2.3	4.0	1.0	4.2	5.0	9.2	
A_u	1430.6	77.3	δ_{ip}(ring) [ν(CC)]; δ_{ip}(CH);	A_g	1429.5	100.6	90.7	9.9	31.9	0.1	19.3	56.0	13.1	87.0	δ_{ip}(ring) [ν(CC)]; δ_{ip}(CH);
A_u	1432.0	257.8	δ_{ip}(NH)	A_g	1431.2	145.5	127.1	18.5	55.3	4.0	30.3	50.5	27.1	127.6	δ_{ip}(NH)
A_u	1432.5	0.8	δ_{ip}(ring) [ν(CC)]; δ_{ip}(CH)	A_g	1433.2	5.9	5.1	0.9	1.7	0.0	0.2	4.5	2.7	2.7	δ_{ip}(ring) [ν(CC)]; δ_{ip}(CH)
A_u	1453.4	8.5	δ_{ip}(ring) [ν(CC)]; δ_{ip}(CH);	A_g	1452.5	41.6	32.8	8.8	0.2	6.6	2.2	31.0	14.3	32.2	δ_{ip}(ring) [ν(CC)]; δ_{ip}(CH);
A_u	1454.3	67.4	δ_{ip}(NH)	A_g	1454.3	42.1	31.9	10.2	3.9	8.3	5.3	5.5	16.6	43.7	δ_{ip}(NH)
A_u	1460.3	13.5	δ_{ip}(ring) [ν(CC)]; δ_{ip}(CH)	A_g	1459.2	63.8	50.5	13.2	0.8	4.3	5.7	26.6	23.0	73.5	δ_{ip}(ring) [ν(CC)]; δ_{ip}(CH)
A_u	1503.4	1.9	δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring)	A_g	1504.1	33.1	19.8	13.3	6.0	13.8	21.0	7.2	1.3	15.4	δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring)

A_u	1505.6	5.3	[ν(CN)]; δ_{ip}(CH)	A_g	1505.9	3.8	2.2	1.6	1.4	1.7	2.2	1.6	0.3	0.1	[ν(CN)]
A_u	1506.8	3.4		A_g	1506.2	39.5	24.4	15.1	3.5	18.3	23.8	1.1	5.3	19.4	
A_u	1530.8	31.2	δ_{ip}(NH); δ_{ip}(ring) [ν(CC)];	A_g	1531.1	58.9	43.8	15.1	0.1	3.8	1.7	35.2	34.6	45.3	δ_{ip}(NH); δ_{ip}(ring) [ν(CC)];
A_u	1535.7	52.6	δ_{ip}(CH)	A_g	1536.8	46.0	32.7	13.3	0.1	9.6	1.4	30.1	27.1	22.5	δ_{ip}(CH)
A_u	1539.8	145.3	δ_{ip}(ring) [ν(CC)]; δ_{ip}(CH)	A_g	1539.4	38.3	26.7	11.7	1.4	2.9	0.1	29.1	26.9	18.4	δ_{ip}(ring) [ν(CC)]; δ_{ip}(CH)
A_u	1614.7	145.8	δ_{ip}(NH); δ_{ip}(ring) [ν(CC)];	A_g	1614.8	22.3	20.1	2.2	15.2	4.4	0.1	24.8	0.7	2.9	δ_{ip}(NH); δ_{ip}(ring) [ν(CC)];
A_u	1615.9	38.0	δ_{ip}(ring) [ν(CN)]; δ_{ip}(CH)	A_g	1615.7	13.2	10.6	2.5	0.0	0.2	0.2	13.3	5.1	9.8	δ_{ip}(ring) [ν(CN)]; δ_{ip}(CH)
A_u	1621.7	38.3	δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]; δ_{ip}(CH)	A_g	1621.4	22.2	18.5	3.8	11.2	9.1	0.0	23.8	0.9	1.3	δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]; δ_{ip}(CH)
A_u	1636.3	211.9	δ_{ip}(NH); δ_{ip}(ring) [ν(CC)];	A_g	1637.0	126.0	72.0	54.0	83.5	72.5	0.0	2.2	53.7	52.8	
A_u	1637.0	73.9	δ_{ip}(ring) [ν(CN)]; δ_{ip}(CH)	A_g	1638.3	119.8	68.5	51.2	55.7	83.4	4.8	0.0	50.5	38.1	
A_u	1637.6	227.8	δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]; δ_{ip}(CH)	A_g	1641.0	41.9	24.4	17.4	12.9	27.7	0.0	0.5	28.8	2.4	δ_{ip}(NH); δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]; δ_{ip}(CH)
A_u	1655.0	49.5	δ_{ip}(NH); δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]; δ_{ip}(CH)	A_g	1655.1	8.1	4.8	3.3	0.0	6.9	2.3	5.4	0.3	0.3	
A_u	1658.3	39.0	δ_{ip}(NH); δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]; δ_{oop}(OH) [γ(OH)]; δ_{ip}(CH)	A_g	1657.1	26.6	18.9	7.7	0.7	0.0	0.1	27.8	18.3	9.3	δ_{ip}(NH); δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]; δ_{oop}(OH) [γ(OH)]; δ_{ip}(CH)
A_u	1660.9	60.8	δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]; δ_{ip}(CH)	A_g	1661.7	23.8	15.3	8.5	2.3	1.1	4.5	34.1	11.1	0.5	δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]; δ_{ip}(CH)
A_u	1673.5	319.1	δ_{ip}(NH); δ_{oop}(NH); δ_{ip}(ring)	A_g	1680.3	9.1	5.6	3.6	0.2	0.5	3.5	15.8	1.0	1.5	δ_{ip}(NH); δ_{oop}(NH); δ_{ip}(ring)
A_u	1683.6	292.3	[ν(CC)]; δ_{ip}(ring) [ν(CN)]; δ_{oop}(OH) [γ(OH)]	A_g	1683.2	36.8	21.0	15.8	20.6	0.5	8.0	21.0	27.9	0.0	[ν(CC)]; δ_{ip}(ring) [ν(CN)]; δ_{oop}(OH) [γ(OH)]
A_u	1698.5	308.4	δ_{ip}(NH); δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]	A_g	1701.0	23.7	13.7	10.0	16.8	0.0	13.3	15.7	5.9	2.1	δ_{ip}(NH); δ_{ip}(ring) [ν(CC)]; δ_{ip}(ring) [ν(CN)]
A_u	1706.7	289.5	δ_{ip}(NH); δ_{oop}(OH) [γ(OH)]; δ_{ip}(ring) [ν(CC)]	A_g	1705.6	7.1	4.1	3.1	1.4	0.8	0.0	0.5	9.1	0.2	δ_{ip}(NH); δ_{oop}(OH) [γ(OH)]; δ_{ip}(ring) [ν(CC)]
A_u	2357.9	10854.2	ν(OH)	A_g	2373.0	329.9	244.7	85.2	28.7	0.8	3.1	145.8	106.5	506.2	ν(OH)
A_u	2776.0	260.0		A_g	2772.2	19.5	11.3	8.2	1.1	6.5	11.9	4.5	5.9	5.9	
A_u	2782.8	229.0	δ_{oop}(NH) [γ(NH)]	A_g	2785.5	1000.0	705.7	294.3	833.9	488.9	251.4	203.2	144.3	4.2	δ_{oop}(NH) [γ(NH)]
A_u	2789.3	24850.8		A_g	2793.9	162.3	123.6	38.7	134.5	58.5	7.1	36.9	58.9	15.9	
A_u	3171.8	11.7		A_g	3171.9	118.3	90.5	27.7	146.2	55.9	1.1	37.1	9.8	0.2	
A_u	3187.2	181.7	ν(CH); δ_{oop}(CH)	A_g	3187.5	211.6	149.9	61.7	175.7	128.6	31.7	33.4	30.0	3.8	ν(CH); δ_{oop}(CH)
A_u	3191.4	171.5		A_g	3191.5	156.0	117.9	38.1	126.5	85.2	16.1	62.5	13.4	3.1	
A_u	3192.8	256.9	ν(CH); δ_{oop}(NH) [γ(NH)]	A_g	3192.6	230.0	157.2	72.8	13.5	25.4	98.0	1.1	51.1	293.7	ν(CH); δ_{oop}(NH) [γ(NH)]
A_u	3200.6	714.1	ν(CH); δ_{oop}(NH) [γ(NH)]; ν(OH)	A_g	3199.1	165.9	97.4	68.4	18.0	5.3	14.0	262.9	78.8	31.4	ν(CH); ν(NH); δ_{oop}(NH) [γ(NH)]
A_u	3200.9	112.0		A_g	3200.9	335.2	236.2	99.0	349.7	197.8	21.6	35.5	58.4	1.9	ν(CH)
A_u	3201.6	173.0	ν(CH)	A_g	3202.0	273.8	207.0	66.9	67.0	54.7	52.5	2.5	5.6	444.9	ν(CH); δ_{oop}(NH) [γ(NH)]
A_u	3203.7	17.2		A_g	3203.7	90.4	52.2	38.2	0.3	68.8	28.3	19.3	10.1	45.2	ν(CH)
A_u	3208.5	618.6		A_g	3207.8	399.1	303.0	96.1	21.6	43.1	103.5	73.0	132.3	422.8	
A_u	3214.9	57.5	ν(CH); δ_{oop}(NH) [γ(NH)]	A_g	3214.9	95.2	71.9	23.3	87.4	63.7	0.1	37.2	2.1	0.7	ν(CH); δ_{oop}(NH) [γ(NH)]
A_u	3215.1	99.4		A_g	3215.3	336.3	245.8	90.6	0.0	12.2	5.6	189.3	241.8	218.6	
A_u	3216.6	6.2		A_g	3217.0	118.6	94.2	24.3	85.5	16.6	59.8	10.1	1.7	58.4	ν(CH); δ_{oop}(CH)
A_u	3219.0	8.9	ν(CH); δ_{oop}(CH)	A_g	3219.4	502.0	367.1	134.9	306.0	26.6	313.3	3.6	10.1	373.6	
A_u	3220.2	46.2		A_g	3222.5	131.6	77.2	54.4	1.6	63.1	20.4	38.1	96.6	3.8	ν(CH); δ_{oop}(CH); δ_{oop}(NH) [γ(NH)]
A_u	3222.0	152.0	ν(CH); δ_{oop}(CH); ν(OH) [water]; δ_{oop}(NH) [γ(NH)]	A_g	3223.5	505.5	416.0	89.5	349.1	135.9	131.4	332.0	13.3	49.8	
A_u	3226.3	124.6	ν(CH)	A_g	3226.7	783.3	659.5	123.8	86.7	35.8	44.5	872.2	264.8	320.8	ν(CH); δ_{oop}(NH) [γ(NH)]
A_u	3230.9	80.4		A_g	3231.5	456.1	408.7	47.4	170.2	119.1	10.7	537.2	0.1	126.0	ν(CH)
A_u	3243.0	2.3	ν(CH)	A_g	3243.1	355.5	264.0	91.5	4.4	63.9	44.8	536.3	92.9	26.7	ν(CH); δ_{oop}(NH) [γ(NH)]; ν(OH) [water]
A_u	3250.7	18.3		A_g	3243.9	162.1	103.1	59.0	123.4	1.0	103.1	46.2	16.6	69.0	δ_{oop}(NH) [γ(NH)]; ν(OH) [water]; ν(CH); ν(NH)
A_u	3255.5	29.5		A_g	3251.2	657.9	561.3	96.5	57.7	5.7	1.0	1000.0	187.3	192.4	ν(CH)

A_u	3257.7	16.7		A_g	3255.9	393.4	331.3	62.1	167.7	2.3	125.1	67.0	67.5	364.7	
A_u	3266.0	2740.7	δ_{oop}(NH) [γ(NH)]; ν(OH) [water]; ν(CH); ν(NH)	A_g	3258.3	974.0	846.3	127.8	189.0	4.8	32.1	911.4	357.7	502.7	
A_u	3328.1	3457.6	ν(OH) [water]; ν(NH); ν(CH)	A_g	3321.5	395.8	310.9	84.9	6.0	7.4	13.0	871.3	55.2	15.3	ν(OH) [water]; ν(NH); ν(CH)

Table S20. Calculated wavenumbers v (cm^{-1}), IR intensities I ($km \cdot mol^{-1}$), Raman polycrystalline isotropic intensities I_tot, I_par, I_perp (arbitrary units) and single crystal directional intensities I_xx, I_xy, I_xz, I_yy, I_yz, I_zz (arbitrary units), and tentative interpretation of the bands in the IR and Raman spectra of **1a·2d**.

IR				Raman										
Mode	v	I	Interpretation	Mode	v	I_tot	I_par	I_perp	I_xx	I_xy	I_xz	I_yy	I_yz	I_zz	Interpretation
B_u	0.0	0.0		B_g	15.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{rock}(ring); δ_{rock}(SeO_4)
A_u	0.0	0.0	acoustic modes	A_g	23.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{rock}(ring); δ_{wagg}(ring); δ_{rock}(SeO_4); δ_{rock}(water)
B_u	0.0	0.0		A_g	31.6	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.1	
B_u	12.3	14.3		B_g	34.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{rock}(ring); δ_{rock}(SeO_4)
A_u	14.2	0.1	δ_{rock}(ring); δ_{wagg}(ring); δ_{rock}(SeO_4)	A_g	36.7	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
A_u	22.3	0.2		B_g	37.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{rock}(ring); δ_{wagg}(ring); δ_{rock}(SeO_4); δ_{rock}(water); ν_β(NH)
B_u	25.0	0.0		B_g	42.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{wagg}(ring); δ_{rock}(SeO_4); δ_{rock}(water)
A_u	30.5	0.0		A_g	44.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{rock}(ring); δ_{rock}(SeO_4); ν_β(OH)
A_u	37.0	0.7	δ_{rock}(ring); δ_{rock}(SeO_4)	A_g	47.0	0.1	0.1	0.0	0.0	0.0	0.0	0.1	0.0	0.1	δ_{rock}(ring); δ_{rock}(SeO_4); δ_{rock}(water); ν_β(OH); ν_β(NH)
B_u	38.0	11.5		B_g	47.0	0.1	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	ν_β(NH); δ_{rock}(SeO_4); δ_{rock}(ring); δ_{wagg}(ring)
B_u	43.6	3.0		A_g	49.0	0.2	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.2	δ_{rock}(ring); δ_{wagg}(ring); δ_{rock}(SeO_4)
A_u	48.9	2.9		B_g	53.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{rock}(ring); δ_{rock}(SeO_4)
A_u	53.0	0.3	δ_{rock}(ring); δ_{wagg}(ring); δ_{rock}(SeO_4)	A_g	55.1	0.1	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	
B_u	54.7	6.4		B_g	63.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{rock}(ring); δ_{wagg}(ring); δ_{rock}(SeO_4)
B_u	58.5	7.0	δ_{rock}(ring); δ_{wagg}(ring); δ_{rock}(SeO_4); ν_β(NH)	A_g	64.8	0.2	0.1	0.1	0.1	0.0	0.0	0.1	0.0	0.1	δ_{rock}(ring); δ_{rock}(SeO_4)
A_u	60.4	1.4	δ_{rock}(ring); δ_{rock}(SeO_4)	B_g	66.4	0.2	0.1	0.1	0.0	0.0	0.0	0.0	0.2	0.0	δ_{rock}(ring); δ_{rock}(SeO_4); ν_β(NH)
B_u	62.0	3.0		A_g	69.3	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{rock}(ring); δ_{rock}(SeO_4); ν_β(OH); ν_β(NH)
A_u	66.4	22.4	δ_{rock}(ring); δ_{wagg}(ring);	A_g	69.5	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{rock}(ring); δ_{wagg}(ring);
B_u	66.9	1.3	δ_{rock}(SeO_4); ν_β(NH)	B_g	70.3	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{rock}(SeO_4)
A_u	67.8	0.5	δ_{rock}(ring); δ_{wagg}(ring); δ_{rock}(SeO_4)	B_g	73.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{rock}(ring); δ_{rock}(SeO_4); δ_{rock}(water); ν_β(OH);
B_u	72.5	11.9	δ_{wagg}(ring); δ_{rock}(SeO_4)	A_g	74.3	0.2	0.1	0.1	0.0	0.0	0.0	0.1	0.0	0.1	ν_β(NH)
A_u	73.1	2.6		B_g	76.6	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{rock}(ring); δ_{wagg}(ring);
A_u	74.3	0.0	δ_{rock}(ring); δ_{wagg}(ring); δ_{rock}(SeO_4)	A_g	77.9	0.3	0.2	0.1	0.2	0.0	0.1	0.0	0.0	0.0	δ_{rock}(SeO_4); δ_{rock}(water); ν_β(OH); ν_β(NH)
B_u	76.2	47.9		B_g	79.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{wagg}(ring); δ_{rock}(ring); δ_{rock}(SeO_4)
B_u	84.3	13.1	δ_{wagg}(ring); δ_{rock}(SeO_4); ν_β(OH)	B_g	81.7	0.4	0.3	0.2	0.0	0.3	0.0	0.0	0.0	0.0	δ_{wagg}(ring); δ_{rock}(ring); δ_{rock}(SeO_4); ν_β(OH)
A_u	85.3	2.4	δ_{wagg}(ring); δ_{rock}(SeO_4); ν_β(NH)	A_g	83.1	0.1	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	δ_{wagg}(ring); δ_{rock}(ring);
A_u	90.7	1.6	δ_{wagg}(ring); δ_{rock}(SeO_4); ν_β(NH); ν_β(OH)	A_g	88.5	0.2	0.1	0.1	0.1	0.0	0.0	0.1	0.0	0.1	δ_{rock}(SeO_4); ν_β(OH); ν_β(NH)
B_u	92.2	3.3		B_g	91.3	0.2	0.1	0.1	0.0	0.1	0.0	0.0	0.1	0.0	δ_{rock}(ring); δ_{rock}(SeO_4); ν_β(OH); ν_β(NH)
B_u	96.4	4.7	δ_{rock}(ring); δ_{rock}(SeO_4); ν_σ(NH);	B_g	95.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{wagg}(ring); δ_{rock}(SeO_4);

			ν_β(OH)												ν_β(NH)
A_u	97.6	2.3	δ_{wagg}(ring); $\delta_{rock}(SeO_4)$; ν_β(NH)	B_g	96.8	0.4	0.3	0.2	0.0	0.1	0.0	0.0	0.3	0.0	δ_{rock}(ring); δ_{wagg}(ring); $\delta_{rock}(SeO_4)$; ν_σ(NH); ν_β(NH)
A_u	98.7	70.0	δ_{rock}(ring); δ_{wagg}(ring); $\delta_{rock}(SeO_4)$; ν_β(OH)	A_g	100.0	0.2	0.2	0.1	0.0	0.0	0.1	0.0	0.0	0.2	δ_{wagg}(ring); $\delta_{rock}(SeO_4)$; ν_σ(NH)
B_u	100.6	7.7	δ_{rock}(ring); δ_{wagg}(ring); $\delta_{rock}(SeO_4)$	A_g	103.6	0.1	0.1	0.1	0.1	0.0	0.0	0.0	0.0	0.0	δ_{rock}(ring); δ_{wagg}(ring); $\delta_{rock}(SeO_4)$; ν_σ(NH)
B_u	103.5	19.4	δ_{wagg}(ring); $\delta_{rock}(SeO_4)$; ν_σ(NH)	B_g	104.1	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	ν_σ(NH); δ_{wagg}(ring); $\delta_{rock}(SeO_4)$
A_u	106.1	2.8	δ_{rock}(ring); δ_{wagg}(ring); $\delta_{rock}(SeO_4)$; δ_{rock}(water)	A_g	107.3	0.4	0.3	0.2	0.0	0.0	0.0	0.0	0.0	0.6	δ_{wagg}(ring); δ_{rock}(ring); $\delta_{rock}(SeO_4)$; δ_{rock}(water); ν_σ(NH)
B_u	106.6	31.3		B_g	108.6	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.1	0.0	δ_{rock}(ring); δ_{wagg}(ring); $\delta_{rock}(SeO_4)$; δ_{rock}(water); ν_β(NH)
A_u	107.5	0.8	δ_{rock}(ring); δ_{wagg}(ring); $\delta_{rock}(SeO_4)$	A_g	112.5	0.1	0.1	0.1	0.1	0.0	0.1	0.0	0.0	0.0	$\delta_{rock}(SeO_4)$; δ_{rock}(water); δ_{wagg}(ring); ν_β(NH); ν_β(OH)
B_u	110.2	23.5		A_g	114.0	0.1	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.2	δ_{wagg}(ring); $\delta_{rock}(SeO_4)$; ν_β(NH)
A_u	115.2	2.3		B_g	114.9	0.2	0.1	0.1	0.0	0.1	0.0	0.0	0.1	0.0	δ_{wagg}(ring); δ_{rock}(water);
B_u	116.1	112.9		A_g	122.8	0.3	0.2	0.1	0.0	0.0	0.1	0.2	0.0	0.0	$\delta_{rock}(SeO_4)$; ν_σ(NH); ν_β(OH)
A_u	124.9	119.4	δ_{wagg}(ring); $\delta_{rock}(SeO_4)$; ν_σ(NH)	B_g	124.5	0.2	0.1	0.1	0.0	0.1	0.0	0.0	0.1	0.0	δ_{wagg}(ring); δ_{twist}(ring); $\delta_{rock}(SeO_4)$; ν_σ(OH)
B_u	129.1	0.7		B_g	129.7	0.3	0.2	0.2	0.0	0.0	0.0	0.0	0.3	0.0	δ_{rock}(water); $\delta_{rock}(SeO_4)$; ν_β(OH)
A_u	132.0	13.5		A_g	129.9	0.3	0.2	0.1	0.1	0.0	0.1	0.1	0.0	0.0	δ_{wagg}(ring); $\delta_{rock}(SeO_4)$; ν_σ(NH)
A_u	134.4	35.3		B_g	139.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{twist}(ring); δ_{wagg}(ring); $\delta_{rock}(SeO_4)$; ν_σ(NH)
B_u	140.4	68.0	δ_{wagg}(ring); $\delta_{rock}(SeO_4)$; ν_σ(OH)	A_g	145.7	0.1	0.1	0.0	0.1	0.0	0.0	0.0	0.0	0.0	δ_{wagg}(ring); $\delta_{rock}(SeO_4)$; ν_σ(OH); ν_σ(NH)
A_u	145.4	7.9	δ_{twist}(ring); δ_{wagg}(ring); $\delta_{rock}(SeO_4)$; ν_σ(NH); δ_{rock}(water)	B_g	148.1	0.2	0.1	0.1	0.0	0.0	0.0	0.0	0.1	0.0	
B_u	151.0	6.4	$\delta_{rock}(SeO_4)$; δ_{wagg}(ring); ν_σ(NH)	A_g	149.3	0.2	0.2	0.1	0.0	0.0	0.0	0.2	0.0	0.0	δ_{wagg}(ring); $\delta_{rock}(SeO_4)$
A_u	153.8	0.4	$\delta_{rock}(SeO_4)$; δ_{wagg}(ring); ν_σ(OH); ν_σ(NH)	A_g	156.2	0.1	0.0	0.0	0.1	0.0	0.0	0.1	0.0	0.0	δ_{twist}(ring); $\delta_{rock}(SeO_4)$; δ_{rock}(water); $\delta_{rock}(CH_2)$; $\delta_{rock}(CH_3)$
B_u	154.7	22.1	δ_{twist}(ring); $\delta_{rock}(SeO_4)$; ν_σ(NH)	B_g	157.7	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{twist}(ring); $\delta_{rock}(SeO_4)$; δ_{rock}(water); $\delta_{rock}(CH_2)$; $\delta_{rock}(CH_3)$; ν_σ(NH)
A_u	157.2	0.6	δ_{twist}(ring)	B_g	161.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{twist}(ring); $\delta_{rock}(SeO_4)$;
B_u	160.8	59.5	δ_{twist}(ring); $\delta_{rock}(SeO_3)$; ν_σ(OH)	A_g	163.2	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.1	$\delta_{rock}(CH_2)$; $\delta_{rock}(CH_3)$; ν_σ(NH)
B_u	169.1	1.5	δ_{twist}(ring)	A_g	177.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{twist}(ring); $\delta_{rock}(CH_2)$;
A_u	169.1	25.2		B_g	178.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	$\delta_{rock}(CH_3)$; ν_σ(NH)
A_u	187.6	27.9	$\delta_{rock}(SeO_4)$; ν_σ(OH)	B_g	187.7	0.6	0.3	0.2	0.0	0.0	0.0	0.0	0.5	0.0	$\delta_{rock}(SeO_4)$; ν_σ(OH)
B_u	187.8	79.2		A_g	188.0	1.0	0.8	0.3	0.0	0.0	0.2	0.0	0.0	1.1	
A_u	210.6	0.1	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$; ν_σ(NH); ν_σ(OH)	B_g	211.0	0.2	0.1	0.1	0.0	0.1	0.0	0.0	0.1	0.0	$\delta_{twist}(CH_3)$; ν_σ(NH); ν_σ(OH)
B_u	211.1	14.9	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$	A_g	211.1	0.4	0.3	0.2	0.2	0.0	0.1	0.3	0.0	0.1	$\delta_{twist}(CH_3)$
B_u	220.2	15.7	ν_σ(OH); $\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$	A_g	213.7	1.1	0.7	0.4	0.9	0.0	0.4	0.0	0.0	0.0	ν_σ(OH)
A_u	221.7	22.4		B_g	214.5	0.8	0.5	0.3	0.0	0.1	0.0	0.0	0.6	0.0	ν_σ(OH); $\delta_{twist}(CH_3)$
B_u	226.2	117.7	ν_σ(OH); $\delta_{twist}(CH_3)$	A_g	221.7	0.2	0.1	0.1	0.1	0.0	0.0	0.0	0.0	0.2	$\delta_{twist}(CH_3)$
A_u	226.8	53.3		B_g	222.0	0.4	0.2	0.2	0.0	0.3	0.0	0.0	0.0	0.0	

B_u	231.4	4.4	$\delta_{twist}(CH_3)$	B_g	230.9	0.6	0.3	0.3	0.0	0.5	0.0	0.0	0.0	0.0	
A_u	234.5	0.1		A_g	234.1	0.4	0.2	0.1	0.0	0.0	0.2	0.0	0.0	0.2	
A_u	243.2	23.8	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$	A_g	243.6	0.3	0.2	0.1	0.0	0.0	0.0	0.0	0.0	0.4	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$
B_u	243.4	18.0		B_g	246.6	1.1	0.6	0.5	0.0	0.0	0.0	0.0	0.0	0.9	0.0
B_u	272.8	5.6	$\delta_{twist}(CH_3)$	B_g	272.8	0.2	0.1	0.1	0.0	0.1	0.0	0.0	0.1	0.0	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$
A_u	273.0	19.1		A_g	273.5	0.7	0.4	0.3	0.1	0.0	0.5	0.1	0.0	0.1	
A_u	275.6	3.5	$\delta_{scissor}(OSeO)$; $\delta_{twist}(OSeO)$; $\delta_{twist}(CH_3)$	A_g	280.7	1.2	0.7	0.5	0.0	0.0	0.6	0.5	0.0	0.3	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$
B_u	276.0	15.2	$\delta_{scissor}(OSeO)$; $\delta_{twist}(OSeO)$	B_g	281.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
B_u	279.3	1.2	$\delta_{rock}(CH_3)$; $\delta_{twist}(CH_3)$	A_g	286.7	2.6	1.5	1.1	2.6	0.0	0.0	0.1	0.0	1.5	
A_u	280.1	20.8		B_g	288.6	1.4	0.8	0.6	0.0	0.9	0.0	0.0	0.3	0.0	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$; $\delta_{twist}(OSeO)$; $\delta_{scissor}(OSeO)$; $\delta_{rock}(CH_2)$
A_u	287.6	7.5	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$; $\delta_{twist}(OSeO)$; $\delta_{scissor}(OSeO)$	B_g	290.0	1.0	0.6	0.4	0.0	0.3	0.0	0.0	0.5	0.0	
B_u	289.3	1.6	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$	A_g	290.1	0.6	0.5	0.1	0.5	0.0	0.1	0.1	0.0	0.0	
B_u	289.9	3.2		A_g	291.6	1.3	0.7	0.6	0.5	0.0	0.4	0.0	0.0	0.8	$\delta_{twist}(CH_3)$; $\delta_{scissor}(OSeO)$
A_u	290.8	3.1	$\delta_{twist}(CH_3)$	B_g	292.7	4.3	2.5	1.8	0.0	3.5	0.0	0.0	0.1	0.0	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{rock}(CH_3)$; $\delta_{twist}(OSeO)$
B_u	292.5	9.0	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_2)$	B_g	293.9	0.8	0.5	0.4	0.0	0.3	0.0	0.0	0.4	0.0	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{rock}(CH_3)$
A_u	293.6	0.9	$\delta_{twist}(CH_3)$	A_g	294.7	0.5	0.3	0.2	0.1	0.0	0.0	0.5	0.0	0.3	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{scissor}(OSeO)$
A_u	298.0	2.5	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$;	A_g	299.0	2.8	1.6	1.2	0.1	0.0	0.4	1.8	0.0	1.9	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$;
B_u	300.2	6.5	$\delta_{scissor}(OSeO)$; $\delta_{twist}(OSeO)$	B_g	299.1	0.8	0.5	0.4	0.0	0.7	0.0	0.0	0.0	0.0	$\delta_{rock}(CH_2)$; $\delta_{twist}(OSeO)$; $\delta_{scissor}(OSeO)$
B_u	301.9	30.1	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$; $\delta_{scissor}(OSeO)$; $\delta_{twist}(OSeO)$	A_g	302.7	7.8	4.5	3.3	2.5	0.0	1.7	0.6	0.0	6.3	$\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{twist}(OSeO)$
A_u	304.0	0.2	$\delta_{rock}(CH_2)$; $\delta_{rock}(CH_3)$; $\delta_{scissor}(OSeO)$; $\delta_{twist}(OSeO)$	B_g	306.5	1.0	0.6	0.4	0.0	0.5	0.0	0.0	0.3	0.0	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{twist}(OSeO)$
A_u	310.3	30.7	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{rock}(CH_3)$	A_g	310.2	0.3	0.3	0.1	0.0	0.0	0.1	0.1	0.0	0.2	
B_u	310.4	0.3		B_g	311.9	0.6	0.3	0.2	0.0	0.1	0.0	0.0	0.4	0.0	$\delta_{rock}(CH_2)$; $\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$
A_u	313.0	1.8	$\delta_{rock}(CH_2)$; $\delta_{rock}(CH_3)$	A_g	315.4	0.6	0.4	0.2	0.8	0.0	0.0	0.0	0.0	0.2	
B_u	316.6	13.7	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{scissor}(OSeO)$; $\delta_{twist}(OSeO)$	A_g	317.5	2.2	1.3	0.9	1.1	0.0	0.1	2.1	0.0	0.1	$\delta_{twist}(CH_3)$; $\delta_{twist}(OSeO)$
A_u	318.8	1.6	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{scissor}(OSeO)$	B_g	317.7	0.6	0.4	0.3	0.0	0.2	0.0	0.0	0.3	0.0	
B_u	320.8	22.6	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{scissor}(OSeO)$	B_g	319.4	0.3	0.2	0.1	0.0	0.2	0.0	0.0	0.1	0.0	$\delta_{rock}(CH_2)$
A_u	322.0	7.1	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$;	B_g	322.0	1.8	1.1	0.8	0.0	1.5	0.0	0.0	0.0	0.0	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$;
B_u	323.4	71.4	$\delta_{scissor}(OSeO)$; $\delta_{twist}(OSeO)$	A_g	322.1	3.8	2.2	1.6	1.7	0.0	1.3	1.9	0.0	0.0	$\delta_{rock}(CH_2)$; $\delta_{scissor}(OSeO)$
A_u	325.2	28.9	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$	A_g	323.7	1.6	0.9	0.7	1.4	0.0	0.0	1.1	0.0	0.1	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{rock}(CH_3)$; $\delta_{twist}(OSeO)$; $\delta_{scissor}(OSeO)$
B_u	327.2	4.9		B_g	325.1	1.2	0.7	0.5	0.0	0.0	0.0	0.0	0.9	0.0	
B_u	328.3	11.7	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{scissor}(OSeO)$	A_g	325.6	4.8	2.8	2.0	3.6	0.0	0.9	2.5	0.0	0.0	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{rock}(CH_3)$; $\delta_{scissor}(OSeO)$
A_u	329.2	0.1	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$	B_g	327.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
B_u	331.4	92.4	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{scissor}(OSeO)$	B_g	328.2	0.2	0.1	0.1	0.0	0.2	0.0	0.0	0.0	0.0	$\delta_{twist}(CH_3)$; $\delta_{twist}(OSeO)$; $\delta_{scissor}(OSeO)$
A_u	331.7	172.8	$\delta_{twist}(CH_3)$; $\delta_{scissor}(OSeO)$	A_g	328.6	1.1	0.6	0.5	0.8	0.0	0.1	0.7	0.0	0.1	
A_u	340.1	53.7		A_g	331.7	0.3	0.2	0.1	0.0	0.0	0.0	0.3	0.0	0.0	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_2)$
B_u	340.6	4.4	$\delta_{twist}(CH_3)$	B_g	332.7	1.1	0.6	0.5	0.0	0.1	0.0	0.0	0.8	0.0	$\delta_{twist}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{twist}(OSeO)$
A_u	343.4	19.5		A_g	340.5	2.8	1.9	0.8	2.4	0.0	0.8	0.1	0.0	0.0	
B_u	344.0	78.6		B_g	340.7	1.8	1.0	0.8	0.0	0.5	0.0	0.0	1.0	0.0	$\delta_{twist}(CH_3)$
B_u	345.8	27.7		A_g	350.6	0.7	0.4	0.3	0.6	0.0	0.0	0.5	0.0	0.1	

A_u	346.4	50.0		B_g	350.7	0.5	0.3	0.2	0.0	0.3	0.0	0.0	0.1	0.0	
B_u	358.9	81.5		B_g	356.2	0.6	0.4	0.3	0.0	0.0	0.0	0.0	0.5	0.0	$\delta_{scissor}$(OSeO);
A_u	359.1	446.6		A_g	356.4	3.8	2.4	1.4	1.3	0.0	0.0	1.9	0.0	2.7	δ_{wagg}(OSeO); δ_{twist}(CH_3)
B_u	367.5	597.8	$\delta_{scissor}$(OSeO); $\delta_{umbrella}$(SeO_3); δ_{wagg}(OSeO); δ_{twist}(CH_3)	B_g	370.5	1.4	0.8	0.6	0.0	0.0	0.0	0.0	1.1	0.0	$\delta_{umbrella}$(SeO_3); δ_{wagg}(OSeO); $\delta_{scissor}$(OSeO); δ_{twist}(CH_3); δ(ring) [6-ring]
A_u	368.7	61.9		A_g	372.0	3.1	1.9	1.1	4.2	0.0	0.0	0.6	0.0	0.0	$\delta_{umbrella}$(SeO_3); δ_{wagg}(OSeO); $\delta_{scissor}$(OSeO)
A_u	372.1	400.4		B_g	373.5	2.5	1.5	1.1	0.0	1.5	0.0	0.0	0.6	0.0	δ_{twist}(CH_3); δ(ring) [6-ring]
B_u	372.7	169.1	$\delta_{umbrella}$(SeO_3); δ_{twist}(CH_3); δ(ring) [6-ring]	A_g	375.2	8.6	7.0	1.7	6.2	0.0	2.0	0.1	0.0	1.6	
B_u	375.6	367.5		B_g	377.4	6.7	3.8	2.9	0.0	0.7	0.0	0.0	4.9	0.0	
A_u	377.7	15.3		A_g	377.4	11.1	6.4	4.8	3.6	0.0	5.7	0.0	0.0	3.3	
A_u	387.9	0.0	$\delta_{umbrella}$(SeO_3); δ_{twist}(CH_3); δ(ring) [6-ring]; δ_{rock}(CH_2)	A_g	386.7	1.9	1.1	0.7	0.0	0.0	0.1	2.3	0.0	0.5	δ_{wagg}(OSeO); $\delta_{scissor}$(OSeO); $\delta_{umbrella}$(SeO_3)
B_u	388.7	227.8	$\delta_{umbrella}$(SeO_3); $\delta_{scissor}$(OSeO); δ_{twist}(CH_3); δ(ring) [6-ring]; δ_{rock}(CH_2)	B_g	387.8	4.2	2.4	1.8	0.0	3.5	0.0	0.0	0.0	0.0	
B_u	389.7	14.0	δ(ring) [6-ring]; δ_{twist}(CH_3);	A_g	395.5	6.6	4.7	1.9	4.0	0.0	2.5	0.0	0.0	0.7	δ(ring) [6-ring]; δ_{twist}(CH_3);
A_u	392.8	3.5	δ_{rock}(CH_2)	B_g	395.6	0.2	0.1	0.1	0.0	0.0	0.0	0.0	0.1	0.0	δ_{rock}(CH_2)
A_u	402.7	0.1		B_g	397.5	1.1	0.6	0.5	0.0	0.3	0.0	0.0	0.6	0.0	δ_{wagg}(OSeO); $\delta_{scissor}$(OSeO); δ(ring) [6-ring]; δ_{rock}(CH_2); δ_{rock}(CH_3)
B_u	402.9	76.1	δ_{rock}(CH_3); δ_{rock}(CH_2); $\delta_{scissor}$(OSeO); $\delta_{umbrella}$(SeO_3)	A_g	402.3	2.1	1.2	0.9	0.5	0.0	0.2	0.9	0.0	1.6	δ_{wagg}(OSeO); $\delta_{umbrella}$(SeO_3); δ(ring) [6-ring]; δ_{rock}(CH_2); δ_{rock}(CH_3)
B_u	404.9	113.0		B_g	405.3	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{rock}(CH_2); δ_{rock}(CH_3); δ(ring) [6-ring]
A_u	406.8	4.5	δ_{rock}(CH_3); δ_{rock}(CH_2)	A_g	405.4	3.7	2.1	1.6	0.6	0.0	0.3	1.4	0.0	3.5	$\delta_{umbrella}$(SeO_3); δ_{rock}(CH_2); δ_{rock}(CH_3); δ(ring) [6-ring]
B_u	407.7	58.0		B_g	409.6	0.9	0.5	0.4	0.0	0.8	0.0	0.0	0.0	0.0	δ_{rock}(CH_2); δ_{rock}(CH_3);
A_u	408.8	16.8	δ_{wagg}(OSeO); $\delta_{scissor}$(OSeO); v_o(OH); δ_{rock}(CH_3)	A_g	410.4	2.2	1.3	0.9	0.3	0.0	1.4	0.0	0.0	0.5	δ(ring) [6-ring]
A_u	413.3	1.9		A_g	411.6	0.6	0.3	0.2	0.1	0.0	0.1	0.5	0.0	0.1	
B_u	414.1	36.3	δ_{rock}(CH_2); δ_{rock}(CH_3)	B_g	415.0	1.2	0.7	0.5	0.0	0.2	0.0	0.0	0.8	0.0	δ_{rock}(CH_2); δ_{rock}(CH_3)
B_u	418.9	41.1		B_g	417.1	0.2	0.1	0.1	0.0	0.0	0.0	0.0	0.1	0.0	
A_u	419.4	1.3		A_g	418.5	3.3	1.9	1.4	1.6	0.0	0.2	3.0	0.0	0.4	
B_u	433.2	260.8		B_g	427.5	0.9	0.5	0.4	0.0	0.6	0.0	0.0	0.1	0.0	
A_u	436.2	1.3	v_o(OH)	A_g	428.3	10.9	6.2	4.6	0.0	0.0	6.1	3.3	0.0	2.3	v_o(OH); $\delta_{umbrella}$(SeO_3)
B_u	456.5	29.6		A_g	450.5	12.1	7.5	4.6	0.6	0.0	3.2	9.3	0.0	3.0	v_o(OH)
A_u	457.1	39.6		B_g	450.5	12.7	7.2	5.4	0.0	0.1	0.0	0.0	10.3	0.0	
A_u	471.5	7.8		A_g	474.3	0.9	0.5	0.4	1.0	0.0	0.0	0.2	0.0	0.2	
B_u	472.2	12.8	δ_{rock}(CH_3); δ_{rock}(CH_2)	B_g	474.5	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	
B_u	475.8	7.3		B_g	475.9	0.5	0.3	0.2	0.0	0.2	0.0	0.0	0.2	0.0	δ(ring) [6-ring]; δ_{twist}(CH_2);
A_u	476.1	1.0		A_g	476.6	0.4	0.3	0.2	0.1	0.0	0.1	0.1	0.0	0.2	δ_{rock}(CH_2); δ_{rock}(CH_3)
B_u	485.0	9.5	δ(ring) [6-ring]; δ_{rock}(CH_3); δ_{rock}(CH_2)	B_g	483.7	0.6	0.4	0.3	0.0	0.3	0.0	0.0	0.2	0.0	
A_u	485.3	44.9		A_g	484.4	1.1	0.6	0.5	0.3	0.0	0.1	1.2	0.0	0.1	
B_u	486.3	4.6		B_g	486.7	0.8	0.5	0.3	0.0	0.3	0.0	0.0	0.3	0.0	
A_u	486.7	1.0		A_g	487.2	1.1	0.7	0.5	1.4	0.0	0.0	0.4	0.0	0.0	
A_u	488.6	24.0		A_g	488.8	3.5	2.1	1.4	0.6	0.0	0.5	2.0	0.0	2.2	δ(ring) [6-ring]; δ_{twist}(CH_2);
B_u	488.9	28.5	δ(ring) [6-ring]; δ_{rock}(CH_3)	B_g	489.3	0.6	0.3	0.2	0.0	0.3	0.0	0.0	0.2	0.0	δ_{rock}(CH_3)
B_u	496.4	5.4		B_g	491.9	2.1	1.2	0.9	0.0	0.9	0.0	0.0	0.8	0.0	
A_u	496.6	0.5		A_g	492.5	1.5	0.9	0.6	1.2	0.0	0.2	0.6	0.0	0.2	
A_u	535.1	36.5	δ(ring) [6-ring]; δ_{ip}(NH);	B_g	536.6	0.8	0.5	0.4	0.0	0.3	0.0	0.0	0.4	0.0	δ(ring) [6-ring]; δ_{rock}(CH_2);

B_u	535.7	40.2	$\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$	A_g	536.8	1.7	1.0	0.7	0.6	0.0	0.6	0.2	0.0	0.6	$\delta_{rock}(CH_3)$; $\delta_{ip}(NH)$
B_u	540.0	35.9		B_g	539.8	0.2	0.1	0.1	0.0	0.1	0.0	0.0	0.1	0.0	
A_u	540.1	5.4		A_g	540.0	3.1	1.9	1.2	1.0	0.0	1.7	0.4	0.0	0.2	
B_u	578.7	5.3		B_g	577.4	0.2	0.1	0.1	0.0	0.1	0.0	0.0	0.1	0.0	
A_u	579.7	20.5	δ(ring) [6-ring]; $\delta_{rock}(CH_2)$;	A_g	579.2	33.3	32.4	0.9	19.4	0.0	0.8	6.0	0.0	12.5	
B_u	583.8	0.7	$\delta_{rock}(CH_3)$	A_g	581.6	2.9	2.8	0.1	2.4	0.0	0.0	0.6	0.0	0.5	δ(ring) [6-ring]; $\delta_{rock}(CH_2)$;
A_u	585.0	17.3		B_g	581.8	0.5	0.3	0.2	0.0	0.1	0.0	0.0	0.3	0.0	$\delta_{rock}(CH_3)$
A_u	692.3	21.6	δ_{oop}(OH) [γ(OH)]	B_g	680.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	δ_{oop}(OH) [γ(OH)]
B_u	692.5	49.5		A_g	680.6	1.6	1.1	0.5	1.3	0.0	0.0	0.7	0.0	0.5	
B_u	721.6	147.0	ν(SeO); δ(ring) [6-ring];	B_g	713.8	1.1	0.7	0.5	0.0	0.8	0.0	0.0	0.1	0.0	δ_{oop}(OH) [γ(OH)]; ν(SeO)
A_u	722.8	686.7	δ_{oop}(OH) [γ(OH)]	A_g	714.3	2.4	2.2	0.2	1.6	0.0	0.0	1.4	0.0	0.0	
B_u	726.4	68.9	δ(ring) [6-ring]	B_g	722.8	1.9	1.1	0.8	0.0	1.6	0.0	0.0	0.0	0.0	ν(SeO); δ_{oop}(OH) [γ(OH)];
B_u	728.4	77.7		A_g	723.4	5.4	5.1	0.3	3.9	0.0	0.1	2.0	0.0	0.4	δ(ring) [6-ring]; $\delta_{rock}(CH_2)$
A_u	728.6	5.4	δ(ring) [6-ring]; ν(SeO)	B_g	726.8	0.1	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	δ(ring) [6-ring]; $\delta_{rock}(CH_2)$; δ_{oop}(OH) [γ(OH)]
A_u	730.2	121.2		B_g	728.4	2.2	1.3	0.9	0.0	1.8	0.0	0.0	0.0	0.0	δ(ring) [6-ring]; $\delta_{rock}(CH_2)$; ν(SeO); δ_{oop}(OH) [γ(OH)]
B_u	752.8	591.2	ν(SeO)	A_g	729.4	57.2	56.5	0.7	15.6	0.0	0.5	32.8	0.0	17.4	δ(ring) [6-ring]; $\delta_{rock}(CH_2)$
A_u	753.4	87.9		A_g	730.3	11.6	11.3	0.3	3.2	0.0	0.0	8.3	0.0	2.2	δ(ring) [6-ring]; $\delta_{rock}(CH_2)$; ν(SeO)
B_u	768.2	5.7	δ(ring) [6-ring]	A_g	754.1	55.5	53.3	2.2	31.5	0.0	2.2	7.9	0.0	22.7	ν(SeO)
A_u	769.1	3.2		B_g	754.3	0.5	0.3	0.2	0.0	0.3	0.0	0.0	0.0	0.0	
B_u	776.6	449.8		B_g	768.5	0.2	0.1	0.1	0.0	0.2	0.0	0.0	0.0	0.0	δ(ring) [ν(CN)]; δ(ring)
A_u	779.7	557.9	δ_{oop}(OH) [γ(OH)]; δ(ring) [6-ring]	A_g	769.2	0.2	0.1	0.1	0.1	0.0	0.0	0.0	0.0	0.1	[ν(CC)]; δ(ring) [6-ring]; $\delta_{rock}(CH_3)$
A_u	783.2	170.5		A_g	779.3	1.4	1.1	0.4	1.7	0.0	0.1	0.2	0.0	0.1	δ_{ip}(OH); δ(ring) [ν(CN)];
B_u	783.5	131.3		B_g	781.0	0.4	0.2	0.2	0.0	0.3	0.0	0.0	0.0	0.0	$\delta_{twist}(CH_2)$; δ(ring) [6-ring]
A_u	802.7	232.2	δ_{ip}(OH)	B_g	788.1	0.1	0.1	0.0	0.0	0.1	0.0	0.0	0.0	0.0	δ_{ip}(OH); δ(ring) [6-ring]
B_u	803.3	14.4		A_g	788.3	2.9	2.6	0.3	1.7	0.0	0.4	0.7	0.0	0.4	
A_u	831.4	971.2	ν(SeO); $\delta_{rock}(CH_3)$;	A_g	831.5	208.9	200.2	8.7	29.6	0.0	4.0	153.8	0.0	59.3	ν(SeO); δ(ring) [ν(CN)];
B_u	831.7	93.7	δ(ring) [6-ring]	B_g	832.3	6.0	3.4	2.6	0.0	0.3	0.0	0.0	4.7	0.0	δ(ring) [6-ring]; δ_{ip}(NH); $\delta_{rock}(CH_3)$
A_u	841.3	66.6	ν(SeO); $\delta_{rock}(CH_3)$;	A_g	841.1	2.2	2.0	0.2	0.5	0.0	0.3	0.5	0.0	1.0	δ(ring) [6-ring]; δ(ring)
B_u	843.1	74.6	δ(ring) [6-ring]; δ_{ip}(NH)	B_g	842.4	0.7	0.4	0.3	0.0	0.0	0.0	0.0	0.6	0.0	[ν(CN)]; $\delta_{rock}(CH_3)$; δ_{ip}(NH)
B_u	848.0	19.6	ν(SeO); $\delta_{rock}(CH_3)$;	A_g	847.7	69.4	68.7	0.7	19.2	0.0	0.9	28.7	0.0	31.1	ν(SeO); $\delta_{rock}(CH_3)$; δ(ring)
A_u	848.0	358.0	δ(ring) [6-ring]	B_g	849.3	1.0	0.6	0.4	0.0	0.2	0.0	0.0	0.6	0.0	[6-ring]; δ_{ip}(NH)
B_u	858.7	467.5	ν(SeO); δ(ring) [6-ring]	A_g	857.9	6.5	6.3	0.3	0.8	0.0	0.1	4.6	0.0	2.2	ν(SeO)
A_u	859.0	408.6		B_g	858.1	7.4	4.2	3.2	0.0	5.0	0.0	0.0	1.1	0.0	
B_u	867.8	1393.1	$\delta_{rock}(CH_2)$; ν(SeO); δ_{ip}(OH)	B_g	866.0	1.2	0.7	0.5	0.0	0.3	0.0	0.0	0.7	0.0	$\delta_{rock}(CH_2)$; δ(ring) [ν(CN)]
A_u	868.5	9.4	$\delta_{rock}(CH_2)$; δ(ring) [ν(CN)]	A_g	866.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
B_u	868.8	215.0	$\delta_{rock}(CH_2)$; δ(ring) [ν(CN)]; ν(SeO)	A_g	874.8	39.7	33.4	6.4	30.1	0.0	4.9	0.0	0.0	13.3	ν(SeO); $\delta_{rock}(CH_2)$; δ_{oop}(OH) [γ(OH)]
A_u	869.8	687.7	ν(SeO); δ_{ip}(OH)	B_g	875.5	3.7	2.1	1.6	0.0	3.1	0.0	0.0	0.0	0.0	
B_u	876.6	18.7	$\delta_{rock}(CH_2)$	B_g	877.8	0.1	0.1	0.0	0.0	0.1	0.0	0.0	0.0	0.0	$\delta_{rock}(CH_2)$; δ(ring) [ν(CN)];
A_u	876.8	5.1		A_g	878.1	4.6	4.1	0.5	0.3	0.0	0.0	0.3	0.0	5.2	δ_{oop}(OH) [γ(OH)]
B_u	883.6	181.7	ν(SeO)	A_g	884.1	76.5	71.0	5.5	8.3	0.0	6.5	26.2	0.0	46.9	ν(SeO); δ_{ip}(NH)
A_u	884.1	947.3		B_g	885.6	22.9	13.1	9.8	0.0	0.3	0.0	0.0	18.6	0.0	
B_u	894.0	20.2		A_g	894.4	9.9	7.3	2.6	2.2	0.0	4.9	1.6	0.0	0.7	
A_u	894.0	1.0	δ(ring) [ν(CC)]; $\delta_{rock}(CH_3)$	B_g	894.7	0.8	0.4	0.3	0.0	0.0	0.0	0.0	0.6	0.0	δ(ring) [ν(CC)]; δ(ring) [6-
A_u	899.4	4.2		B_g	899.3	1.3	0.7	0.5	0.0	0.8	0.0	0.0	0.3	0.0	ring]; $\delta_{rock}(CH_2)$
B_u	899.7	2.3		A_g	899.6	9.9	8.1	1.8	3.2	0.0	3.4	2.3	0.0	1.3	
A_u	918.5	0.9	δ(ring) [ν(CN)]; δ(ring) [6-ring];	A_g	918.6	9.4	5.4	4.0	7.4	0.0	0.0	0.2	0.0	7.8	δ(ring) [ν(CN)]; δ(ring)
B_u	919.0	83.0	$\delta_{rock}(CH_3)$	B_g	919.4	1.9	1.1	0.8	0.0	1.6	0.0	0.0	0.0	0.0	[ν(CC)]; $\delta_{rock}(CH_3)$
A_u	922.8	49.1	δ_{ip}(NH); δ(ring) [6-ring]; $\delta_{rock}(CH_3)$; δ_{oop}(OH) [γ(OH)]	A_g	922.1	10.8	6.9	3.8	3.9	0.0	4.3	1.3	0.0	2.9	δ_{ip}(NH); δ(ring) [6-ring]; δ_{oop}(OH) [γ(OH)];

B_u	924.0	46.4		A_g	924.9	2.6	1.6	1.1	0.7	0.0	0.6	1.1	0.0	1.2	$\delta_{rock}(CH_3)$ δ(ring) [ν(CN)]; δ(ring) [6-ring]; $\delta_{rock}(CH_3)$
A_u	925.7	2.5	δ(ring) [ν(CN)]; δ(ring) [6-ring]; $\delta_{rock}(CH_3)$	B_g	925.4	14.8	8.5	6.4	0.0	2.3	0.0	0.0	9.9	0.0	$\delta_{ip}(NH)$; $\delta_{rock}(CH_3)$; δ(ring) [6-ring]; $\delta_{oop}(OH)$ [γ(OH)]
B_u	926.2	115.1		B_g	925.6	2.7	1.5	1.1	0.0	0.3	0.0	0.0	1.9	0.0	δ(ring) [ν(CN)]; δ(ring) [6-ring]; $\delta_{rock}(CH_3)$; $\delta_{ip}(NH)$
A_u	931.8	0.8	$\delta_{ip}(NH)$; δ(ring) [6-ring];	A_g	930.8	11.9	9.4	2.5	0.3	0.0	2.6	0.7	0.0	10.4	$\delta_{ip}(NH)$; δ(ring) [6-ring];
B_u	934.5	76.2	$\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$	B_g	933.2	8.5	4.9	3.7	0.0	2.3	0.0	0.0	4.7	0.0	$\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$
B_u	942.0	422.0	$\delta_{oop}(OH)$ [γ(OH)]; ν(SeO);	B_g	941.6	0.8	0.5	0.4	0.0	0.1	0.0	0.0	0.6	0.0	$\delta_{oop}(OH)$ [γ(OH)]; ν(SeO)
A_u	942.2	450.5	$\delta_{rock}(CH_3)$	A_g	942.1	7.6	5.6	2.1	6.6	0.0	2.1	0.0	0.0	0.3	$\delta_{oop}(OH)$ [γ(OH)]; ν(SeO);
B_u	944.8	1427.2		B_g	946.8	0.4	0.2	0.2	0.0	0.2	0.0	0.0	0.1	0.0	$\delta_{rock}(CH_3)$
A_u	947.5	25.0	δ(ring) [6-ring]; $\delta_{rock}(CH_3)$; $\delta_{oop}(OH)$ [γ(OH)]	A_g	947.3	7.8	6.2	1.5	4.8	0.0	1.9	0.0	0.0	2.1	$\delta_{rock}(CH_3)$; ν(SeO); ν(CC); δ(ring) [6-ring]
A_u	948.6	10.4	ν(SeO)	B_g	947.7	0.4	0.2	0.2	0.0	0.0	0.0	0.0	0.3	0.0	
B_u	948.9	357.7	$\delta_{oop}(OH)$ [γ(OH)]; $\delta_{rock}(CH_3)$;	A_g	948.3	55.2	40.9	14.3	0.1	0.0	4.1	0.0	0.0	71.8	ν(SeO); ν(CC); $\delta_{rock}(CH_3)$
B_u	949.5	522.0	δ(ring) [6-ring]; ν(SeO)	B_g	952.4	1.1	0.6	0.5	0.0	0.4	0.0	0.0	0.6	0.0	$\delta_{oop}(OH)$ [γ(OH)]; ν(SeO);
A_u	954.0	186.0	$\delta_{oop}(OH)$ [γ(OH)]; ν(SeO)	A_g	953.2	27.7	19.0	8.7	9.5	0.0	12.9	0.3	0.0	6.3	$\delta_{rock}(CH_3)$
B_u	958.8	15.2	δ(ring) [6-ring]; $\delta_{rock}(CH_3)$; $\delta_{oop}(OH)$ [γ(OH)]	B_g	956.8	0.2	0.1	0.1	0.0	0.0	0.0	0.0	0.1	0.0	$\delta_{oop}(OH)$ [γ(OH)]; $\delta_{rock}(CH_3)$; δ(ring) [6-ring]; $\delta_{oop}(NH)$ [γ(NH)]
A_u	961.2	12.5		A_g	959.8	8.1	4.6	3.5	4.4	0.0	1.9	0.1	0.0	5.2	$\delta_{rock}(CH_3)$; δ(ring) [6-ring]; $\delta_{oop}(NH)$ [γ(NH)]
B_u	965.2	9.1	$\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{ip}(NH)$	B_g	963.0	3.3	1.9	1.4	0.0	0.2	0.0	0.0	2.6	0.0	$\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{ip}(NH)$
A_u	965.5	0.1	$\delta_{rock}(CH_3)$; $\delta_{oop}(OH)$ [γ(OH)]	B_g	964.8	0.5	0.3	0.2	0.0	0.0	0.0	0.0	0.4	0.0	$\delta_{rock}(CH_3)$; $\delta_{ip}(NH)$
B_u	965.5	47.5		A_g	966.2	1.7	1.0	0.6	0.3	0.0	0.5	1.3	0.0	0.1	$\delta_{rock}(CH_3)$
A_u	966.9	7.1	$\delta_{rock}(CH_3)$; $\delta_{twist}(CH_2)$; $\delta_{ip}(NH)$	A_g	967.9	4.2	2.4	1.8	1.8	0.0	0.5	3.9	0.0	0.2	$\delta_{rock}(CH_3)$; $\delta_{oop}(NH)$ [γ(NH)]
B_u	969.2	34.1	$\delta_{rock}(CH_3)$;	A_g	969.4	0.3	0.2	0.1	0.3	0.0	0.0	0.1	0.0	0.1	$\delta_{rock}(CH_3)$; $\delta_{twist}(CH_2)$
A_u	970.0	0.9	$\delta_{rock}(CH_3)$; $\delta_{twist}(CH_2)$	B_g	970.1	1.1	0.6	0.5	0.0	0.2	0.0	0.0	0.7	0.0	
B_u	977.5	73.6		A_g	977.8	4.7	2.7	2.0	2.7	0.0	0.1	4.7	0.0	0.2	
A_u	978.5	13.3	$\delta_{rock}(CH_3)$; $\delta_{wagg}(CH_2)$	B_g	978.5	0.9	0.5	0.4	0.0	0.7	0.0	0.0	0.0	0.0	$\delta_{rock}(CH_3)$; $\delta_{wagg}(CH_2)$
B_u	989.4	0.7		B_g	988.9	1.9	1.1	0.8	0.0	0.7	0.0	0.0	0.9	0.0	
A_u	990.2	30.1	$\delta_{rock}(CH_3)$; $\delta_{twist}(CH_2)$; $\delta_{ip}(NH)$	A_g	990.4	0.5	0.4	0.0	0.5	0.0	0.0	0.0	0.0	0.1	
A_u	992.0	0.7	$\delta_{rock}(CH_3)$; $\delta_{twist}(CH_2)$; $\delta_{rock}(CH_2)$; $\delta_{ip}(NH)$	A_g	992.3	14.2	9.9	4.3	10.1	0.0	0.0	4.1	0.0	7.0	$\delta_{rock}(CH_3)$; $\delta_{wagg}(CH_2)$; $\delta_{ip}(NH)$
B_u	993.7	6.4	$\delta_{rock}(CH_3)$; $\delta_{wagg}(CH_2)$	B_g	992.9	0.9	0.5	0.4	0.0	0.0	0.0	0.0	0.7	0.0	$\delta_{rock}(CH_3)$; $\delta_{wagg}(CH_2)$
A_u	995.9	22.7		A_g	995.7	9.0	6.7	2.3	0.0	0.0	0.3	12.3	0.0	0.0	$\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$;
A_u	999.6	0.0		A_g	1000.9	4.5	3.6	0.8	0.0	0.0	0.0	5.2	0.0	0.8	$\delta_{ip}(NH)$
B_u	1002.9	38.0	$\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{ip}(NH)$	B_g	1003.1	0.3	0.2	0.1	0.0	0.2	0.0	0.0	0.0	0.0	$\delta_{rock}(CH_3)$; $\delta_{twist}(CH_2)$; $\delta_{ip}(NH)$
B_u	1005.1	32.9		B_g	1007.3	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	$\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{ip}(NH)$
A_u	1031.8	7.3		A_g	1033.2	0.2	0.1	0.1	0.1	0.0	0.1	0.0	0.0	0.0	$\delta_{rock}(CH_3)$; $\delta_{twist}(CH_2)$
B_u	1033.4	17.2	$\delta_{rock}(CH_3)$; $\delta_{twist}(CH_2)$	B_g	1033.9	0.1	0.1	0.0	0.0	0.1	0.0	0.0	0.0	0.0	
A_u	1035.1	1.7		A_g	1036.0	0.5	0.3	0.2	0.0	0.0	0.4	0.0	0.0	0.0	$\delta_{rock}(CH_3)$; $\delta_{twist}(CH_2)$;
B_u	1035.9	13.6	$\delta_{rock}(CH_3)$; $\delta_{twist}(CH_2)$; $\delta_{oop}(OH)$ [γ(OH)]	B_g	1038.3	3.6	2.1	1.5	0.0	1.5	0.0	0.0	1.4	0.0	$\delta_{oop}(OH)$ [γ(OH)]
B_u	1052.2	6.4	δ(ring) [6-ring]; $\delta_{ip}(NH)$;	A_g	1051.1	3.5	2.7	0.8	0.0	0.0	0.1	4.7	0.0	0.0	$\delta_{ip}(NH)$; $\delta_{rock}(CH_3)$;
A_u	1052.3	0.0	$\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$	B_g	1053.0	0.1	0.1	0.1	0.0	0.0	0.0	0.0	0.1	0.0	$\delta_{rock}(CH_2)$; δ(ring) [6-ring]
B_u	1058.3	621.4	$\delta_{oop}(OH)$ [γ(OH)]; $\delta_{ip}(NH)$; $\delta_{rock}(CH_3)$	A_g	1059.0	1.5	0.9	0.5	0.4	0.0	0.7	0.4	0.0	0.1	$\delta_{oop}(OH)$ [γ(OH)]; $\delta_{ip}(NH)$; $\delta_{rock}(CH_3)$
A_u	1062.4	203.4	δ(ring) [6-ring]; $\delta_{ip}(NH)$;	B_g	1062.4	0.4	0.2	0.2	0.0	0.2	0.0	0.0	0.1	0.0	
A_u	1065.9	184.0	$\delta_{rock}(CH_3)$; $\delta_{oop}(OH)$ [γ(OH)]	B_g	1067.7	0.2	0.1	0.1	0.0	0.1	0.0	0.0	0.1	0.0	$\delta_{oop}(OH)$ [γ(OH)]; $\delta_{ip}(NH)$;

B_u	1067.9	103.8		A_g	1067.8	4.5	3.7	0.8	1.5	0.0	0.6	3.4	0.0	0.0	δ(ring) [6-ring]; $\delta_{rock}(CH_3)$
B_u	1078.3	10.5	δ(ring) [ν(CC)]; $\delta_{rock}(CH_3)$	B_g	1078.6	1.3	0.8	0.6	0.0	0.1	0.0	0.0	1.0	0.0	
A_u	1078.8	0.1		A_g	1078.9	7.9	4.6	3.4	6.6	0.0	0.4	0.4	0.0	5.2	δ(ring) [ν(CC)]; $\delta_{wagg}(CH_2)$
A_u	1081.3	0.1	δ(ring) [ν(CC)]	B_g	1081.4	1.1	0.6	0.5	0.0	0.3	0.0	0.0	0.6	0.0	
B_u	1081.4	5.1		A_g	1081.4	3.1	1.8	1.3	1.6	0.0	1.3	0.1	0.0	0.8	
B_u	1084.4	9.5	$\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{oop}(OH)$ [γ(OH)]	B_g	1084.6	0.1	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	$\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{oop}(OH)$ [γ(OH)]
B_u	1087.3	14.3		B_g	1087.9	4.7	2.7	2.0	0.0	1.6	0.0	0.0	2.3	0.0	
A_u	1088.6	39.2	$\delta_{rock}(CH_3)$	A_g	1090.3	5.4	3.1	2.3	0.0	0.0	1.5	3.4	0.0	2.6	$\delta_{rock}(CH_3)$; $\delta_{twist}(CH_2)$
A_u	1089.4	14.5	$\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{oop}(OH)$ [γ(OH)]	A_g	1090.8	8.0	4.6	3.4	0.1	0.0	3.3	3.7	0.0	2.9	$\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{oop}(OH)$ [γ(OH)]
A_u	1114.8	0.0	$\delta_{rock}(CH_3)$; $\delta_{twist}(CH_2)$; $\delta_{oop}(NH)$ [γ(NH)]	A_g	1114.9	1.5	0.8	0.6	0.4	0.0	1.0	0.0	0.0	0.1	$\delta_{twist}(CH_2)$; $\delta_{rock}(CH_3)$
B_u	1115.1	42.6		A_g	1115.6	5.1	2.9	2.2	3.7	0.0	0.5	0.3	0.0	3.5	$\delta_{twist}(CH_2)$; $\delta_{rock}(CH_3)$;
A_u	1115.7	0.0	$\delta_{twist}(CH_2)$; $\delta_{rock}(CH_3)$; $\delta_{oop}(NH)$ [γ(NH)]; $\delta_{oop}(OH)$ [γ(OH)]	B_g	1116.0	2.8	1.6	1.2	0.0	1.1	0.0	0.0	1.2	0.0	$\delta_{oop}(NH)$ [γ(NH)]; $\delta_{oop}(OH)$ [γ(OH)]
B_u	1116.1	154.5		B_g	1116.6	0.7	0.4	0.3	0.0	0.4	0.0	0.0	0.2	0.0	
A_u	1142.4	6.6	δ(ring) [ν(CN)]; $\delta_{rock}(CH_3)$; $\delta_{twist}(CH_2)$; $\delta_{oop}(NH)$ [γ(NH)]; $\delta_{wagg}(CH_2)$	A_g	1142.7	0.6	0.4	0.3	0.7	0.0	0.0	0.0	0.0	0.2	$\delta_{twist}(CH_2)$; δ(ring) [6-ring]; $\delta_{oop}(NH)$ [γ(NH)]; $\delta_{rock}(CH_3)$
B_u	1144.7	105.8	δ(ring) [ν(CN)]; $\delta_{rock}(CH_3)$; $\delta_{twist}(CH_2)$; $\delta_{oop}(NH)$ [γ(NH)]	B_g	1145.6	2.8	1.6	1.2	0.0	1.6	0.0	0.0	0.7	0.0	
A_u	1148.1	0.1		A_g	1147.5	1.3	0.8	0.5	0.2	0.0	0.8	0.2	0.0	0.2	
B_u	1149.4	168.5		B_g	1150.8	5.1	2.9	2.2	0.0	2.4	0.0	0.0	1.7	0.0	
B_u	1209.9	108.5	δ(ring) [ν(CN)]; $\delta_{rock}(CH_3)$	A_g	1210.6	2.6	1.6	0.9	2.4	0.0	0.3	0.7	0.0	0.2	
A_u	1210.8	0.5	δ(ring) [ν(CN)]; $\delta_{rock}(CH_3)$; $\delta_{twist}(CH_2)$	B_g	1211.4	1.4	0.8	0.6	0.0	0.7	0.0	0.0	0.4	0.0	δ(ring) [6-ring]; δ(ring) [ν(CN)]; $\delta_{rock}(CH_3)$
A_u	1213.8	8.2	δ(ring) [6-ring]; $\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$	A_g	1213.7	1.8	1.0	0.8	1.0	0.0	0.1	1.6	0.0	0.2	
B_u	1214.5	25.4	δ(ring) [6-ring]; $\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$; $\delta_{oop}(NH)$ [γ(NH)]	B_g	1214.3	1.5	0.9	0.6	0.0	0.4	0.0	0.0	0.9	0.0	δ(ring) [6-ring]; δ(ring) [ν(CN)]; $\delta_{oop}(NH)$ [γ(NH)]
B_u	1216.3	27.3		B_g	1215.5	0.7	0.4	0.3	0.0	0.2	0.0	0.0	0.4	0.0	$\delta_{rock}(CH_3)$; $\delta_{oop}(NH)$ [γ(NH)]; δ(ring) [ν(CC)]
A_u	1217.0	1.1		A_g	1216.3	0.1	0.1	0.0	0.1	0.0	0.0	0.0	0.0	0.0	
A_u	1219.9	1.5	$\delta_{oop}(NH)$ [γ(NH)]; δ(ring) [ν(CC)]; $\delta_{rock}(CH_3)$; $\delta_{rock}(CH_2)$	B_g	1219.5	0.6	0.3	0.3	0.0	0.1	0.0	0.0	0.4	0.0	$\delta_{rock}(CH_3)$; $\delta_{oop}(NH)$ [γ(NH)]; δ(ring) [ν(CC)]; ν(CC)
B_u	1221.3	5.0		A_g	1220.0	1.0	0.6	0.4	0.0	0.0	0.4	0.2	0.0	0.6	
B_u	1251.5	237.7	$\delta_{twist}(CH_2)$; $\delta_{oop}(NH)$ [γ(NH)]; ν(CC); $\delta_{rock}(CH_3)$	B_g	1250.7	1.9	1.1	0.8	0.0	1.1	0.0	0.0	0.5	0.0	$\delta_{twist}(CH_2)$; $\delta_{oop}(NH)$ [γ(NH)]; $\delta_{rock}(CH_3)$; ν(CC)
A_u	1252.8	0.6		A_g	1252.5	1.0	0.6	0.4	0.1	0.0	0.0	0.5	0.0	1.1	
B_u	1257.1	49.5	$\delta_{rock}(CH_2)$; $\delta_{twist}(CH_2)$; $\delta_{ip}(NH)$; $\delta_{rock}(CH_3)$	B_g	1257.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	$\delta_{twist}(CH_2)$; ν(CC); $\delta_{oop}(NH)$ [γ(NH)]
B_u	1257.3	74.6	ν(CC); $\delta_{twist}(CH_2)$; $\delta_{oop}(NH)$ [γ(NH)]; $\delta_{rock}(CH_3)$	B_g	1258.3	16.1	9.2	6.9	0.0	2.3	0.0	0.0	10.9	0.0	
A_u	1259.2	0.1		A_g	1259.0	15.0	9.0	5.9	10.8	0.0	0.5	9.3	0.0	3.0	$\delta_{twist}(CH_2)$; ν(CC)
A_u	1260.0	0.0		A_g	1259.6	0.5	0.3	0.2	0.2	0.0	0.0	0.0	0.0	0.6	$\delta_{twist}(CH_2)$
B_u	1260.6	212.0		B_g	1260.6	2.9	1.7	1.2	0.0	1.7	0.0	0.0	0.7	0.0	
A_u	1261.8	0.7		B_g	1262.1	1.2	0.7	0.5	0.0	0.4	0.0	0.0	0.6	0.0	
B_u	1261.9	4.0	$\delta_{twist}(CH_2)$; $\delta_{oop}(NH)$ [γ(NH)]; $\delta_{rock}(CH_3)$	A_g	1262.1	2.8	1.6	1.2	2.3	0.0	0.3	0.1	0.0	1.6	$\delta_{twist}(CH_2)$; $\delta_{oop}(NH)$ [γ(NH)]; $\delta_{rock}(CH_3)$
A_u	1264.2	3.3		A_g	1263.4	5.8	3.6	2.2	6.0	0.0	0.9	0.0	0.0	1.4	
B_u	1267.1	101.3		B_g	1266.4	2.5	1.5	1.1	0.0	1.7	0.0	0.0	0.4	0.0	
A_u	1267.5	0.2		A_g	1267.1	8.0	4.6	3.4	5.0	0.0	1.2	0.0	0.0	5.6	
A_u	1293.9	86.0		A_g	1294.5	13.3	7.6	5.6	7.1	0.0	3.2	7.7	0.0	0.6	
B_u	1295.3	12.3	δ(ring) [ν(CC)]; $\delta_{ip}(NH)$; $\delta_{twist}(CH_2)$; $\delta_{rock}(CH_3)$	B_g	1295.0	3.3	1.9	1.4	0.0	1.7	0.0	0.0	1.0	0.0	
A_u	1302.4	60.1		A_g	1300.2	8.7	5.0	3.7	3.2	0.0	2.0	6.7	0.0	0.4	$\delta_{twist}(CH_2)$; $\delta_{ip}(NH)$; $\delta_{rock}(CH_3)$
B_u	1303.0	22.2		B_g	1301.2	7.6	4.3	3.2	0.0	0.6	0.0	0.0	5.6	0.0	
A_u	1344.3	4.5	$\delta_{twist}(CH_2)$; $\delta_{ip}(NH)$	A_g	1344.4	12.6	7.2	5.4	0.2	0.0	9.0	0.4	0.0	2.2	
B_u	1345.7	19.9		B_g	1345.5	1.4	0.8	0.6	0.0	0.6	0.0	0.0	0.6	0.0	
A_u	1351.5	6.7	$\delta_{twist}(CH_2)$; $\delta_{ip}(NH)$; $\delta_{ip}(OH)$	A_g	1351.5	27.4	15.7	11.7	0.9	0.0	18.0	1.9	0.0	6.3	$\delta_{twist}(CH_2)$; $\delta_{ip}(NH)$; $\delta_{ip}(OH)$
B_u	1352.2	16.8		B_g	1352.2	0.1	0.1	0.0	0.0	0.1	0.0	0.0	0.0	0.0	
B_u	1364.4	242.7	$\delta_{ip}(OH)$; $\delta_{wagg}(CH_2)$	A_g	1365.0	0.5	0.3	0.2	0.3	0.0	0.3	0.1	0.0	0.0	$\delta_{ip}(OH)$; $\delta_{wagg}(CH_2)$

A_u	1365.0	146.1		B_g	1365.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
A_u	1373.2	2.8	$\delta_{wagg}(CH_2)$; $\delta_{oop}(NH)$ [γ(NH)];	A_g	1373.1	1.1	0.7	0.5	0.8	0.0	0.1	0.3	0.0	0.6	$\delta_{wagg}(CH_2)$; $\delta_{oop}(NH)$
B_u	1373.5	19.4	$\delta_{ip}(OH)$	B_g	1373.4	2.4	1.4	1.0	0.0	1.1	0.0	0.0	0.9	0.0	[γ(NH)]; $\delta_{ip}(OH)$
A_u	1378.4	0.6	$\delta_{wagg}(CH_2)$; $\delta_{oop}(NH)$ [γ(NH)]	A_g	1379.3	2.2	1.3	0.9	0.7	0.0	0.2	0.9	0.0	1.6	$\delta_{wagg}(CH_2)$; $\delta_{oop}(NH)$
B_u	1378.9	0.6		B_g	1379.7	3.3	1.9	1.4	0.0	2.5	0.0	0.0	0.2	0.0	[γ(NH)]
A_u	1384.9	18.9		A_g	1384.6	0.8	0.5	0.3	0.3	0.0	0.3	0.1	0.0	0.3	
B_u	1386.4	10.4	$\delta_{wagg}(CH_2)$	B_g	1386.2	0.2	0.1	0.1	0.0	0.1	0.0	0.0	0.0	0.0	$\delta_{wagg}(CH_2)$
A_u	1389.1	50.7		A_g	1388.4	0.9	0.5	0.3	0.3	0.0	0.4	0.2	0.0	0.2	
B_u	1390.6	1.9		B_g	1390.0	0.5	0.3	0.2	0.0	0.4	0.0	0.0	0.0	0.0	
A_u	1390.9	0.2	$\delta_{wagg}(CH_2)$; $\delta_{twist}(CH_2)$; $\delta_{oop}(NH)$	A_g	1390.8	0.9	0.5	0.4	0.5	0.0	0.1	0.0	0.0	0.7	
B_u	1392.5	5.4	[γ(NH)]	B_g	1392.0	3.1	1.8	1.3	0.0	1.7	0.0	0.0	0.8	0.0	$\delta_{wagg}(CH_2)$; $\delta_{oop}(NH)$
A_u	1395.2	1.3	$\delta_{wagg}(CH_2)$; $\delta_{oop}(NH)$ [γ(NH)]	A_g	1395.9	1.0	0.6	0.4	0.5	0.0	0.4	0.2	0.0	0.0	[γ(NH)]
B_u	1396.5	10.0		B_g	1396.5	4.1	2.3	1.8	0.0	2.6	0.0	0.0	0.8	0.0	
B_u	1414.7	42.9		B_g	1414.7	0.7	0.4	0.3	0.0	0.4	0.0	0.0	0.2	0.0	
A_u	1414.8	4.0		A_g	1414.9	3.2	1.9	1.3	1.3	0.0	0.2	0.0	0.0	3.5	
A_u	1416.4	0.1		B_g	1415.5	0.2	0.1	0.1	0.0	0.1	0.0	0.0	0.1	0.0	
B_u	1416.9	78.7	$\delta_{umbrella}(CH_3)$	A_g	1416.6	0.3	0.2	0.1	0.0	0.0	0.2	0.0	0.0	0.0	$\delta_{umbrella}(CH_3)$
A_u	1420.7	0.0		A_g	1420.2	0.3	0.2	0.1	0.1	0.0	0.0	0.2	0.0	0.2	
B_u	1421.7	20.8		B_g	1420.4	1.4	0.8	0.6	0.0	0.0	0.0	0.0	1.1	0.0	
A_u	1422.2	19.3		A_g	1421.5	0.2	0.1	0.1	0.1	0.0	0.1	0.1	0.0	0.0	
B_u	1422.6	163.2		B_g	1424.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
A_u	1430.6	3.2		A_g	1432.0	1.0	0.6	0.4	0.3	0.0	0.2	0.4	0.0	0.4	
B_u	1432.3	0.7		B_g	1433.1	6.9	3.9	2.9	0.0	4.5	0.0	0.0	1.2	0.0	$\delta_{umbrella}(CH_3)$; $\delta_{oop}(NH)$
B_u	1432.9	327.1	$\delta_{umbrella}(CH_3)$; $\delta_{oop}(NH)$ [γ(NH)]	B_g	1434.3	1.2	0.7	0.5	0.0	0.8	0.0	0.0	0.2	0.0	[γ(NH)]
A_u	1435.0	15.0		A_g	1437.0	0.5	0.3	0.1	0.4	0.0	0.0	0.2	0.0	0.1	$\delta_{umbrella}(CH_3)$; $\delta_{oop}(NH)$ [γ(NH)]; $\delta_{scissor}(HCH)$
A_u	1442.4	25.4	$\delta_{umbrella}(CH_3)$; $\delta_{scissor}(HCH)$; $\delta_{oop}(NH)$ [γ(NH)]	A_g	1441.9	0.4	0.3	0.1	0.0	0.0	0.1	0.1	0.0	0.3	$\delta_{umbrella}(CH_3)$; $\delta_{scissor}(HCH)$
B_u	1443.4	76.1	$\delta_{umbrella}(CH_3)$; $\delta_{oop}(NH)$ [γ(NH)]	A_g	1446.5	1.2	1.1	0.1	0.7	0.0	0.2	0.2	0.0	0.3	
A_u	1445.8	42.5	$\delta_{umbrella}(CH_3)$	B_g	1446.5	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.1	0.0	$\delta_{umbrella}(CH_3)$; $\delta_{oop}(NH)$
B_u	1449.6	10.9	$\delta_{umbrella}(CH_3)$; $\delta_{oop}(NH)$ [γ(NH)]	B_g	1449.0	2.3	1.3	1.0	0.0	0.5	0.0	0.0	1.4	0.0	[γ(NH)]
A_u	1449.8	12.5		B_g	1450.7	5.3	3.0	2.3	0.0	2.7	0.0	0.0	1.7	0.0	
B_u	1450.0	20.0	$\delta_{scissor}(HCH)$; $\delta_{umbrella}(CH_3)$; $\delta_{oop}(NH)$ [γ(NH)];	A_g	1451.5	4.0	2.3	1.7	1.6	0.0	0.6	0.5	0.0	3.4	$\delta_{scissor}(HCH)$; $\delta_{oop}(NH)$ [γ(NH)]
A_u	1456.6	0.1	$\delta_{scissor}(HCH)$; $\delta_{oop}(NH)$ [γ(NH)]; $\delta_{ip}(OH)$	B_g	1460.3	29.5	16.9	12.6	0.0	14.1	0.0	0.0	10.2	0.0	$\delta_{scissor}(HCH)$; $\delta_{oop}(NH)$ [γ(NH)]; $\delta_{ip}(OH)$
B_u	1457.7	10.3	$\delta_{scissor}(HCH)$; $\delta_{oop}(NH)$ [γ(NH)]	A_g	1461.1	2.2	1.3	1.0	2.8	0.0	0.0	0.5	0.0	0.4	$\delta_{scissor}(HCH)$; $\delta_{oop}(NH)$ [γ(NH)]
B_u	1477.2	314.7		A_g	1474.7	1.0	0.7	0.2	1.2	0.0	0.0	0.1	0.0	0.0	
A_u	1477.7	16.9	$\delta_{scissor}(HCH)$; $\delta_{ip}(OH)$; $\delta_{oop}(NH)$ [γ(NH)]	B_g	1477.9	5.5	3.2	2.4	0.0	4.4	0.0	0.0	0.1	0.0	$\delta_{scissor}(HCH)$; $\delta_{oop}(NH)$
A_u	1479.5	4.6		A_g	1479.4	2.9	1.6	1.2	0.1	0.0	0.8	1.2	0.0	1.9	[γ(NH)]; $\delta_{ip}(OH)$
B_u	1480.7	18.8	$\delta_{scissor}(HCH)$	B_g	1480.3	29.0	16.6	12.4	0.0	18.6	0.0	0.0	5.3	0.0	
A_u	1483.5	19.4		A_g	1482.3	3.7	2.1	1.6	2.7	0.0	1.3	0.7	0.0	0.2	$\delta_{scissor}(HCH)$; $\delta_{ip}(OH)$
B_u	1484.1	77.4		B_g	1483.8	1.6	0.9	0.7	0.0	0.5	0.0	0.0	0.9	0.0	
A_u	1485.7	6.0	$\delta_{scissor}(HCH)$; $\delta_{oop}(NH)$ [γ(NH)]	A_g	1485.4	8.2	4.7	3.5	6.8	0.0	0.1	0.0	0.0	6.5	$\delta_{scissor}(HCH)$; $\delta_{oop}(NH)$ [γ(NH)]; $\delta_{ip}(OH)$
B_u	1485.8	5.7		B_g	1485.4	11.7	6.7	5.0	0.0	9.5	0.0	0.0	0.1	0.0	
B_u	1486.8	17.9	$\delta_{scissor}(HCH)$; $\delta_{oop}(NH)$ [γ(NH)];	B_g	1486.6	1.2	0.7	0.5	0.0	0.8	0.0	0.0	0.1	0.0	$\delta_{scissor}(HCH)$; $\delta_{oop}(NH)$
A_u	1487.5	0.0	$\delta_{ip}(OH)$	A_g	1487.9	2.3	1.4	1.0	0.1	0.0	1.4	0.3	0.0	0.7	[γ(NH)]
B_u	1489.3	52.4	$\delta_{scissor}(HCH)$; $\delta_{oop}(NH)$ [γ(NH)]	A_g	1489.1	0.7	0.4	0.2	0.8	0.0	0.1	0.0	0.0	0.0	
A_u	1489.9	11.0	$\delta_{scissor}(HCH)$; $\delta_{oop}(NH)$ [γ(NH)]; $\delta_{ip}(OH)$	B_g	1490.3	20.9	12.0	9.0	0.0	12.7	0.0	0.0	4.5	0.0	
A_u	1492.3	6.9	$\delta_{scissor}(HCH)$; $\delta_{ip}(OH)$	B_g	1491.2	1.9	1.1	0.8	0.0	0.7	0.0	0.0	0.9	0.0	$\delta_{scissor}(HCH)$; $\delta_{oop}(NH)$
B_u	1492.5	30.5	$\delta_{scissor}(HCH)$; $\delta_{oop}(NH)$ [γ(NH)]	A_g	1492.2	9.4	5.4	4.0	0.1	0.0	5.2	1.4	0.0	3.6	[γ(NH)]; $\delta_{ip}(OH)$
B_u	1493.6	70.8	$\delta_{scissor}(HCH)$; $\delta_{oop}(NH)$ [γ(NH)];	A_g	1493.9	14.2	8.1	6.1	1.0	0.0	10.0	1.7	0.0	0.5	

A_u	1494.0	17.8	δ_{ip}(OH)	B_g	1495.2	8.5	4.8	3.6	0.0	0.7	0.0	0.0	6.2	0.0	
A_u	1495.9	10.4		A_g	1497.0	5.9	3.4	2.5	6.5	0.0	0.1	1.4	0.0	1.6	
A_u	1497.3	4.4	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]	B_g	1497.9	0.3	0.2	0.1	0.0	0.2	0.0	0.0	0.1	0.0	
B_u	1497.4	73.7		B_g	1498.7	18.6	10.7	8.0	0.0	0.0	0.0	0.0	15.3	0.0	
B_u	1501.3	186.3		A_g	1500.9	24.1	13.8	10.3	5.3	0.0	8.1	2.1	0.0	16.0	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]
A_u	1501.5	6.9		B_g	1502.1	3.2	1.8	1.4	0.0	0.2	0.0	0.0	2.5	0.0	
B_u	1501.9	8.1		A_g	1503.6	5.1	3.1	2.0	3.8	0.0	1.8	0.7	0.0	0.0	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]
A_u	1502.7	89.8	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]; δ_{ip}(OH)	A_g	1505.4	14.9	8.8	6.1	3.8	0.0	0.1	1.0	0.0	19.2	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]; δ_{ip}(OH)
B_u	1504.0	43.7		A_g	1506.3	14.4	8.2	6.2	3.5	0.0	8.0	3.8	0.0	0.2	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]
A_u	1504.7	3.8		B_g	1508.0	10.3	5.9	4.4	0.0	6.6	0.0	0.0	1.9	0.0	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]; δ_{ip}(OH)
B_u	1506.8	51.0	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]	B_g	1509.5	8.6	4.9	3.7	0.0	2.1	0.0	0.0	5.0	0.0	
A_u	1508.0	1.6	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)];	A_g	1511.4	3.5	2.6	0.9	0.2	0.0	1.2	2.4	0.0	0.0	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]
B_u	1508.9	32.1	δ_{ip}(OH)	B_g	1513.7	13.8	7.9	5.9	0.0	3.7	0.0	0.0	7.6	0.0	
A_u	1509.7	4.9	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]	A_g	1514.2	0.4	0.3	0.2	0.3	0.0	0.1	0.2	0.0	0.1	
B_u	1513.4	63.5		B_g	1514.8	15.4	8.8	6.6	0.0	0.2	0.0	0.0	12.5	0.0	
A_u	1514.5	5.8	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)];	A_g	1515.8	3.5	2.6	0.9	0.1	0.0	0.6	0.3	0.0	3.5	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]; δ_{ip}(OH)
B_u	1517.1	7.1	δ_{ip}(OH)	B_g	1516.5	6.8	3.9	2.9	0.0	5.5	0.0	0.0	0.0	0.0	
A_u	1518.4	38.4		B_g	1519.6	5.5	3.1	2.3	0.0	4.5	0.0	0.0	0.0	0.0	
B_u	1518.9	118.9		A_g	1520.7	0.6	0.3	0.2	0.0	0.0	0.4	0.0	0.0	0.1	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]
B_u	1520.2	145.4		B_g	1523.1	4.3	2.4	1.8	0.0	3.1	0.0	0.0	0.4	0.0	
A_u	1524.4	93.3	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]	A_g	1524.5	5.9	3.4	2.5	2.0	0.0	0.0	0.7	0.0	7.0	
B_u	1526.7	186.6		B_g	1528.0	1.1	0.6	0.5	0.0	0.0	0.0	0.0	0.9	0.0	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]; δ_{ip}(OH)
B_u	1527.9	52.9	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]; δ_{ip}(OH)	B_g	1529.1	2.4	1.4	1.0	0.0	1.9	0.0	0.0	0.1	0.0	
B_u	1528.5	28.4	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]	A_g	1529.8	12.7	7.4	5.4	3.7	0.0	7.7	0.0	0.0	1.7	
A_u	1529.7	1.0	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)];	A_g	1531.5	6.1	3.5	2.6	5.1	0.0	0.1	0.1	0.0	4.6	
A_u	1532.0	0.7	δ_{ip}(OH)	B_g	1531.5	5.0	2.8	2.1	0.0	1.4	0.0	0.0	2.7	0.0	δ_{oop}(NH) [γ(NH)];
A_u	1534.8	0.9	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]	A_g	1535.7	35.7	20.9	14.9	0.3	0.0	22.2	3.3	0.0	10.2	$\delta_{scissor}$(HCH)
B_u	1536.2	53.4	$\delta_{scissor}$(HCH); δ_{oop}(NH) [γ(NH)]; δ_{ip}(OH)	B_g	1537.9	15.9	9.1	6.8	0.0	3.3	0.0	0.0	9.8	0.0	
A_u	1538.3	21.9	δ_{oop}(NH) [γ(NH)]; $\delta_{scissor}$(HCH)	A_g	1538.9	7.6	4.3	3.2	3.0	0.0	4.2	0.4	0.0	0.5	
B_u	1540.5	0.0		A_g	1540.1	2.0	1.2	0.8	0.9	0.0	0.9	0.1	0.0	0.3	
A_u	1541.1	3.0	δ_{oop}(NH) [γ(NH)]; $\delta_{scissor}$(HCH); δ_{ip}(OH)	B_g	1540.8	25.1	14.3	10.8	0.0	12.6	0.0	0.0	8.1	0.0	$\delta_{scissor}$(HCH); δ_{ip}(OH);
A_u	1541.8	52.3		A_g	1544.8	14.6	8.5	6.1	0.0	0.0	8.8	1.8	0.0	4.6	δ_{oop}(NH) [γ(NH)]
B_u	1545.0	55.0		B_g	1545.8	0.4	0.2	0.2	0.0	0.1	0.0	0.0	0.3	0.0	δ_{oop}(NH) [γ(NH)];
B_u	1550.1	15.0	δ_{oop}(NH) [γ(NH)]; $\delta_{scissor}$(HCH)	A_g	1551.4	4.5	2.6	1.9	4.2	0.0	0.0	1.0	0.0	2.0	$\delta_{scissor}$(HCH)
A_u	1551.7	0.0	δ_{oop}(NH) [γ(NH)]; $\delta_{scissor}$(HCH); δ_{ip}(OH)	B_g	1552.6	30.2	17.3	13.0	0.0	19.8	0.0	0.0	5.0	0.0	δ_{oop}(NH) [γ(NH)]; $\delta_{scissor}$(HCH); δ_{ip}(OH)
A_u	1650.7	2.4	δ_{ip}(OH)	A_g	1681.1	7.4	4.9	2.6	0.6	0.0	2.9	4.4	0.0	0.8	
B_u	1650.7	232.4		B_g	1681.2	0.1	0.1	0.1	0.0	0.0	0.0	0.0	0.1	0.0	δ_{ip}(NH)
B_u	1681.1	53.2		B_g	1693.4	1.9	1.1	0.8	0.0	0.6	0.0	0.0	1.0	0.0	
A_u	1681.2	201.9	δ_{ip}(NH)	A_g	1693.6	3.1	2.1	1.0	0.1	0.0	1.3	1.3	0.0	0.7	
B_u	1693.6	886.2		B_g	1709.6	1.9	1.1	0.8	0.0	1.3	0.0	0.0	0.2	0.0	δ_{ip}(OH)
A_u	1694.8	144.6		A_g	1709.8	2.4	1.8	0.6	1.2	0.0	1.0	0.2	0.0	0.1	
B_u	2208.1	13394.2		B_g	2243.3	29.6	16.9	12.7	0.0	17.1	0.0	0.0	7.2	0.0	
A_u	2208.9	3060.7	v(OH)	A_g	2248.3	211.9	193.6	18.3	200.4	0.0	7.2	23.6	0.0	26.8	v(OH)
B_u	2736.2	11663.6		B_g	2740.0	194.5	111.1	83.4	0.0	37.3	0.0	0.0	122.8	0.0	
A_u	2747.9	4361.6		A_g	2742.4	221.5	185.0	36.5	9.5	0.0	29.8	16.6	0.0	211.6	
B_u	3024.2	20.1		B_g	3024.4	16.8	9.6	7.2	0.0	10.9	0.0	0.0	3.0	0.0	
A_u	3024.2	23.5	v(CH)	A_g	3024.9	7.0	5.7	1.3	0.5	0.0	2.3	2.9	0.0	1.6	v(CH)
A_u	3027.1	49.6		B_g	3027.8	80.3	45.9	34.4	0.0	19.9	0.0	0.0	46.2	0.0	
B_u	3027.1	68.2		A_g	3028.0	204.6	185.5	19.1	24.2	0.0	28.5	63.0	0.0	113.6	

B_u	3034.4	35.2	
A_u	3034.8	62.2	
A_u	3036.9	0.9	
B_u	3037.3	122.8	
A_u	3038.6	5.6	
B_u	3038.8	38.0	
B_u	3042.0	8.7	
A_u	3042.0	5.1	
A_u	3045.4	4.7	
B_u	3045.6	5.0	
B_u	3046.2	3.4	
A_u	3046.2	88.3	
B_u	3049.7	83.0	
A_u	3049.8	2.9	
A_u	3051.3	58.5	
B_u	3051.4	69.0	
A_u	3056.9	5.3	
B_u	3057.9	9.9	
A_u	3066.2	232.3	
B_u	3070.2	2.2	
B_u	3073.6	8.6	
B_u	3074.0	39.8	
A_u	3074.3	69.5	
A_u	3075.3	230.6	v(CH); v(NH)
B_u	3084.6	835.0	v(NH)
A_u	3086.1	6549.1	
B_u	3090.4	214.9	v(CH); v(NH)
A_u	3090.7	108.1	
A_u	3093.7	3891.2	v(NH); v(CH); v(OH)
B_u	3094.7	175.9	v(CH); v(NH)
A_u	3094.8	14.8	v(CH)
B_u	3095.1	548.9	v(NH); v(CH); v(OH)
B_u	3101.2	17.9	
A_u	3101.2	1.2	
A_u	3104.0	91.7	
B_u	3104.2	43.6	
A_u	3105.2	46.2	
B_u	3105.4	28.5	
B_u	3106.2	22.3	
A_u	3106.3	73.5	
B_u	3108.4	37.5	
A_u	3108.5	1.7	
A_u	3119.3	28.1	v(CH)
B_u	3119.3	26.1	
A_u	3125.8	2.9	
B_u	3125.9	31.2	
B_u	3127.4	7.2	
A_u	3127.5	55.3	
A_u	3130.7	0.4	
B_u	3130.9	11.3	
B_u	3131.9	0.6	
A_u	3132.4	4.7	
B_u	3135.0	8.5	
A_u	3135.6	10.4	v(CH); v(NH)
A_u	3137.9	8.7	

B_g	3034.5	3.6	2.1	1.5	0.0	2.8	0.0	0.0	0.2	0.0	
A_g	3034.8	79.9	78.8	1.1	16.0	0.0	0.1	46.5	0.0	30.6	
B_g	3037.2	2.1	1.2	0.9	0.0	0.0	0.0	0.0	1.7	0.0	
A_g	3037.4	25.2	23.2	2.0	5.6	0.0	3.0	4.6	0.0	15.2	
A_g	3038.2	265.0	263.4	1.6	94.7	0.0	2.8	93.5	0.0	113.5	
B_g	3038.3	11.8	6.8	5.1	0.0	5.2	0.0	0.0	4.6	0.0	
A_g	3041.4	16.8	10.1	6.6	4.7	0.0	2.2	8.8	0.0	9.2	
B_g	3042.6	2.5	1.4	1.1	0.0	1.7	0.0	0.0	0.3	0.0	
B_g	3045.4	15.1	8.6	6.5	0.0	10.4	0.0	0.0	2.1	0.0	
A_g	3046.1	1000.0	990.2	9.9	298.7	0.0	3.3	572.8	0.0	285.4	
B_g	3047.4	28.5	16.3	12.2	0.0	14.4	0.0	0.0	9.1	0.0	
A_g	3047.6	141.7	134.2	7.6	118.8	0.0	2.0	31.7	0.0	17.5	
A_g	3051.2	347.0	340.9	6.1	81.9	0.0	1.4	97.4	0.0	224.8	
B_g	3051.2	37.2	21.3	16.0	0.0	7.9	0.0	0.0	22.7	0.0	
A_g	3051.5	204.6	203.3	1.3	104.7	0.0	0.7	75.2	0.0	56.1	
B_g	3051.8	7.6	4.3	3.3	0.0	3.4	0.0	0.0	2.9	0.0	
A_g	3059.8	461.6	451.1	10.5	224.7	0.0	7.9	224.1	0.0	79.3	
B_g	3060.5	9.5	5.5	4.1	0.0	7.3	0.0	0.0	0.6	0.0	
A_g	3068.1	224.8	184.5	40.3	55.8	0.0	62.5	115.3	0.0	9.3	
B_g	3069.7	21.1	12.1	9.1	0.0	2.0	0.0	0.0	15.4	0.0	
B_g	3073.6	19.3	11.1	8.3	0.0	7.2	0.0	0.0	8.7	0.0	
B_g	3074.2	10.6	6.1	4.6	0.0	0.8	0.0	0.0	8.0	0.0	
A_g	3074.3	310.8	275.5	35.3	49.1	0.0	63.5	112.3	0.0	110.1	
A_g	3076.0	810.0	780.0	29.9	152.5	0.0	33.1	489.9	0.0	259.0	
A_g	3083.9	703.7	536.9	166.8	0.4	0.0	1.0	1000.0	0.0	0.5	v(NH)
B_g	3085.2	41.2	23.6	17.7	0.0	0.2	0.0	0.0	33.8	0.0	
B_g	3090.3	51.0	29.2	21.9	0.0	0.0	0.0	0.0	42.0	0.0	v(CH); v(NH)
A_g	3090.3	197.7	190.1	7.6	23.2	0.0	5.4	98.4	0.0	104.1	
B_g	3093.4	44.3	25.3	19.0	0.0	30.6	0.0	0.0	5.9	0.0	v(NH); v(CH); v(OH)
A_g	3093.5	123.0	92.2	30.8	1.6	0.0	1.7	171.0	0.0	1.1	
A_g	3094.8	70.7	40.8	30.0	24.0	0.0	8.7	3.3	0.0	71.2	
B_g	3094.8	20.5	11.7	8.8	0.0	14.3	0.0	0.0	2.6	0.0	
B_g	3101.1	42.6	24.4	18.3	0.0	4.6	0.0	0.0	30.4	0.0	
A_g	3101.2	203.9	175.5	28.5	43.7	0.0	51.1	33.7	0.0	88.1	
A_g	3104.1	44.5	26.2	18.3	2.8	0.0	33.1	0.7	0.0	2.7	
B_g	3104.2	34.7	19.9	14.9	0.0	21.4	0.0	0.0	7.2	0.0	
A_g	3105.3	208.5	128.2	80.3	27.0	0.0	20.6	94.1	0.0	170.4	
B_g	3105.6	41.4	23.7	17.7	0.0	32.4	0.0	0.0	1.6	0.0	
B_g	3106.3	25.9	14.8	11.1	0.0	1.3	0.0	0.0	19.9	0.0	
A_g	3106.4	121.4	91.0	30.4	68.6	0.0	0.1	19.3	0.0	86.7	
B_g	3108.5	46.9	26.8	20.1	0.0	17.0	0.0	0.0	21.6	0.0	v(CH)
A_g	3108.7	19.6	11.2	8.4	2.4	0.0	13.7	2.4	0.0	0.0	
B_g	3116.8	63.0	36.0	27.0	0.0	16.5	0.0	0.0	35.3	0.0	
A_g	3116.8	80.5	46.1	34.5	68.2	0.0	5.7	49.8	0.0	3.1	
A_g	3125.7	141.0	129.6	11.4	109.2	0.0	2.9	3.5	0.0	57.2	
B_g	3125.9	12.2	7.0	5.2	0.0	9.6	0.0	0.0	0.5	0.0	
A_g	3127.3	240.3	156.0	84.3	9.2	0.0	1.3	350.4	0.0	11.7	
B_g	3127.4	9.3	5.3	4.0	0.0	1.4	0.0	0.0	6.3	0.0	
A_g	3130.7	131.4	78.2	53.2	13.7	0.0	81.1	13.0	0.0	23.9	
B_g	3130.7	32.1	18.4	13.8	0.0	3.5	0.0	0.0	22.9	0.0	
B_g	3131.9	6.4	3.7	2.8	0.0	4.0	0.0	0.0	1.3	0.0	
A_g	3132.5	205.0	143.2	61.9	0.8	0.0	2.0	299.0	0.0	3.6	
A_g	3134.1	180.2	156.4	23.9	112.6	0.0	21.6	1.8	0.0	77.6	v(CH); v(NH)
B_g	3134.2	5.0	2.9	2.1	0.0	1.4	0.0	0.0	2.8	0.0	v(CH)
A_g	3137.5	185.2	111.4	73.7	140.6	0.0	62.5	32.3	0.0	0.3	

B_u	3138.0	5.6		B_g	3137.7	0.2	0.1	0.1	0.0	0.1	0.0	0.0	0.1	0.0	
A_u	3140.8	9.9		B_g	3141.9	27.6	15.8	11.9	0.0	4.6	0.0	0.0	18.1	0.0	
B_u	3142.1	175.4	v(CH)	A_g	3142.2	177.0	101.2	75.8	140.4	0.0	0.0	150.8	0.0	0.0	
A_u	3147.9	53.8		A_g	3148.2	587.2	516.6	70.6	442.4	0.0	34.7	2.5	0.0	243.5	
B_u	3148.0	210.6		B_g	3148.3	33.1	18.9	14.2	0.0	26.5	0.0	0.0	0.7	0.0	
B_u	3148.8	140.6		A_g	3150.5	340.6	198.2	142.4	80.9	0.0	152.9	2.0	0.0	167.8	
A_u	3150.1	485.4		B_g	3150.8	32.2	18.4	13.8	0.0	0.1	0.0	0.0	26.4	0.0	v(CH); v(NH)
A_u	3156.1	1.6	v(CH); v(NH)	A_g	3156.0	202.2	177.2	25.1	30.8	0.0	11.6	6.5	0.0	201.3	
B_u	3156.3	167.4		B_g	3156.5	44.6	25.5	19.1	0.0	9.8	0.0	0.0	26.9	0.0	
B_u	3160.0	1247.1		B_g	3160.2	10.1	5.8	4.3	0.0	6.5	0.0	0.0	1.7	0.0	
A_u	3161.0	0.0		A_g	3161.0	306.0	240.3	65.7	383.2	0.0	19.5	1.9	0.0	4.1	
B_u	3161.8	3971.1		B_g	3163.5	86.8	49.6	37.2	0.0	21.0	0.0	0.0	50.5	0.0	
A_u	3165.0	196.6		A_g	3164.4	54.2	36.4	17.8	0.7	0.0	2.0	1.7	0.0	76.5	
B_u	3165.6	94.5	v(CH)	B_g	3165.6	4.7	2.7	2.0	0.0	1.4	0.0	0.0	2.5	0.0	v(CH)
A_u	3166.5	209.9		A_g	3166.1	177.2	112.6	64.7	6.1	0.0	21.4	8.3	0.0	221.5	
B_u	3169.2	274.3	v(CH); v(NH)	B_g	3170.4	157.8	90.2	67.6	0.0	56.7	0.0	0.0	73.1	0.0	v(CH); v(NH)
A_u	3169.9	73.3		A_g	3170.4	123.7	87.0	36.7	2.5	0.0	61.8	7.3	0.0	51.4	
A_u	3176.9	4.7		A_g	3176.9	240.0	179.8	60.2	64.5	0.0	87.0	0.0	0.0	107.3	
B_u	3177.1	34.0	v(CH)	B_g	3177.2	0.4	0.2	0.2	0.0	0.3	0.0	0.0	0.0	0.0	v(CH)
B_u	3184.4	31.4		B_g	3184.4	12.5	7.1	5.4	0.0	3.3	0.0	0.0	7.0	0.0	
A_u	3185.6	35.3		A_g	3185.5	159.8	101.9	57.9	8.7	0.0	101.8	0.0	0.0	38.6	
B_u	3348.9	2512.0		A_g	3349.1	159.7	102.0	57.8	71.6	0.0	8.9	56.9	0.0	104.3	
A_u	3350.2	493.0	v(OH) [water]	B_g	3349.2	95.6	54.6	41.0	0.0	0.9	0.0	0.0	77.7	0.0	v(OH) [water]
B_u	3424.8	6300.0		A_g	3384.3	472.2	433.5	38.7	483.2	0.0	0.3	65.8	0.0	39.0	
A_u	3425.8	2902.0		B_g	3385.8	66.2	37.8	28.4	0.0	39.6	0.0	0.0	14.8	0.0	

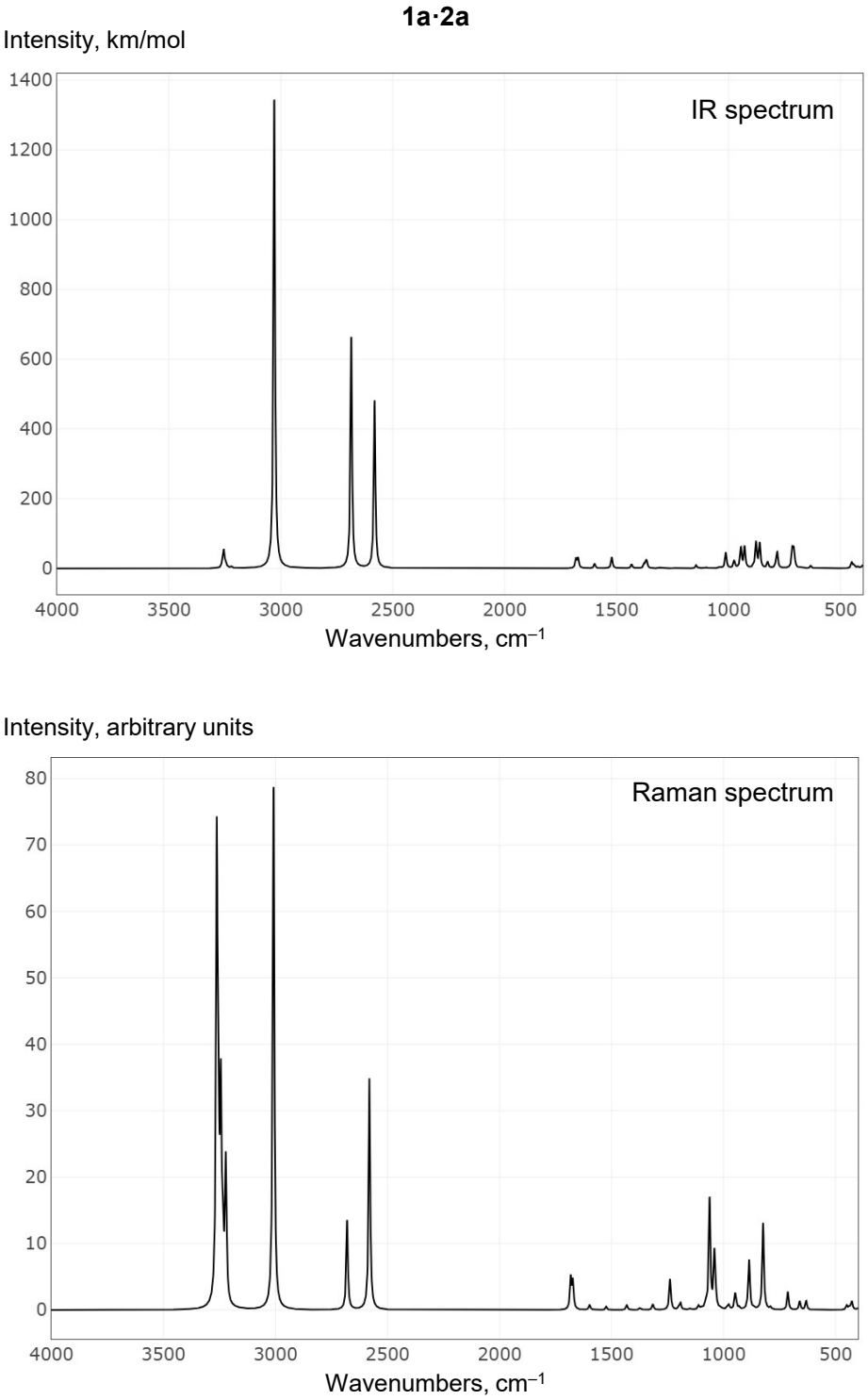


Figure S14. Computed vibrational spectra of **1a·2a**.

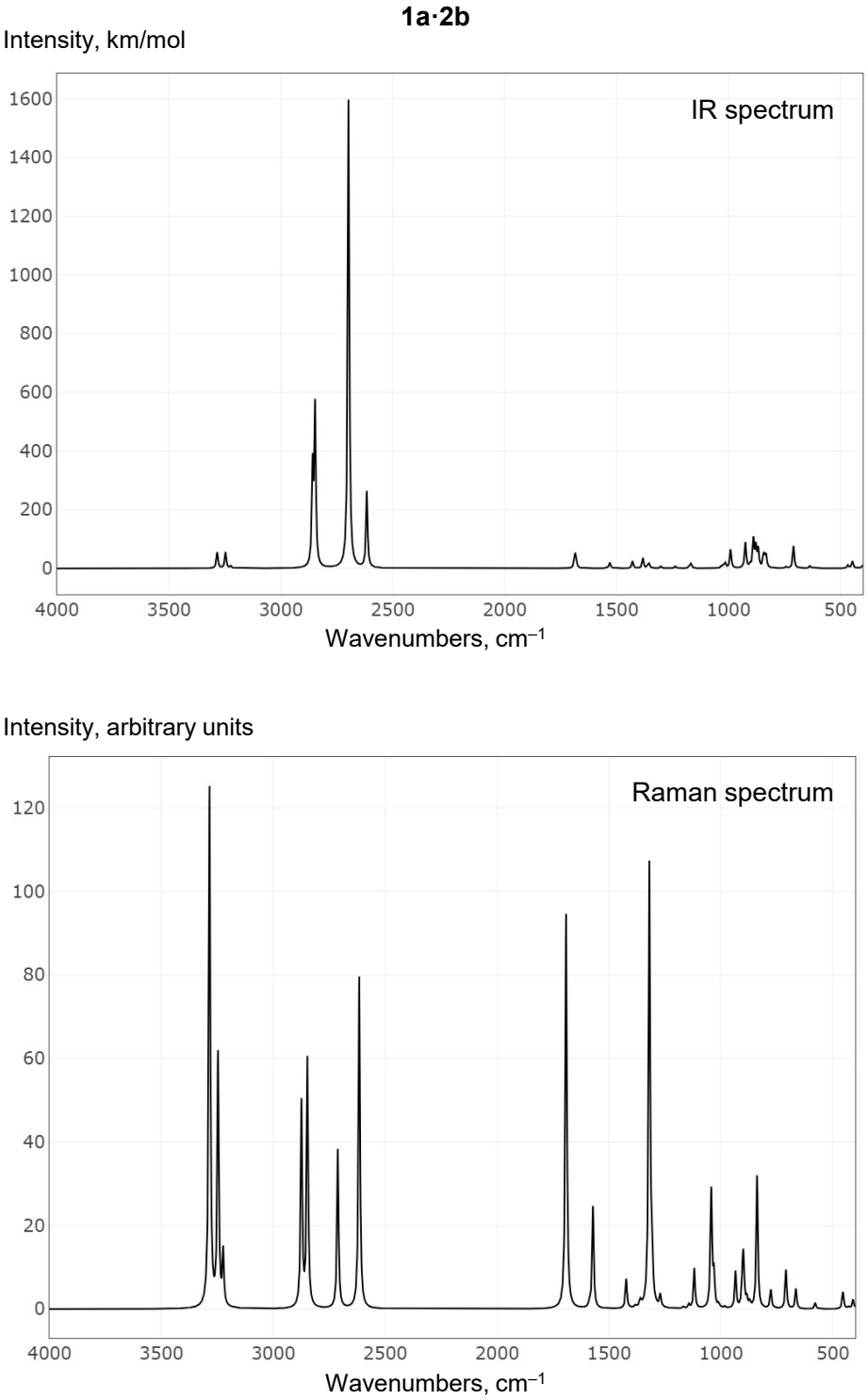


Figure S15. Computed vibrational spectra of **1a·2b**.

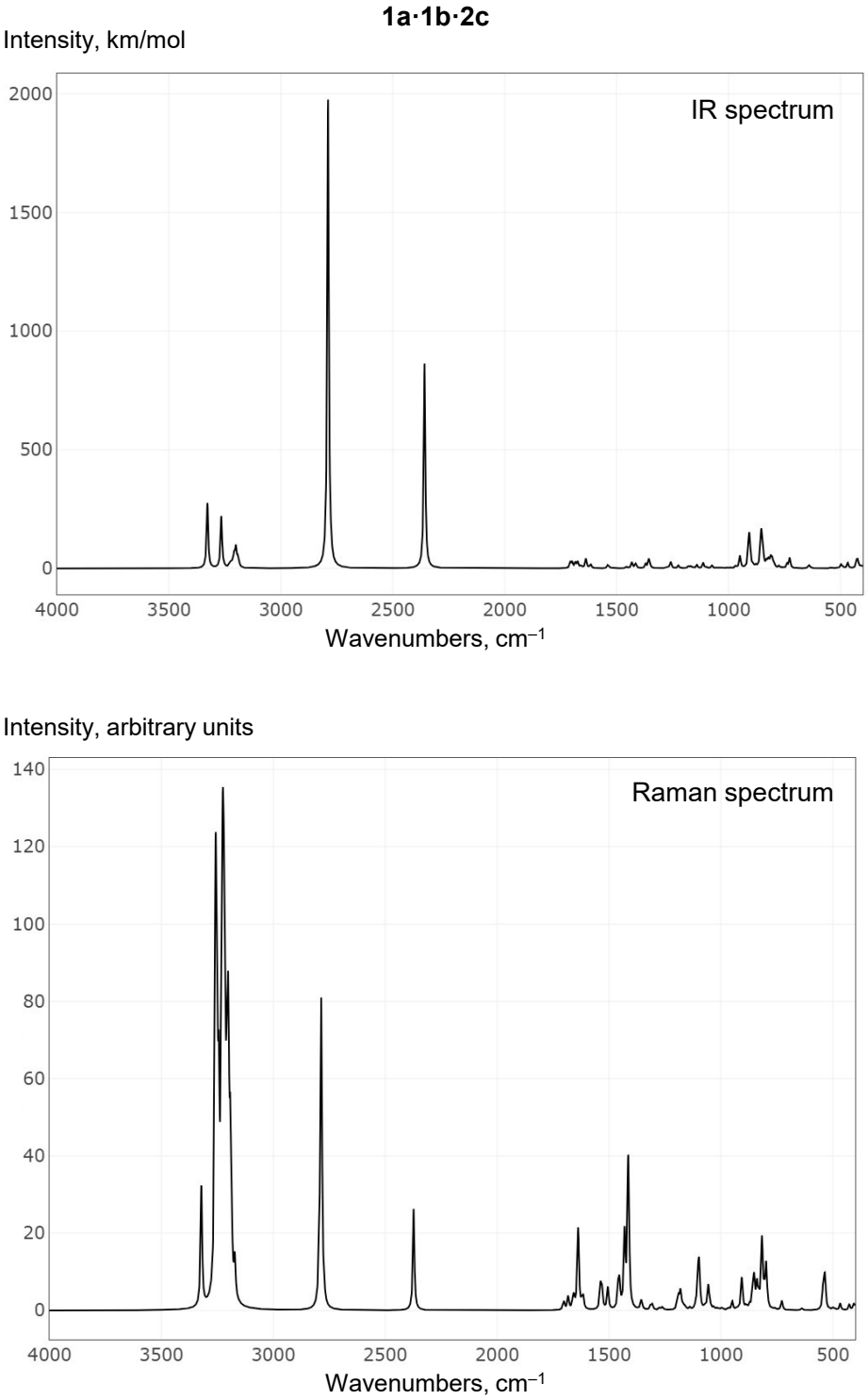


Figure S16. Computed vibrational spectra of **1a·1b·2c**.

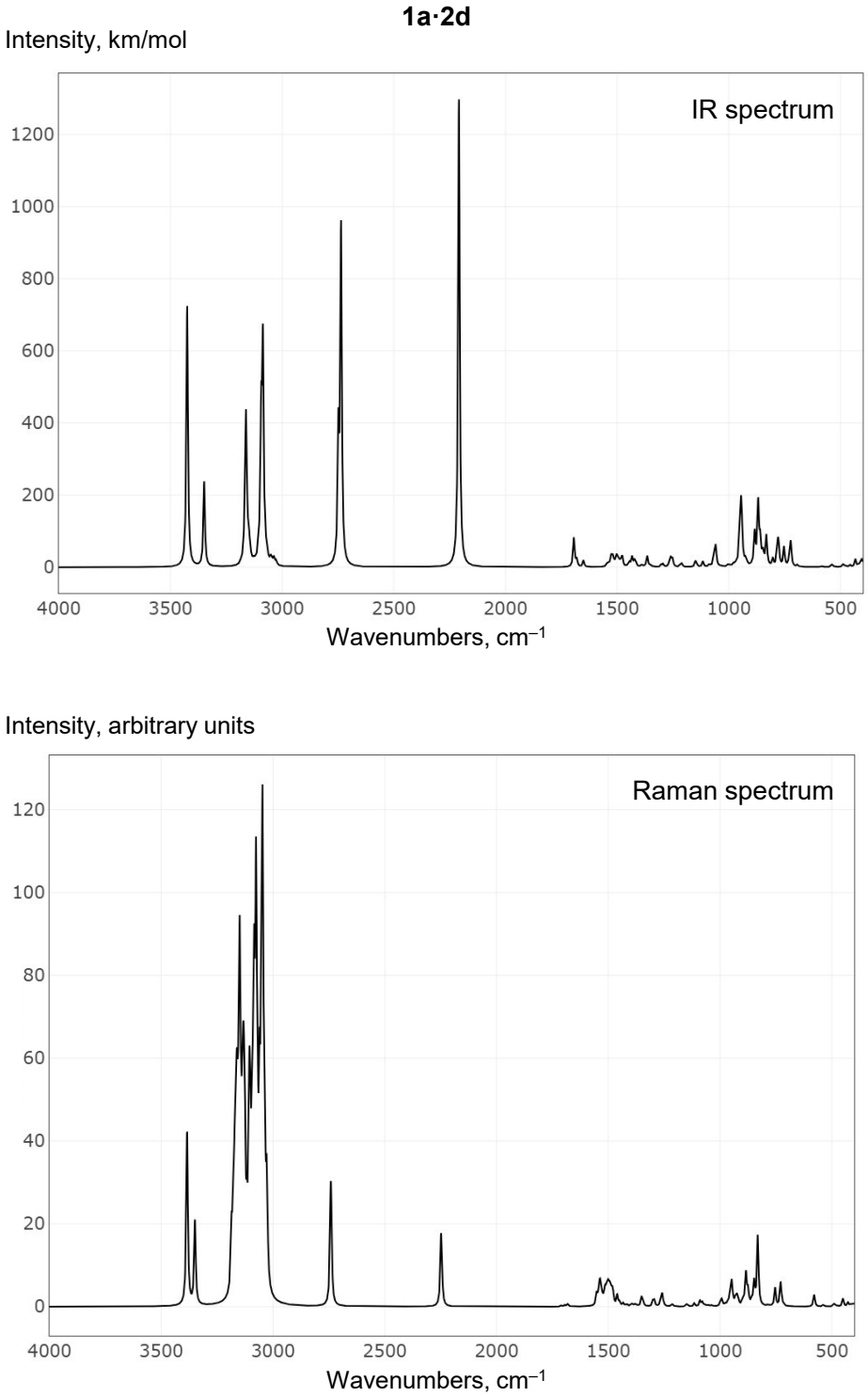


Figure S17. Computed vibrational spectra of **1a·2d**.

Here, isotropic intensities in both IR and Raman spectra are plotted with the CRYSPLOT tool.[17] As the structural model in each case consists of a periodic unit cell containing the same set of atoms as the experimental one, the computed IR and Raman peaks provide direct correspondence to the experimental fundamental peaks. B3LYP is a well-established hybrid functional for simulation of IR and Raman spectra of crystalline solids within the harmonic approximation (see, *e.g.*, Refs. 18–24). Nevertheless, the predicted frequencies are possibly all over-estimated due to the more contracted 0 K optimized structures exhibiting stiffer interatomic potentials in comparison to what can be found at the experimental conditions.

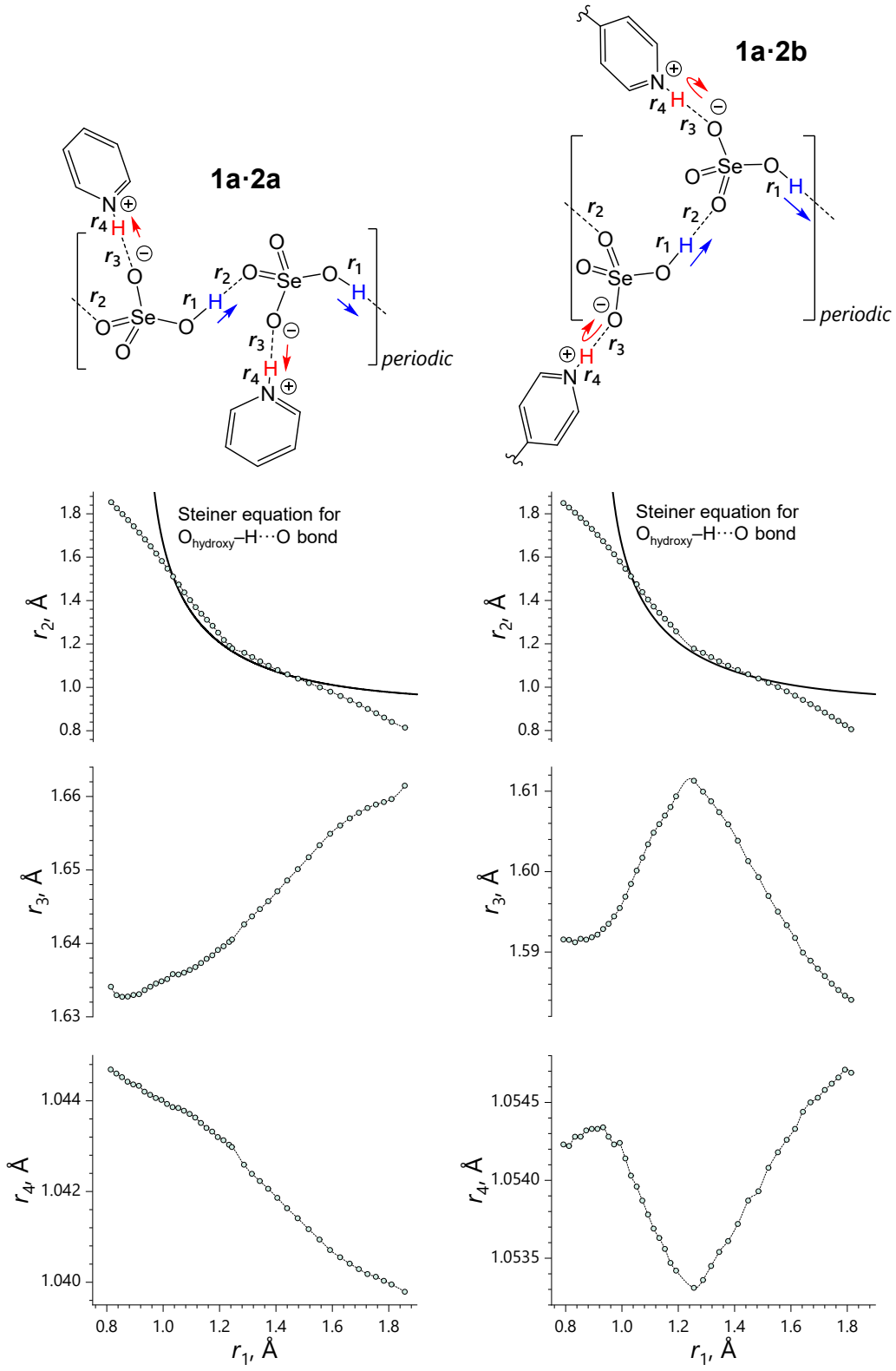


Figure S18. Interdependencies of the SeO–H···OSe and SeO···H–N bond geometries upon the coherent quasi-adiabatic transfer of the SeO–H···OSe bridging protons in **1a·2a** and **1a·2b**.

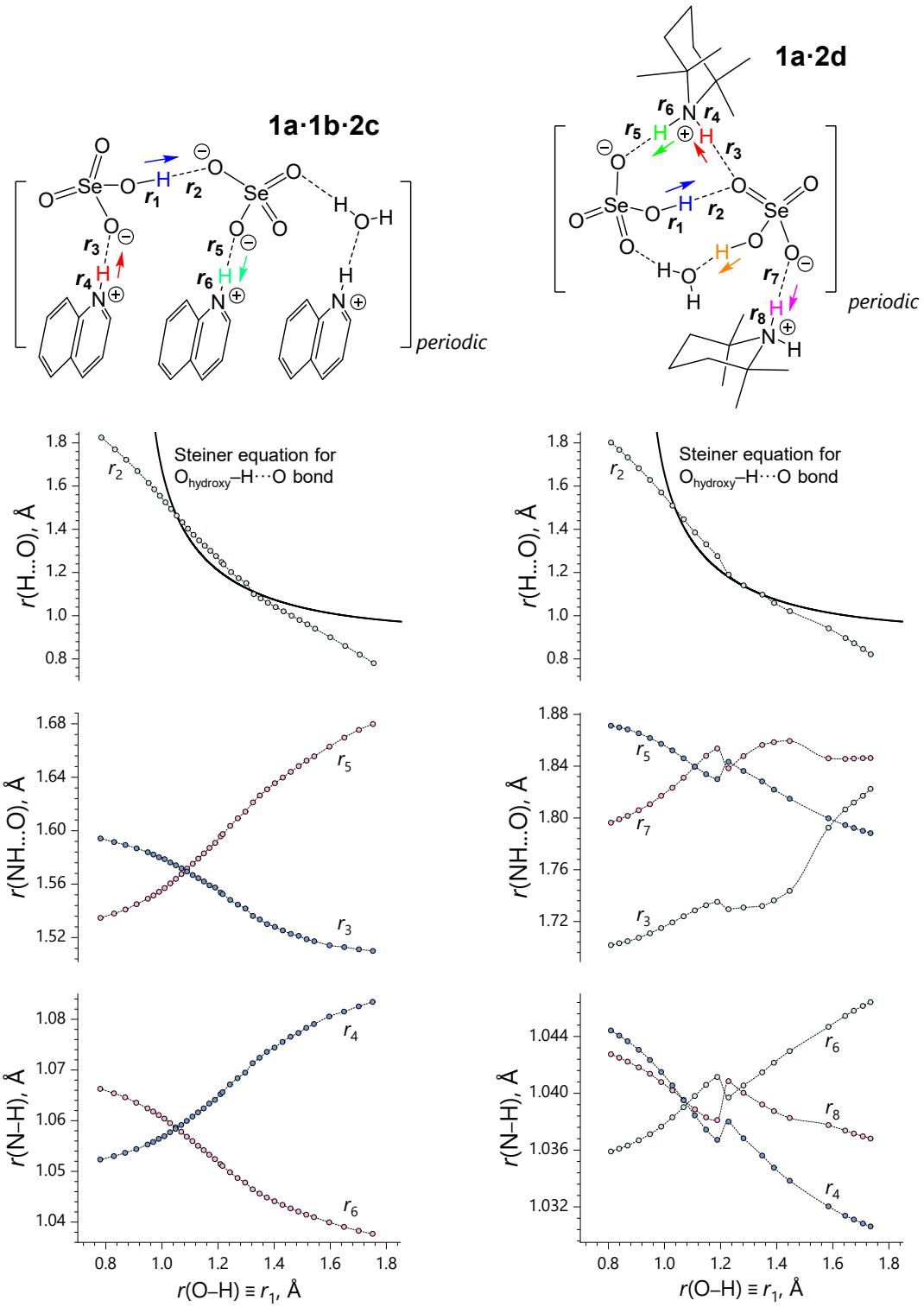


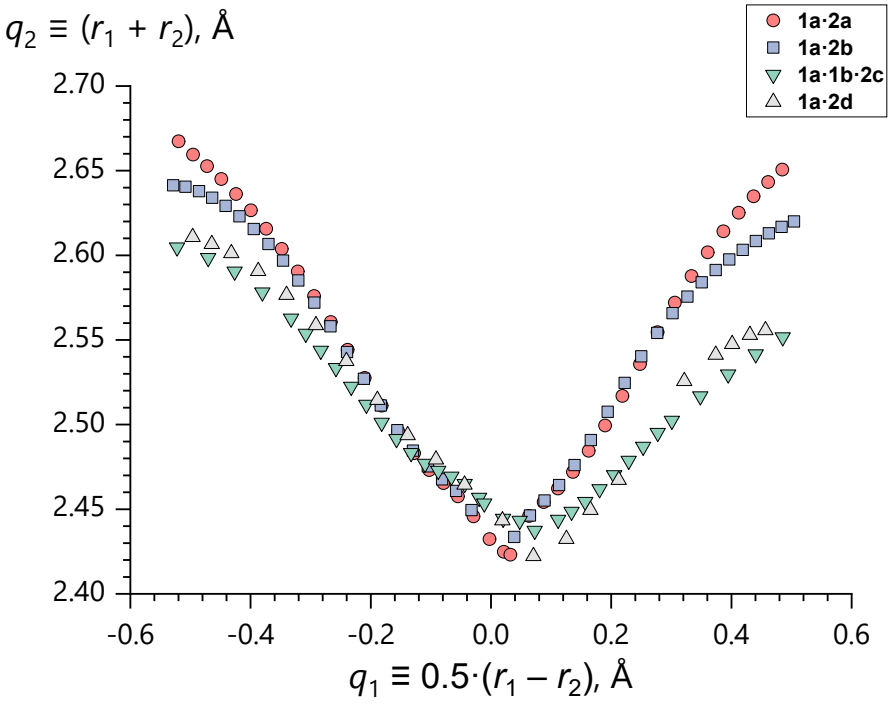
Figure S19. Interdependencies of the SeO–H···OSe and SeO···H–N bond geometries upon the coherent quasi-adiabatic transfer of the SeO–H···OSe bridging protons in **1a·1b·2c** and **1a·2d**.

Figs. S18,S19 show the dependencies of the O–H···O and O···H–N interatomic distances on the SeO–H r_1 distance. As expected, the r_1 and r_2 distances are strongly interdependent and in the vicinity of the H-bond center can be approximated by Steiner equation for O–H···O bonds in the solid state.[25] In all four cases there is no double proton transfer in O–H···O and O···H–N bonds: the H-bond between selenate and protonated N-heterocycle remains in an O···H–N configuration upon the whole proton transfer in the O–H···O bond ($r_3 > r_4$, $r_5 > r_6$, $r_7 > r_8$; see also numerical values in Tables S8–S11). In a way, the interdependence between r_1 and r_3/r_5/r_7 could be read 'backwards': the pronounced proton shift in the O–H···O bond can be induced by a relatively weak perturbation in a form of slight change of the O…N separation controlled by the proton-accepting ability of the given N-heterocycle.[26]

It is interesting to see how the O–H···O and O···H–N bonds can be classified into cooperative or anti-cooperative ones. Anti-cooperativity means that the strengthening (weakening) of one H-bond causes the weakening (strengthening) of the other one. In opposite, cooperativity means a symbatic strengthening or weakening of the coupled H-bonds. Apart of energetic cooperativity (in terms of strengthening/weakening), the geometric cooperativity is often considered (in terms of shortening/lengthening of H-bonds). Here, each crystal should be addressed individually. In **1a·2b**, the coupling scheme remains anti-cooperative over the entire proton transfer pathway. In **1a·2a**, the coupling scheme of two H-bonds changes from anti-cooperative to cooperative one after the SeO–H proton crossed the H-bond center. In **1a·1b·2c**, in the first half of the proton transfer pathway between selenate moieties, the O–H···O bond is coupled cooperatively with the r_3-r_4 O···H–N bond and anti-cooperatively with the r_5-r_6 O···H–N bond. In the second half of the proton transfer pathway, *i.e*. when the SeO–H proton crossed the H-bond center, the footing is reversed: the O···H–O bond interacts cooperatively with the r_5-r_6 bond and anti-cooperatively with the r_3-r_4 one. Finally, in **1a·2d**, the situation is similar: the cooperativity and anti-cooperativity with each one of the three O···H–N bonds reverses along the SeO–H proton transfer pathway, and the H-bond geometrical rearrangements are followed by the protonation of water molecule by the $HSeO_4^{\ominus}$ moiety (not shown, see Table S11). We shall point out that due to the extreme complexity of **1a·2d** and utmost shallow character of the proton transfer potential in the vicinity of the SeO–H···OSe bond's center, the obtained geometric interdependencies are not as smooth as one would expect.

Apparently, the geometric effects of H-bond coupling are most vivid in the case of systems with the 'isolated' SeO–H···OSe bonds, namely, **1a·1b·2c** and **1a·2d**, indicating their proneness of charge relay upon the gradual proton transfer.

Correlation between q_1 and q_2.



Potential energy surfaces for **1a·2a**, **1a·2b**, **1a·1b·2c** and **1a·2d** were calculated by varying the r_1 coordinate and optimizing all other internal coordinates in relaxed conditions; they are plotted in the main text in Figures 7 and 8 as functions of the q_1 coordinate.

The question arises as to how the q_1 and q_2 coordinates are related. The Figure above shows that for all studied crystalline systems, a universal correlation seems to be fulfilled: the q_2 coordinate decreases approximately up to the H-bond center and commences to increase once the bridging proton (deuteron) is preferentially located on the other side. Such correlation has been previously observed by Steiner[25] and reproduced computationally numerous times, see, *e.g.*, Refs. 26–29.

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