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DFT Calculation of IR Absorption Spectra for PCE- n H₂O, TCE- n H₂O, DCE- n H₂O, VC- n H₂O for Small and Water-Dominated Molecular Clusters

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14. ABSTRACT Calculations are presented of vibrational absorption spectra for energy minimized structures of PCE-nH ₂ O, TCE-nH ₂ O, DCE-nH ₂ O, and VC-nH ₂ O molecular clusters using density function theory (DFT). DFT can provide interpretation of absorption spectra with respect to molecular structure for excitation by electromagnetic waves at frequencies within the IR range. The absorption spectrum corresponding to excitation states of these molecular clusters, which consist of relatively small numbers of atoms, should be associated with response features that are intermediate between that of isolated molecules and that of bulk systems. DFT calculated absorption spectra represent quantitative estimates that can be correlated with additional information obtained from laboratory measurements. The DFT software GAUSSIAN was used for the calculations of excitation states presented here.					
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Introduction

The properties of PCE- $n\text{H}_2\text{O}$, TCE- $n\text{H}_2\text{O}$, DCE- $n\text{H}_2\text{O}$ and VC- $n\text{H}_2\text{O}$ molecular clusters are of major importance for monitoring and detection of chlorinated hydrocarbons in water. This follows in that tetrachloroethylene (PCE), trichloroethylene (TCE), dichloroethylene (DCE) and vinyl chloride (VC), which are part of a specific chemical transformation sequence ending in ethene, are among toxic and carcinogenic contaminants commonly found in the environment, e.g., ground water. The transformation sequence for PEC to ethane is shown in Fig. (1). The detection of these hydrocarbons, especially in the presence of water, using methods based on infrared (IR) spectroscopy is of particular interest. Specifically, IR spectral signatures, i.e., fingerprint spectra, can be correlated with the presence of these hydrocarbons (see reference [1]). Accordingly, the molecular structure and IR absorption spectra of these clusters is important for understanding the scattering and absorption of radiation transmitted through ambient environments, which is for purposes of detecting target materials of interest. For example, detection methodologies using lasers require knowledge of IR absorption spectra associated with different types of ambient molecules, e.g., H_2O , in order to apply background subtraction or spectral-signature-correlation algorithms, which would enhance spectral features associated with specific materials targeted for detection. The present study presents investigation of structures and properties of PCE- $n\text{H}_2\text{O}$, TCE- $n\text{H}_2\text{O}$, DCE- $n\text{H}_2\text{O}$ and VC- $n\text{H}_2\text{O}$ molecular clusters using DFT. The molecular-level dielectric response of these clusters, within the IR range of frequencies for vibrational excitation by electromagnetic waves, should be of interest for interpretation of spectral signatures associated with detection methodologies.

Density functional theory (DFT) is applied to determine energy optimized structures and absorption spectra for PCE- $n\text{H}_2\text{O}$, TCE- $n\text{H}_2\text{O}$, DCE- $n\text{H}_2\text{O}$ and VC- $n\text{H}_2\text{O}$ molecular clusters. DFT applied for the determination of equilibrium molecular structures and absorption spectra provides information complementary to that of experimental results. In this study, DFT calculated vibrational modes are associated with different structures of molecular clusters. In particular, DFT is used for calculation of ground state resonance structure to enable physical interpretation of absorption spectra associated with molecular structures excited by IR electromagnetic waves. Such spectra are attributed to optically active vibrational modes. In these studies the DFT calculations were implemented using the computer program GAUSSIAN09 (G09) [2].

The report is organized as follows. First, a general review of vibrational analysis needed for calculation of absorption spectra is presented. Second, DFT calculations of energy-minimized structures and vibration resonance structure for PCE-nH₂O, TCE-nH₂O, DCE-nH₂O and VC-nH₂O molecular clusters are presented. The vibration resonance structure of these molecular clusters provides estimates of their IR spectra and interpretation of spectral features with respect to molecular structure. Finally, a conclusion is presented.

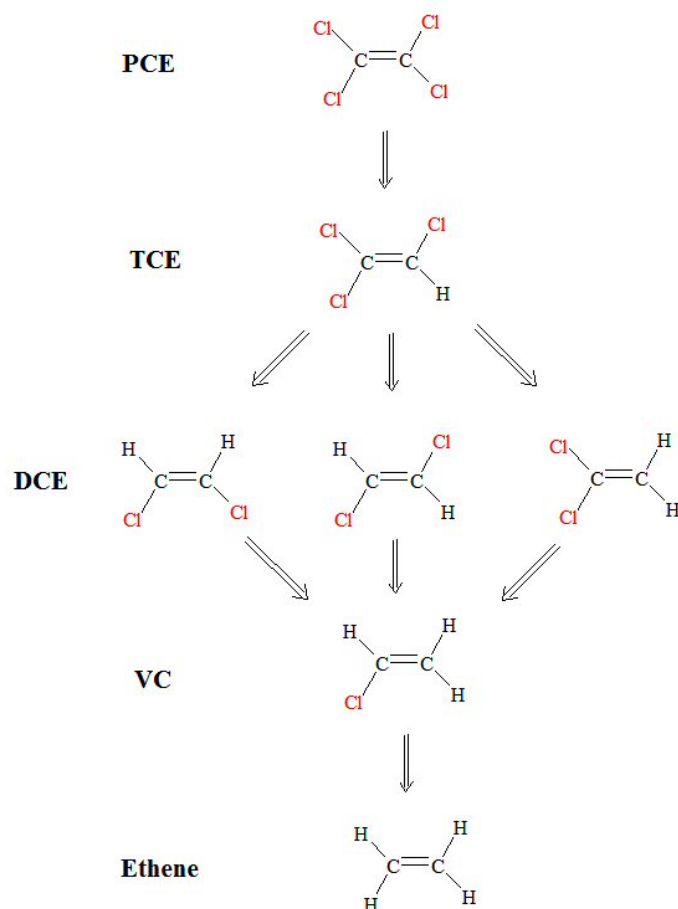


Figure 1. Transformation sequence for PCE to Ethene.

Calculation of Absorption Spectra using DFT

This section describes the formalism underlying DFT calculations and the procedure for calculation of absorption spectra corresponding to vibrational states, which the present study considers. Although descriptions of this formalism have been presented many times previously, a review of vibrational analysis needed for calculation of absorption spectra is given again for

completeness. The DFT software GAUSSIAN09 (G09) can be used to compute an approximation of the IR absorption spectrum of a molecule or molecule [2, 3]. This program calculates vibrational frequencies by determining second derivatives of the energy with respect to the Cartesian nuclear coordinates, and then transforming to mass-weighted coordinates at a stationary point of the geometry. The IR absorption spectrum is obtained using density functional theory to compute the ground state electronic structure in the Born-Oppenheimer approximation using Kohn-Sham density functional theory [4-9]. GAUSSIAN uses specified orbital basis functions to describe the electronic wavefunctions and density. For a given set of nuclear positions, the calculation directly gives the electronic charge density of the molecule, the potential energy V , and the displacements in Cartesian coordinates of each atom. The procedure for vibrational analysis used in GAUSSIAN is described in reference [3], and is reviewed in reference [9].

The procedure followed by GAUSSIAN is based on the fact the vibrational spectrum depends on the Hessian matrix $\mathbf{f}_{\text{CART}}$, which is constructed using the second partial derivatives of the potential energy V with respect to displacements of the atoms in Cartesian coordinates. Accordingly, the elements of the $3N \times 3N$ matrix $\mathbf{f}_{\text{CART}}$ are given by

$$f_{\text{CART}ij} = \left(\frac{\partial^2 V}{\partial \xi_i \partial \xi_j} \right)_0 \quad (\text{Eq 1})$$

where $\{\xi_1, \xi_2, \xi_3, \xi_4, \xi_5, \xi_6, \dots, \xi_{3N}\} = \{\Delta x_1, \Delta y_1, \Delta z_1, \Delta x_2, \Delta y_2, \Delta z_2, \dots, \Delta z_N\}$, which are displacements in Cartesian coordinates, and N is the number of atoms. As discussed above, the zero subscript in Eq.(1) indicates that the derivatives are taken at the equilibrium positions of the atoms, and that the first derivatives are zero. Given the Hessian matrix defined by Eq.(1) the operations for calculation of the vibrational spectrum require that the Hessian matrix Eq.(1) be transformed to mass-weighted Cartesian coordinates according to the relation

$$f_{\text{MWC}ij} = \frac{f_{\text{CART}ij}}{\sqrt{m_i m_j}} = \left(\frac{\partial^2 V}{\partial q_i \partial q_j} \right)_0, \quad (\text{Eq 2})$$

where $\{q_1, q_2, q_3, q_4, q_5, q_6, \dots, q_{3N}\} = \{\sqrt{m_1} \Delta x_1, \sqrt{m_1} \Delta y_1, \sqrt{m_1} \Delta z_1, \sqrt{m_2} \Delta x_2, \sqrt{m_2} \Delta y_2, \sqrt{m_2} \Delta z_2, \dots, \sqrt{m_N} \Delta z_N\}$ are the mass-weighted Cartesian coordinates. GAUSSIAN computes the energy second derivatives Eq.(2), thus computing the forces for displacement perturbations of each atom

along each Cartesian direction. The first derivatives of the dipole moment with respect to atomic positions $\partial \vec{\mu} / \partial \xi_i$ are also computed. Each vibrational eigenmode leads to one peak in the absorption spectrum, at a frequency equal to the mode's eigenfrequency ν_n . The absorption intensity corresponding to a particular eigenmode n , whose eigenfrequency is ν_n , is given by

$$I_n = \frac{\pi}{3c} \left| \sum_{i=1}^{3N} \frac{\partial \vec{\mu}}{\partial \xi_i} l_{\text{CART}im} \right|^2, \quad (\text{Eq 3})$$

where $\mathbf{l}_{\text{CART}}$ is the matrix whose elements are the displacements of the atoms in Cartesian coordinates, and is determined as follows. First,

$$\mathbf{l}_{\text{CART}} = \mathbf{M} \mathbf{l}_{\text{MWC}}, \quad (\text{Eq 4})$$

where $\mathbf{l}_{\text{MWC}}$ is the matrix whose elements are the displacements of the atoms in mass-weighted Cartesian coordinates and $\mathbf{M}$ is a diagonal matrix defined by the elements

$$M_{ii} = \frac{1}{\sqrt{m_i}}. \quad (\text{Eq 5})$$

The matrix $\mathbf{l}_{\text{MWC}}$ is needed to diagonalize $\mathbf{f}_{\text{MWC}}$ defined by Eq.(2) such that

$$(\mathbf{l}_{\text{MWC}})^T \mathbf{f}_{\text{MWC}} (\mathbf{l}_{\text{MWC}}) = \mathbf{\Lambda}, \quad (\text{Eq 6})$$

where $\mathbf{\Lambda}$ is the diagonal matrix with eigenvalues λ_i . The procedure for diagonalizing Eq.(6) consists of the operations

$$\mathbf{f}_{\text{INT}} = (\mathbf{D})^T \mathbf{f}_{\text{MWC}} (\mathbf{D}) \quad (\text{Eq 7})$$

and

$$(\mathbf{L})^T \mathbf{f}_{\text{MWC}} (\mathbf{L}) = \mathbf{\Lambda}, \quad (\text{Eq 8})$$

where $\mathbf{D}$ is a matrix transformation to coordinates where rotation and translation have been separated out and $\mathbf{L}$ is the transformation matrix composed of eigenvectors calculated according to Eq.(8). The eigenfrequencies in units of (cm^{-1}) are calculated using the eigenvalues λ_n by the expression

$$\nu_{n0} = \frac{\sqrt{\lambda_n}}{2\pi c}, \quad (\text{Eq 9})$$

where c is the speed of light. The elements of $\mathbf{l}_{\text{CART}}$ are given by

$$l_{\text{CART}ki} = \sum_{j=1}^{3N} \frac{D_k L_{ji}}{\sqrt{m_j}}, \quad (\text{Eq 10})$$

where $k, i=1, \dots, 3N$, and the column vectors of these elements are the normal modes in Cartesian coordinates.

The intensity Eq.(3) must then be multiplied by the number density of molecules to give an absorption-line intensity in the non-interacting molecule approximation. It follows that the absorption spectrum calculated by GAUSSIAN is a sum of delta functions, whose line positions and coefficients correspond to the vibrational-transition frequencies and the absorption-line intensities, respectively. It should be noted that, in principle, these spectral components must be broadened and shifted to account for anharmonic effects such as finite mode lifetimes and inter-mode couplings.

Energy-Minimized Structures and Their IR Spectra

Results of a computational investigation using DFT concerning PCE-nH₂O, TCE-nH₂O, DCE-nH₂O and VC-nH₂O molecular structures are presented. These results include the energy-minimized configuration of these molecular structures, their ground-state oscillation frequencies and their IR intensities. The DFT calculations have resulted in molecular cluster geometries corresponding to energetically stable structures. For these calculations geometry energy optimization and vibrational analysis was effected using the DFT model B3LYP [10,11] and basis functions 6-311+G(d) [12,13]. These basis functions designate the 6-311G basis set supplemented by diffuse functions, indicated by the sign +, and polarization functions (d), having one set of d functions on heavy atoms [14]. Graphical representations of molecular geometries for stable molecular clusters consisting of PCE-nH₂O, TCE-nH₂O, DCE-nH₂O and VC-nH₂O and their IR spectra are shown in Figs. (2) through (54). The ground-state energies of these molecular clusters are given in Table 1. IR intensities as a function of frequency, for the molecular clusters and IR spectra shown in Figs. (2) through (54), are given in Tables 2 through 7 of appendices 1 through 6, respectively.

Conclusion

The DFT calculated absorption spectra given here provide information concerning molecular level dielectric response structure. The calculations of vibrational excited states associated with PCE-nH₂O, TCE-nH₂O, DCE-nH₂O and VC-nH₂O molecular clusters using DFT

are meant to serve as reasonable estimates of molecular level response characteristics, providing interpretation of dielectric response features with respect to molecular structure, for comparison with experimental measurements. We have studied here PCE-nH₂O, TCE-nH₂O, DCE-nH₂O and VC-nH₂O molecular clusters in order to quantify interpretation of their absorption spectra.

Acknowledgments

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Table 1. Ground-State Energies of Molecular Clusters

PCE+nH₂O energies after optimization (B3LYP/6-311++G(2d,2p))

	Energy [a.u.]	Imaginary Frequencies
PCE	-1917.09662	0
PCE+ 2H ₂ O	-2070.03241	0
PCE+ 5H ₂ O	-2299.44518	0
PCE+ 7H ₂ O	-2452.38532	0
PCE+ 10H ₂ O	-2681.82356	0
PCE+ 12H ₂ O	-2834.77528	0
PCE+ 16H ₂ O	-3140.70336	0
PCE+ 24H ₂ O	-3752.52865	0
PCE+ 39H ₂ O	-4899.71779	0

TCE+nH₂O energies after optimization (B3LYP/6-311++G(2d,2p))

	Energy [a.u.]	Imaginary Frequencies
TCE	-1457.48367	0
TCE+ 2H ₂ O	-1610.41917	0
TCE+ 5H ₂ O	-1839.84710	0
TCE+ 7H ₂ O	-1992.80605	0
TCE+ 10H ₂ O	-2222.20985	0
TCE+ 12H ₂ O	-2375.16146	0
TCE+ 16H ₂ O	-2681.09090	0
TCE+ 24H ₂ O	-3292.91835	0
TCE+ 39H ₂ O	-4440.10601	0

DCE1+nH₂O energies after optimization (B3LYP/6-311++G(2d,2p))

	Energy [a.u.]	Imaginary Frequencies
DCE1	-997.86746	0
DCE1+ 2H ₂ O	-1150.80346	0
DCE1+ 5H ₂ O	-1380.21935	0
DCE1+ 7H ₂ O	-1533.17591	0
DCE1+ 10H ₂ O	-1762.61288	0
DCE1+ 12H ₂ O	-1915.56197	0
DCE1+ 16H ₂ O	-2221.47471	0
DCE1+ 24H ₂ O	-2833.30587	0
DCE1+ 39H ₂ O	-3980.49129	0

DCE2+nH₂O energies after optimization (B3LYP/6-311++G(2d,2p))

	Energy [a.u.]	Imaginary Frequencies
DCE2	-997.86718	0
DCE2+ 2H ₂ O	-1150.80618	0
DCE2+ 5H ₂ O	-1380.23066	0
DCE2+ 7H ₂ O	-1533.18736	0
DCE2+ 10H ₂ O	-1762.61095	0
DCE2+ 12H ₂ O	-1915.57488	0
DCE2+ 16H ₂ O	-2221.47548	0
DCE2+ 24H ₂ O	-2833.30384	0
DCE2+ 39H ₂ O	-3980.49227	0

DCE3+nH₂O energies after optimization (B3LYP/6-311++G(2d,2p))

	Energy [a.u.]	Imaginary Frequencies
DCE3	-997.86479	0
DCE3+ 2H ₂ O	-1150.80283	0
DCE3+ 5H ₂ O	-1380.22515	0
DCE3+ 7H ₂ O	-1533.15484	0
DCE3+ 10H ₂ O	-1762.61277	0
DCE3+ 12H ₂ O	-1915.57015	0
DCE3+ 16H ₂ O	-2221.47192	0
DCE3+ 24H ₂ O	-2833.29831	0
DCE3+ 39H ₂ O	-3980.48844	0

VC+nH₂O energies after optimization (B3LYP/6-311++G(2d,2p))

	Energy [a.u.]	Imaginary Frequencies
VC	-538.24588	0
VC+ 2H ₂ O	-691.18428	0
VC+ 5H ₂ O	-920.59791	0
VC+ 7H ₂ O	-1073.56330	0
VC+ 10H ₂ O	-1302.98080	0
VC+ 12H ₂ O	-1455.93290	1
VC+ 16H ₂ O	-1761.85351	0
VC+ 24H ₂ O	-2373.68116	0
VC+ 39H ₂ O	-3520.86869	0

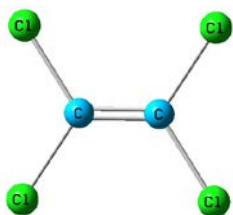


Figure 2A. Equilibrium geometry of isolated PCE molecule.

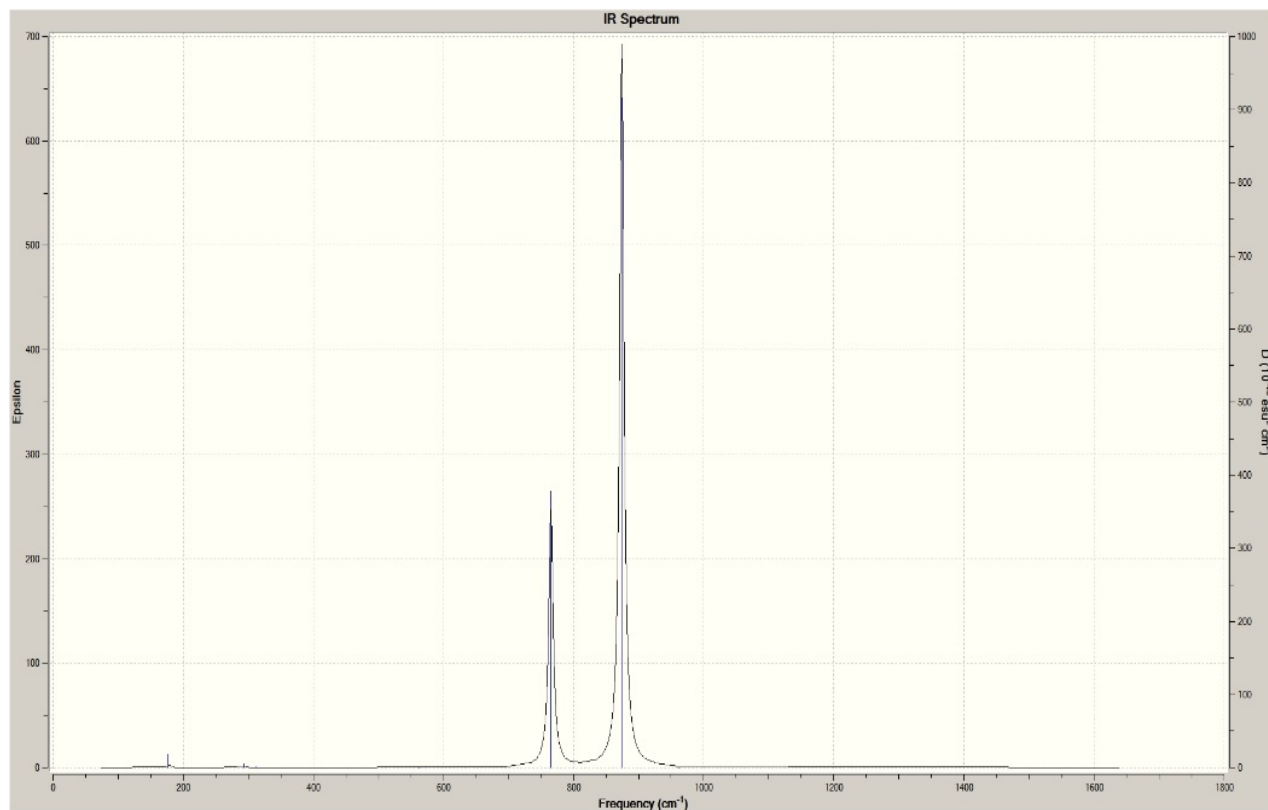


Figure 2B. IR spectrum of isolated PCE molecule.

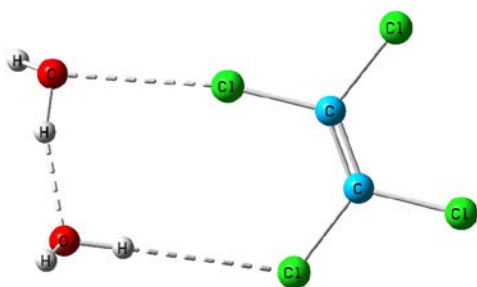


Figure 3A. Equilibrium geometry of PCE and 2 water molecules.

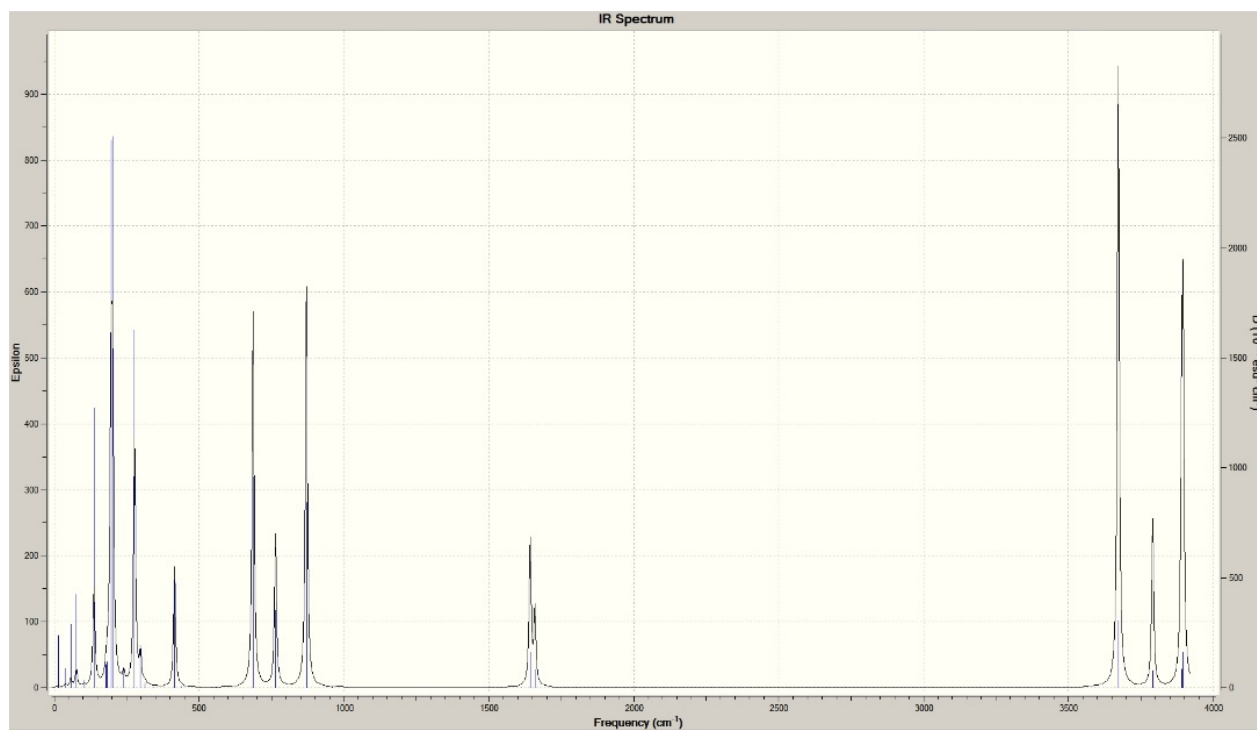


Figure 3B. IR spectrum of PCE and 2 water molecules.

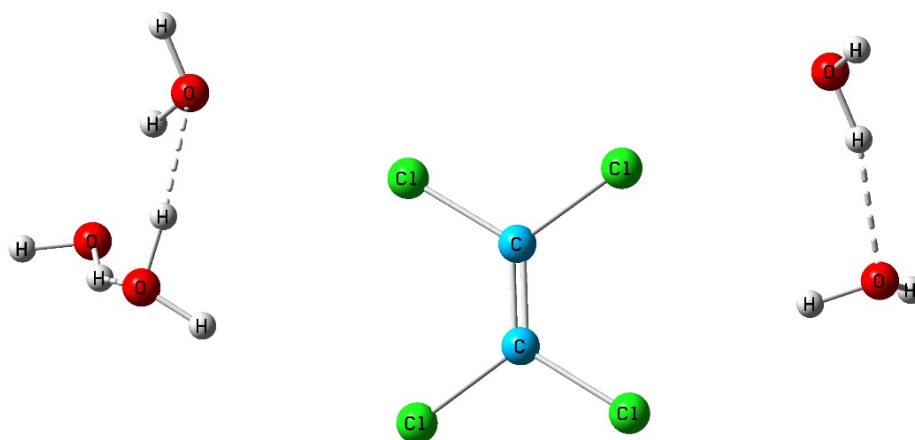


Figure 4A. Equilibrium geometry of PCE and 5 water molecules.

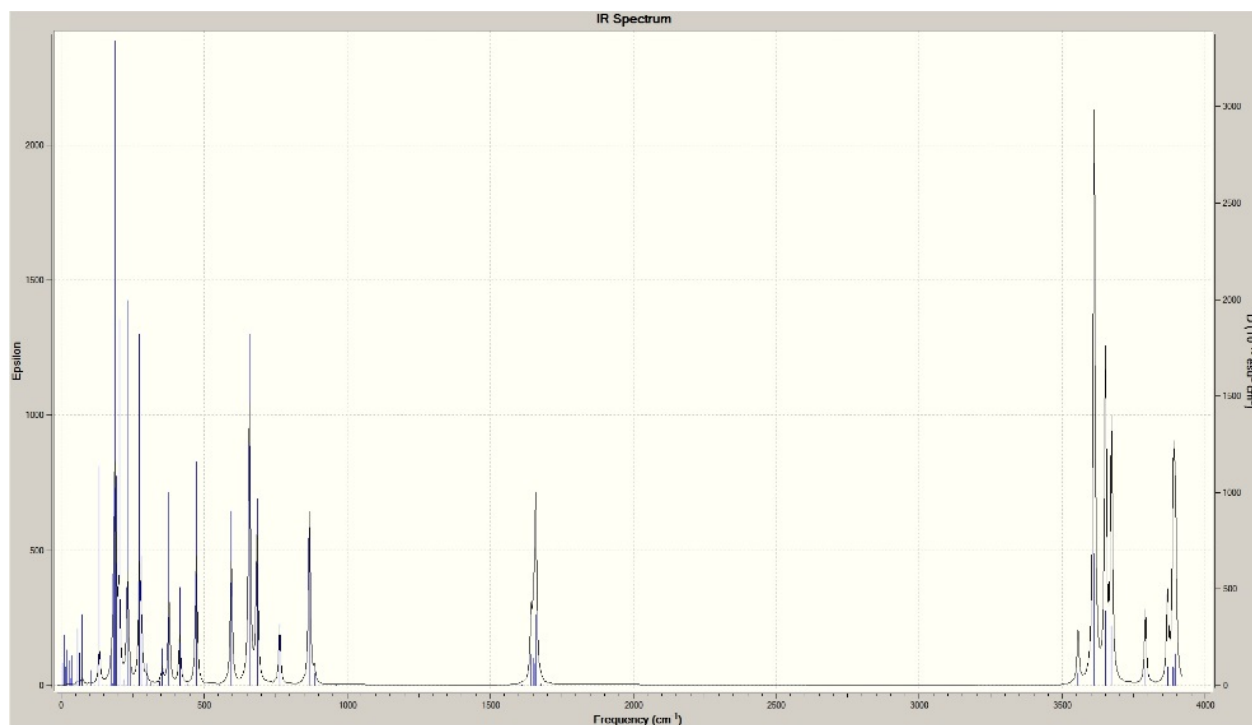


Figure 4B. IR spectrum of PCE and 5 water molecules.

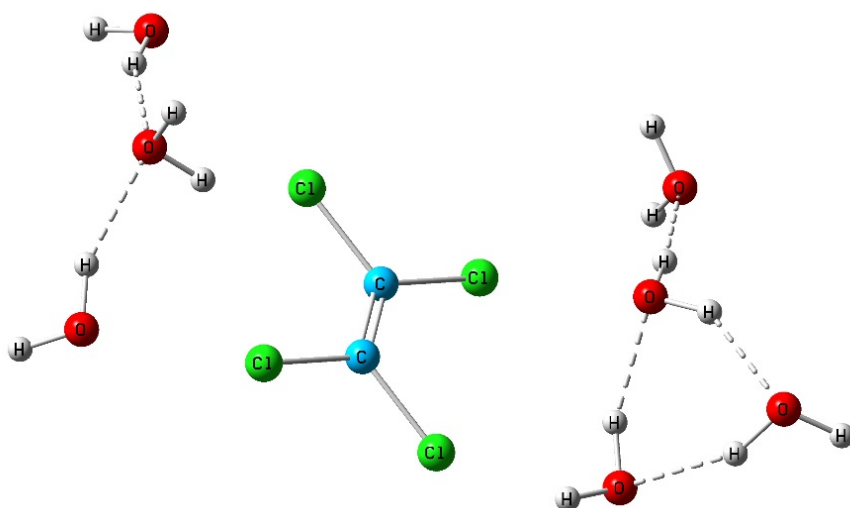


Figure 5A. Equilibrium geometry of PCE and 7 water molecules.

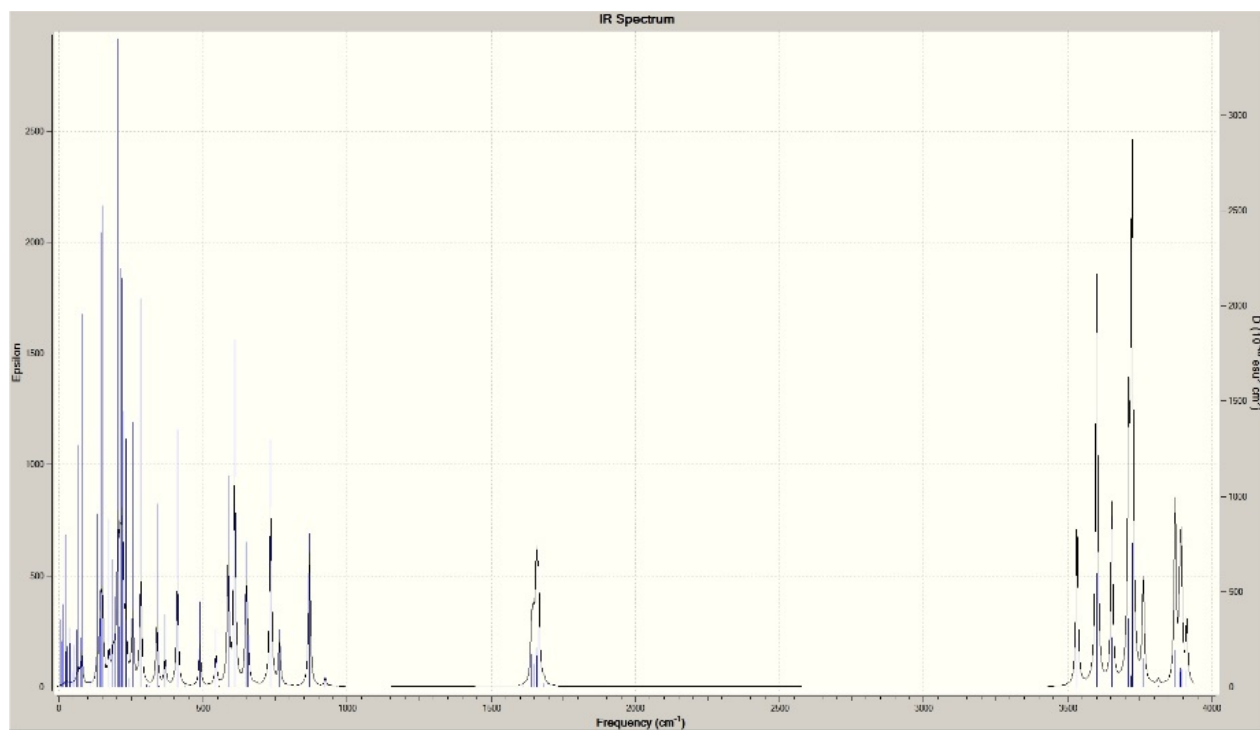


Figure 5B. IR spectrum of PCE and 7 water molecules.

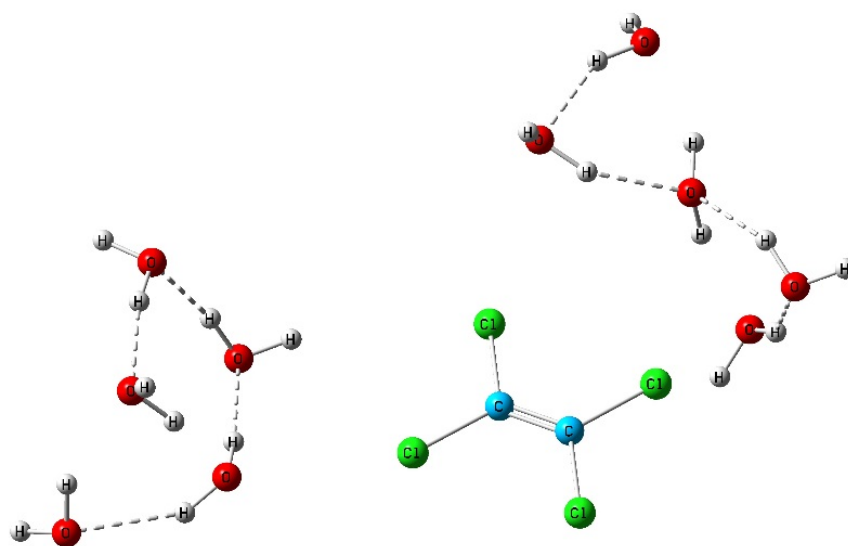


Figure 6A. Equilibrium geometry of PCE and 10 water molecules.

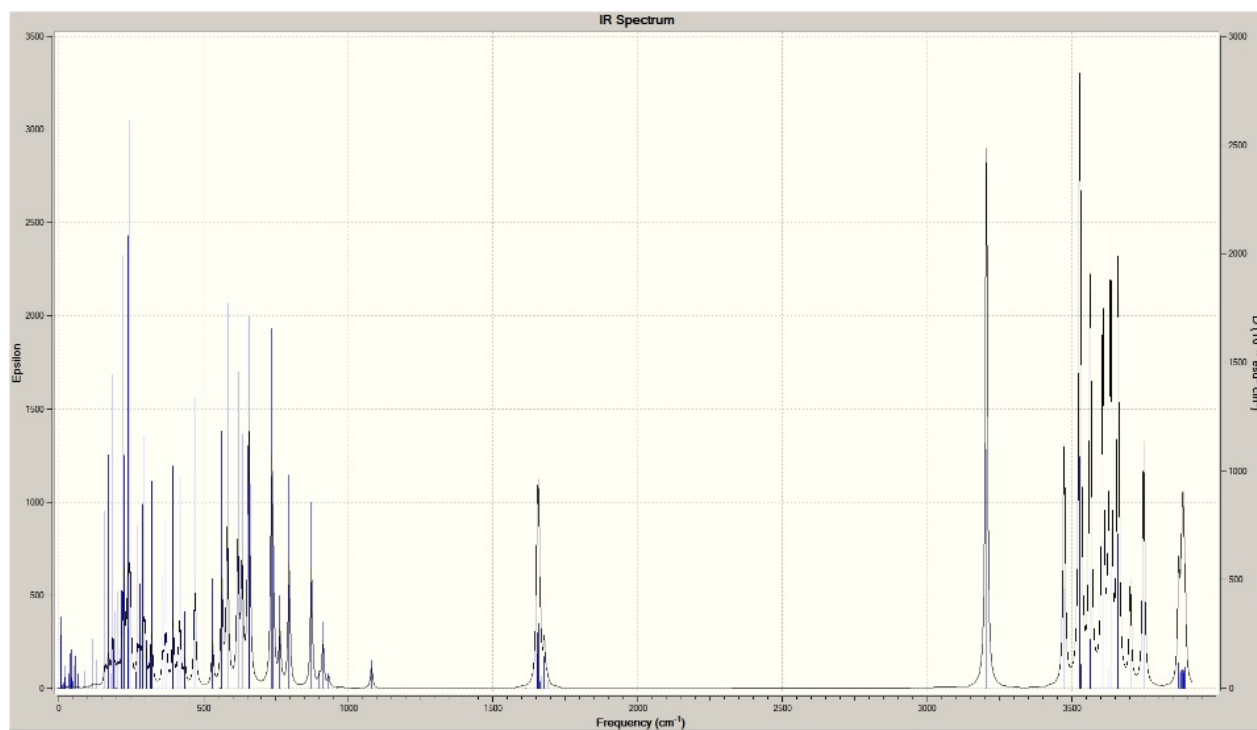


Figure 6B. IR spectrum of PCE and 10 water molecules.

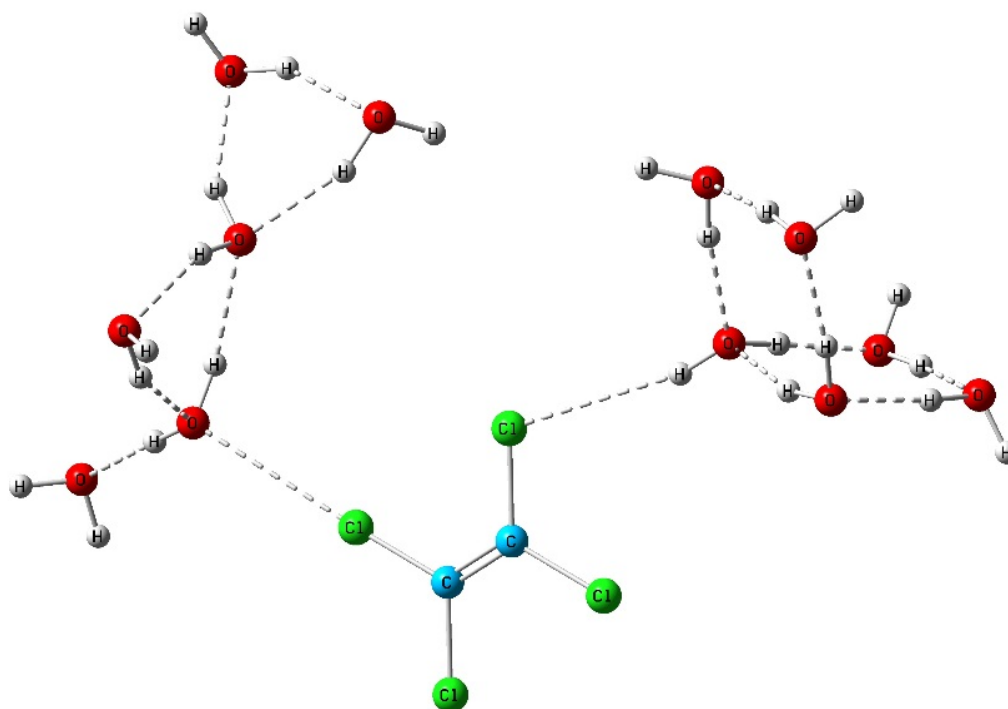


Figure 7A. Equilibrium geometry of PCE and 12 water molecules.

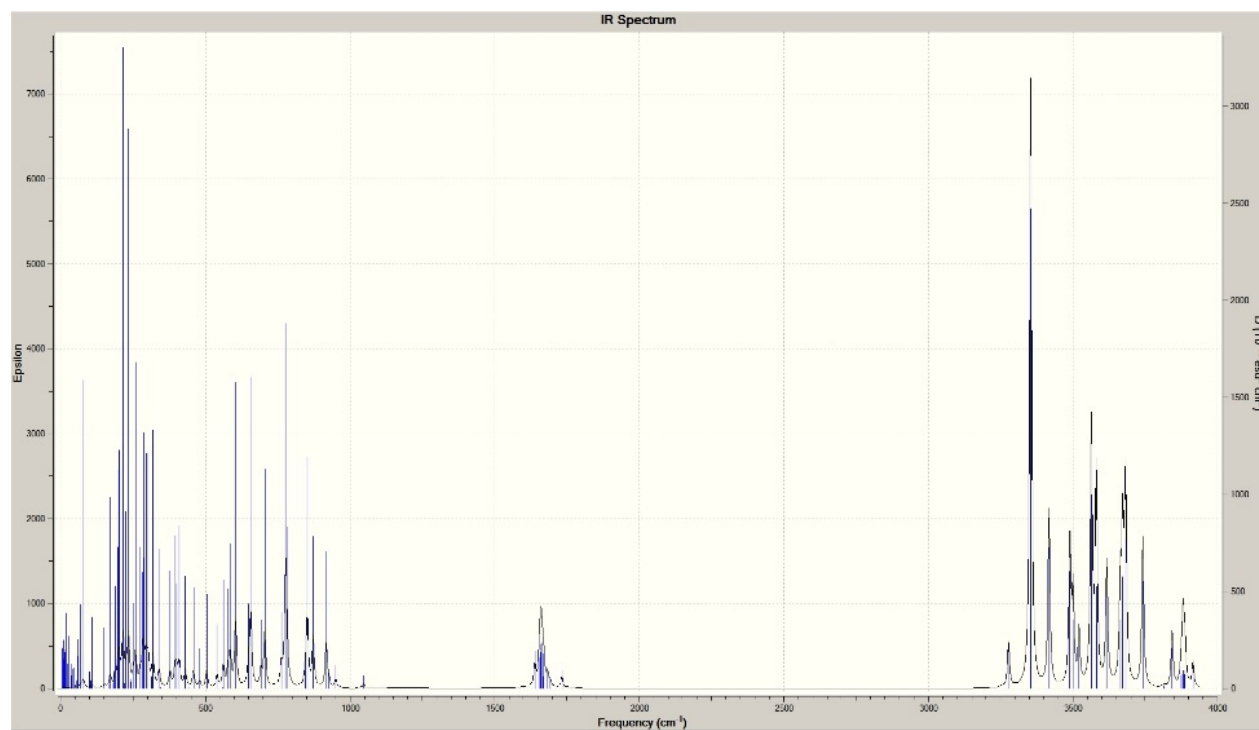


Figure 7B. IR spectrum of PCE and 12 water molecules.

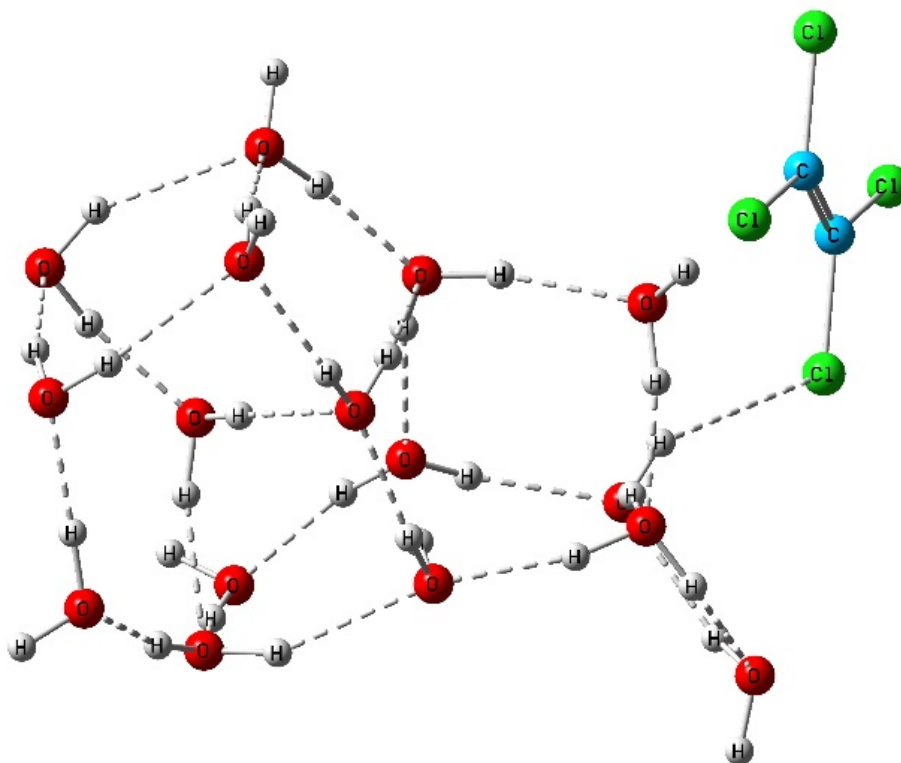


Figure 8A. Equilibrium geometry of PCE and 16 water molecules.

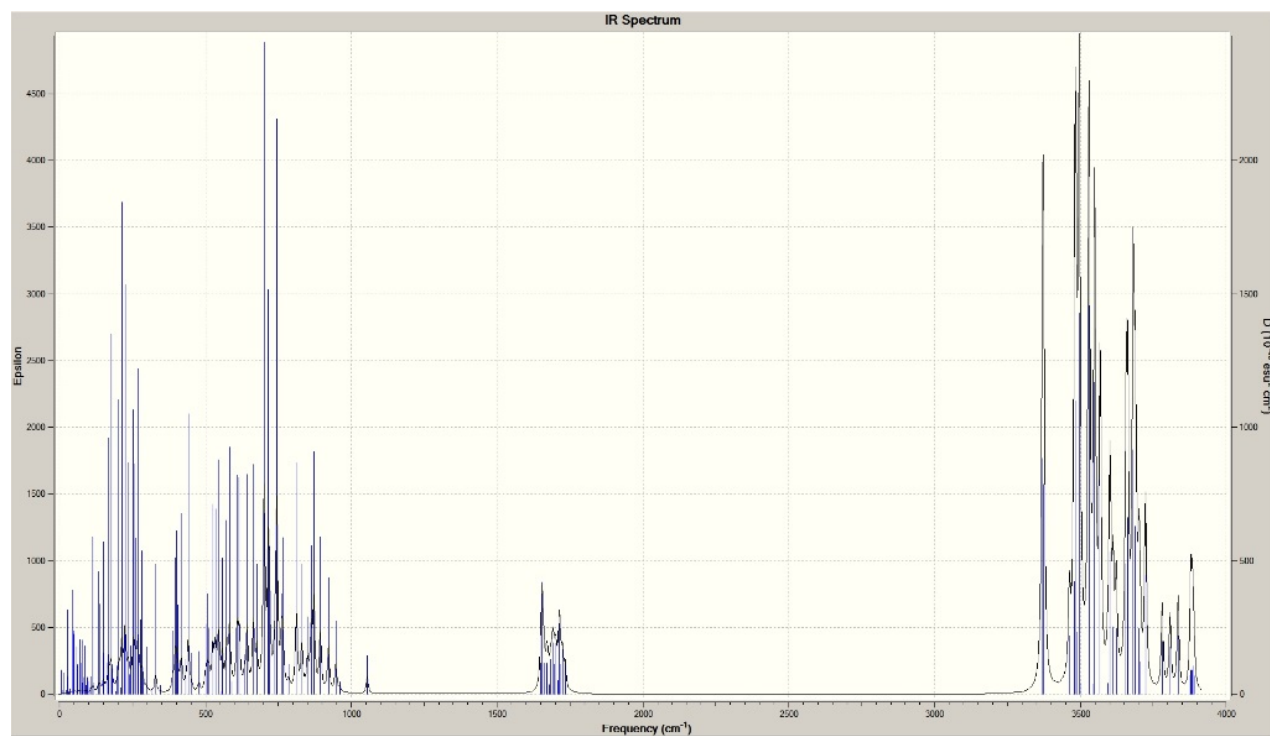


Figure 8B. IR spectrum of PCE and 16 water molecules.

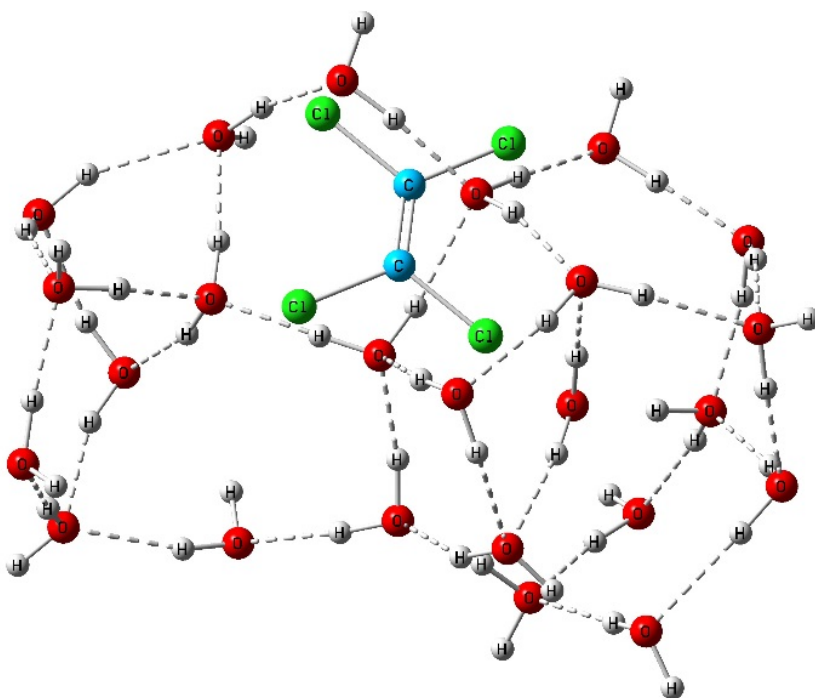


Figure 9A. Equilibrium geometry of PCE and 24 water molecules.

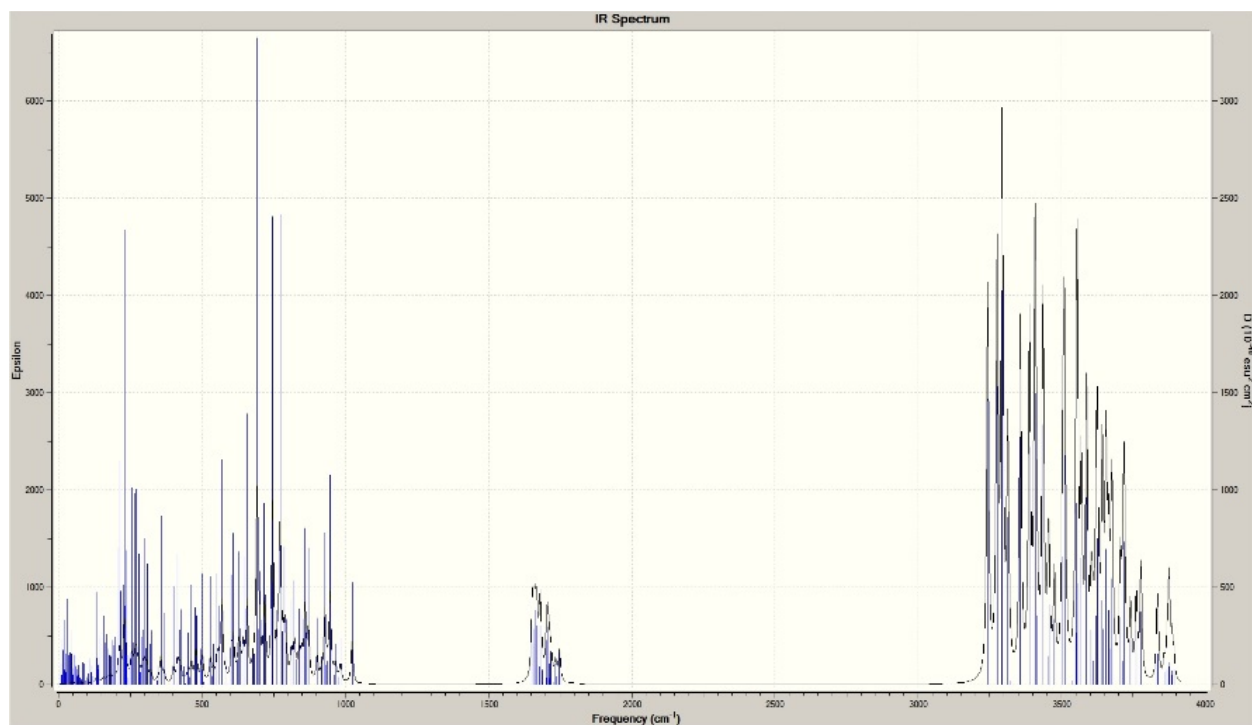


Figure 9B. IR spectrum of PCE and 24 water molecules.

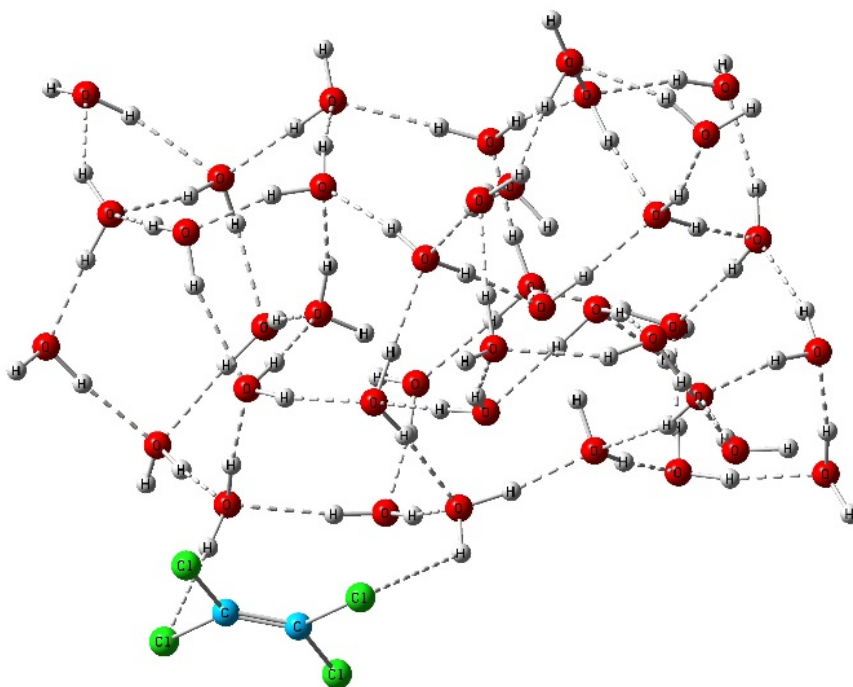


Figure 10A. Equilibrium geometry of PCE and 39 water molecules.

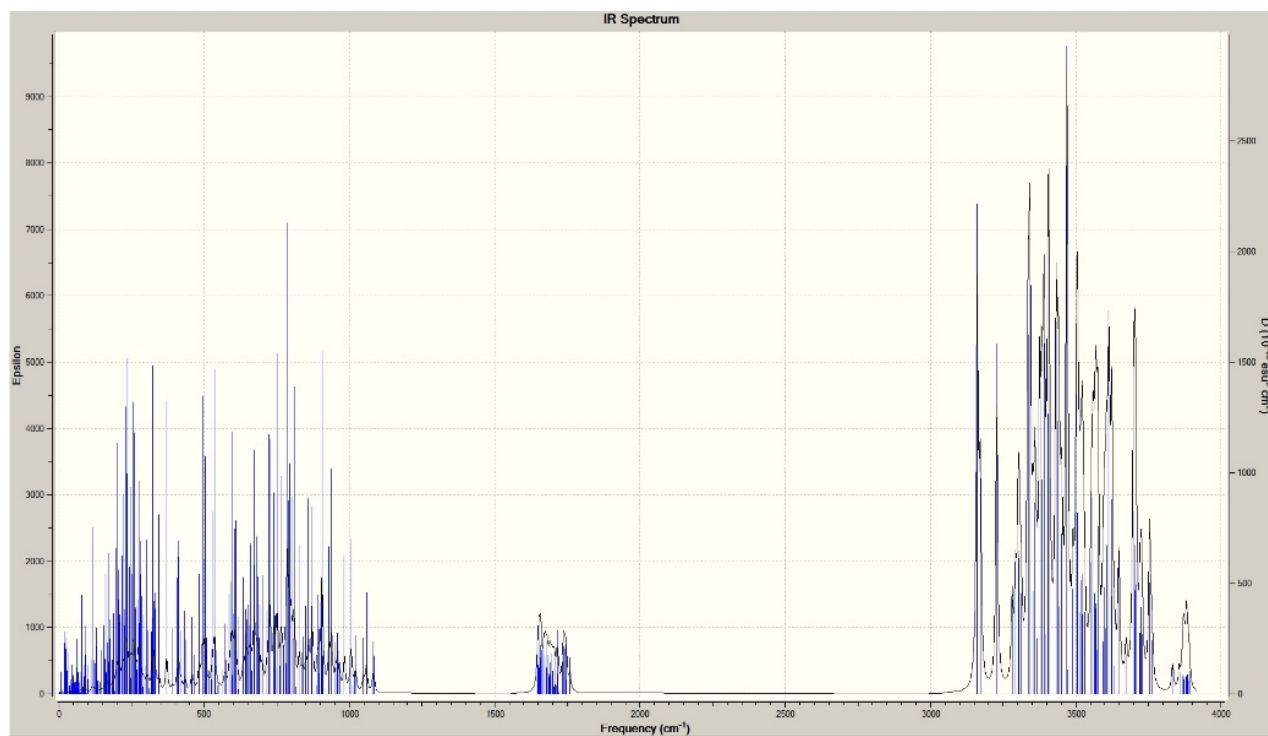


Figure 10B. IR spectrum of PCE and 39 water molecules.

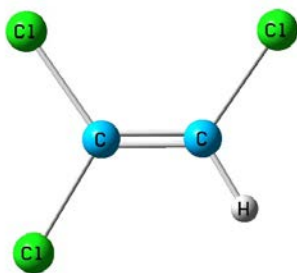


Figure 11A. Equilibrium geometry of isolated TCE molecule.

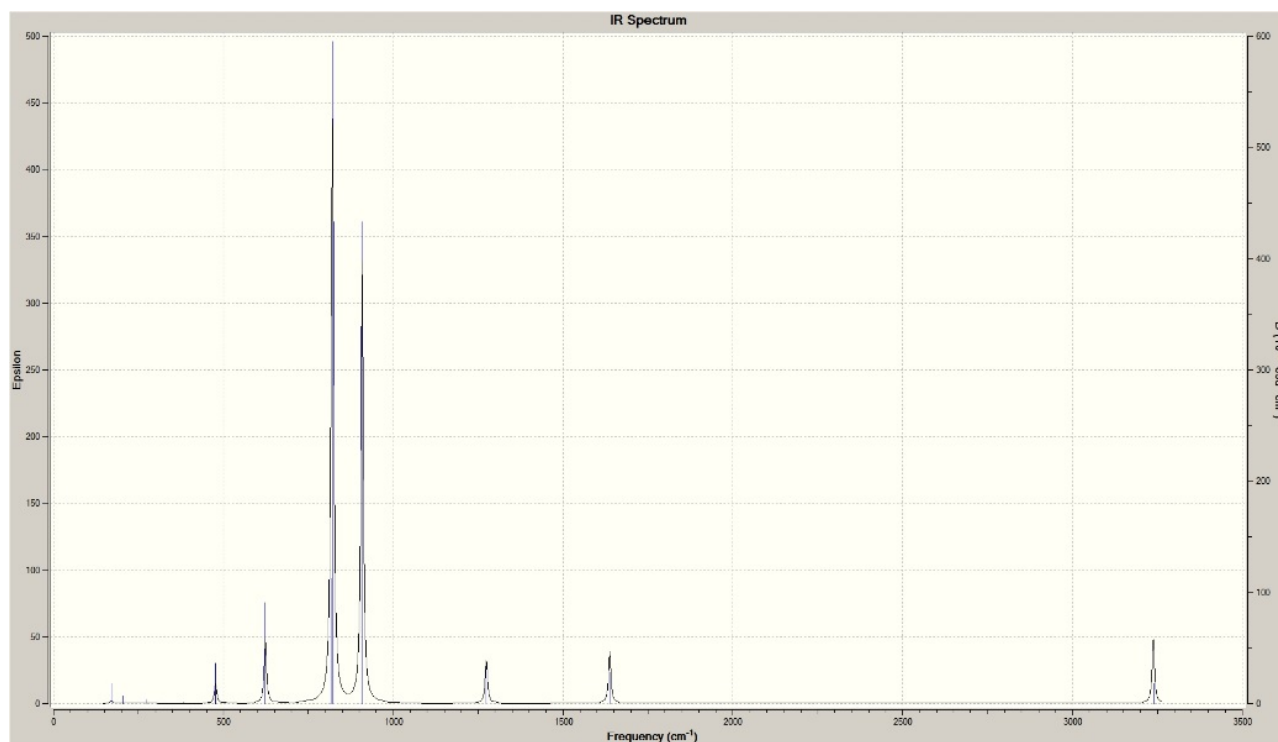


Figure 11B. IR spectrum of isolated TCE molecule.

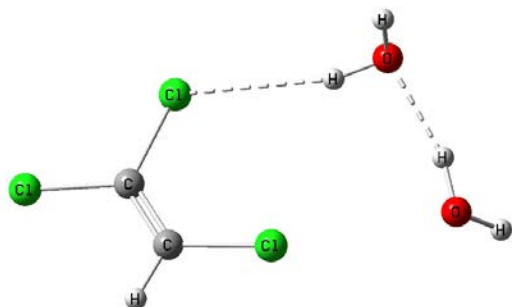


Figure 12A. Equilibrium geometry of TCE and 2 water molecules.

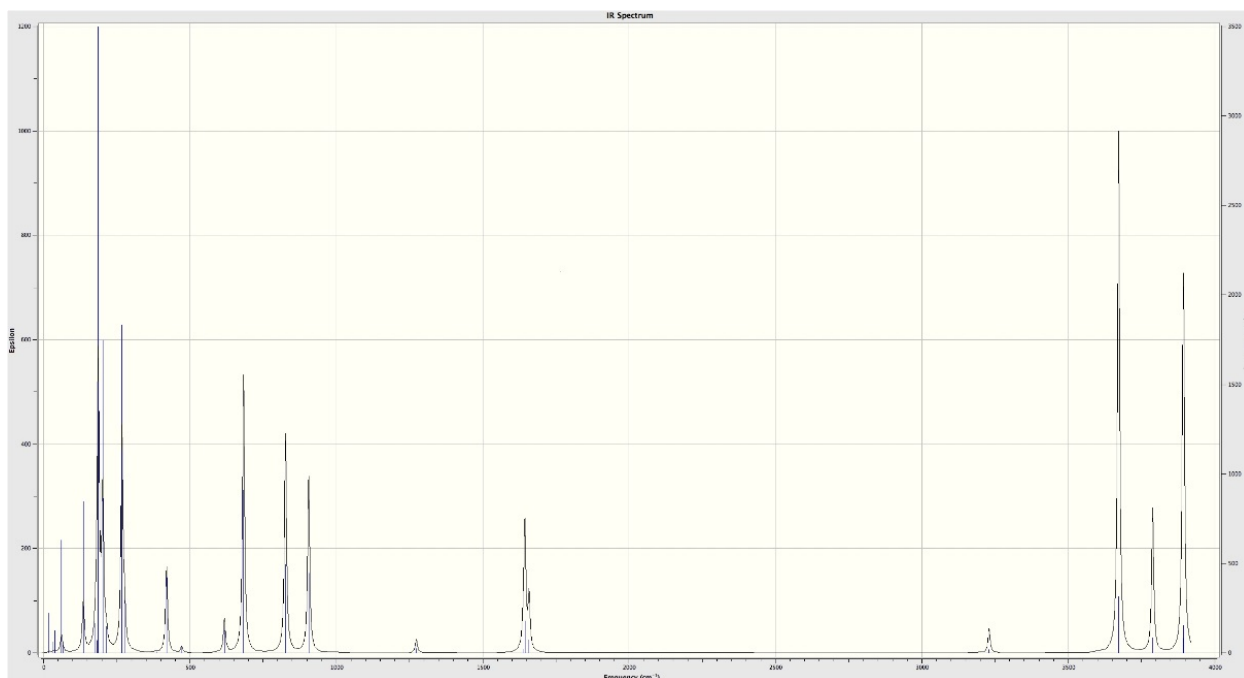


Figure 12B. IR spectrum of TCE and 2 water molecules.

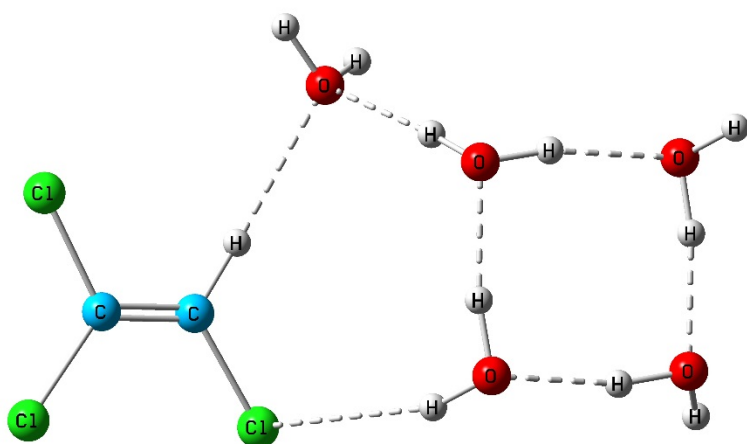


Figure 13A. Equilibrium geometry of TCE and 5 water molecules.

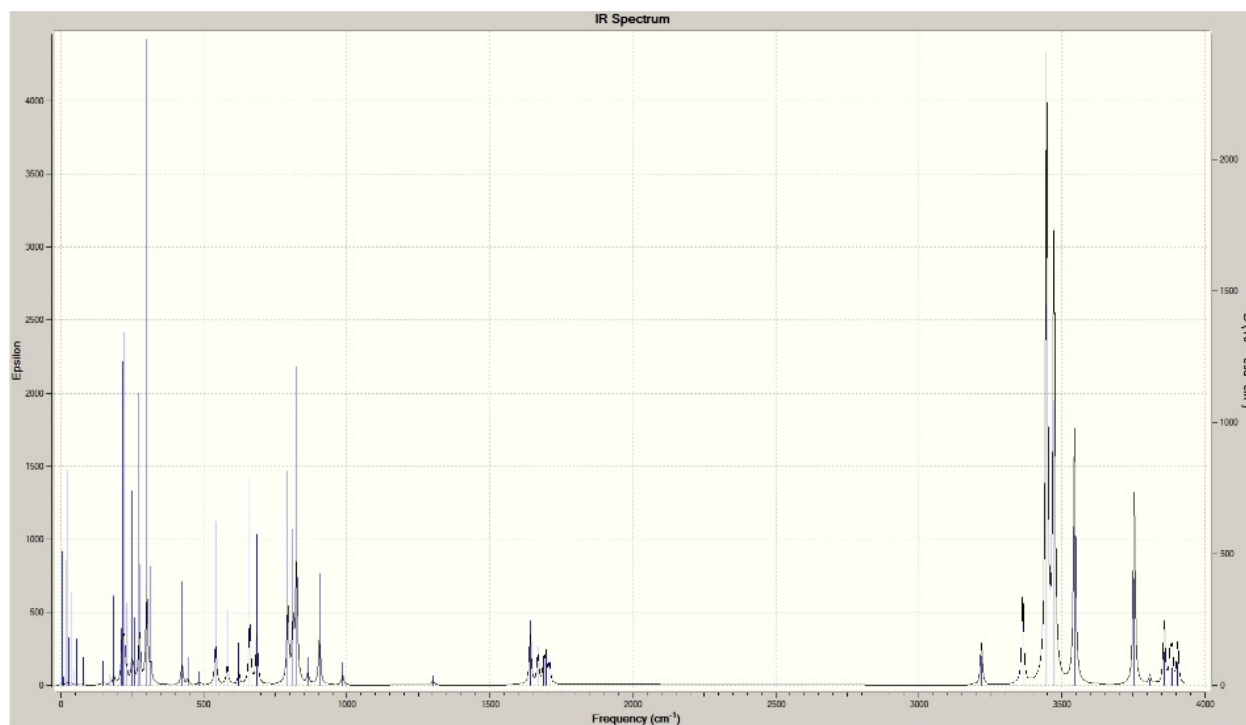


Figure 13B. IR spectrum of TCE and 5 water molecules.

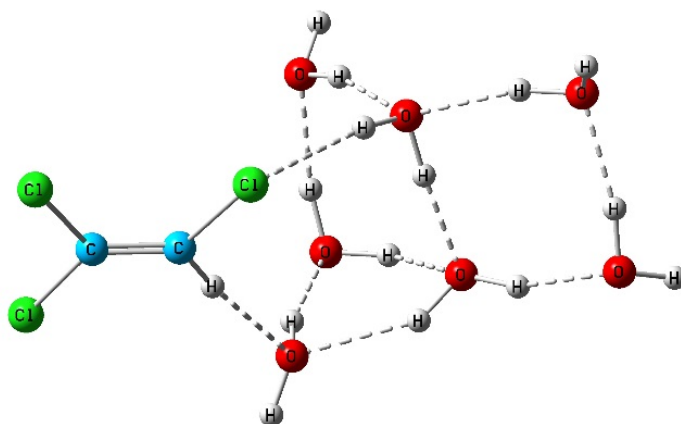


Figure 14A. Equilibrium geometry of TCE and 7 water molecules.

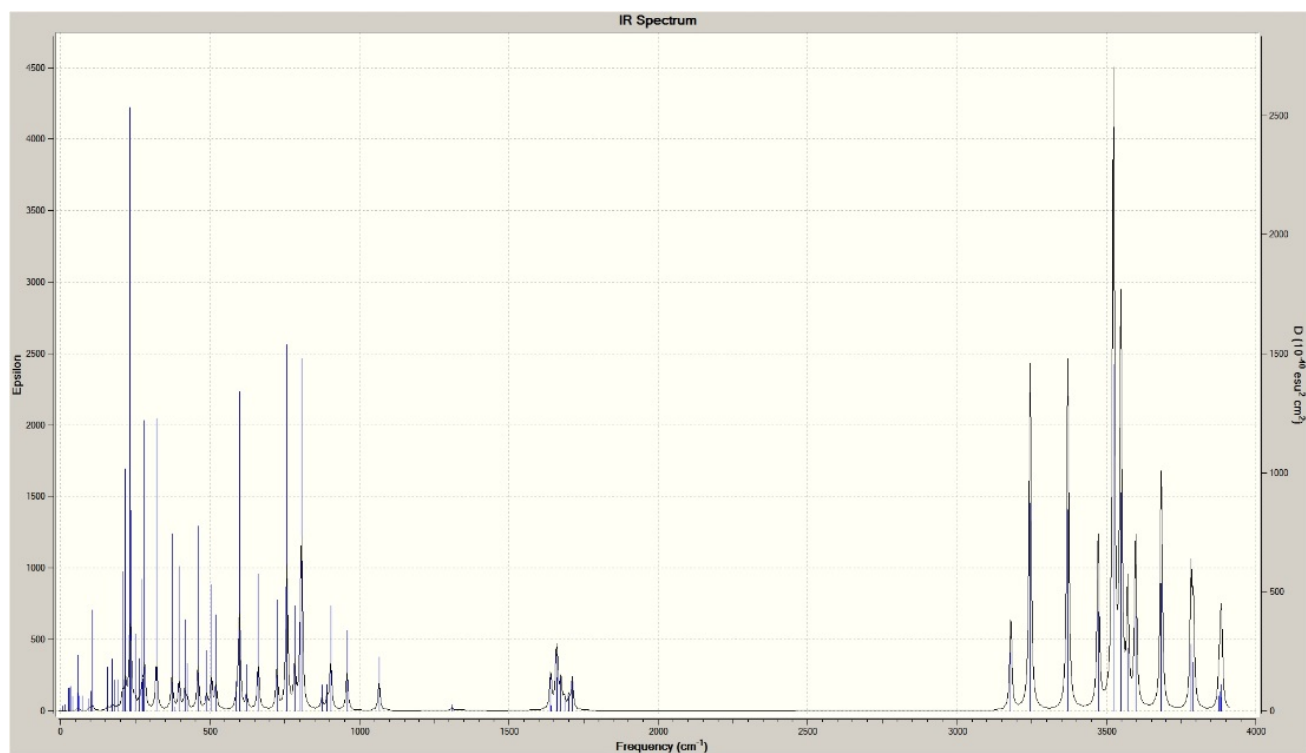


Figure 14B. IR spectrum of TCE and 7 water molecules.

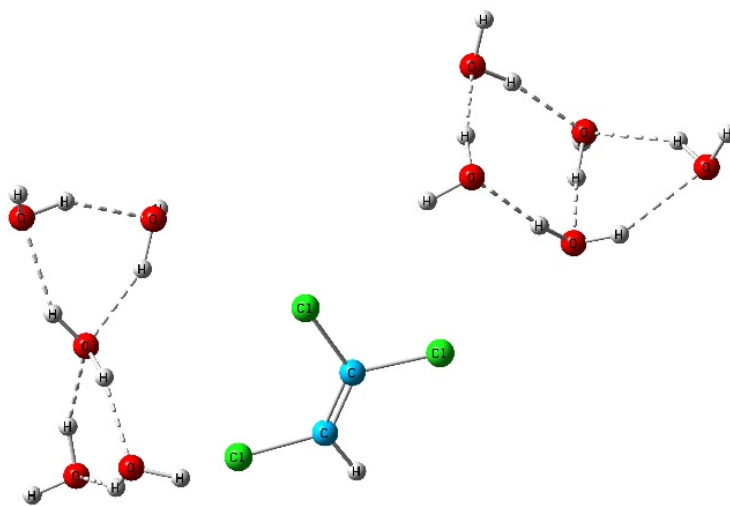


Figure 15A. Equilibrium geometry of TCE and 10 water molecules.

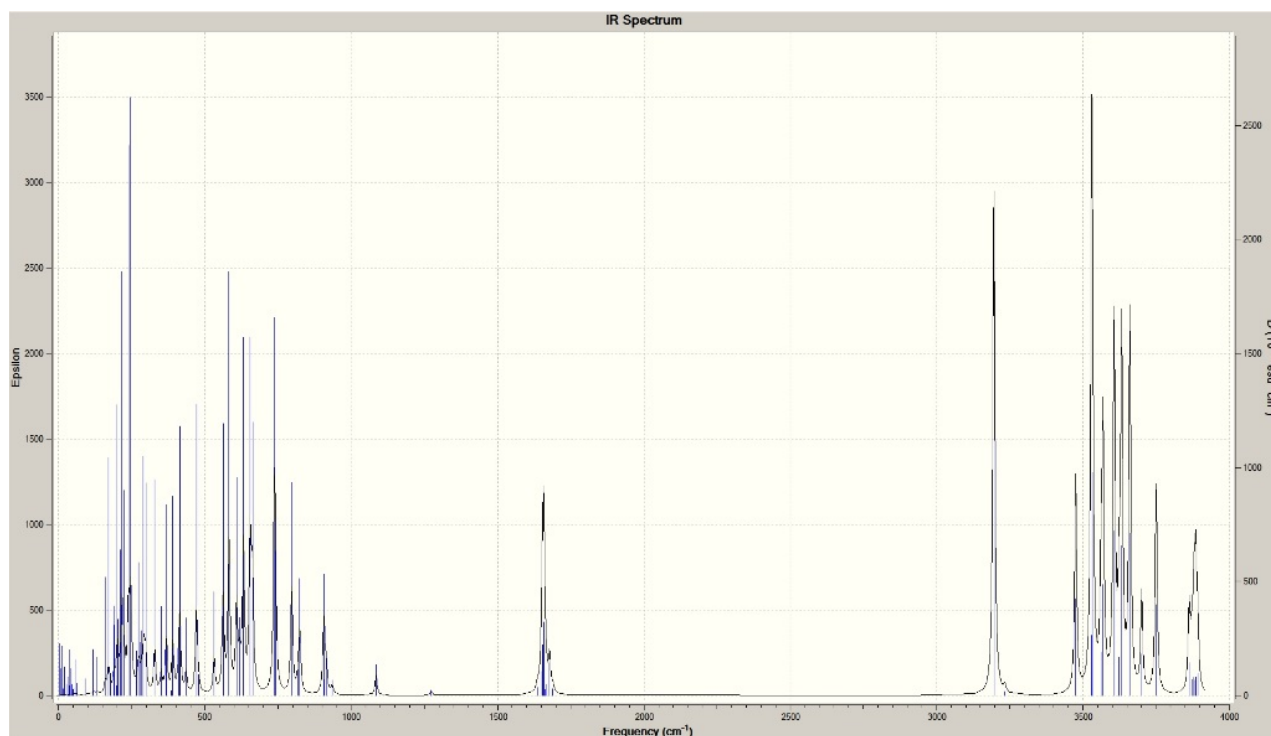


Figure 15B. IR spectrum of TCE and 10 water molecules.

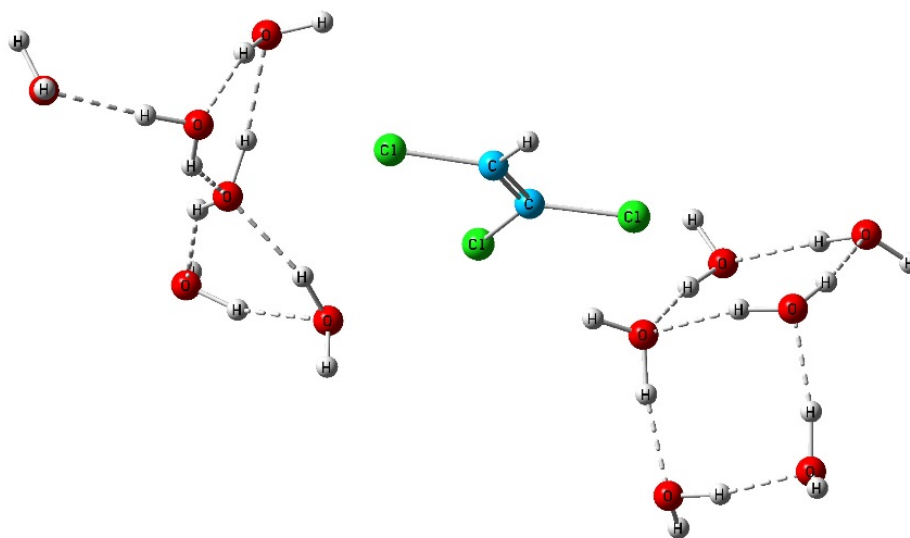


Figure 16A. Equilibrium geometry of TCE and 12 water molecules.

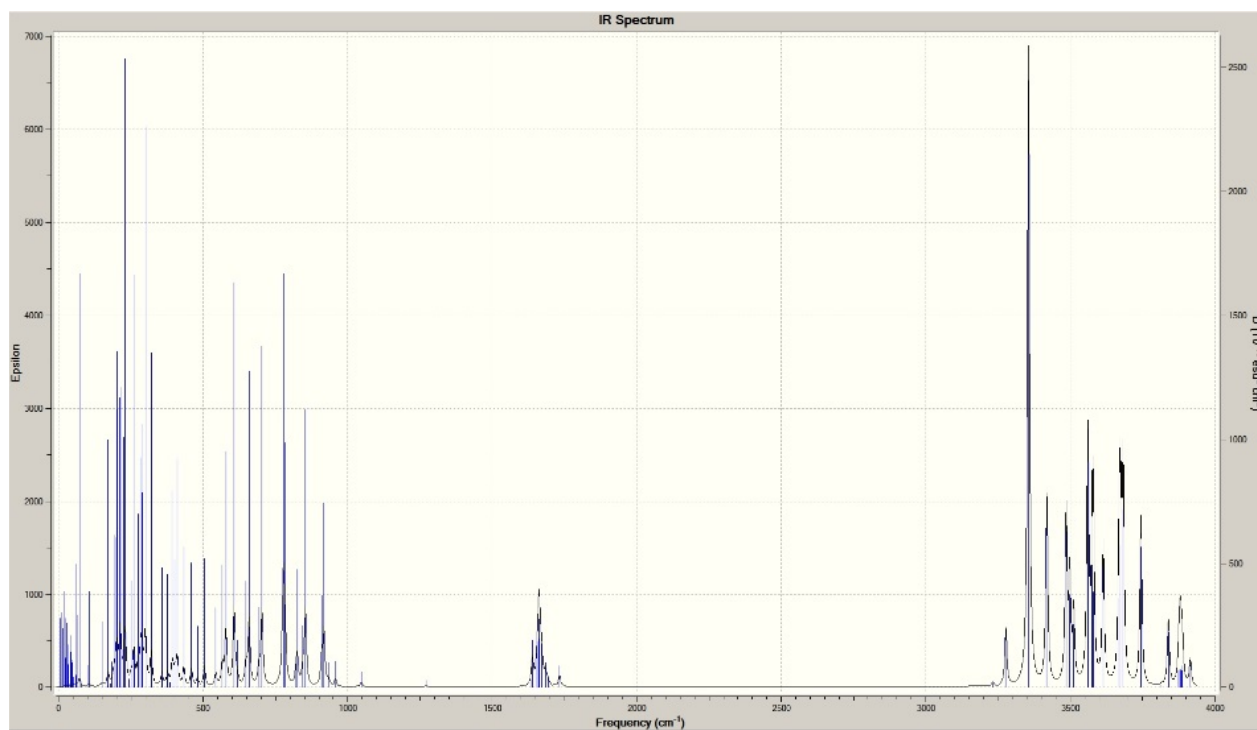


Figure 16B. IR spectrum of TCE and 12 water molecules.

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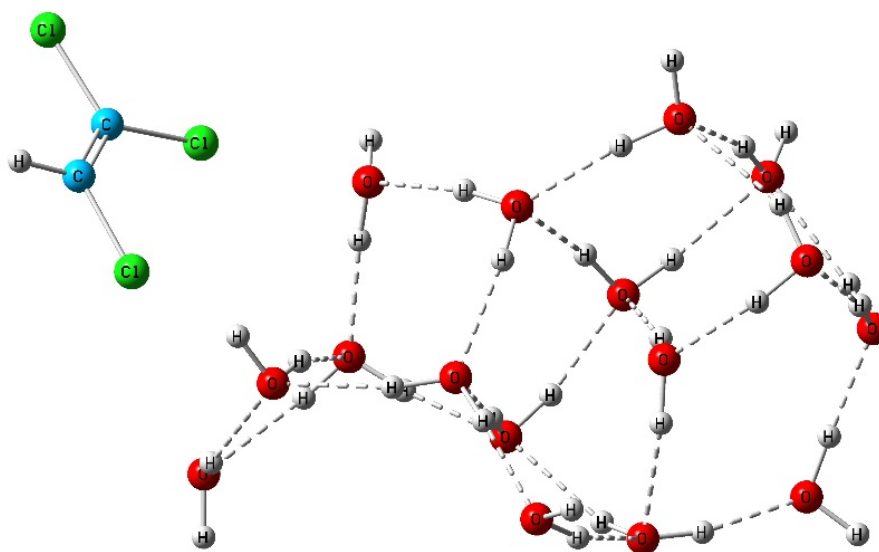


Figure 17A. Equilibrium geometry of TCE and 16 water molecules.

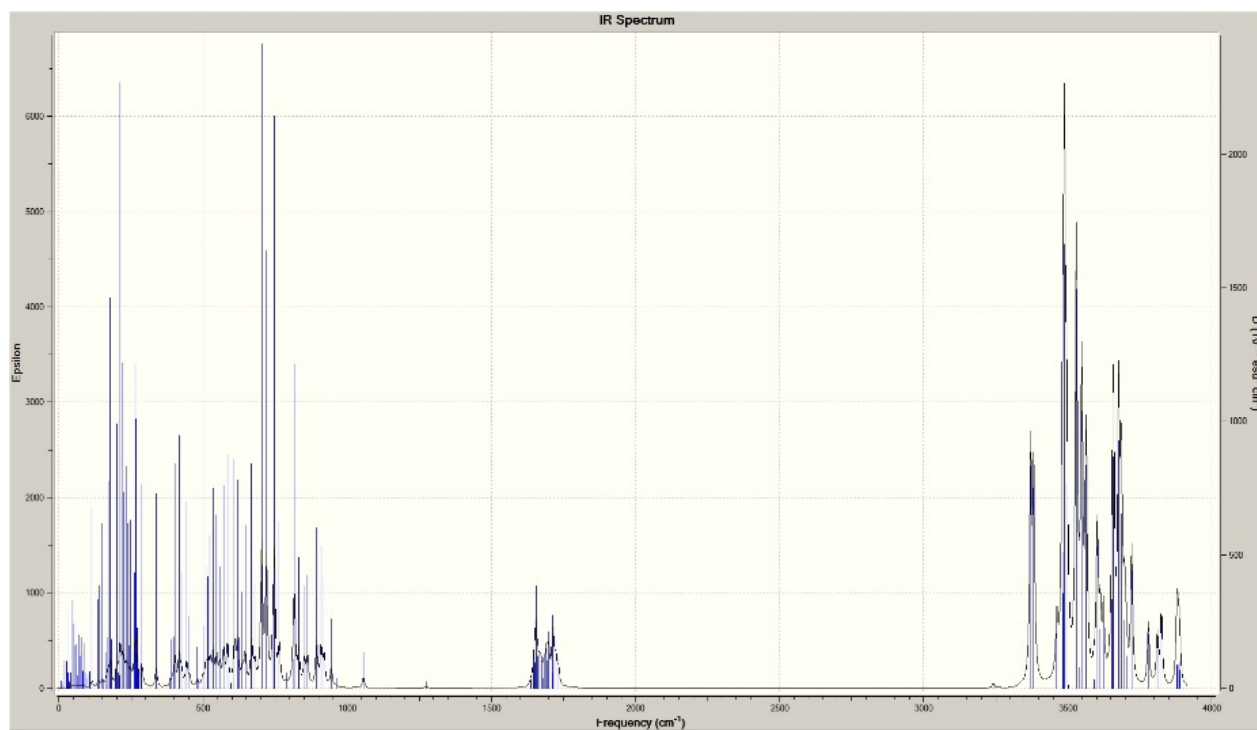


Figure 17B. IR spectrum of TCE and 16 water molecules.

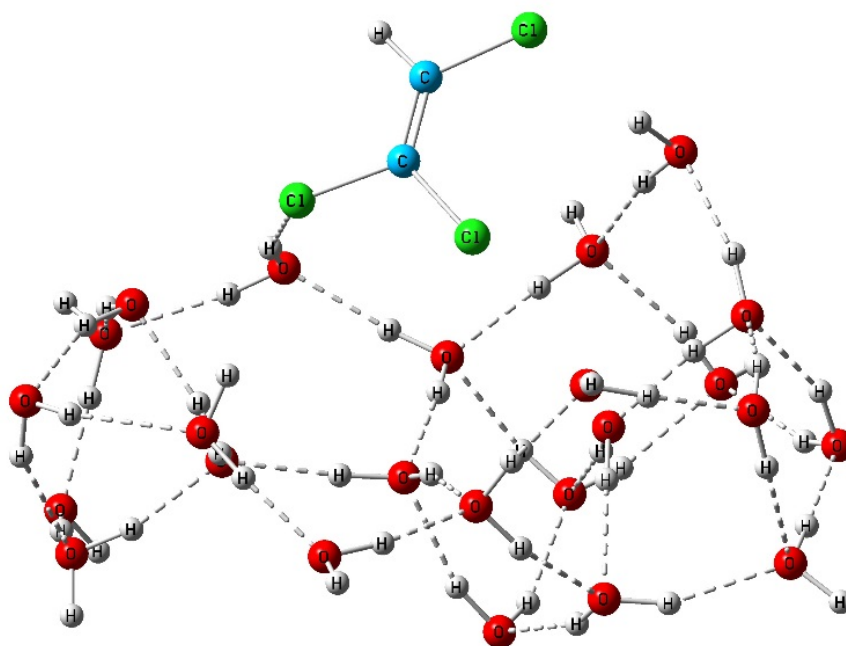


Figure 18A. Equilibrium geometry of TCE and 24 water molecules.

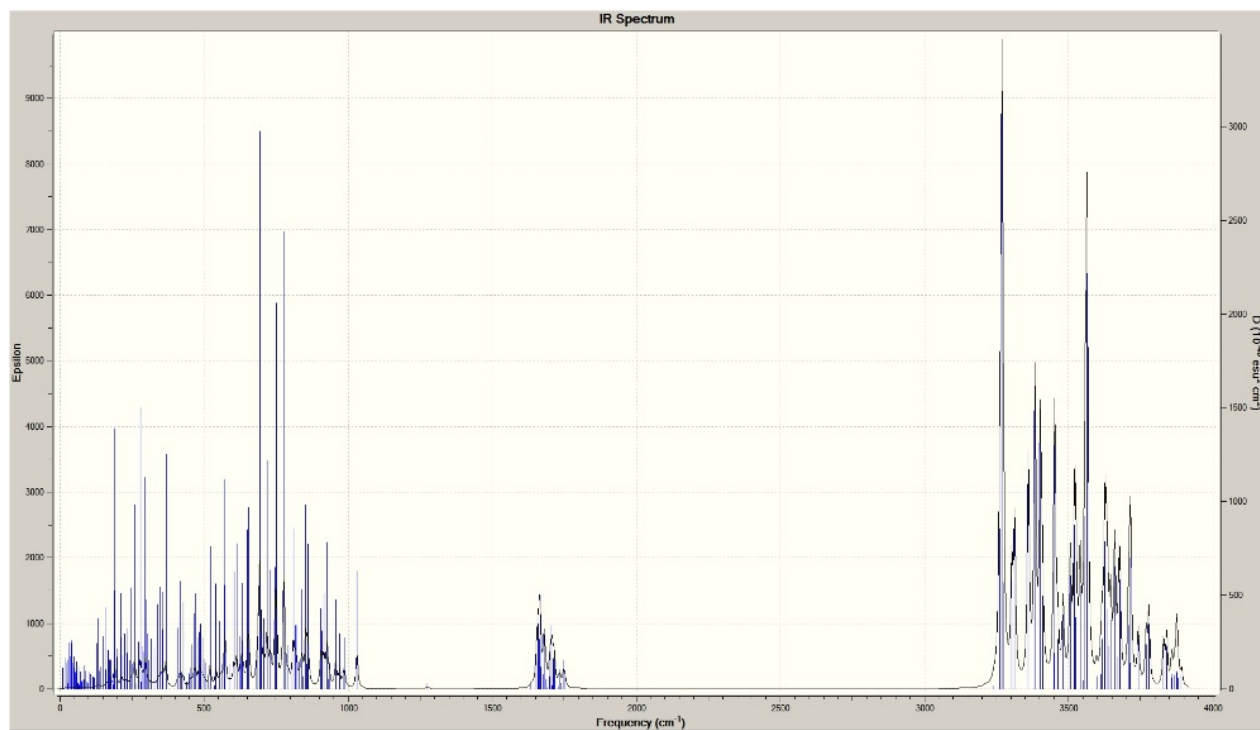


Figure 18B. IR spectrum of TCE and 24 water molecules.

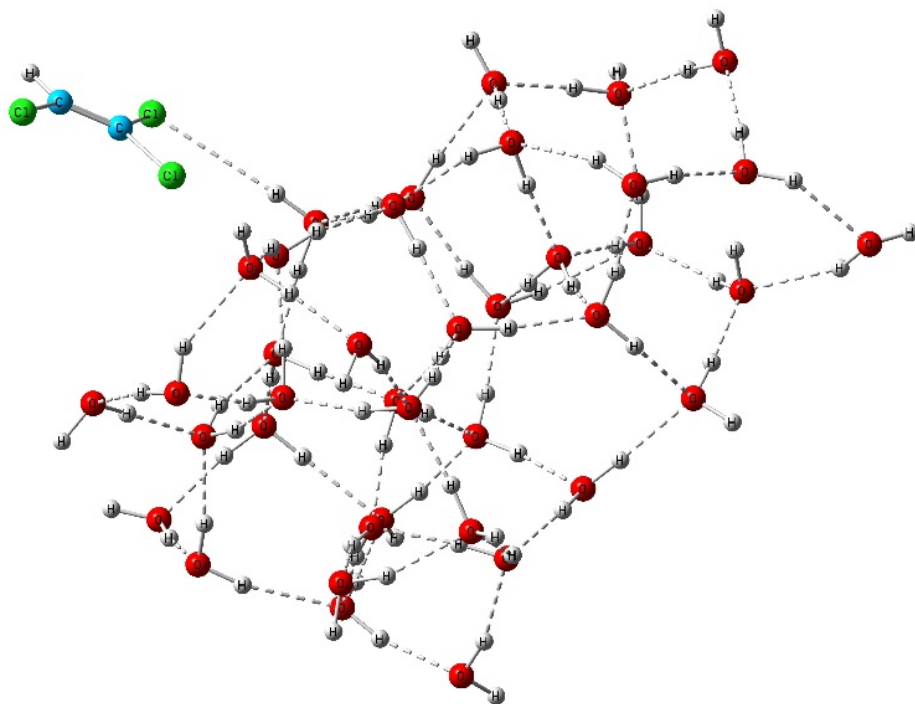


Figure 19A. Equilibrium geometry of TCE and 39 water molecules.

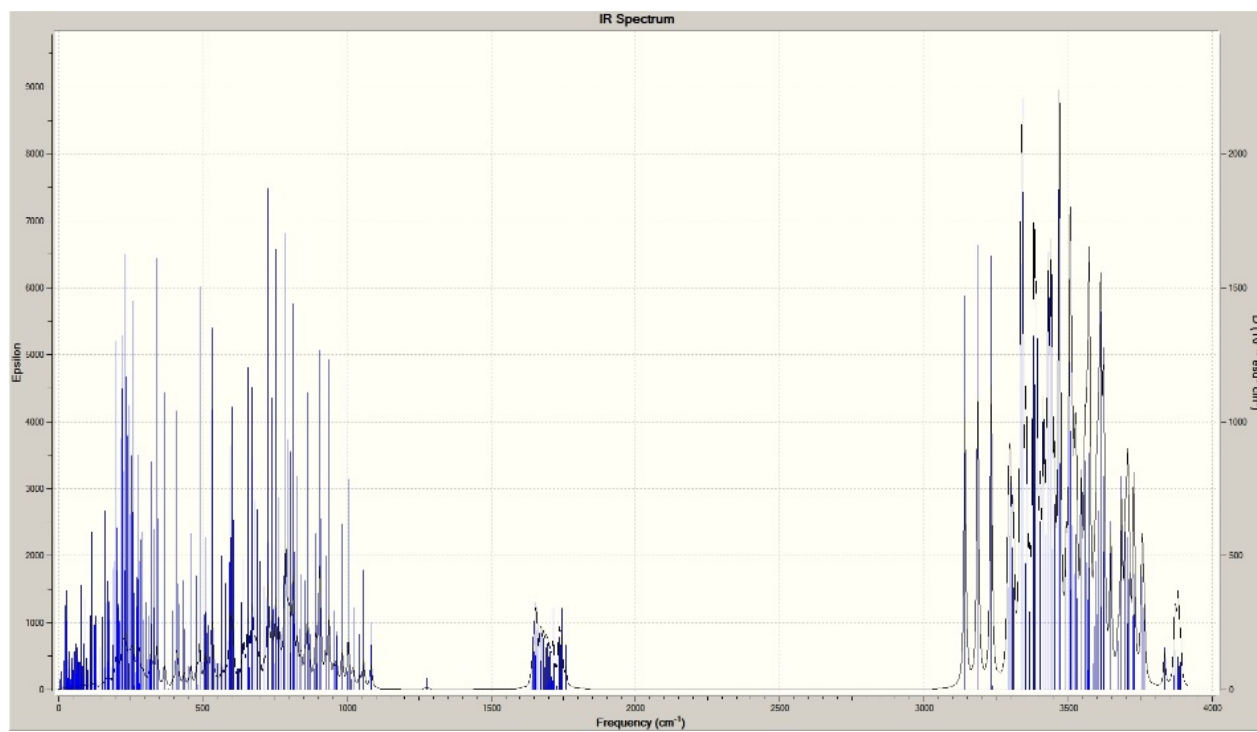


Figure 19B. IR spectrum of TCE and 39 water molecules.

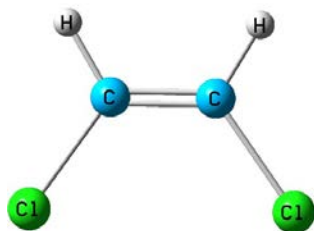


Figure 20A. Equilibrium geometry of isolated DCE1 molecule.

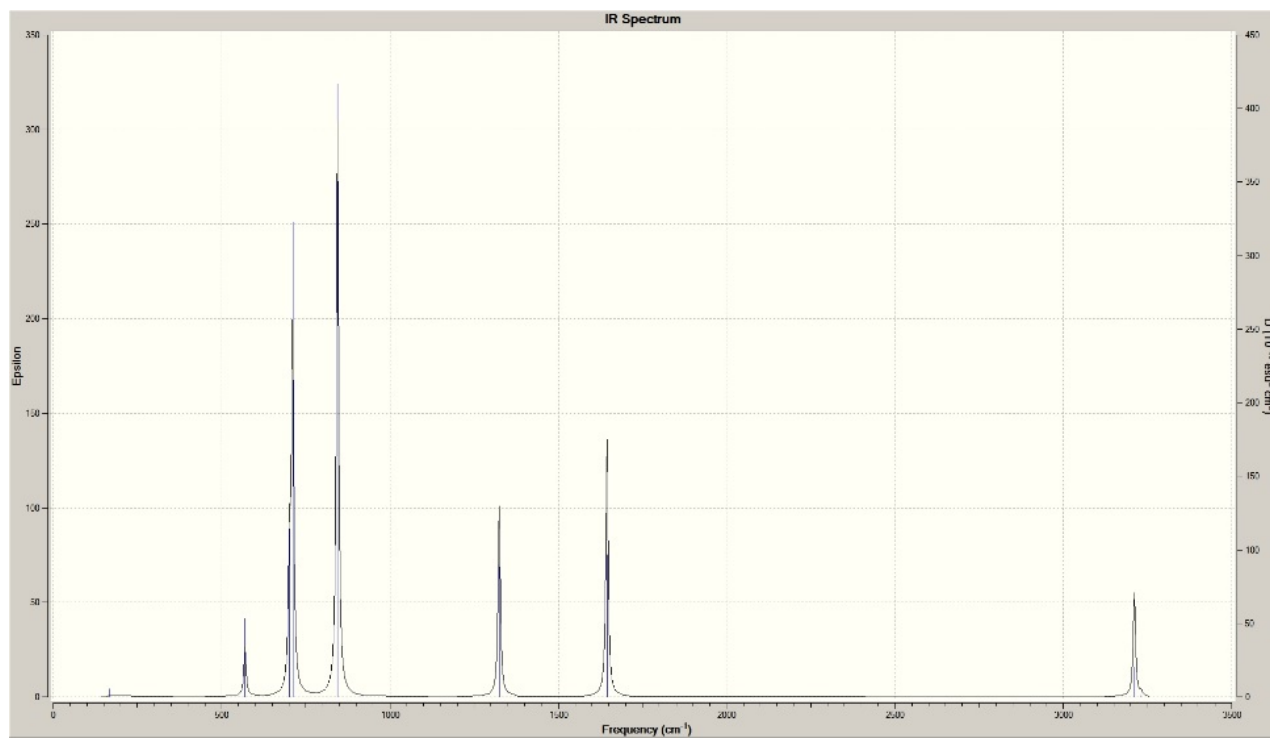


Figure 20B. IR spectrum of isolated DCE1 molecule.

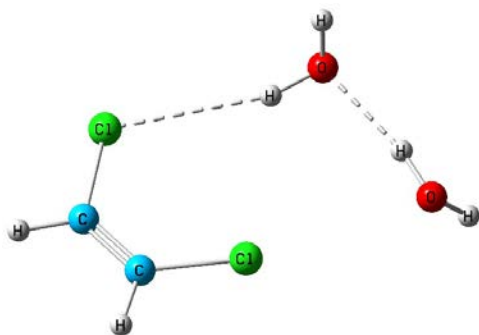


Figure 21A. Equilibrium geometry of DCE1 and 2 water molecules.

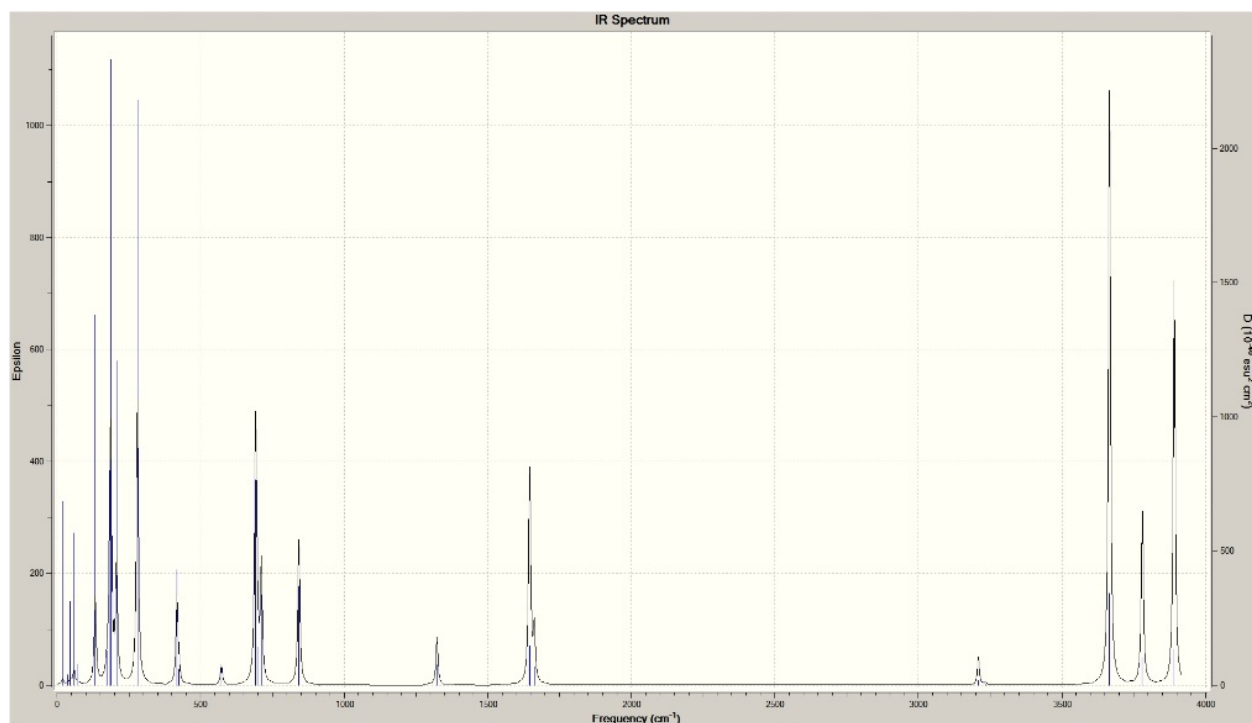


Figure 21B. IR spectrum of DCE1 and 2 water molecules.

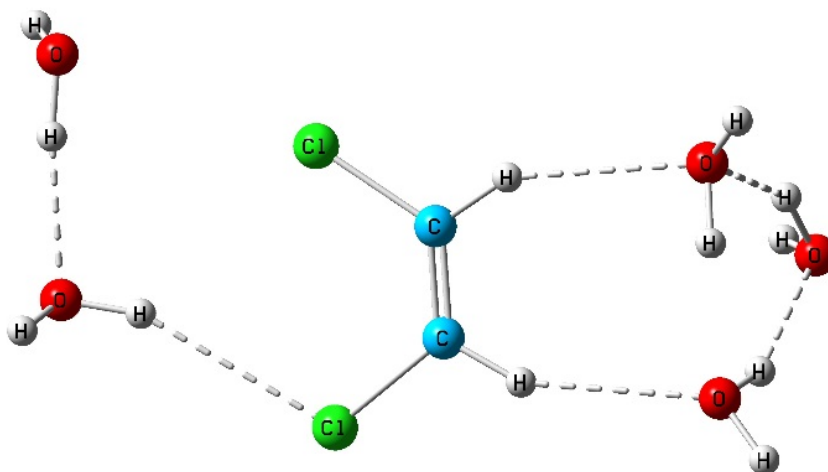


Figure 22A. Equilibrium geometry of DCE1 and 5 water molecules.

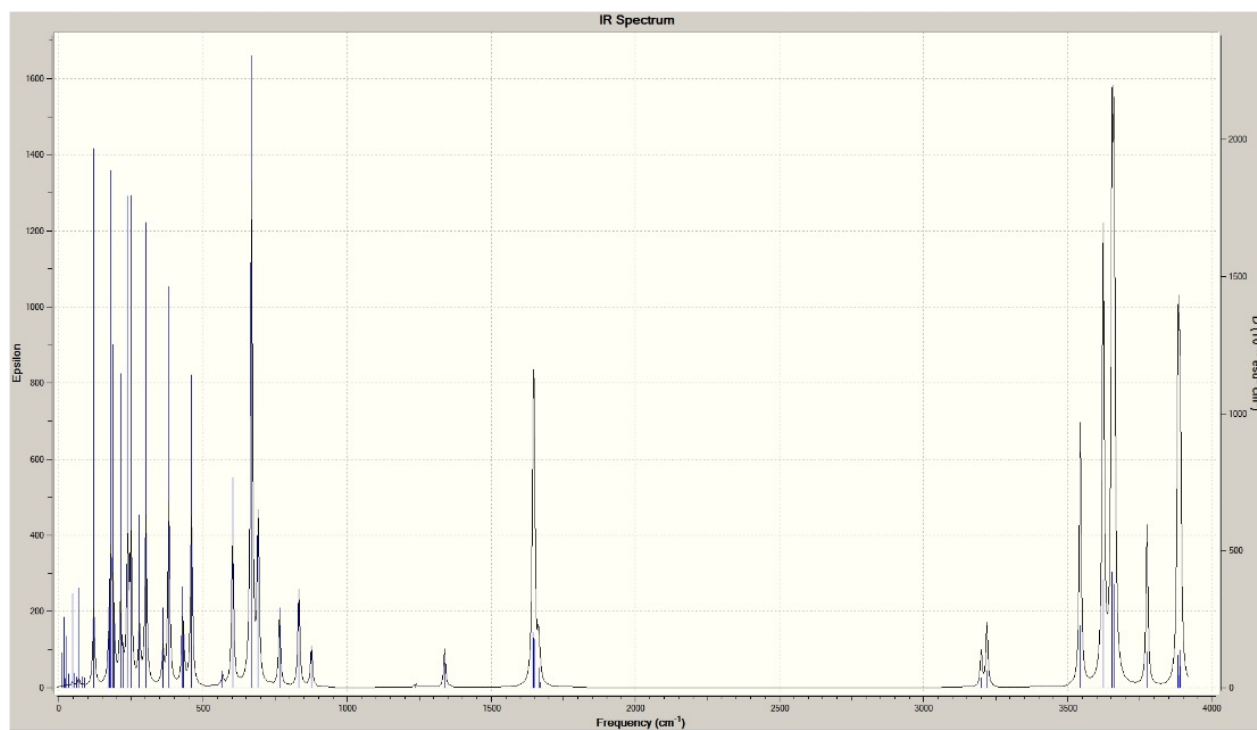


Figure 22B. IR spectrum of DCE1 and 5 water molecules.

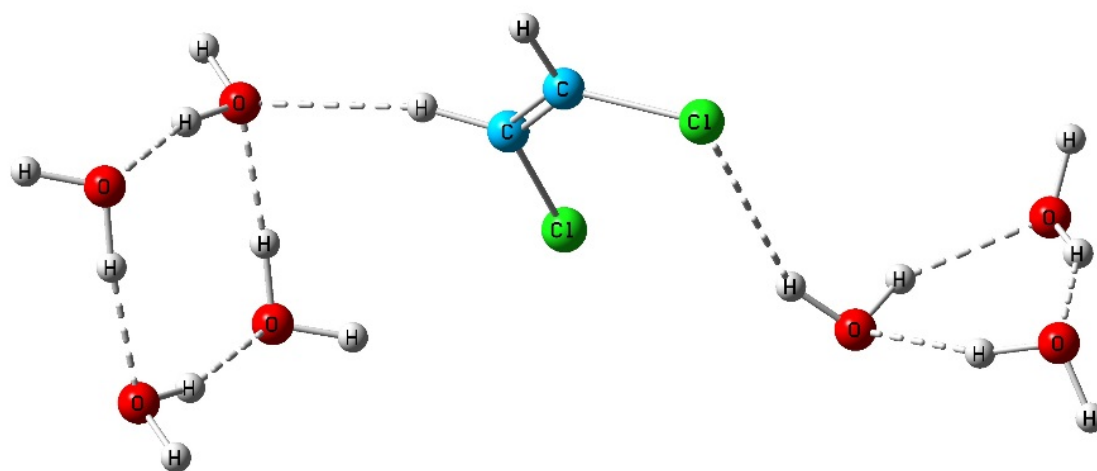


Figure 23A. Equilibrium geometry of DCE1 and 7 water molecules.

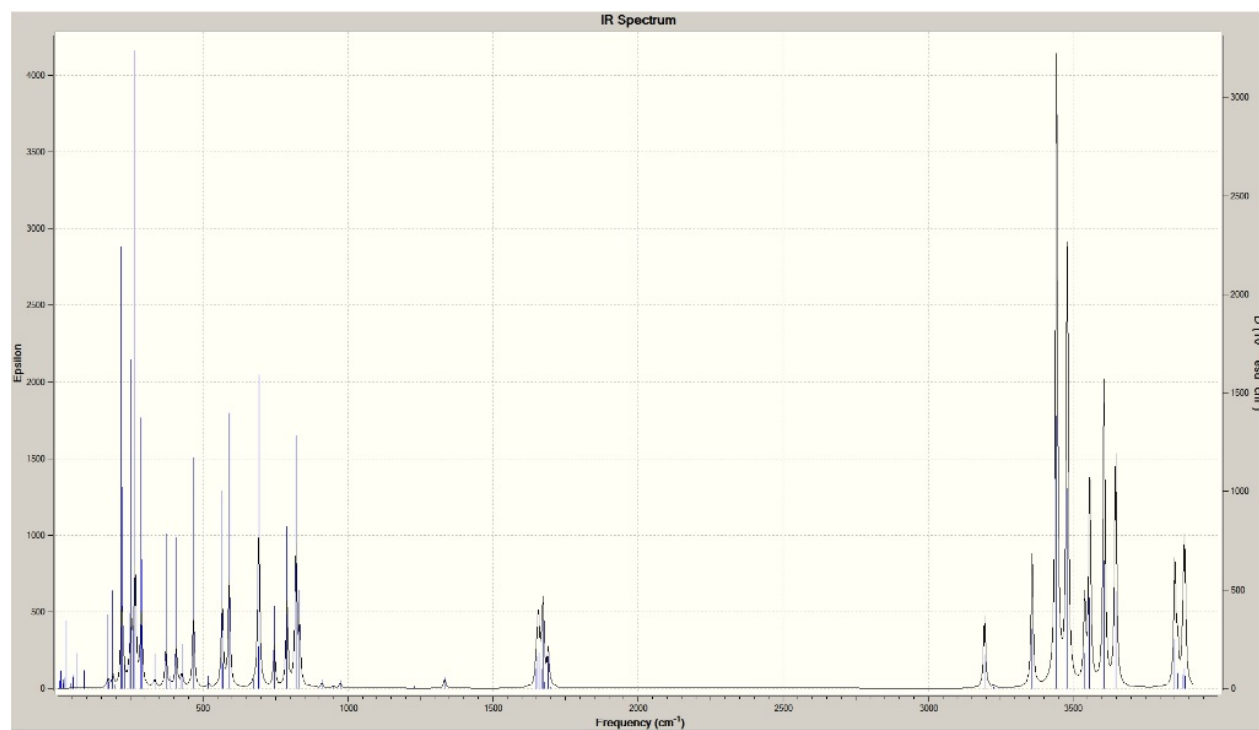


Figure 23B. IR spectrum of DCE1 and 7 water molecules.

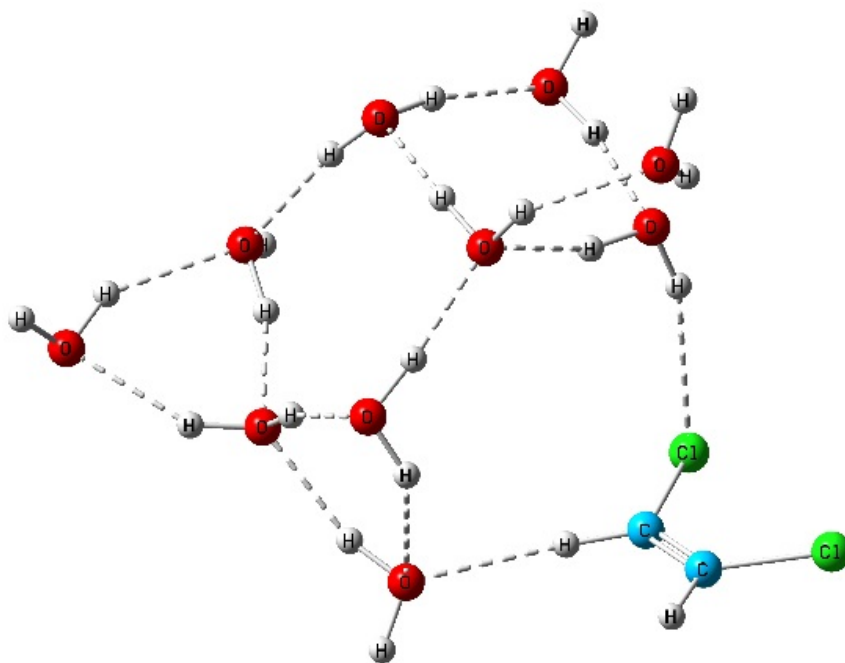


Figure 24A. Equilibrium geometry of DCE1 and 10 water molecules.

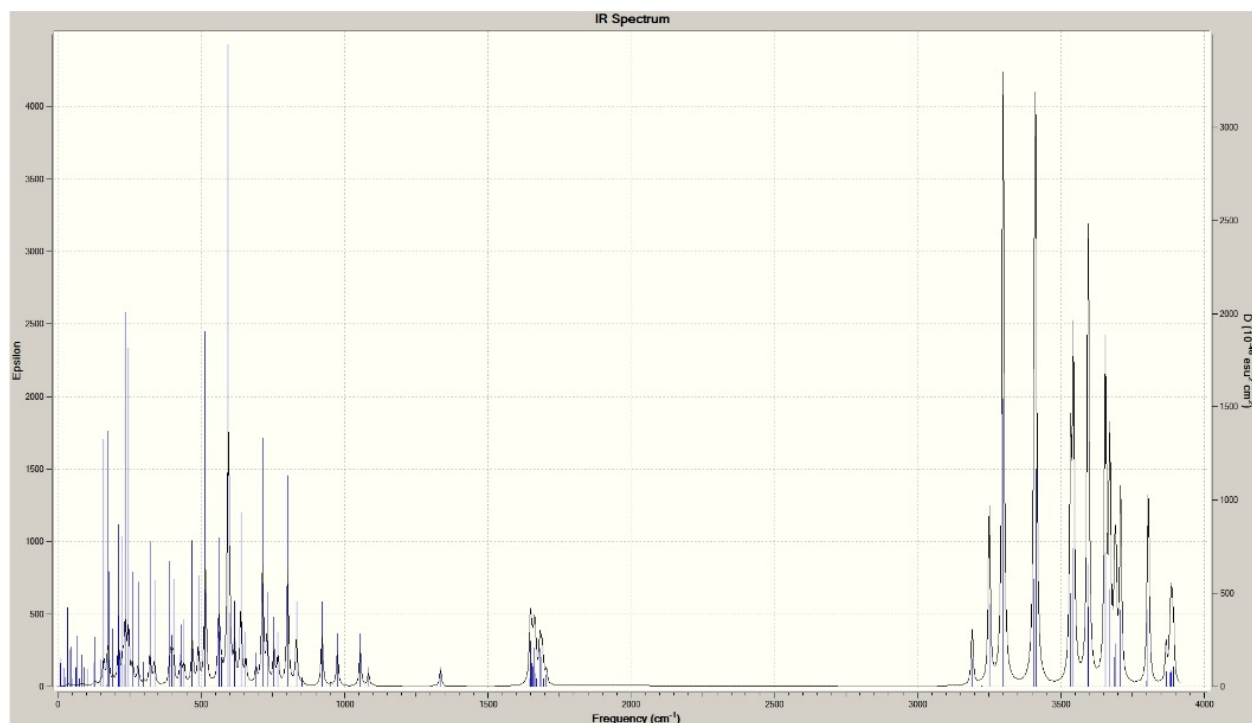


Figure 24B. IR spectrum of DCE1 and 10 water molecules.

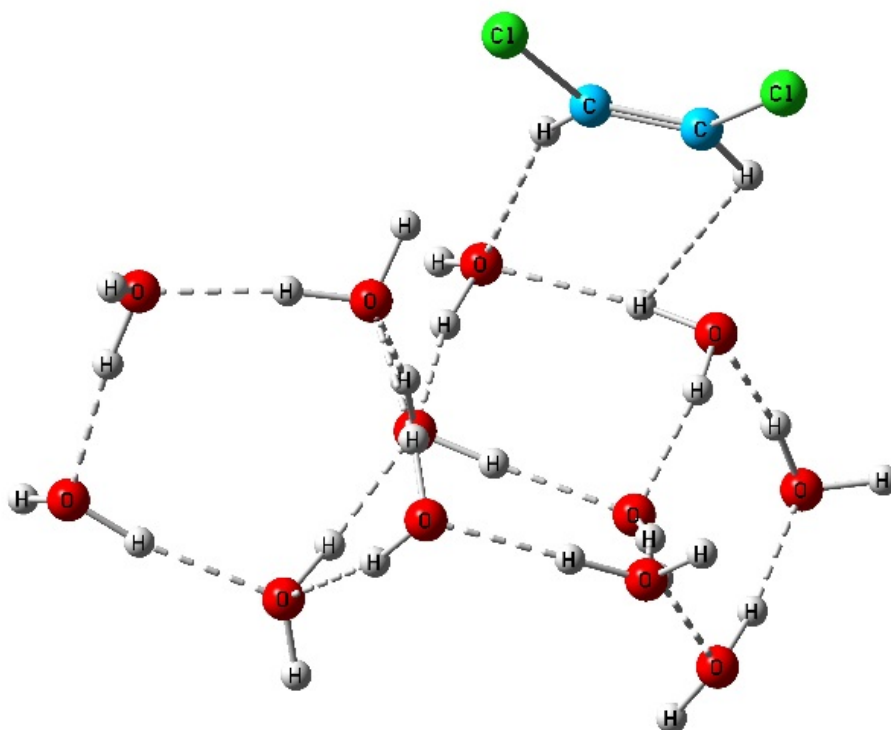


Figure 25A. Equilibrium geometry of DCE1 and 12 water molecules.

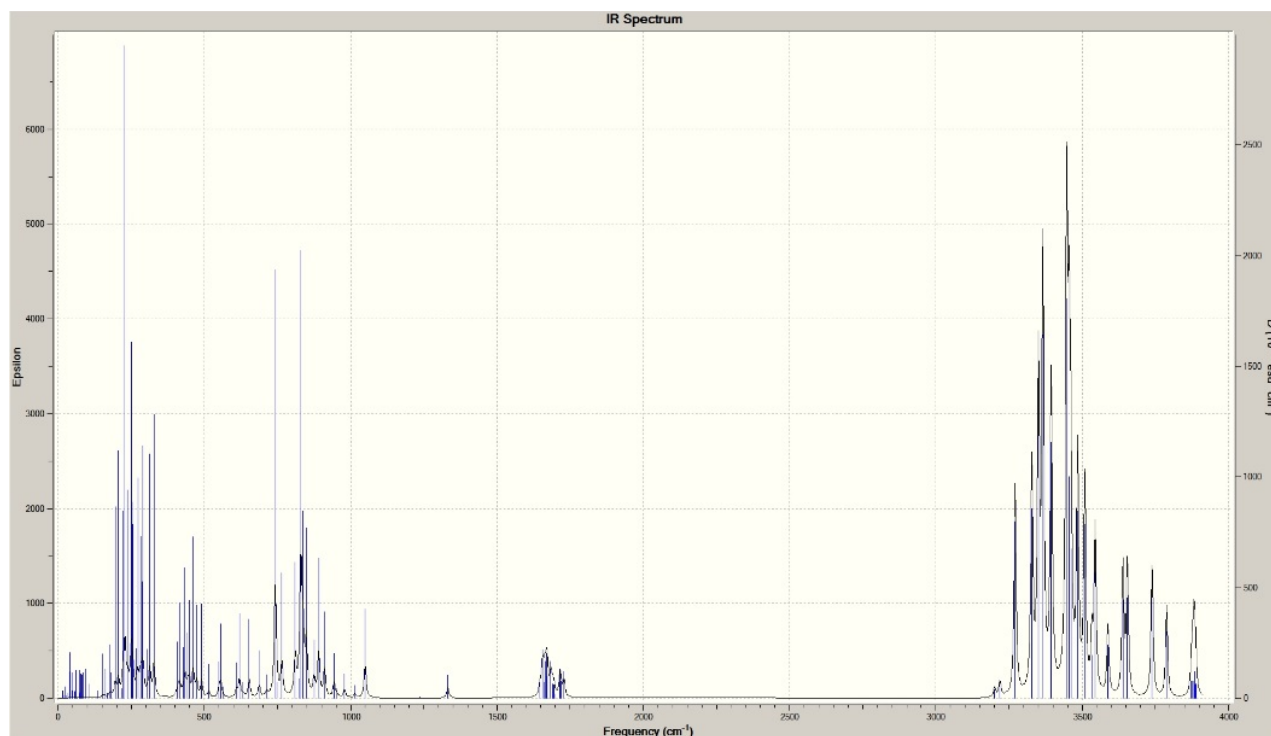


Figure 25B. IR spectrum of DCE1 and 12 water molecules.

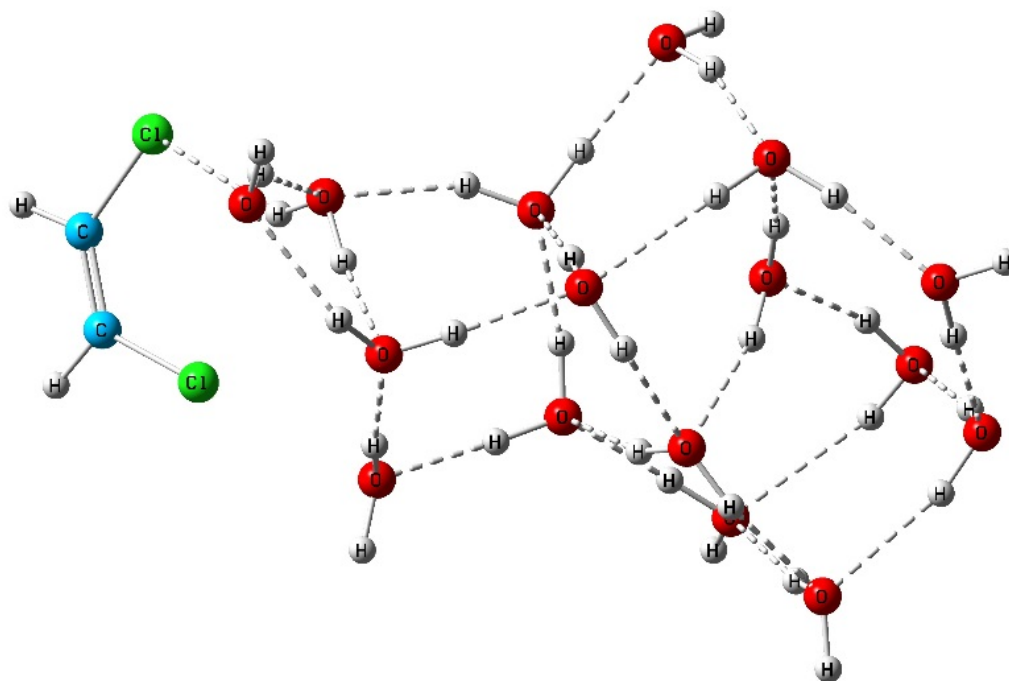


Figure 26A. Equilibrium geometry of DCE1 and 16 water molecules.

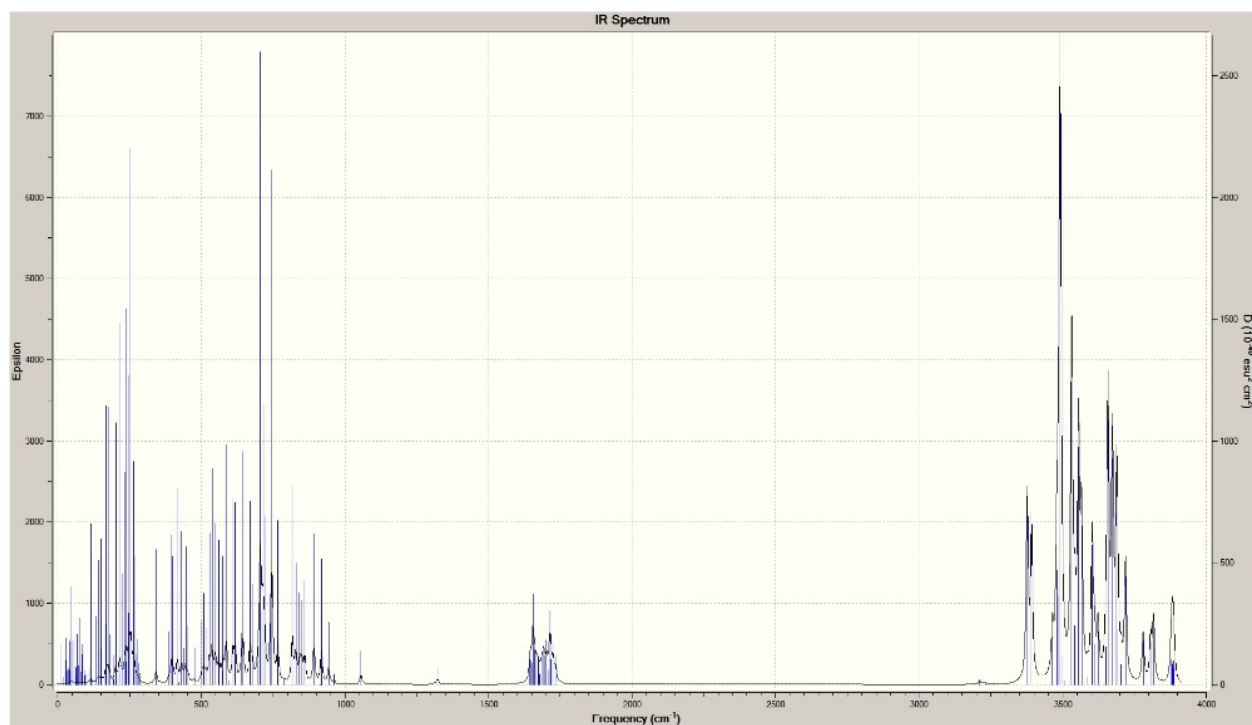


Figure 26B. IR spectrum of DCE1 and 16 water molecules.

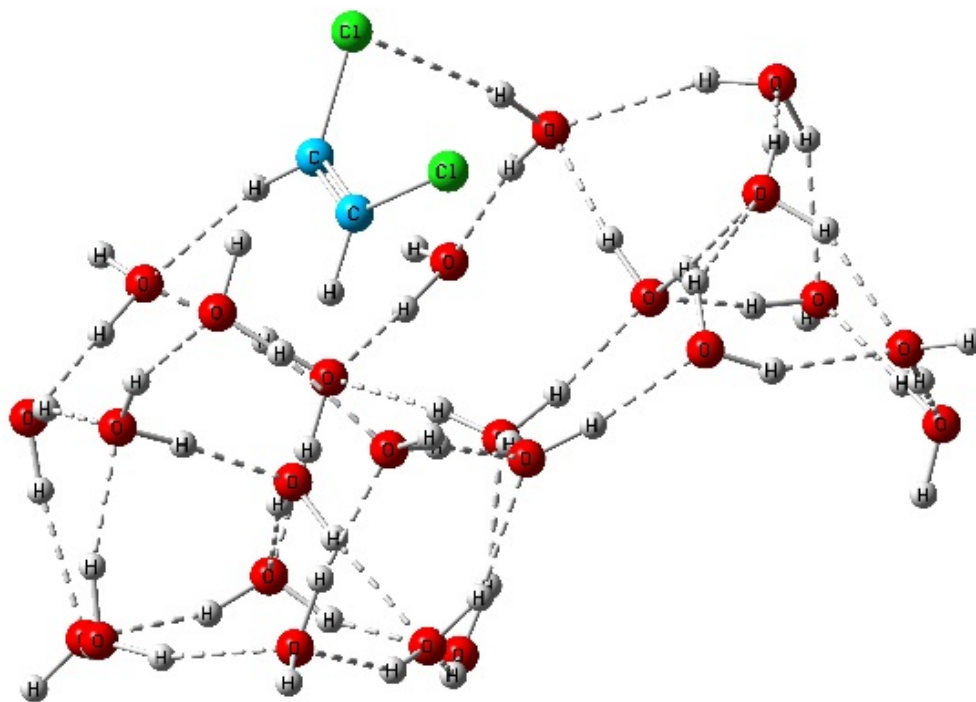


Figure 27A. Equilibrium geometry of DCE1 and 24 water molecules.

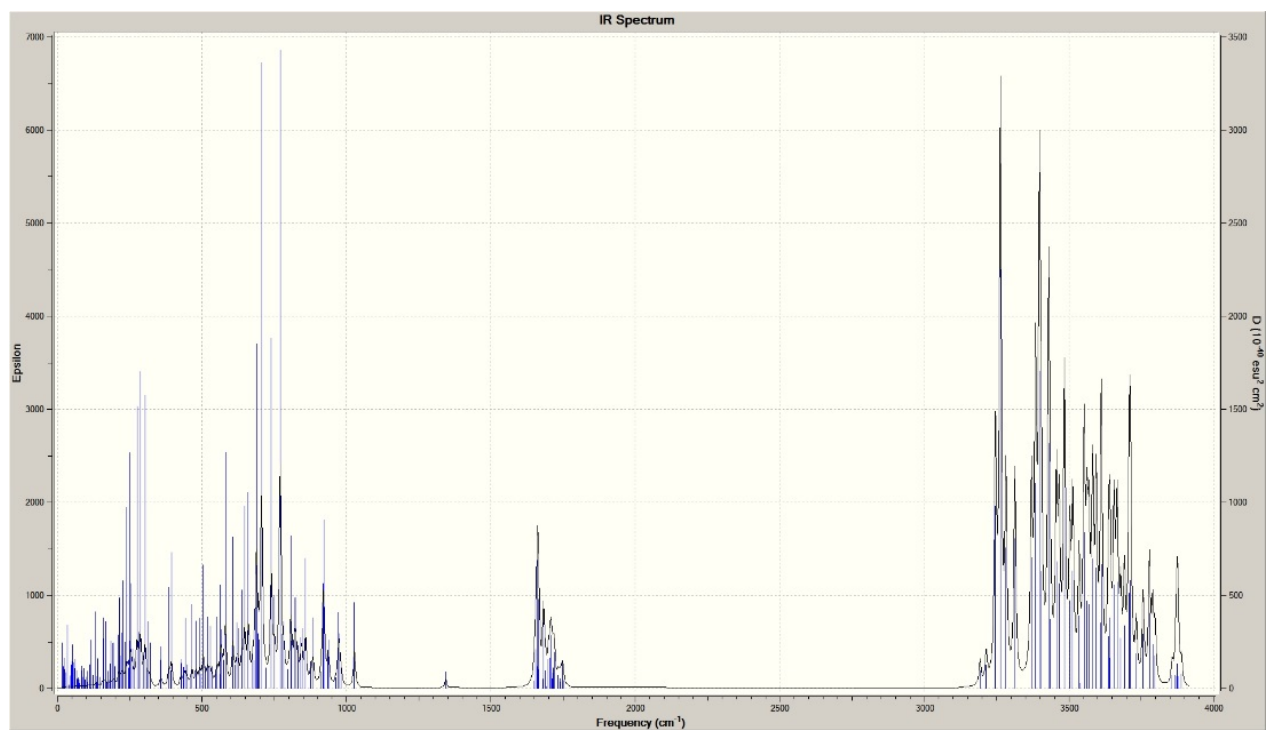


Figure 27B. IR spectrum of DCE1 and 24 water molecules.

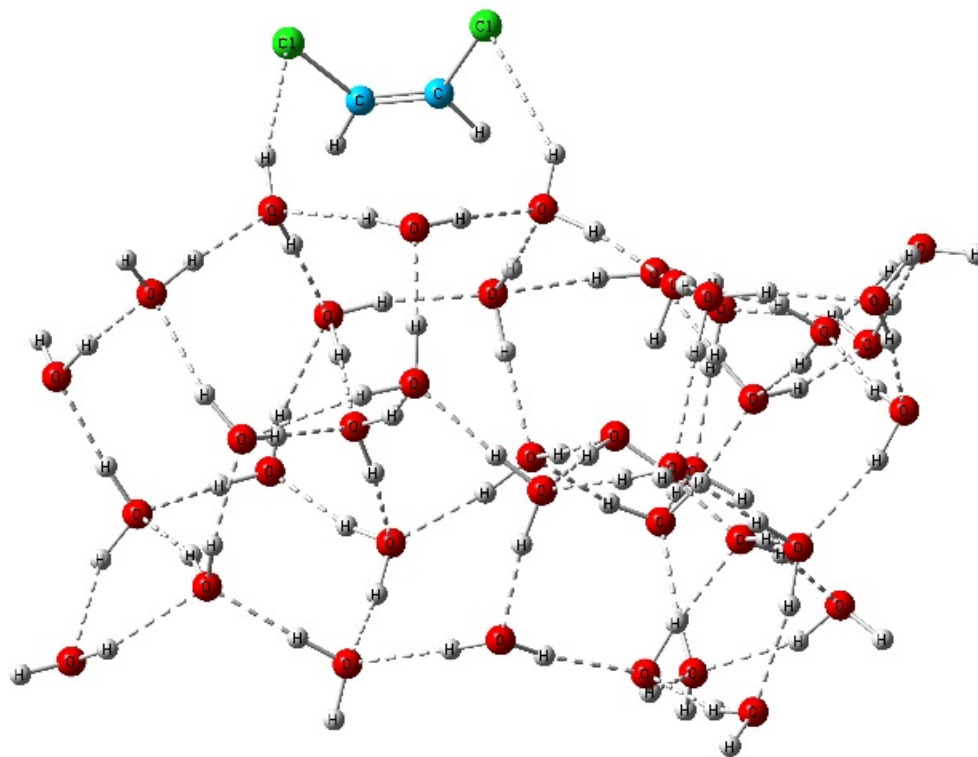


Figure 28A. Equilibrium geometry of DCE1 and 39 water molecules.

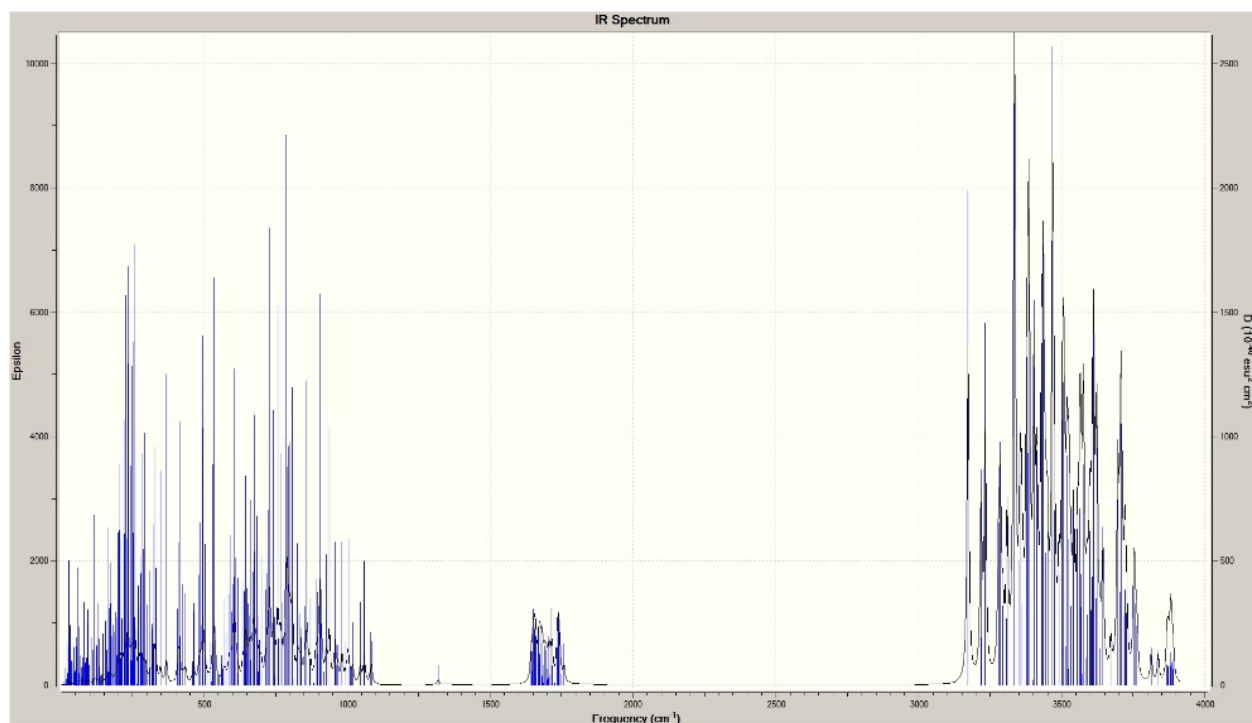


Figure 28B. IR spectrum of DCE1 and 39 water molecules.

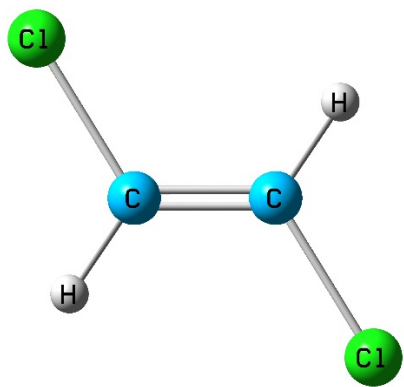


Figure 29A. Equilibrium geometry of isolated DCE2 molecule.

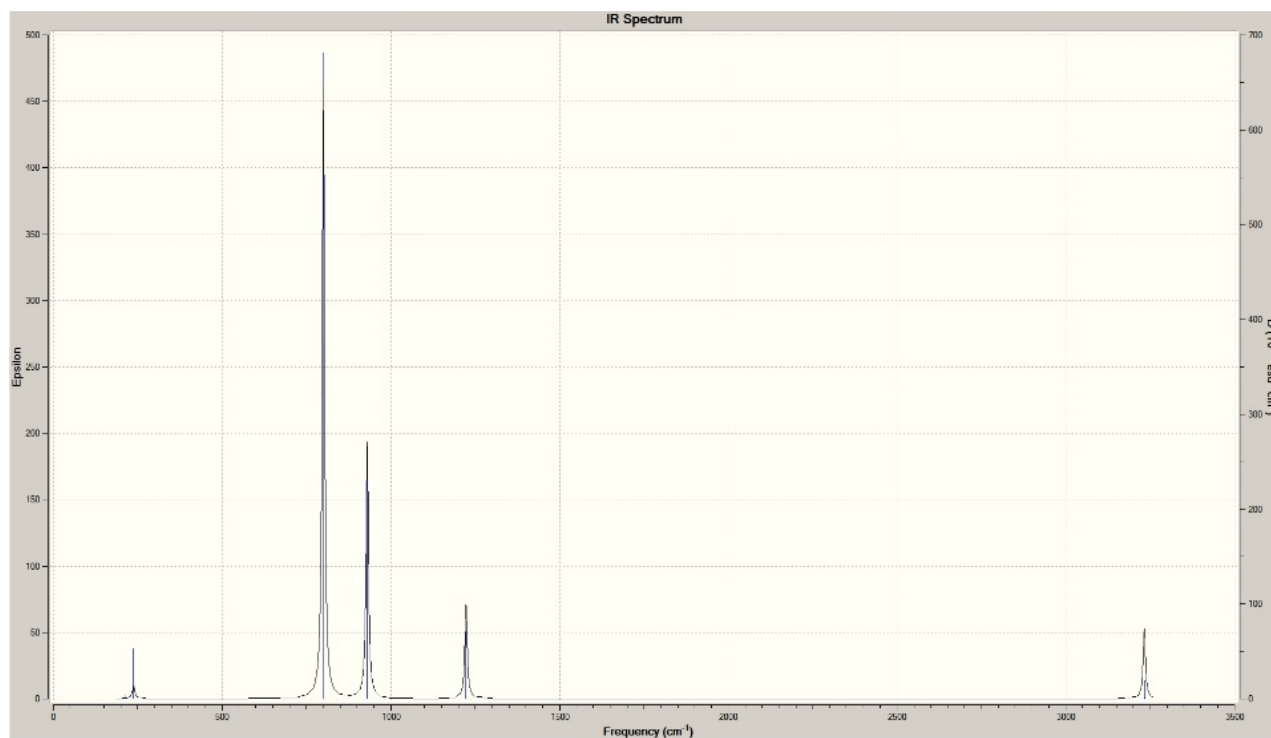


Figure 29B. IR spectrum of isolated DCE2 molecule.

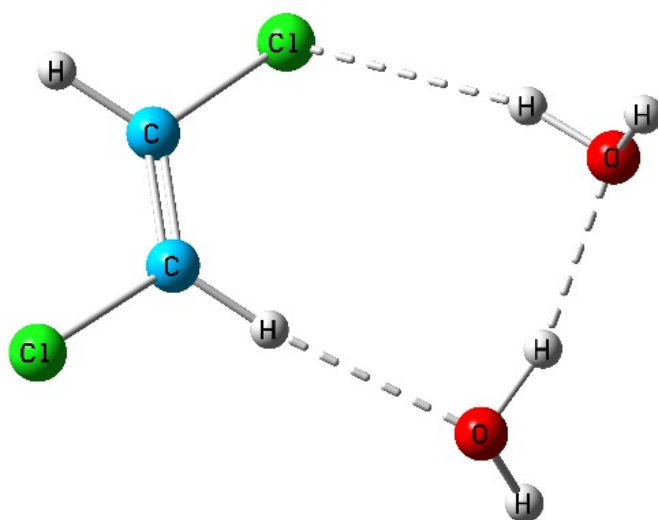


Figure 30A. Equilibrium geometry of DCE2 and 2 water molecules.

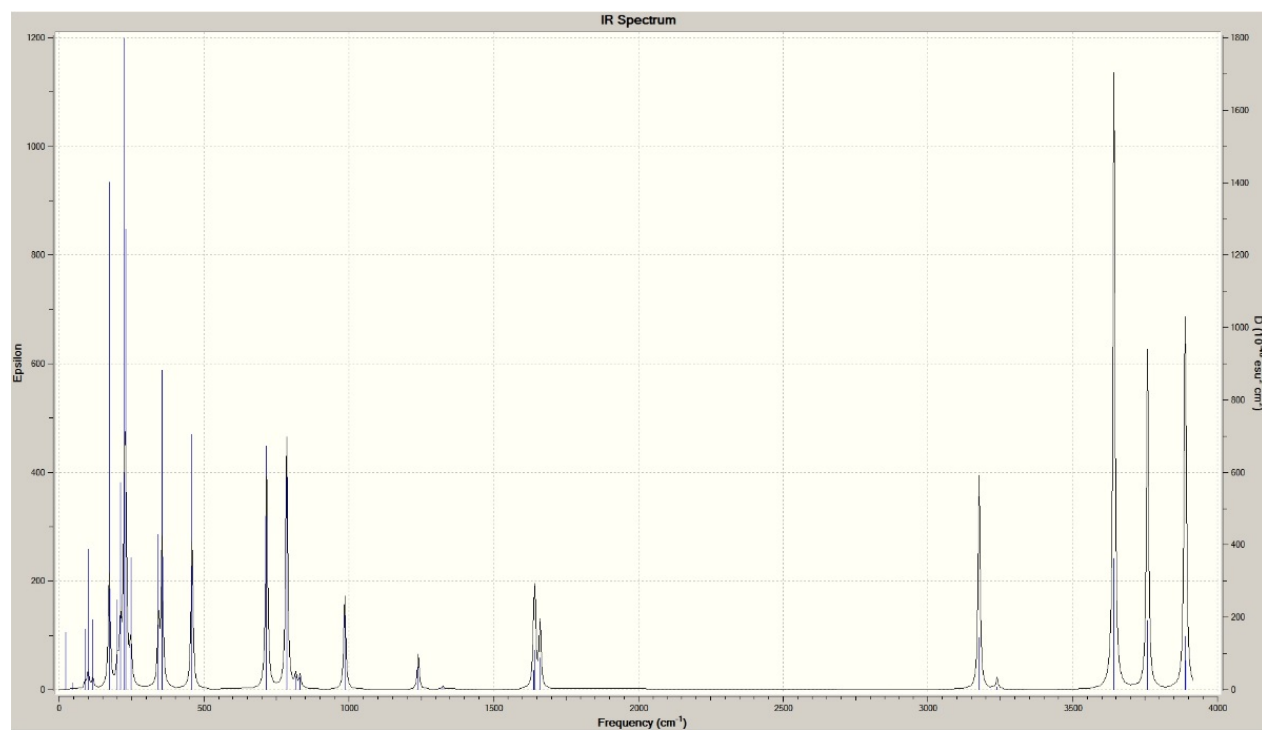


Figure 30B. IR spectrum of DCE2 and 2 water molecules.

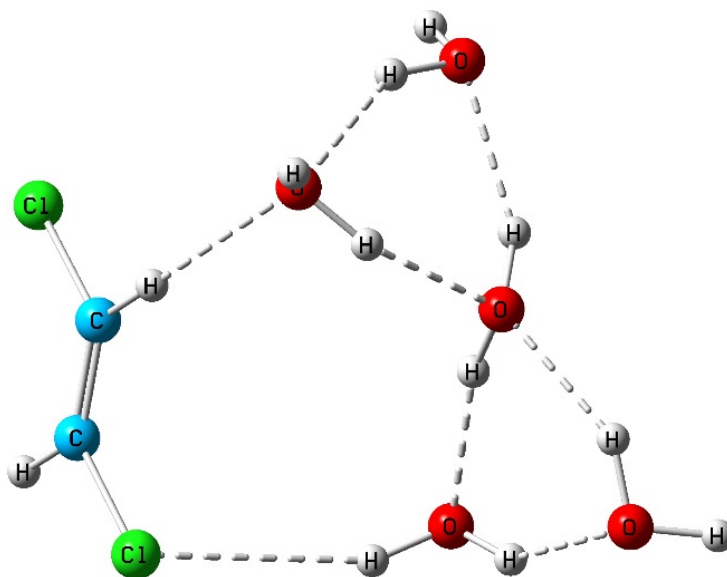


Figure 31A. Equilibrium geometry of DCE2 and 5 water molecules.

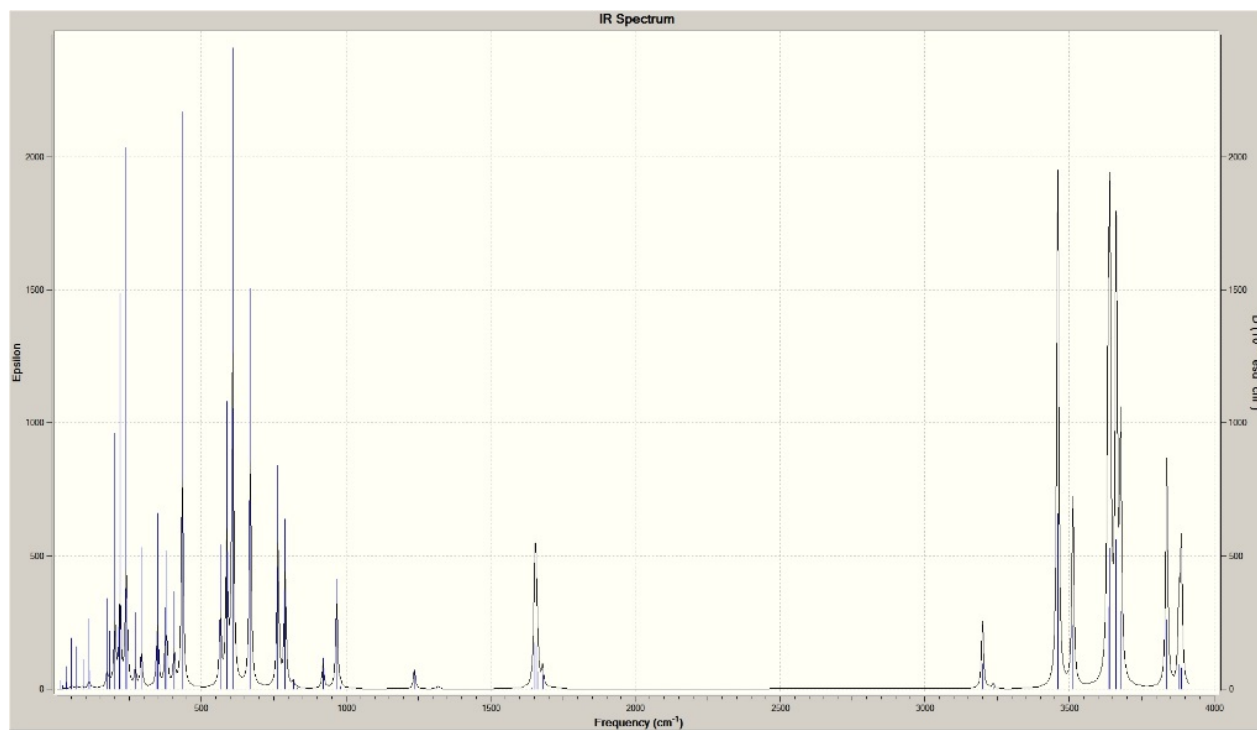


Figure 31B. IR spectrum of DCE2 and 5 water molecules.

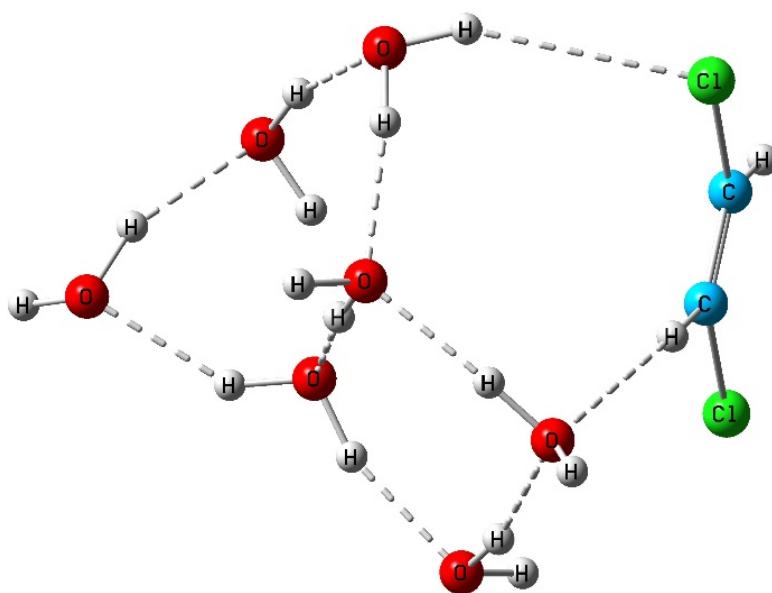


Figure 32A. Equilibrium geometry of DCE2 and 7 water molecules.

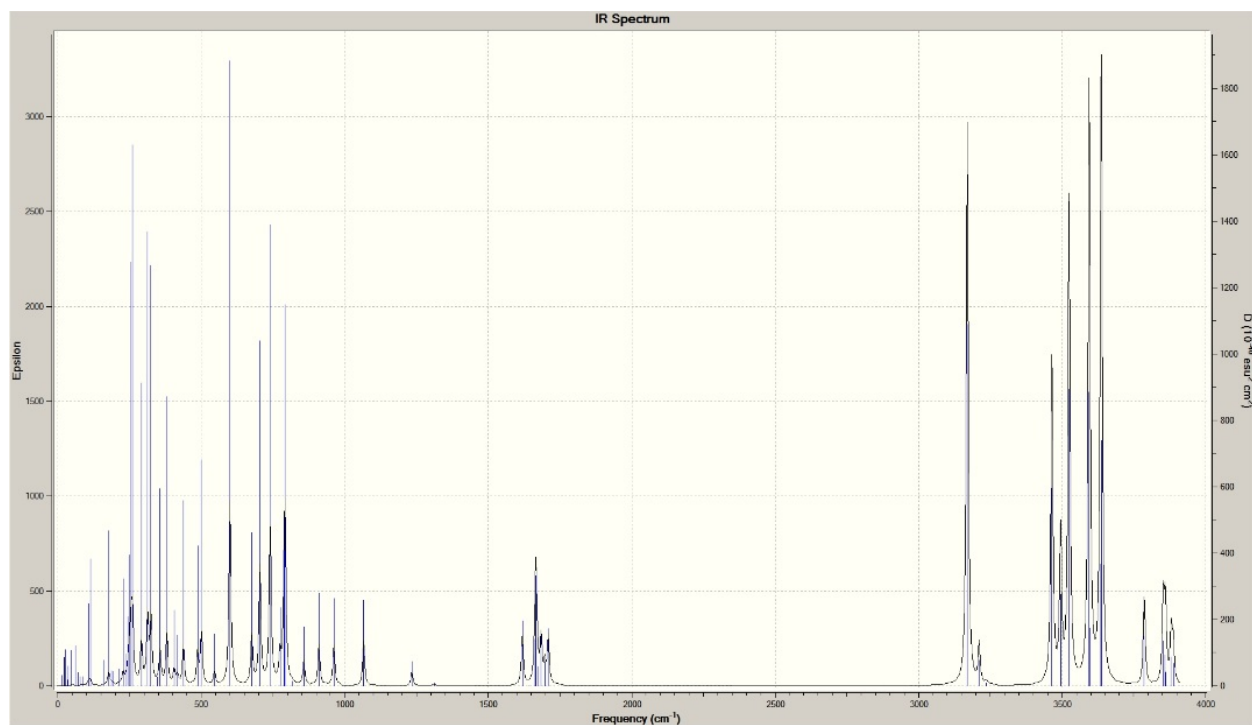


Figure 32B. IR spectrum of DCE2 and 7 water molecules.

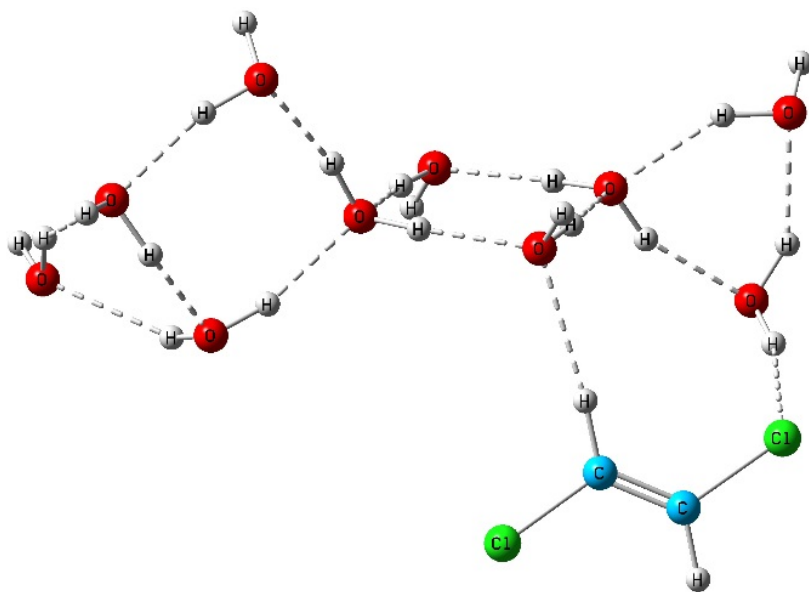


Figure 33A. Equilibrium geometry of DCE2 and 10 water molecules.

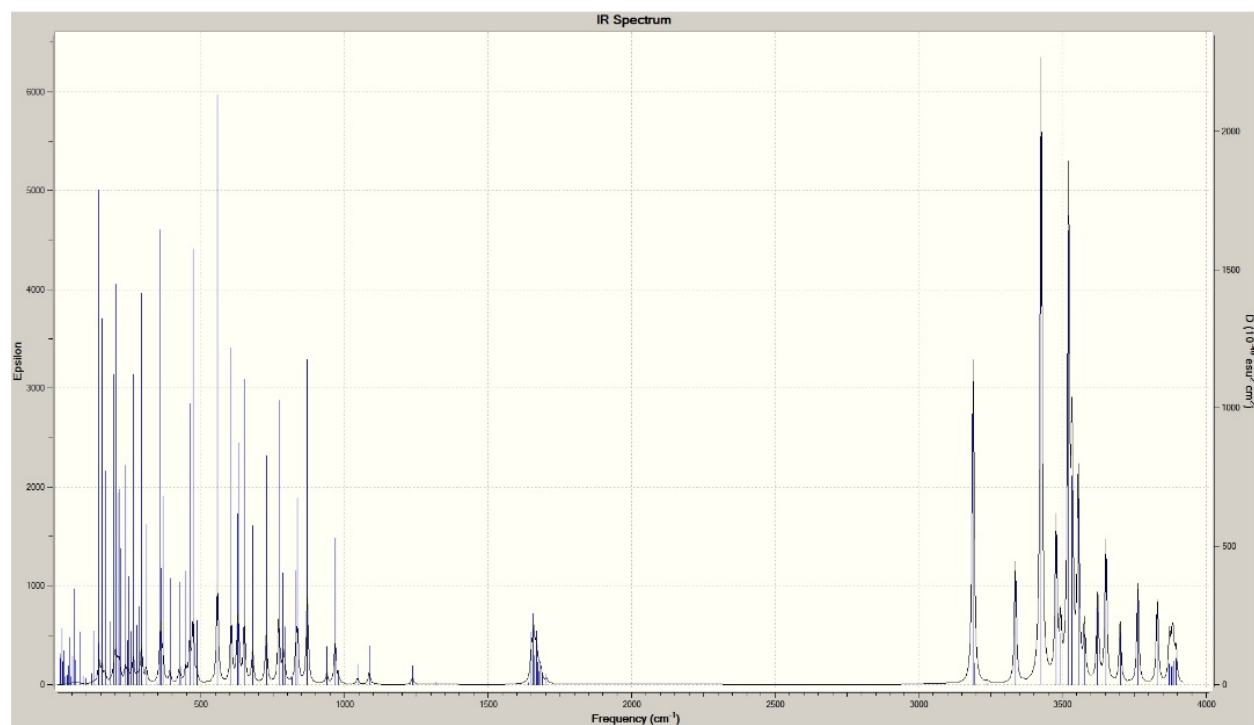


Figure 33B. IR spectrum of DCE2 and 10 water molecules.

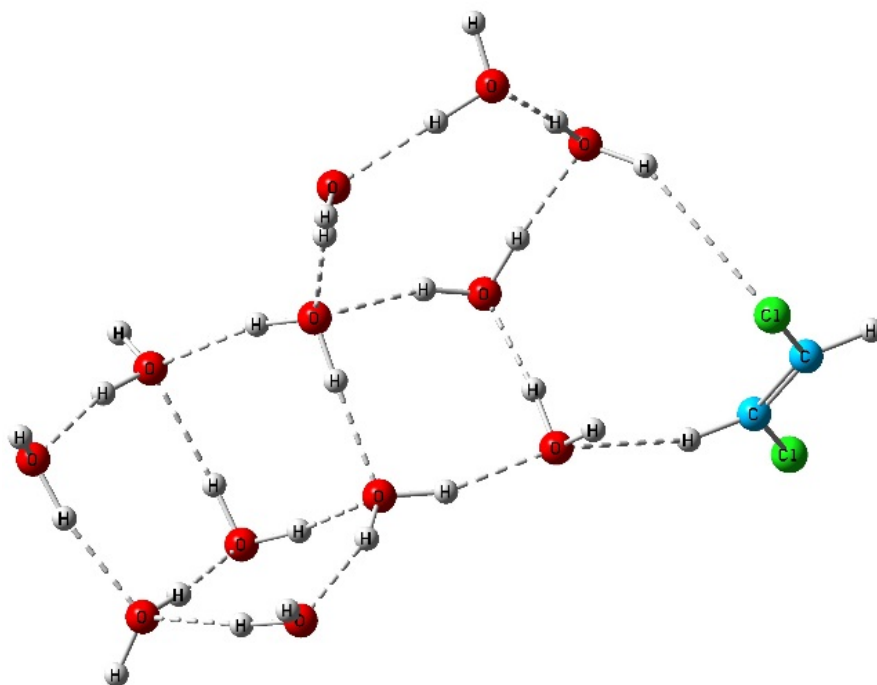


Figure 34A. Equilibrium geometry of DCE2 and 12 water molecules.

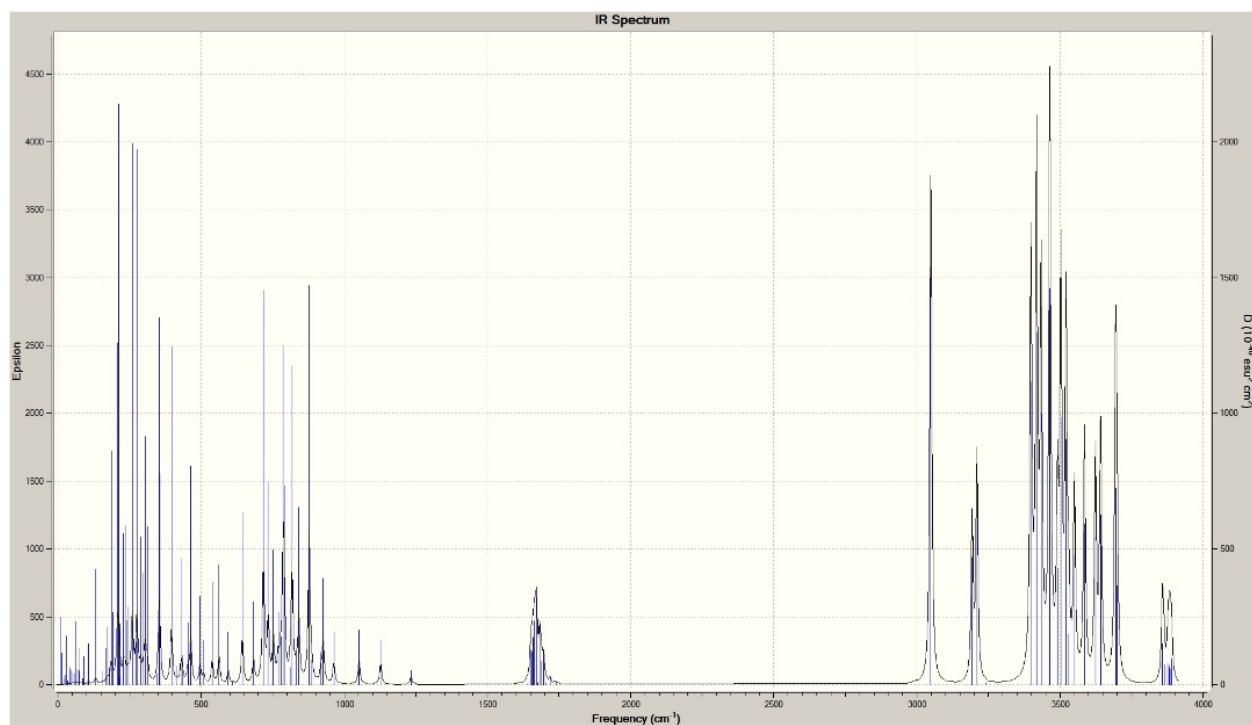


Figure 34B. IR spectrum of DCE2 and 12 water molecules.

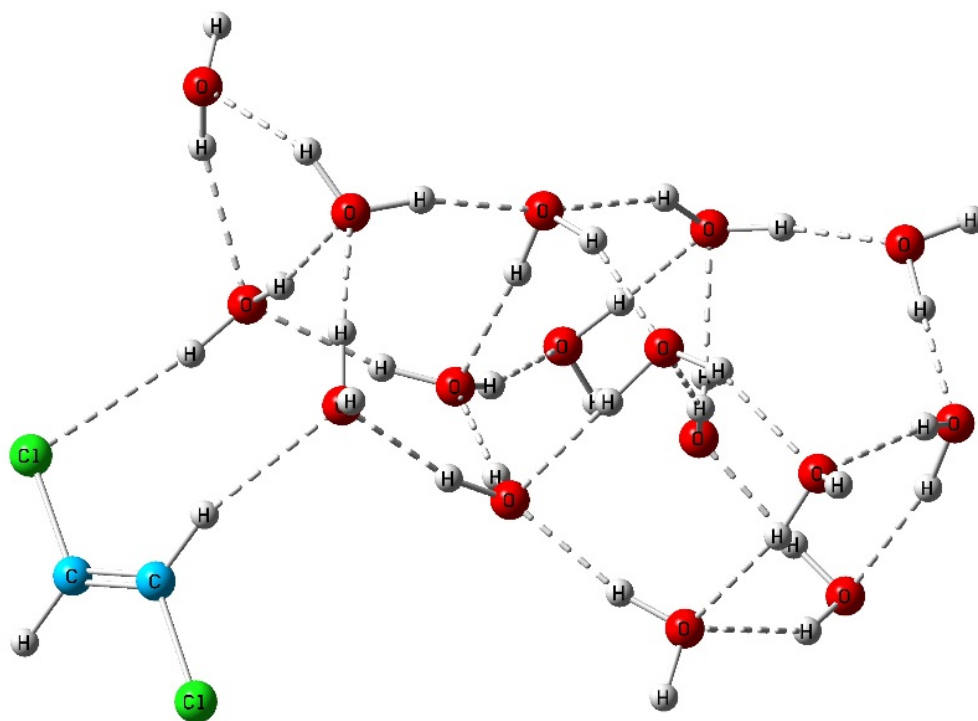


Figure 35A. Equilibrium geometry of DCE2 and 16 water molecules.

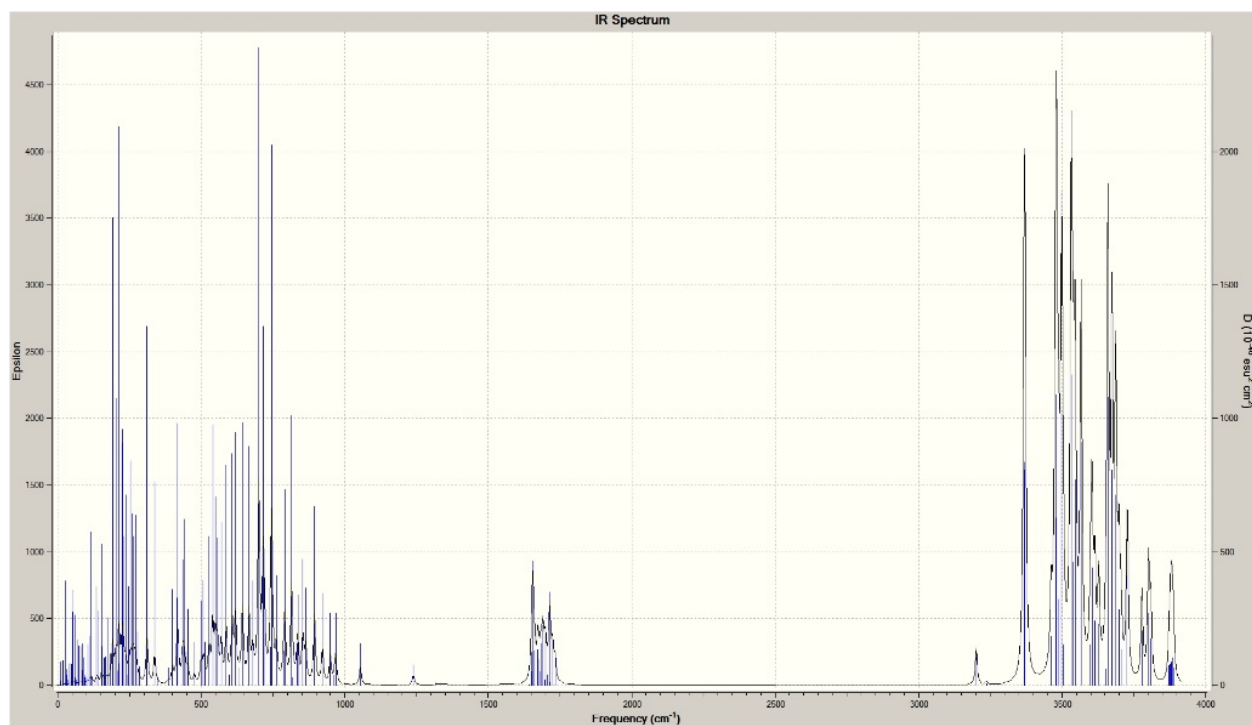


Figure 35B. IR spectrum of DCE2 and 16 water molecules.

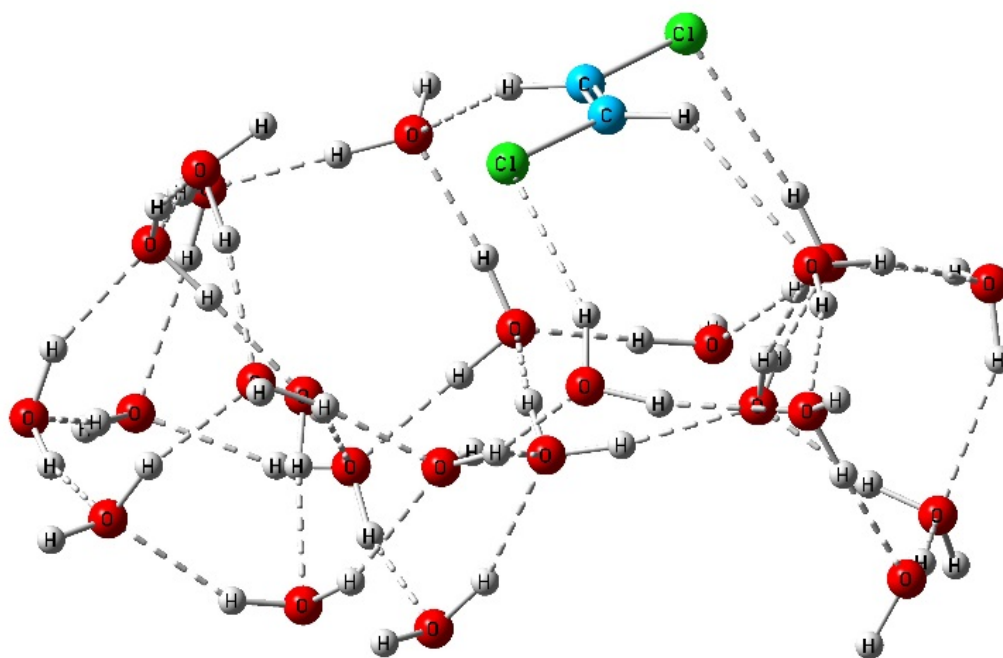


Figure 36A. Equilibrium geometry of DCE2 and 24 water molecules.

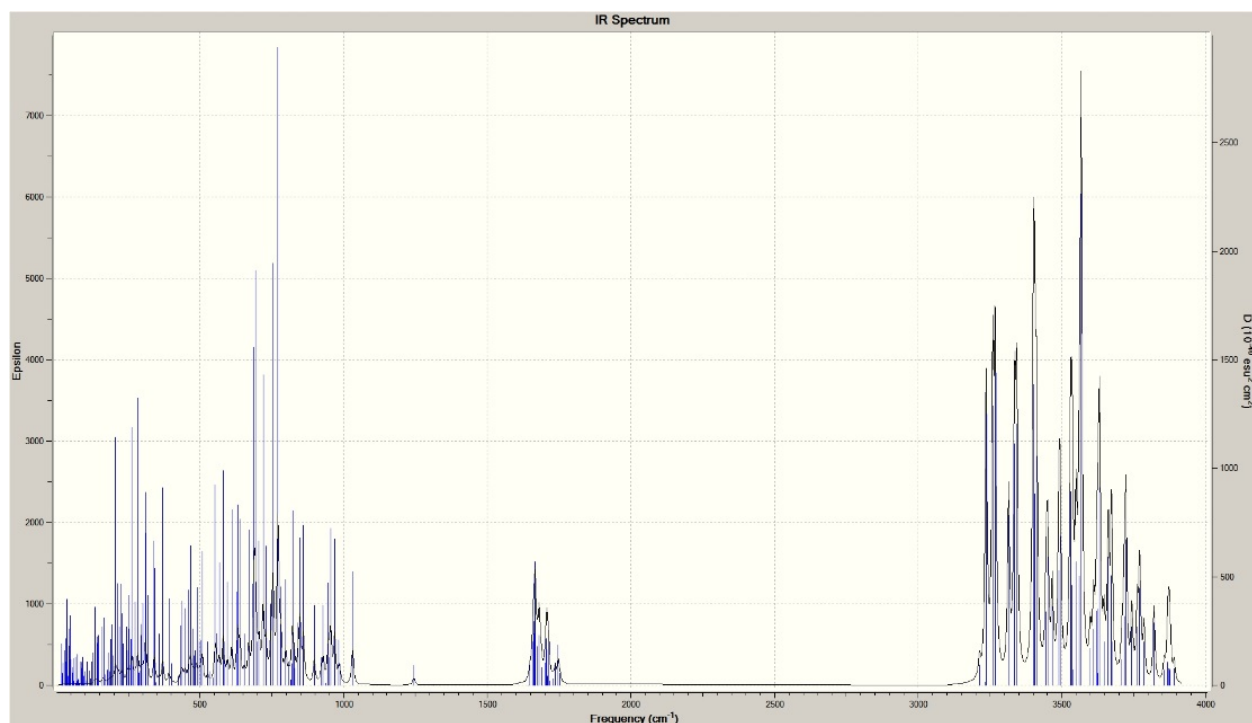


Figure 36B. IR spectrum of DCE2 and 24 water molecules.

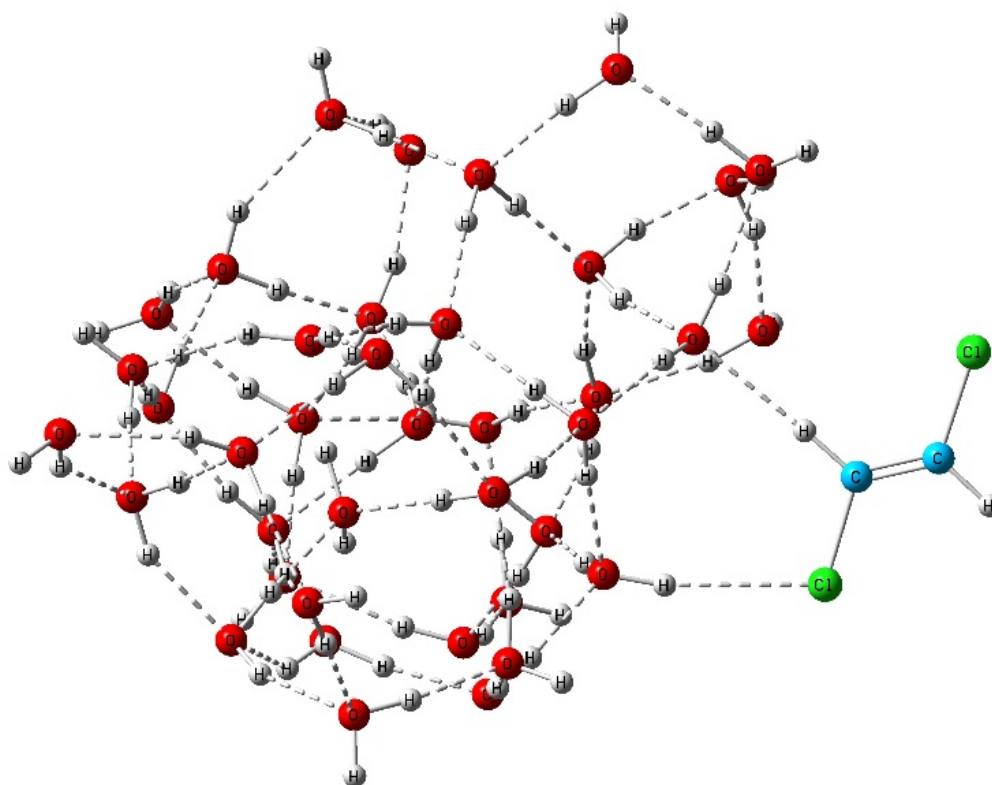


Figure 37A. Equilibrium geometry of DCE2 and 39 water molecules.

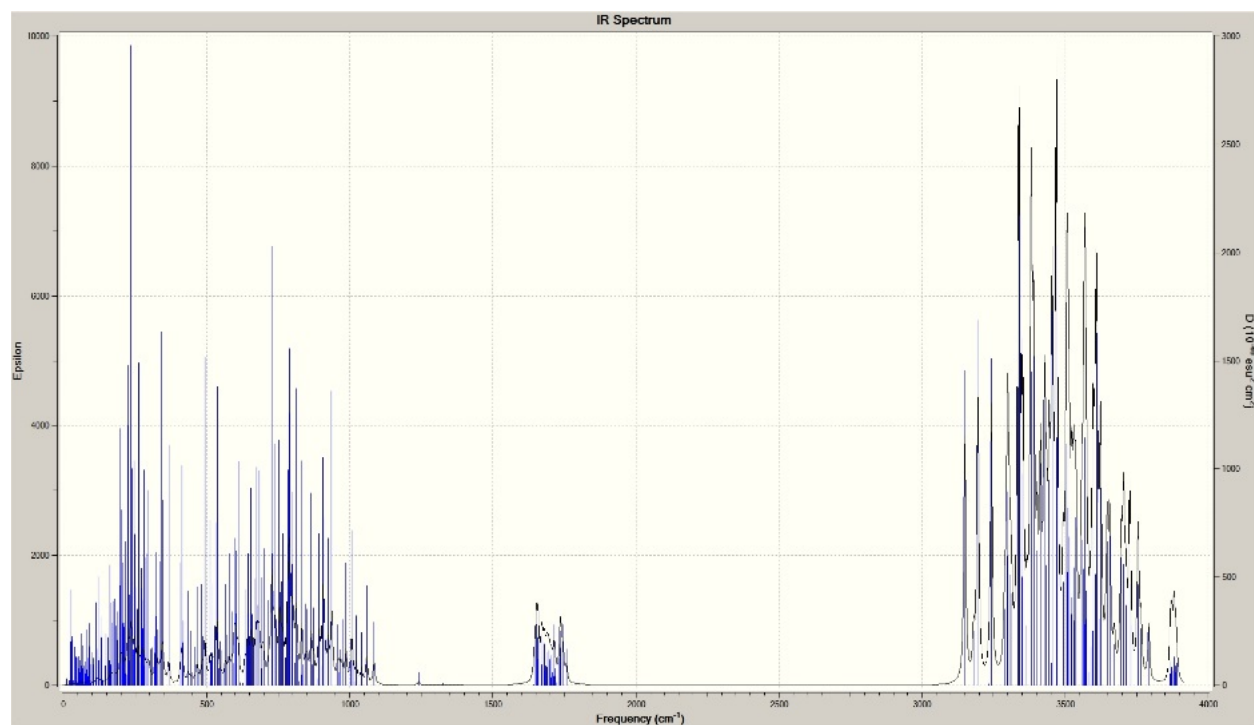


Figure 37B. IR spectrum of DCE2 and 39 water molecules.

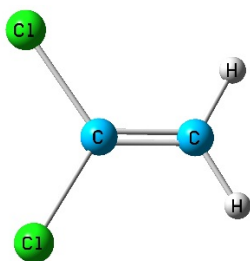


Figure 38A. Equilibrium geometry of isolated DCE3 molecule.

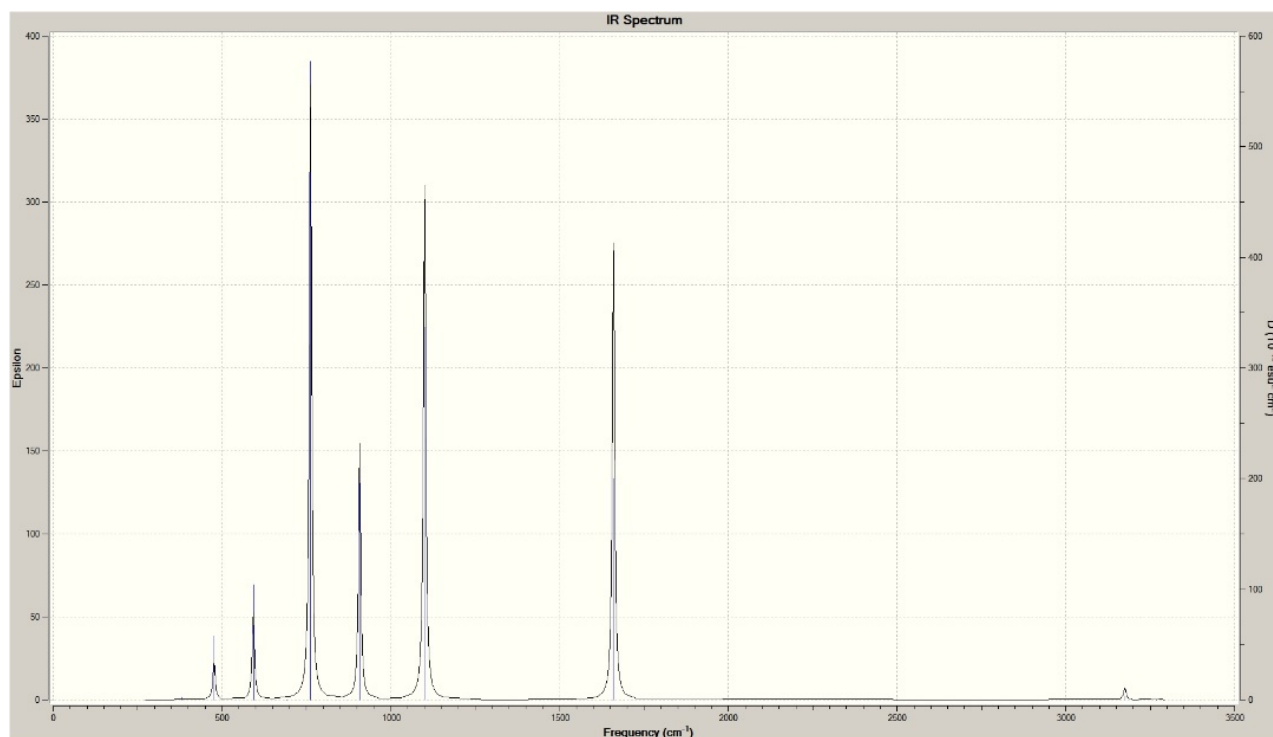


Figure 38B. IR spectrum of isolated DCE3 molecule.

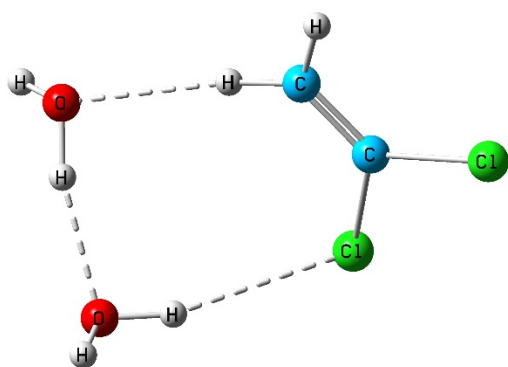


Figure 39A. Equilibrium geometry of DCE3 and 2 water molecules.

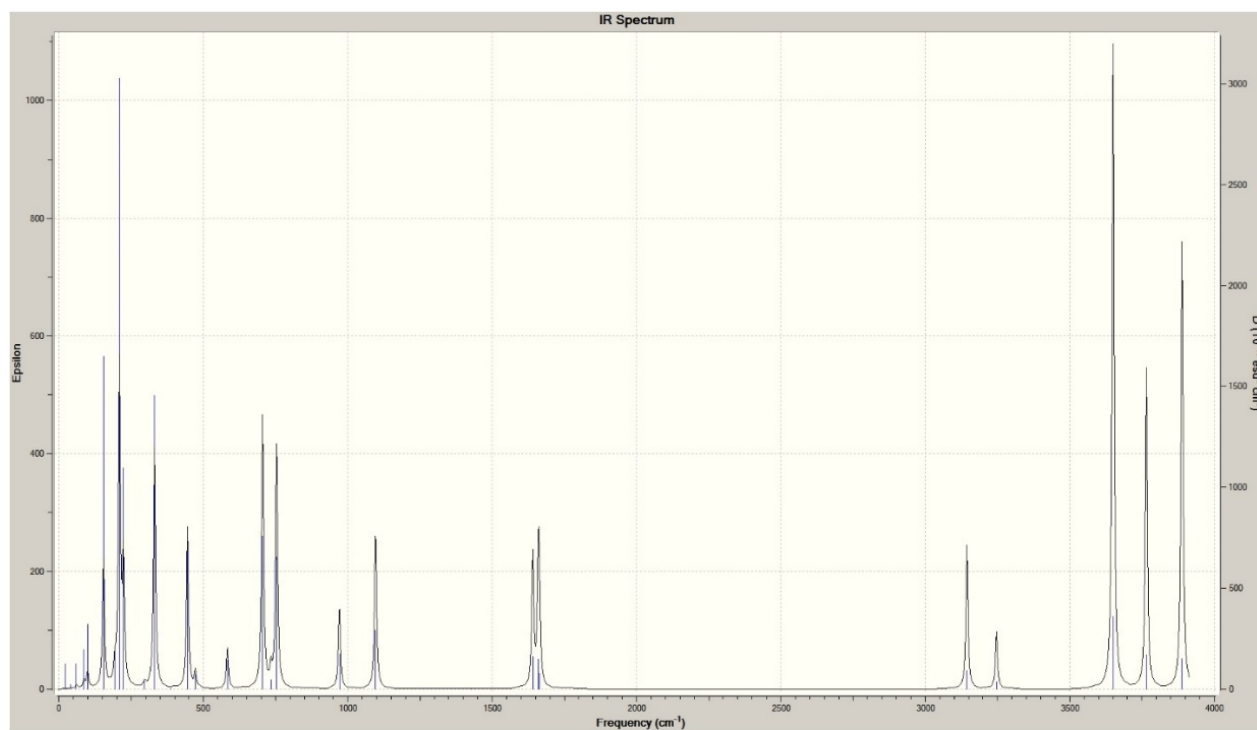


Figure 39B. IR spectrum of DCE3 and 2 water molecules.

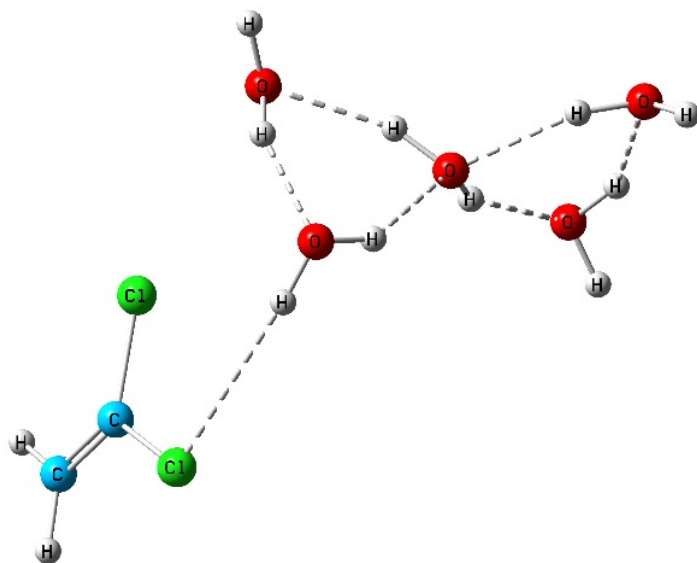


Figure 40A. Equilibrium geometry of DCE3 and 5 water molecules.

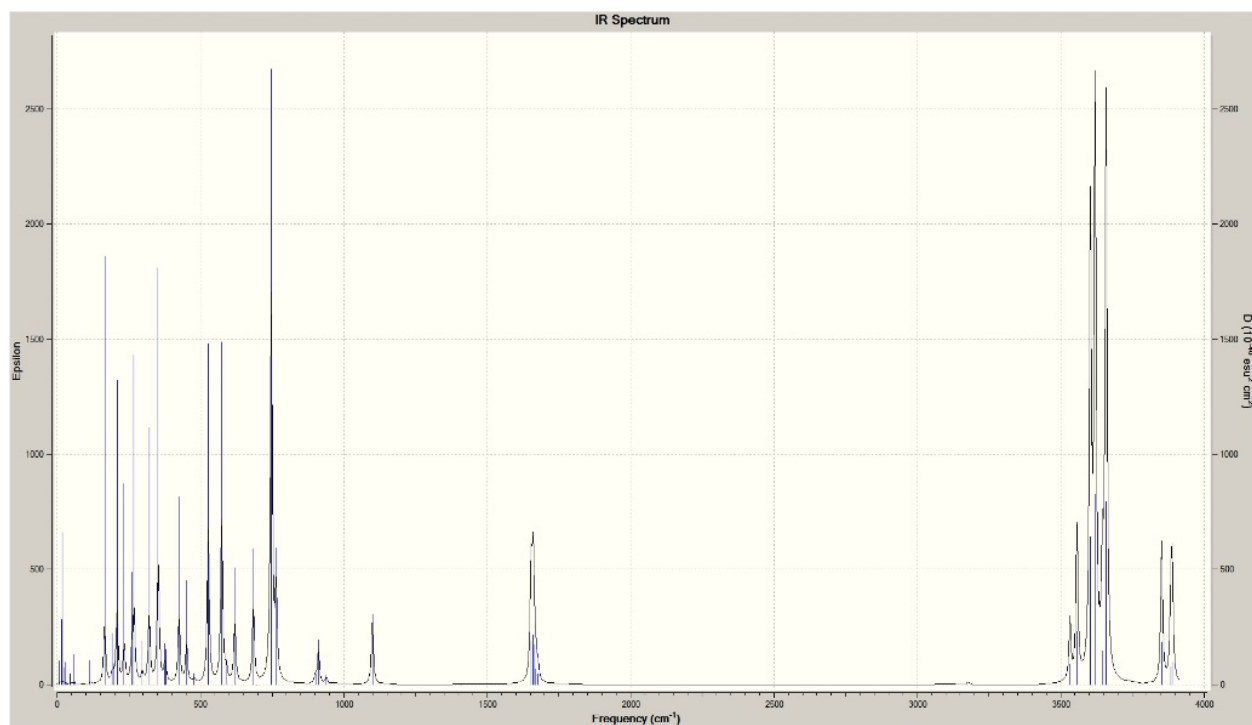


Figure 40B. IR spectrum of DCE3 and 5 water molecules.

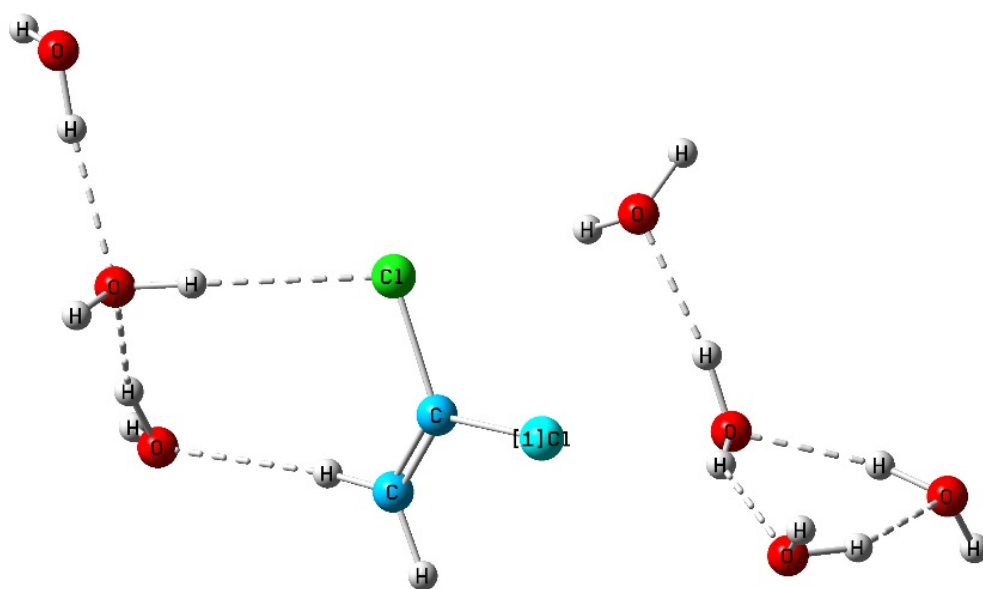


Figure 41A. Equilibrium geometry of DCE3 and 7 water molecules.

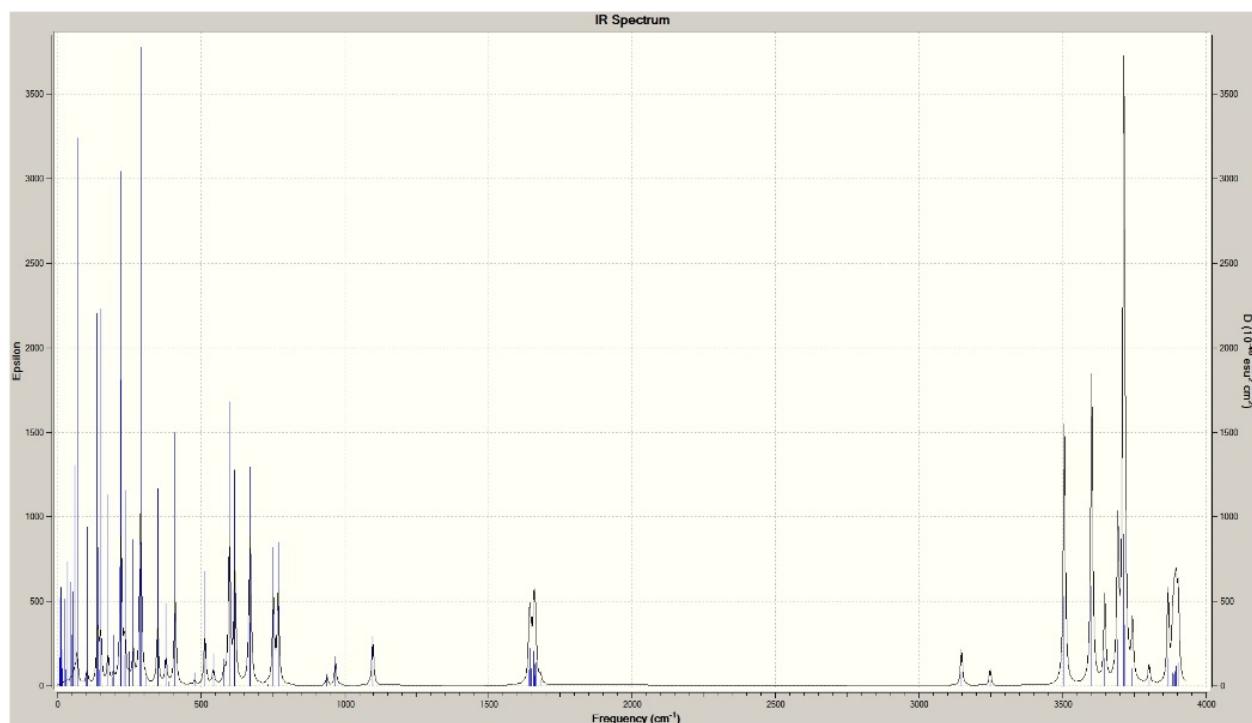


Figure 41B. IR spectrum of DCE3 and 7 water molecules.

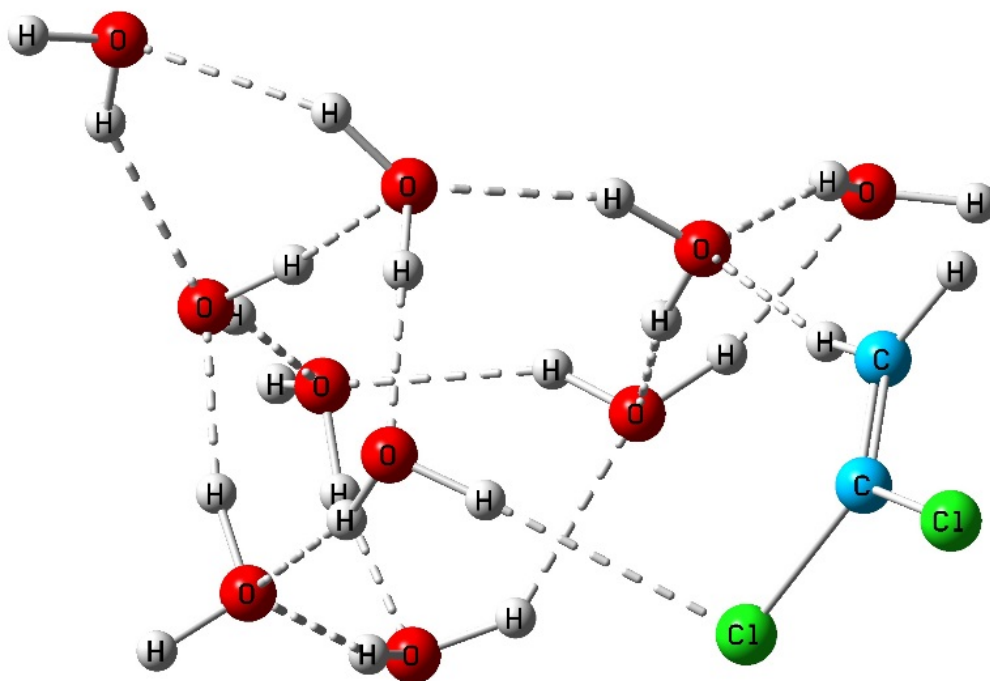


Figure 42A. Equilibrium geometry of DCE3 and 10 water molecules.

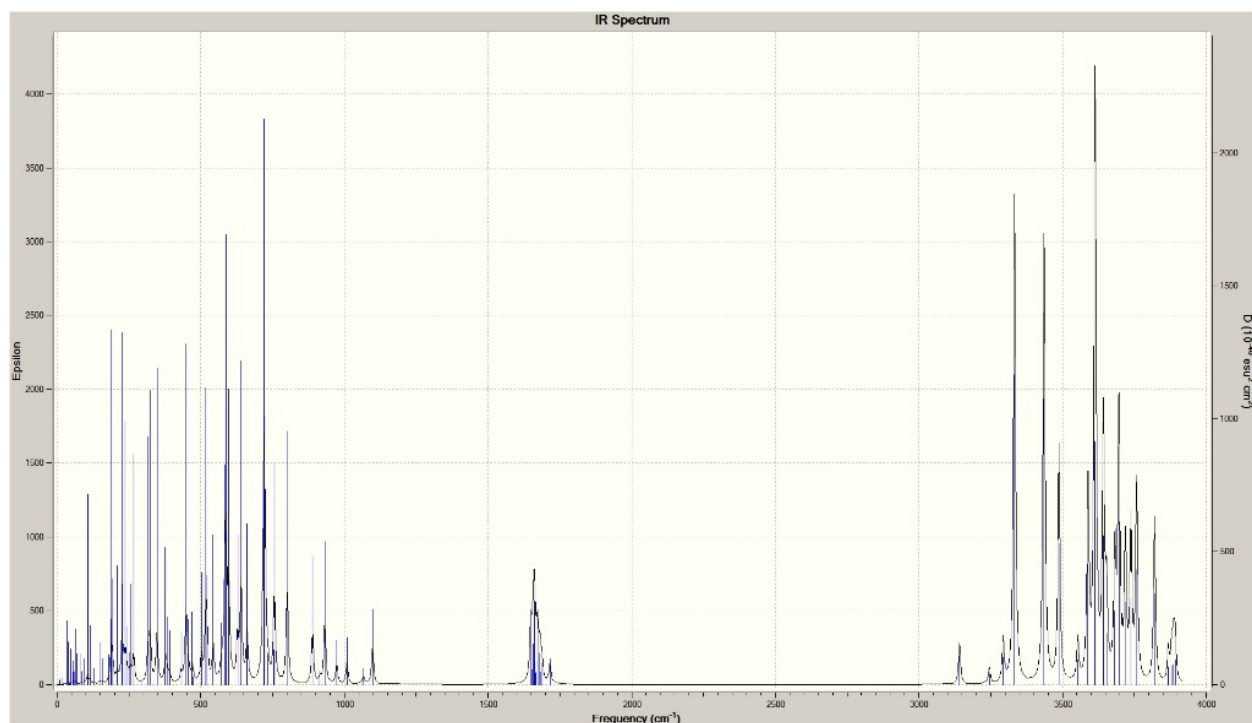


Figure 42B. IR spectrum of DCE3 and 10 water molecules.

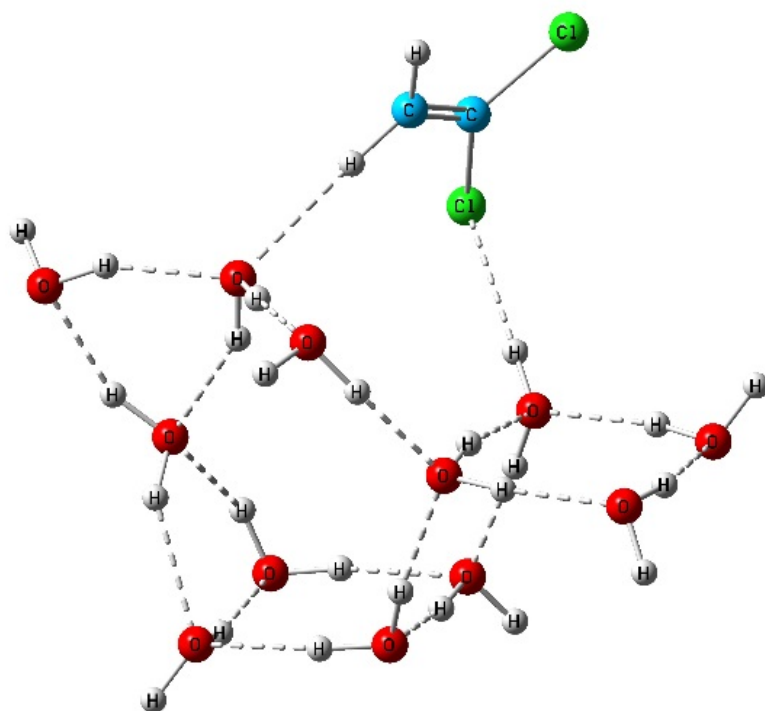


Figure 43A. Equilibrium geometry of DCE3 and 12 water molecules.

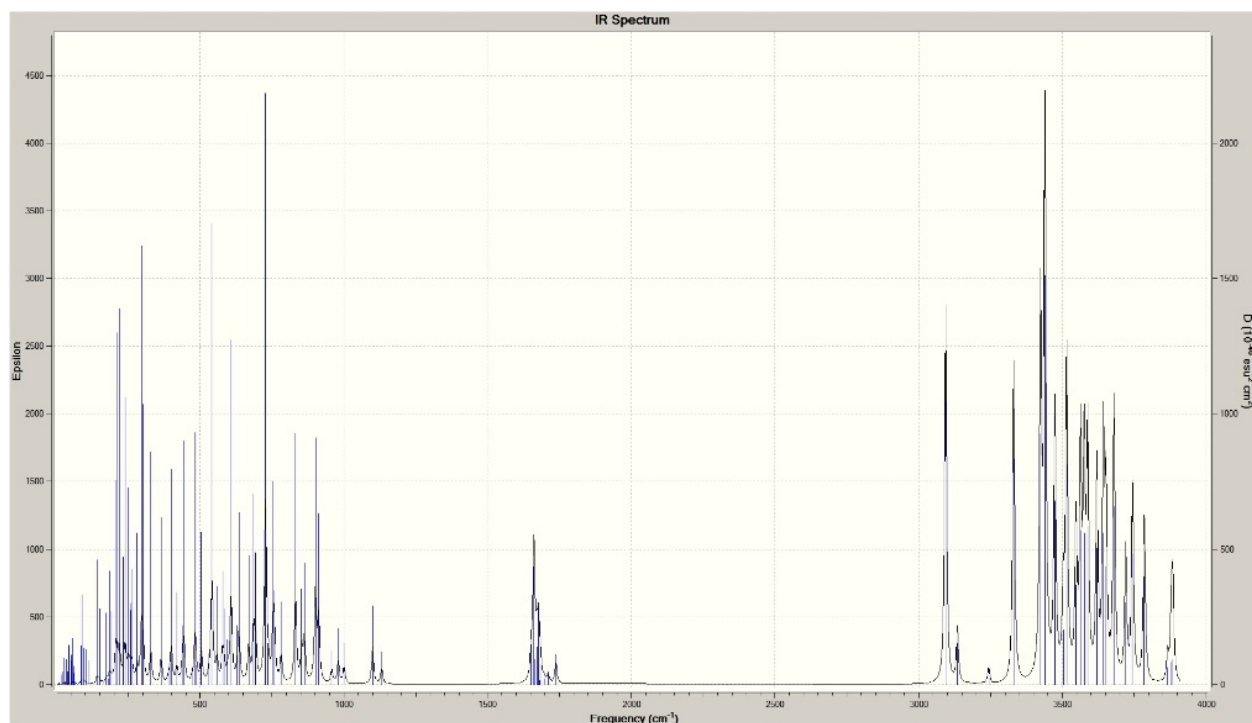


Figure 43B. IR spectrum of DCE3 and 12 water molecules.

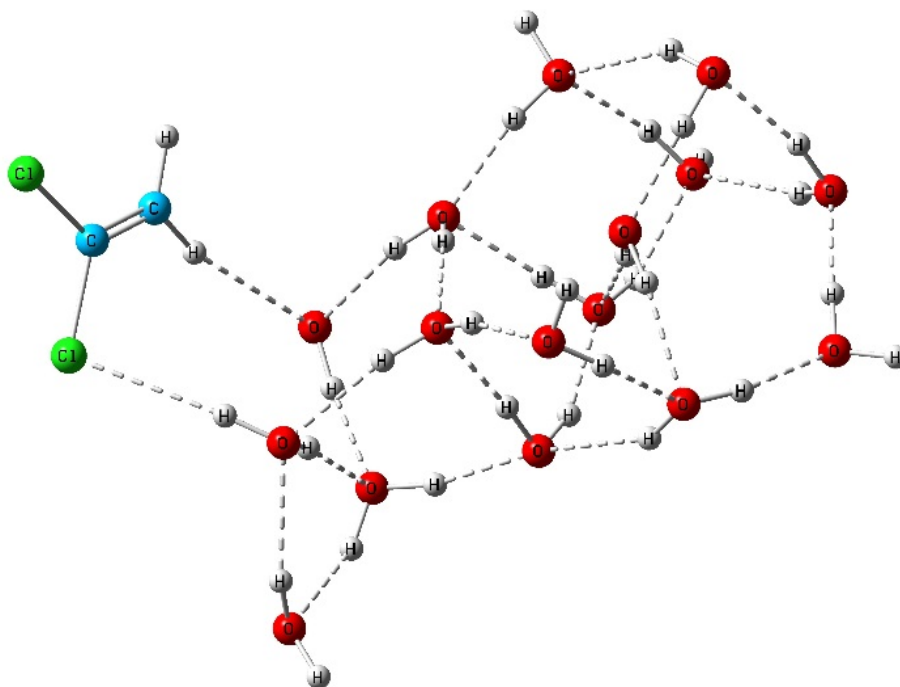


Figure 44A. Equilibrium geometry of DCE3 and 16 water molecules.

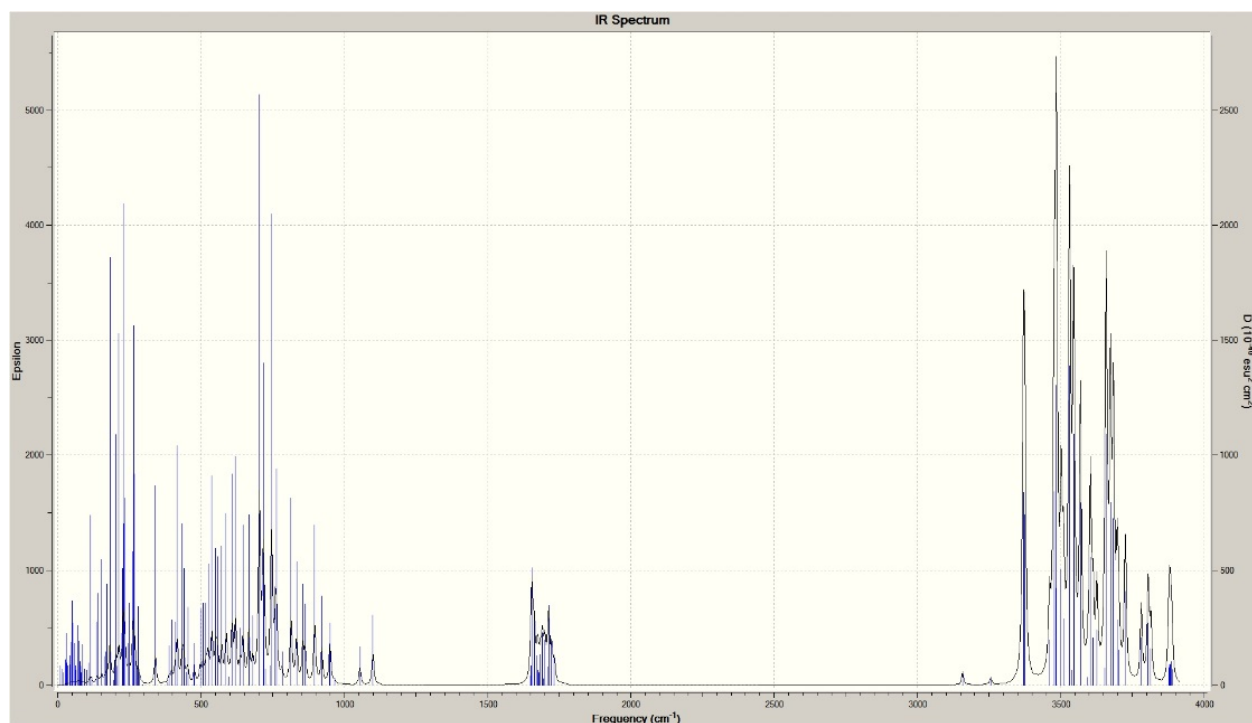


Figure 44B. IR spectrum of DCE3 and 16 water molecules.

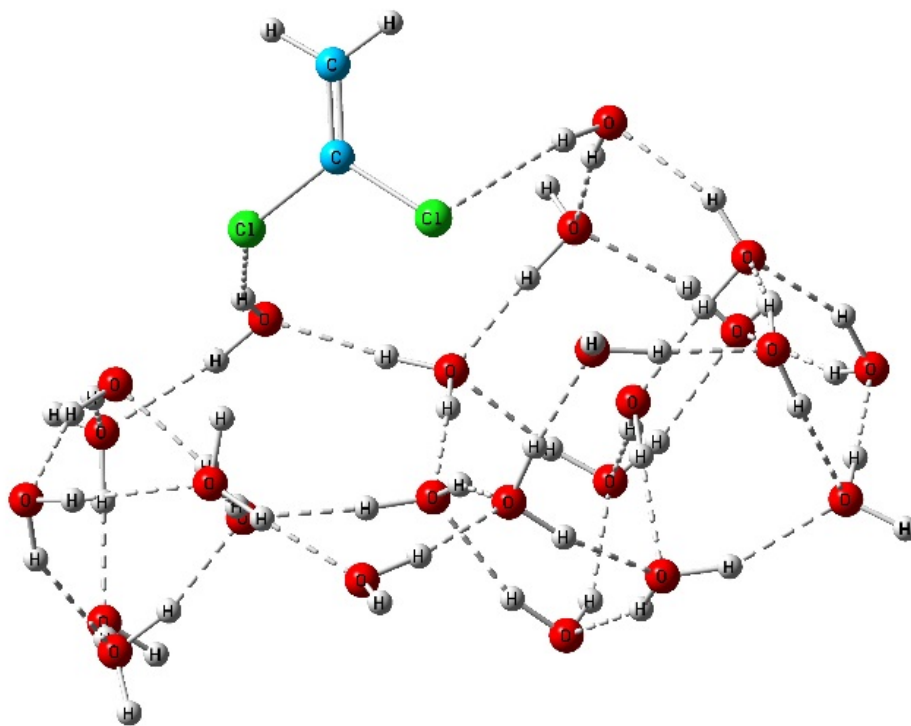


Figure 45A. Equilibrium geometry of DCE3 and 24 water molecules.

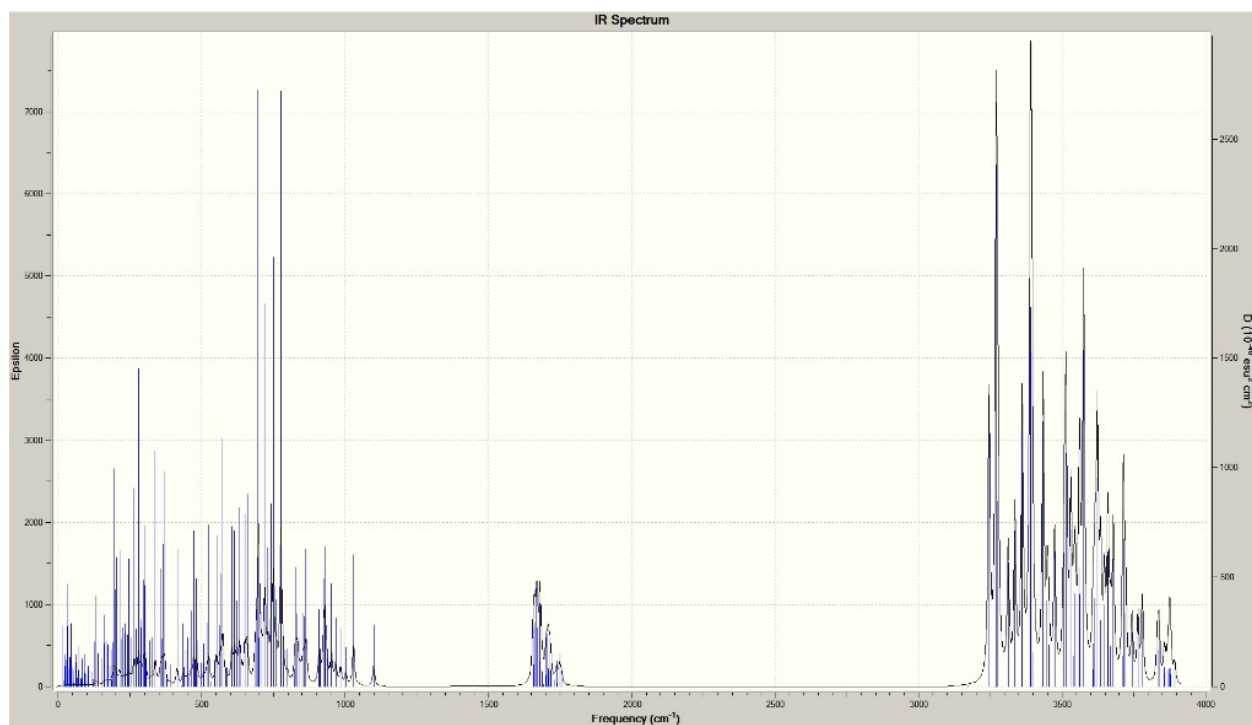


Figure 45B. IR spectrum of DCE3 and 24 water molecules.

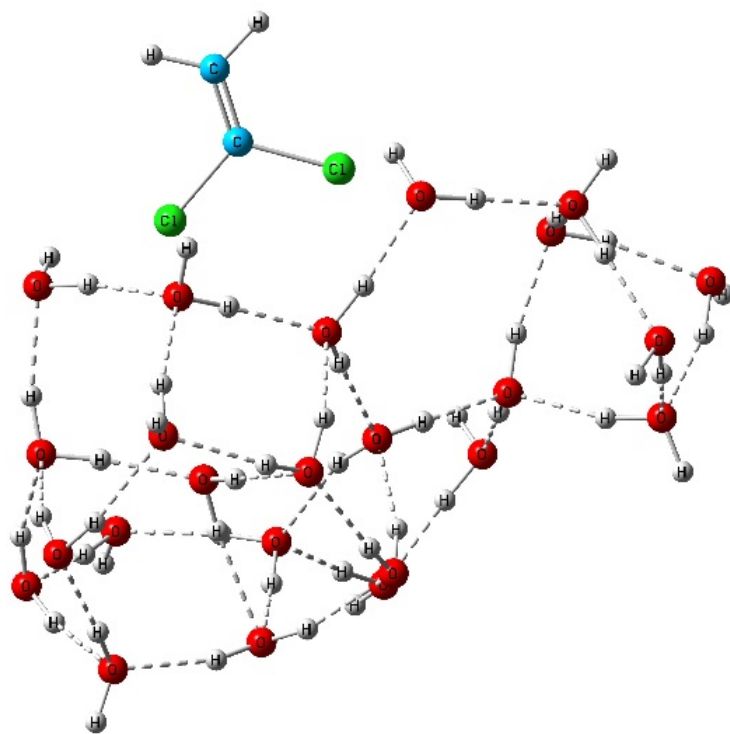


Figure 46A. Equilibrium geometry of DCE3 and 39 water molecules.

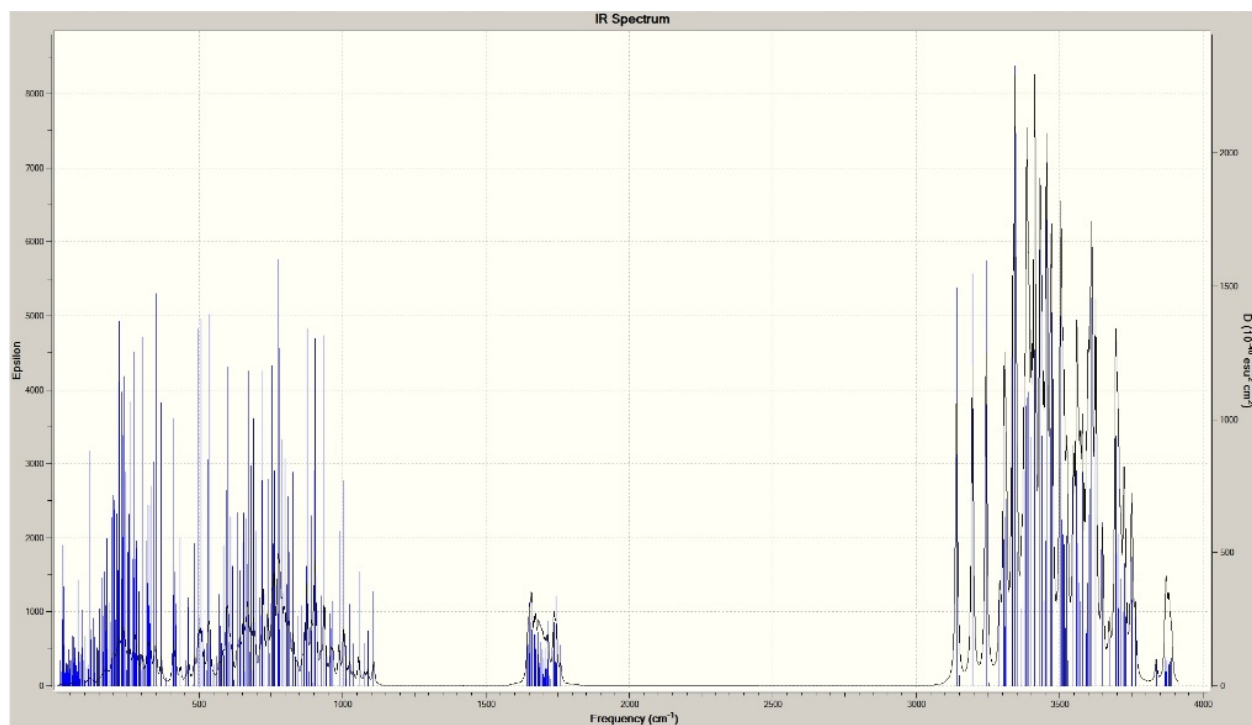


Figure 46B. IR spectrum of DCE3 and 39 water molecules.

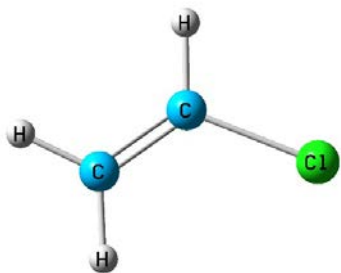


Figure 47A. Equilibrium geometry of isolated VC molecule.

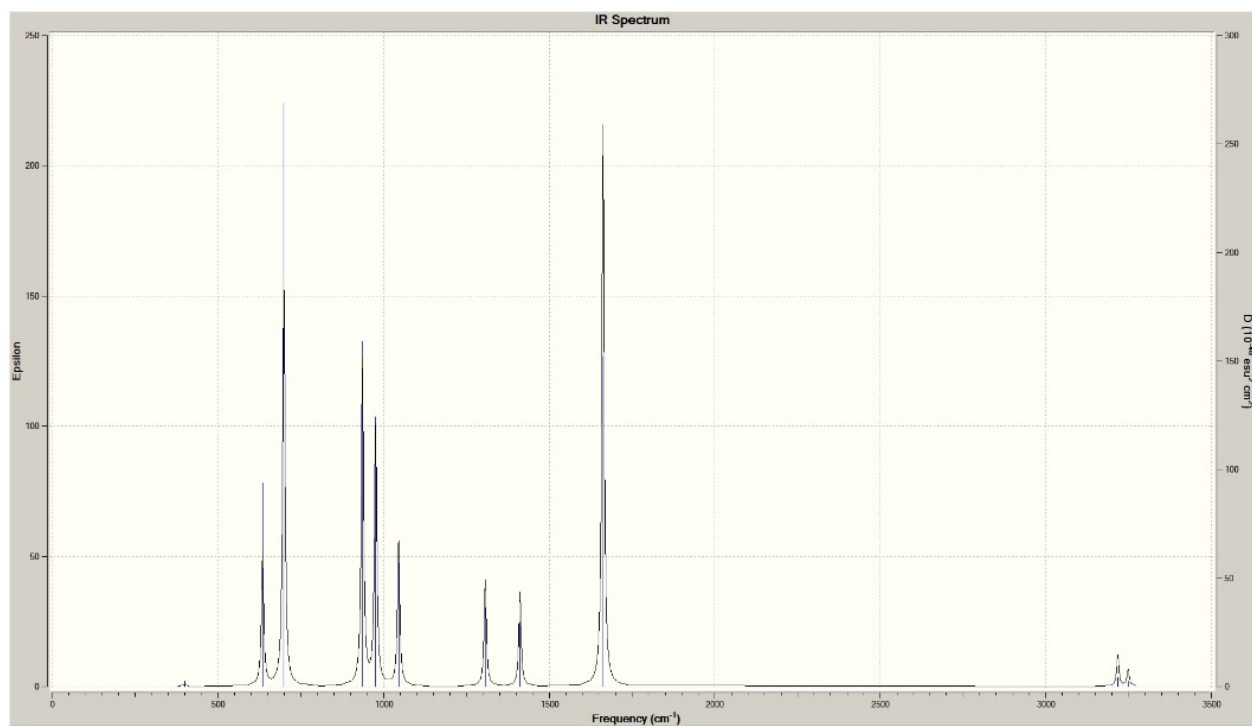


Figure 47B. IR spectrum of isolated VC molecule.

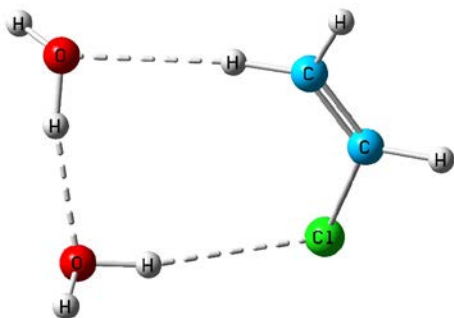


Figure 48A. Equilibrium geometry of VC and 2 water molecules.

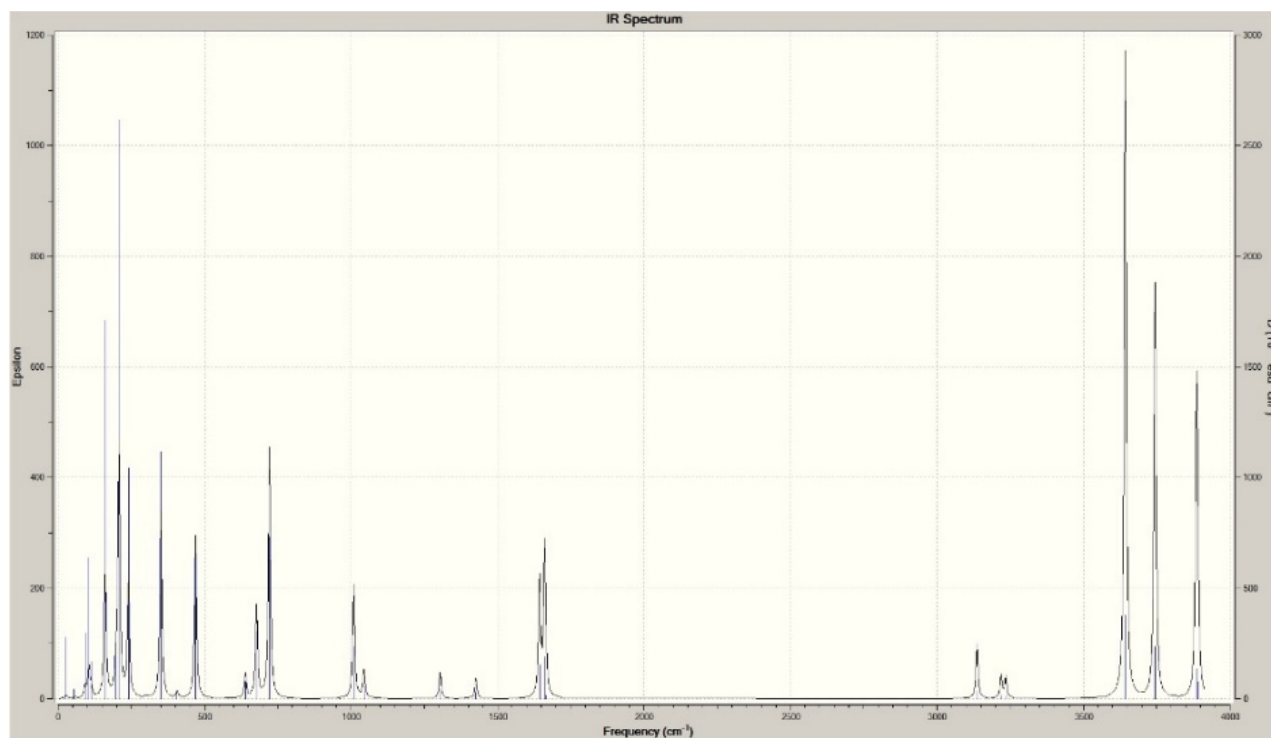


Figure 48B. IR spectrum of VC and 2 water molecules.

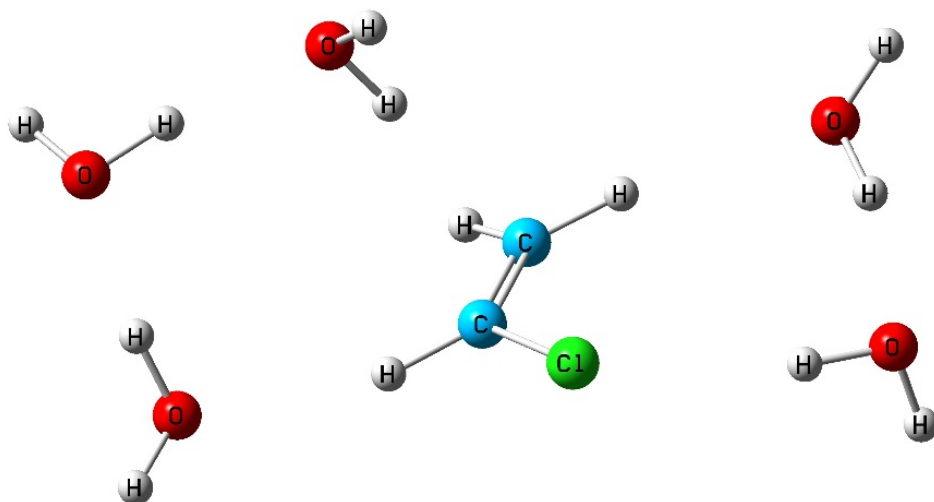


Figure 49A. Equilibrium geometry of VC and 5 water molecules.

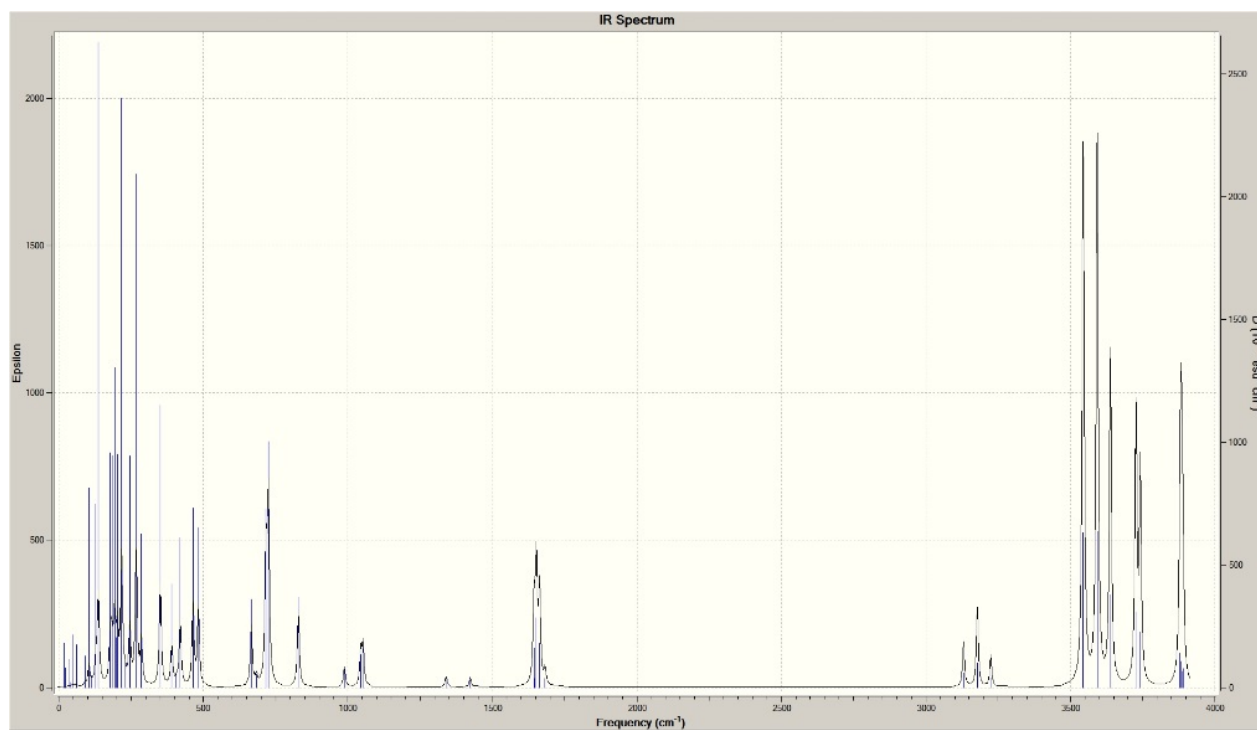


Figure 49B. IR spectrum of VC and 5 water molecules.

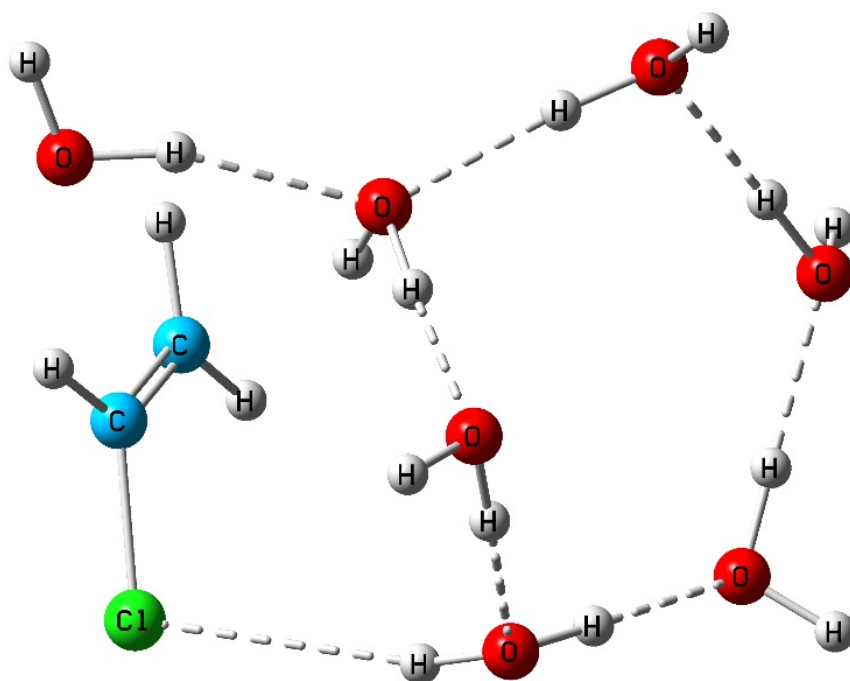


Figure 50A. Equilibrium geometry of VC and 7 water molecules.

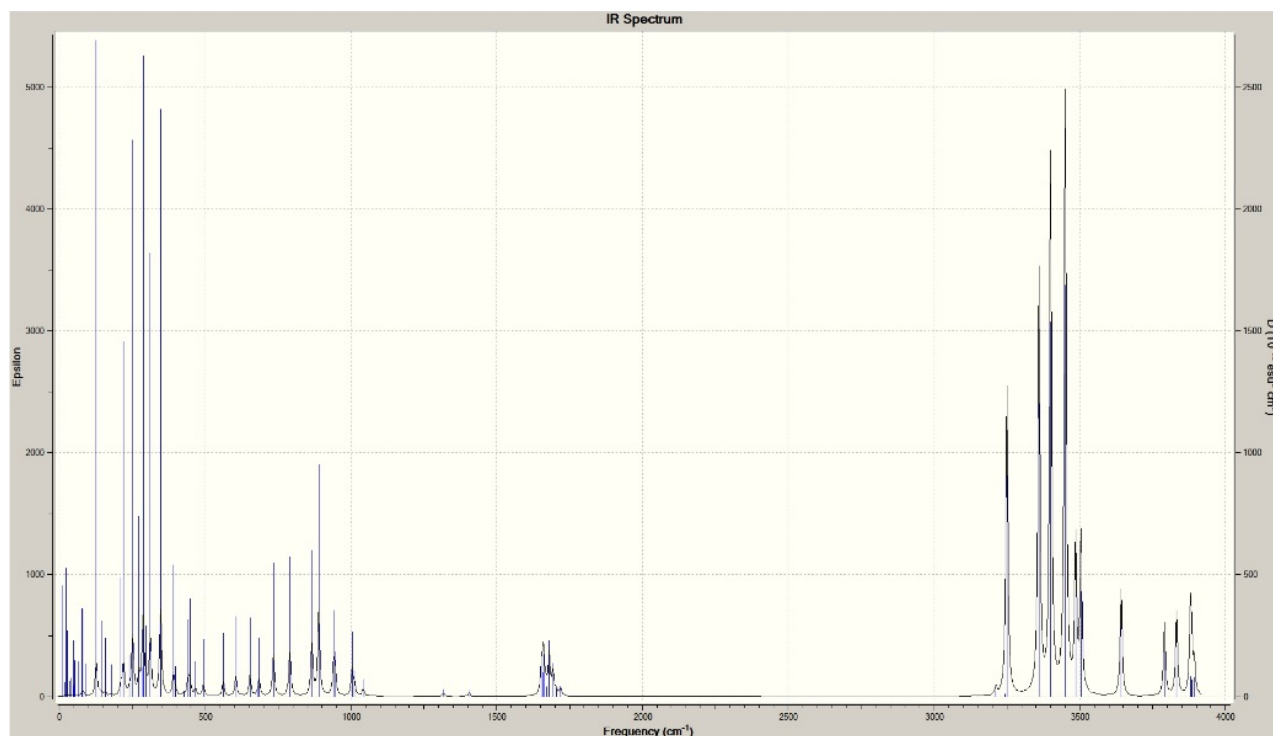


Figure 50B. IR spectrum of VC and 7 water molecules.

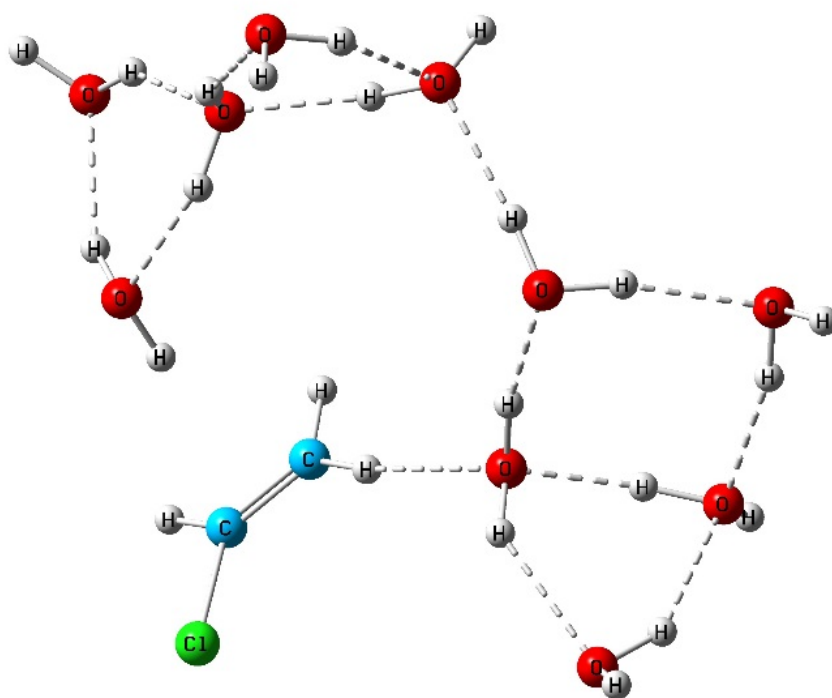


Figure 51A. Equilibrium geometry of VC and 10 water molecules.

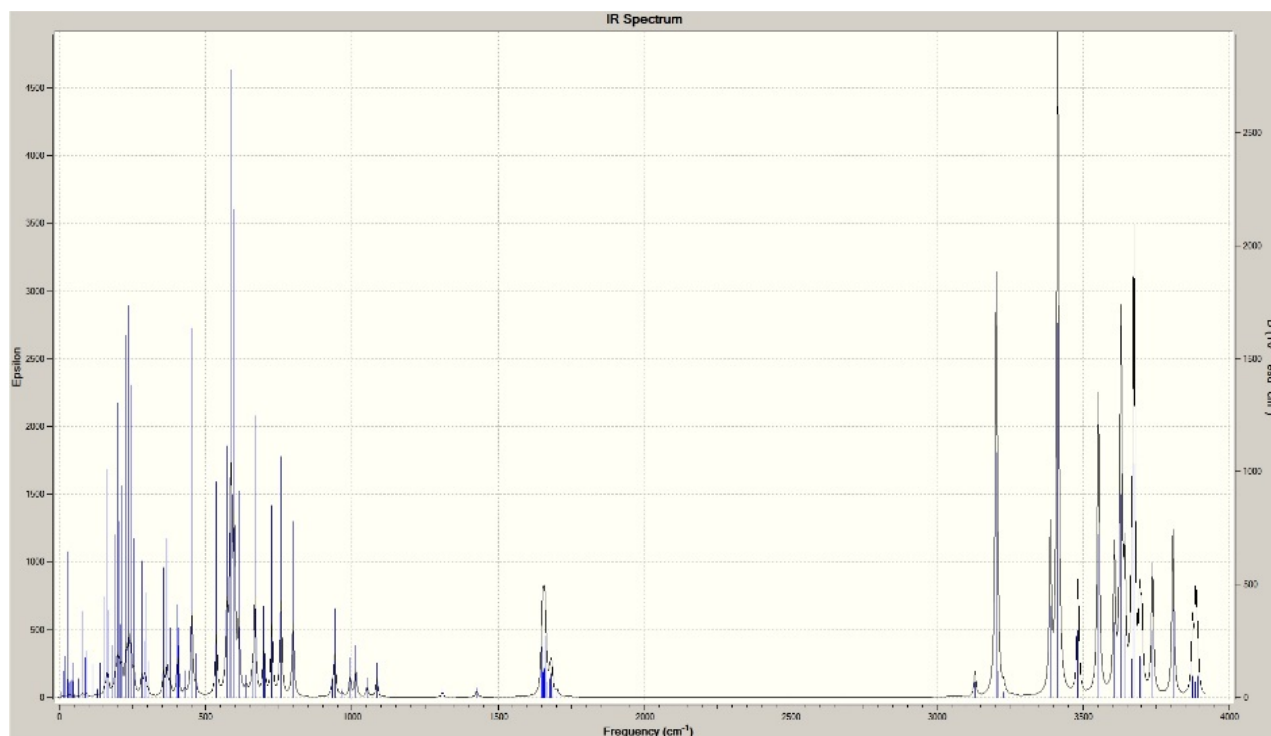


Figure 51B. IR spectrum of VC and 10 water molecules.

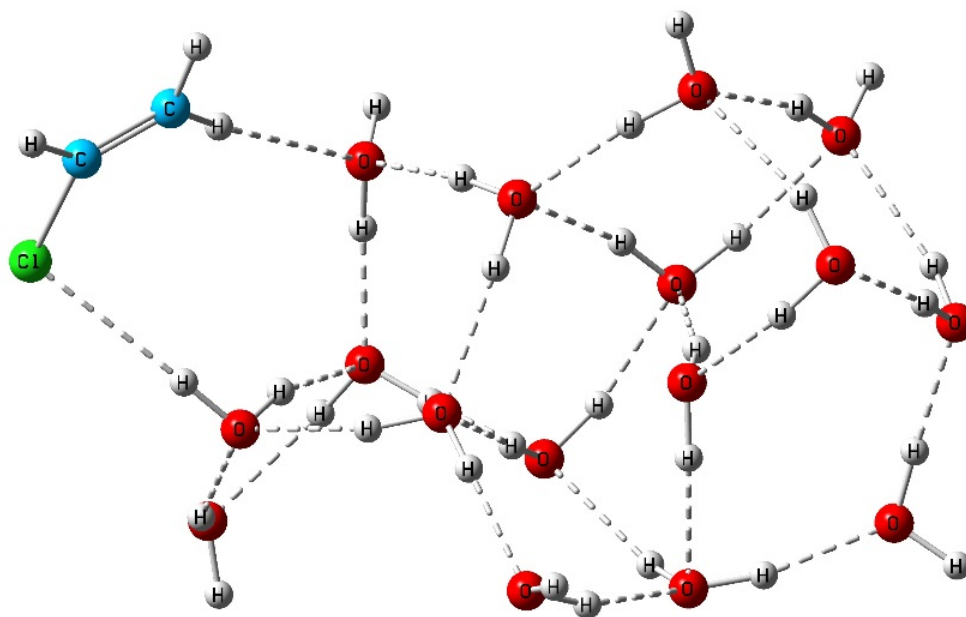


Figure 52A. Equilibrium geometry of VC and 16 water molecules.

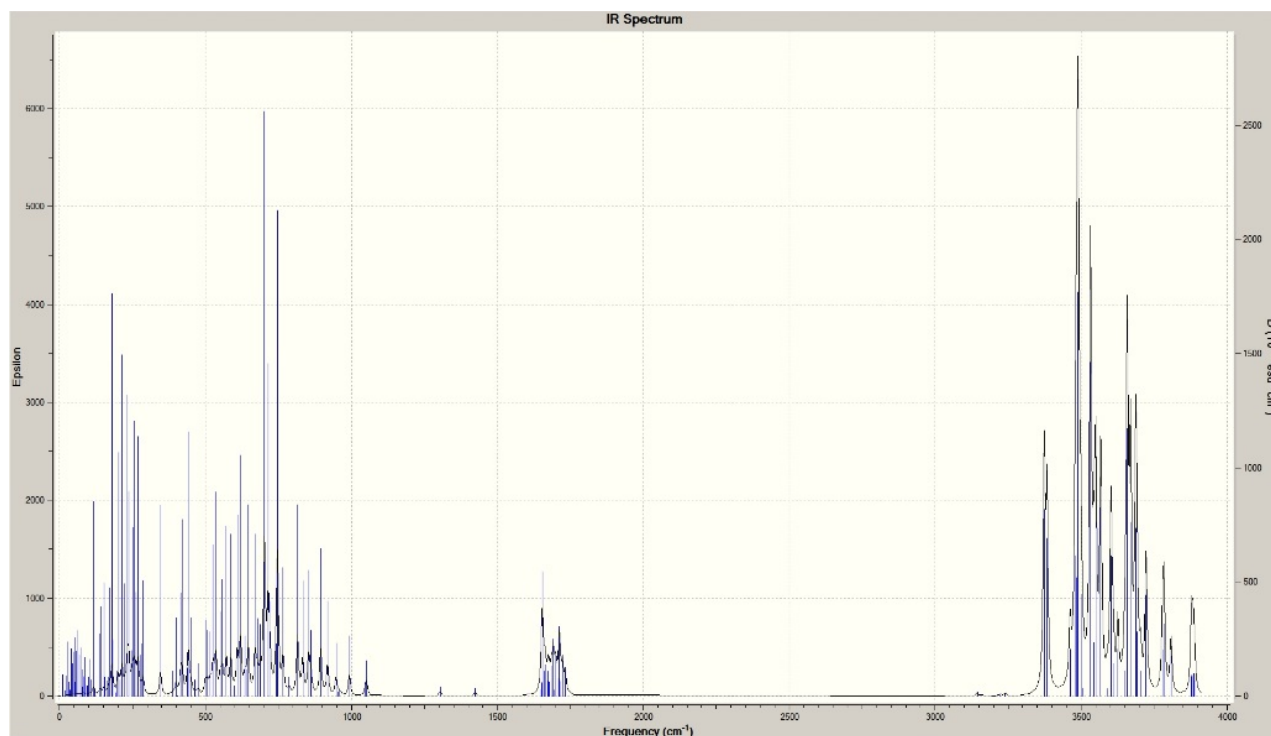


Figure 52B. IR spectrum of VC and 16 water molecules.

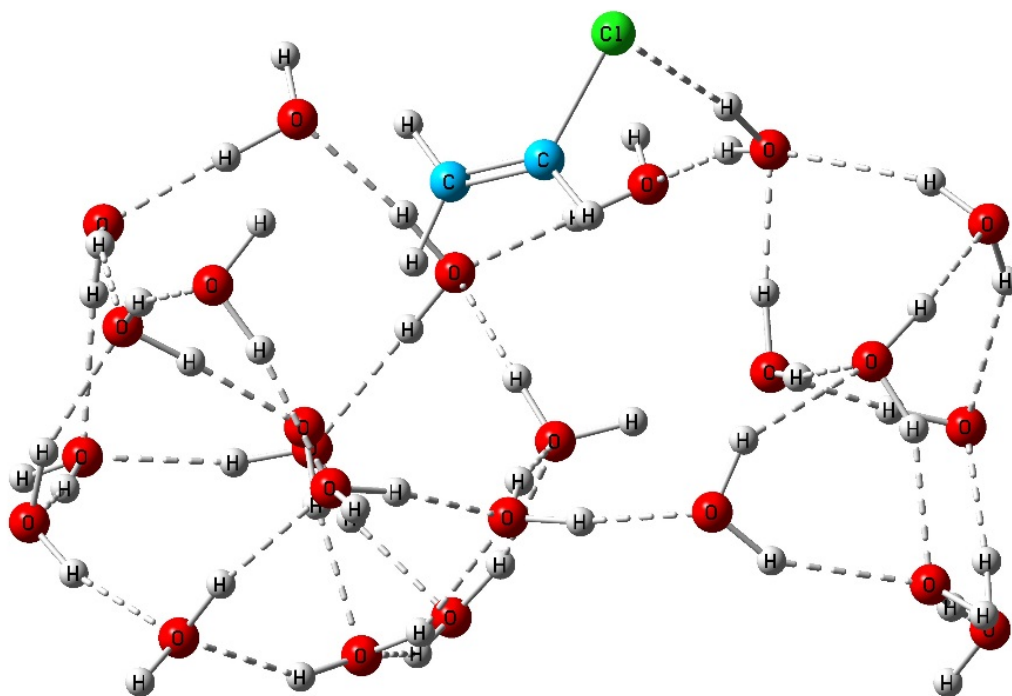


Figure 53A. Equilibrium geometry of VC and 24 water molecules.

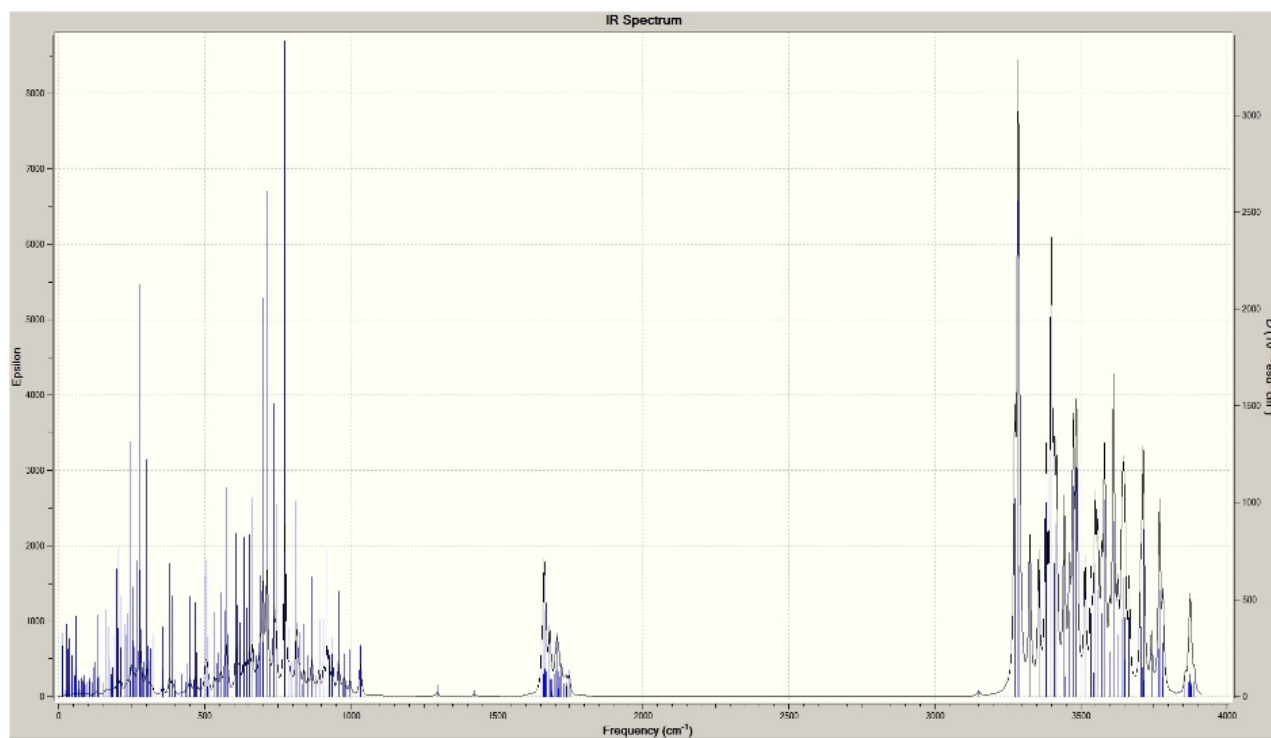


Figure 53B. IR spectrum of VC and 24 water molecules.

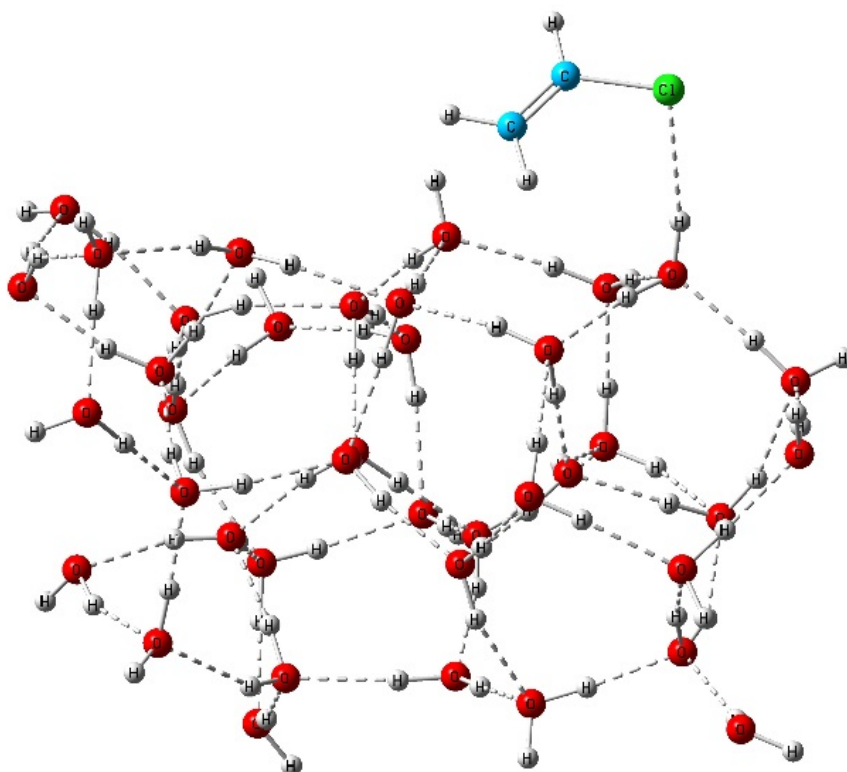


Figure 54A. Equilibrium geometry of VC and 39 water molecules.

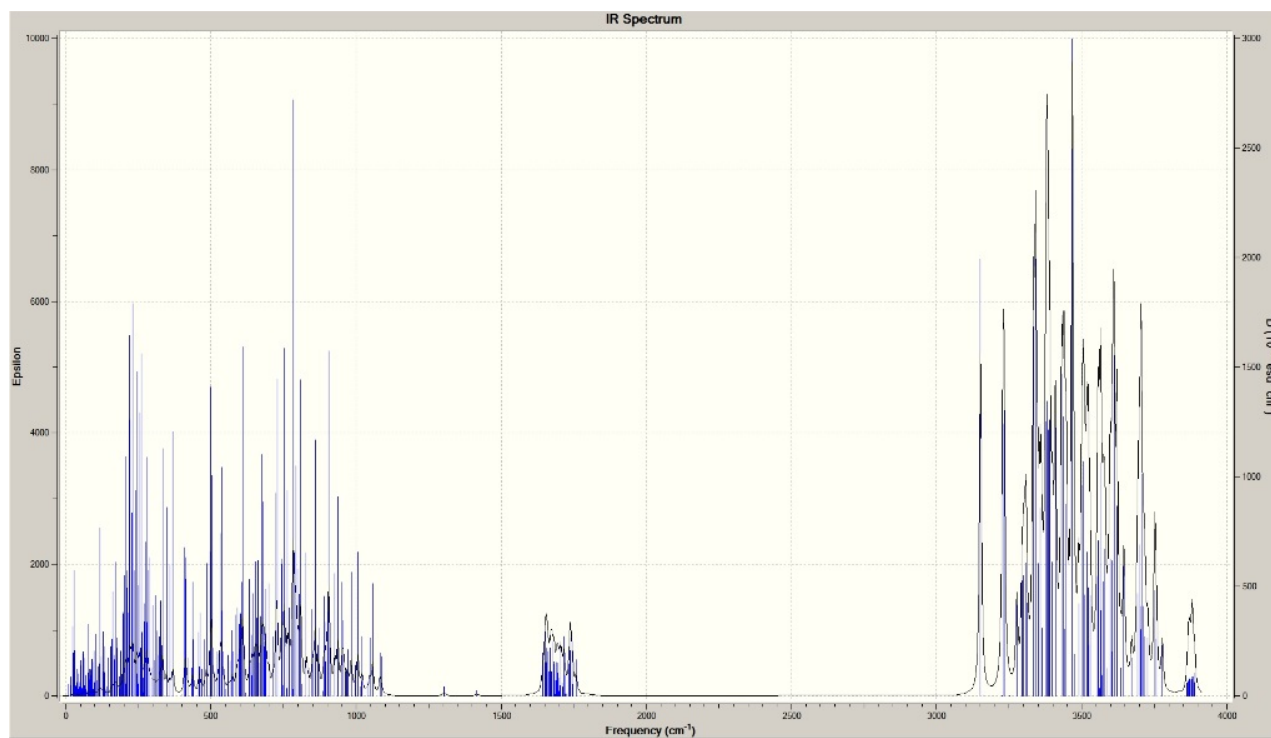


Figure 54B. IR spectrum of VC and 39 water molecules.

Appendix 1

Table 2. IR Intensity as a function of frequency (PCE-nH₂O)

Freq (1/cm) IR Intensity (KM/Mol)

PCE

	Freq	Intensity
1	97.4052	0.0000
2	176.9738	0.7846
3	237.2065	0.0000
4	292.6512	0.4060
5	312.5606	0.1440
6	344.9862	0.0000
7	443.8465	0.0000
8	562.9521	0.0000
9	765.1821	72.4375
10	874.1623	200.8051
11	961.6063	0.0053
12	1613.8350	0.0000

PCE-2H₂O

	Freq	Intensity		Freq	Intensity
1	14.6693	0.8719	16	345.5780	0.3211
2	37.1983	0.6321	17	415.5933	52.8226
3	37.9652	0.8221	18	441.0161	0.7110
4	57.7056	4.1540	19	558.7822	0.1049
5	76.7864	8.1508	20	686.5062	165.2064
6	101.1820	0.8482	21	763.8178	67.3072
7	137.3210	43.7920	22	870.3889	183.6898
8	179.1177	4.6987	23	961.0447	0.5817
9	184.4908	5.4652	24	1612.6975	0.5010
10	196.1845	122.3527	25	1642.6360	66.2819
11	201.8012	126.7467	26	1658.8431	33.8188
12	239.9720	5.1791	27	3672.2212	279.7097
13	277.4537	113.0391	28	3791.0459	73.8527
14	298.0093	13.8295	29	3890.9680	82.4258
15	313.7544	1.5959	30	3895.6245	158.5114

PCE-5H₂O

	Freq	Intensity		Freq	Intensity
1	6.2832	0.1808	30	377.9800	94.7050
2	13.0028	0.8483	31	415.4098	53.0250
3	16.3477	0.3840	32	440.1139	0.7421

4	20.2597	0.9341	33	473.0953	137.4757
5	29.4588	0.9579	34	553.7298	0.0335
6	34.9711	0.3293	35	595.5542	135.0325
7	37.8943	1.4428	36	658.6855	300.6377
8	44.9858	0.0173	37	685.4688	166.4789
9	57.0060	4.1679	38	764.6177	60.8313
10	64.3647	2.7129	39	868.2363	187.3666
11	74.8082	6.9250	40	886.3386	14.6461
12	103.8895	1.9994	41	962.0909	1.2867
13	134.2817	38.1640	42	1611.8728	1.2103
14	174.3633	7.9307	43	1643.3655	66.0703
15	179.5367	0.4398	44	1651.5393	57.9076
16	184.2079	26.8526	45	1658.0052	46.4482
17	188.0826	50.1404	46	1659.9761	153.2966
18	188.1448	157.4097	47	1677.1108	3.4299
19	194.3695	52.8063	48	3555.2358	58.7571
20	203.7048	96.8239	49	3611.2681	616.1510
21	218.1132	1.6321	50	3651.1299	353.3160
22	232.6908	116.2682	51	3671.9419	281.9516
23	241.4033	5.7455	52	3790.7070	80.3373
24	274.4463	125.2047	53	3867.7522	93.8285
25	281.5265	47.4371	54	3886.7869	91.8876
26	298.9418	8.2982	55	3888.9709	66.6456
27	315.4575	1.4315	56	3890.2825	84.9675
28	345.8584	1.6296	57	3895.5017	159.6163
29	353.9639	16.8162			

PCE-7H₂O

	Freq	Intensity		Freq	Intensity
1	5.8012	0.5120	39	368.1403	35.2824
2	9.9034	0.5912	40	410.9134	139.0266
3	12.9658	1.4118	41	438.9867	0.3317
4	21.9240	4.3900	42	488.7250	54.9556
5	24.6774	1.1297	43	544.3362	41.4239
6	27.9060	1.4794	44	555.7084	0.2377
7	28.9235	0.9919	45	586.6712	163.2128
8	34.6946	2.6870	46	609.3306	277.8301
9	37.8314	2.1802	47	649.2601	123.3078
10	44.4120	1.6423	48	655.3818	45.3823
11	50.3814	1.0159	49	734.3413	238.6764
12	53.9341	2.9532	50	765.2789	57.9582
13	60.1548	4.4750	51	869.0850	175.5658
14	67.5701	21.5058	52	923.9311	12.7830
15	77.5913	4.9592	53	963.0779	0.5488
16	79.0933	38.7677	54	1612.0240	0.6359
17	106.2095	1.0020	55	1640.0420	71.0861

18	132.3356	30.1314	56	1645.8713	19.8458
19	144.1808	12.9426	57	1647.0916	48.6955
20	144.5203	86.3750	58	1655.5978	84.0665
21	151.0069	95.5983	59	1657.2505	67.5579
22	173.3310	38.2482	60	1663.9891	125.4322
23	186.0276	4.8145	61	1682.4320	7.4302
24	186.9925	31.2766	62	3532.0212	227.0473
25	195.0601	22.9633	63	3600.6318	537.2494
26	204.8446	174.6632	64	3653.1038	236.7693
27	209.4079	16.4941	65	3711.4580	336.6137
28	212.8087	117.1634	66	3718.7896	55.0245
29	218.9165	117.5731	67	3723.4929	703.8751
30	221.6689	80.4286	68	3762.0481	139.5973
31	231.5558	75.5161	69	3814.4233	7.2444
32	244.9083	2.7990	70	3872.6660	185.5894
33	255.5162	89.0950	71	3873.1189	51.0806
34	283.6629	144.6836	72	3888.1448	74.5141
35	302.5620	0.8905	73	3892.5166	96.6589
36	315.9906	0.2035	74	3894.7524	89.7639
37	339.6161	81.7105	75	3913.0339	84.1657
38	346.3423	0.6530			

PCE-10H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity
1	6.3402	0.5226	35	245.4767	160.6792	69	932.1206	16.5643
2	8.6823	0.5384	36	266.2258	5.0087	70	963.3929	1.7120
3	11.3888	0.0455	37	272.1462	50.9983	71	1080.2321	34.4901
4	14.6457	0.0888	38	279.5327	33.7049	72	1613.2322	0.0235
5	18.6684	0.2424	39	289.1195	61.3540	73	1651.1699	38.0285
6	21.1609	0.5544	40	295.7785	85.9488	74	1651.8199	65.5533
7	26.3641	0.0709	41	301.2162	16.7208	75	1653.5889	105.6119
8	32.5615	0.1889	42	315.0497	13.3939	76	1657.6930	124.6944
9	33.8853	0.5794	43	320.3080	76.5359	77	1657.9763	104.1192
10	36.9253	0.3580	44	345.1076	1.0525	78	1663.7601	12.8273
11	38.6313	1.5619	45	358.7910	47.1799	79	1665.6934	22.9323
12	42.3749	1.8892	46	368.3815	71.9123	80	1677.0931	1.9140
13	45.3686	0.5701	47	373.4520	22.3331	81	1677.2245	61.5089
14	47.7921	0.4069	48	394.2082	101.1347	82	1687.7004	12.5737
15	54.8447	1.4013	49	410.2791	19.5462	83	3205.5164	883.9435
16	56.7959	2.1380	50	417.7586	101.4929	84	3474.3767	397.2254
17	66.3272	1.1178	51	435.0123	38.2532	85	3528.7209	943.0229
18	89.7528	1.7448	52	441.5398	0.8882	86	3532.5002	97.2157
19	104.2905	0.3965	53	469.8601	157.0789	87	3563.2649	201.7562
20	118.6100	6.7770	54	530.9739	67.0014	88	3565.5681	474.4690
21	130.9330	4.3361	55	557.8703	0.4984	89	3608.0381	617.1833
22	158.7791	32.4981	56	563.0902	167.3114	90	3625.1853	79.5844

23	170.8476	46.0396	57	581.9046	258.7017	91	3635.0264	669.9727
24	180.6068	2.9807	58	618.3089	226.0976	92	3660.4614	652.3037
25	185.6679	67.0646	59	632.7222	185.3787	93	3702.8821	161.0938
26	187.9593	8.0947	60	654.9704	281.3299	94	3748.9478	378.8463
27	195.8976	17.3357	61	658.0876	187.8731	95	3869.4453	114.5038
28	198.1289	0.0933	62	734.8991	304.7953	96	3871.6365	67.7707
29	204.4639	22.9180	63	740.1057	139.7574	97	3878.7498	77.1672
30	216.5697	24.5174	64	763.4897	81.5097	98	3882.5012	86.2950
31	223.6721	111.6461	65	795.4478	195.6994	99	3884.6338	64.0926
32	224.5188	60.2844	66	872.3452	187.2887	100	3885.3787	68.5636
33	237.5704	124.0783	67	900.3145	17.2673	101	3887.3374	80.7999
34	241.3636	16.6077	68	912.6056	70.4055	102	3892.2634	94.9674

PCE-12H₂O

	Freq	intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	5.1253	0.2645	31	188.9675	24.9481	61	479.7958	24.5662	91	1668.2167	25.1337
2	8.2077	0.3084	32	196.7786	35.9336	62	504.5323	61.3792	92	1670.4240	75.3524
3	9.1691	0.5717	33	199.8270	56.2251	63	540.3048	44.4058	93	1683.0826	36.1581
4	12.5743	0.6253	34	202.9028	62.3851	64	559.5810	0.2177	94	1683.4872	7.1767
5	15.4775	0.7222	35	214.9998	177.9228	65	562.4354	78.5711	95	1692.9054	19.3747
6	19.2420	0.5691	36	219.3913	1.5457	66	578.9137	74.3927	96	1732.7982	39.6547
7	19.7492	1.9102	37	225.9307	51.6362	67	586.0339	109.4861	97	3277.4475	163.1469
8	23.0730	0.7208	38	234.2411	169.2118	68	604.6043	239.2716	98	3354.0073	2077.0686
9	27.8011	1.4503	39	240.2573	2.7866	69	649.3738	70.8040	99	3417.2917	619.7453
10	29.0142	1.9605	40	244.0019	1.9647	70	657.0479	263.7449	100	3489.7495	527.2867
11	35.0583	0.5222	41	251.0574	27.5398	71	692.4419	61.0313	101	3500.5396	310.7519
12	35.8836	1.1419	42	258.0938	108.6733	72	705.5682	199.6618	102	3521.2344	189.9020
13	38.5559	0.6172	43	261.0892	8.1298	73	762.8470	74.9541	103	3563.9641	890.5185
14	40.9765	0.9985	44	274.7136	49.9789	74	777.4226	366.1221	104	3579.8745	296.6551
15	44.5999	1.1763	45	282.5237	42.2549	75	781.0856	162.7716	105	3581.2612	468.6879
16	49.5708	0.2568	46	285.7519	94.1626	76	845.5399	34.9850	106	3617.1406	429.0779
17	53.7355	0.5255	47	289.5139	48.8781	77	852.4918	254.1840	107	3664.1428	324.1724
18	58.8558	3.7100	48	296.3018	89.9843	78	872.7622	170.6824	108	3672.4668	527.1813
19	60.4601	2.5151	49	302.7291	92.1510	79	917.7573	161.4503	109	3682.1877	707.3292
20	67.5000	7.2885	50	313.6526	4.9074	80	926.6843	22.1143	110	3741.7151	514.9896
21	77.8404	30.9928	51	318.7713	106.1326	81	950.7780	28.2576	111	3816.0664	7.9250
22	78.2532	1.1369	52	339.8056	61.1307	82	963.4823	4.6451	112	3843.4053	199.9238
23	99.3644	2.1461	53	345.5583	0.6170	83	1047.3188	16.6125	113	3874.1960	65.6374
24	104.4679	1.0574	54	377.7919	57.2994	84	1613.3475	0.1652	114	3879.3992	69.3696
25	107.9165	9.9334	55	395.3904	77.6878	85	1639.2115	78.6053	115	3880.7834	53.9751
26	149.8308	11.7810	56	401.5299	53.9229	86	1654.5360	64.1323	116	3881.7654	38.7546
27	167.6064	0.7101	57	410.0785	85.8438	87	1658.2448	94.3487	117	3881.8799	90.2703
28	170.7941	42.2005	58	430.6224	62.4515	88	1659.6385	76.8920	118	3885.7935	69.9357
29	182.0806	1.2117	59	440.5374	0.5481	89	1663.3169	97.3674	119	3888.9001	88.0628
30	183.7734	3.9840	60	458.8221	59.8714	90	1663.7113	46.0955	120	3915.1204	87.0400

PCE-16H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	5.4647	0.1218	40	196.8398	5.1771	79	557.4886	71.1125	118	1695.0000	47.5755
2	7.4529	0.0290	41	202.6923	55.9658	80	572.6282	93.3271	119	1701.3358	80.4750
3	13.9694	0.2785	42	208.5625	1.1851	81	582.2596	135.0104	120	1709.0413	21.1628
4	21.7517	0.0744	43	212.7296	98.2782	82	590.8162	7.0498	121	1713.3647	113.5354
5	25.7038	2.0170	44	222.4044	13.9079	83	608.1917	125.0370	122	1716.3578	48.1864
6	28.9524	0.4735	45	224.0243	86.1856	84	615.5088	125.1727	123	1724.2570	75.7880
7	29.7598	0.4627	46	224.9602	37.6997	85	633.5429	23.3645	124	1733.3274	54.3314
8	31.2757	0.0508	47	235.5334	51.3169	86	642.6666	132.5742	125	3370.6963	746.7098
9	36.6319	0.1774	48	239.9208	4.3000	87	664.3595	143.2611	126	3374.2146	665.1998
10	45.6297	4.4613	49	244.3960	11.0214	88	675.8706	82.2748	127	3462.6384	188.7979
11	46.7962	2.7647	50	252.2475	67.2915	89	700.9987	429.0461	128	3479.5378	368.6256
12	49.8177	2.8026	51	255.7864	55.3120	90	715.8072	271.9528	129	3483.2783	958.2065
13	58.3817	2.5828	52	261.8667	38.3556	91	719.0759	100.0011	130	3487.8652	202.2565
14	59.8664	1.6312	53	268.2208	82.0246	92	737.7427	44.8465	131	3496.2810	1251.4318
15	61.5949	0.3496	54	271.5216	15.1347	93	744.3986	402.2648	132	3502.7146	35.9827
16	69.2340	3.5342	55	277.3545	19.5068	94	760.4257	71.8265	133	3529.6287	1288.5023
17	71.8582	2.0528	56	283.0745	38.1364	95	764.9538	112.2585	134	3542.8643	33.1154
18	76.8905	3.9154	57	285.7841	4.6559	96	785.3471	21.9441	135	3549.1177	1039.2397
19	79.9314	0.8369	58	297.1761	13.2047	97	811.9839	176.8489	136	3567.9143	718.4783
20	83.1858	1.3102	59	314.7939	1.6031	98	830.4283	101.0443	137	3594.6394	36.3546
21	87.0871	3.9303	60	329.0665	40.1918	99	850.1614	61.6314	138	3601.6113	482.3520
22	90.3491	0.7537	61	345.2430	2.7664	100	862.3858	119.9913	139	3612.3323	229.1516
23	95.8791	1.4951	62	387.4479	23.0072	101	871.6414	198.4623	140	3623.1990	223.6920
24	98.2860	1.1947	63	395.6035	50.6947	102	893.8725	131.6788	141	3656.8303	447.2750
25	101.6130	0.5463	64	399.8193	61.3197	103	921.8106	101.1158	142	3662.1340	607.8609
26	106.9432	1.7686	65	405.9955	33.9625	104	946.8253	65.0386	143	3681.2783	844.5456
27	113.4574	16.7454	66	417.2882	70.5966	105	960.9859	10.9621	144	3688.8181	580.3676
28	118.3685	1.2473	67	432.2759	14.0957	106	961.9073	0.7041	145	3700.8716	229.5795
29	133.5311	15.3494	68	441.0513	116.2376	107	1054.7278	38.0224	146	3704.8008	111.2338
30	137.6774	11.6391	69	441.9037	0.1266	108	1614.4397	0.0577	147	3723.6055	414.2251
31	150.0271	21.4921	70	451.1713	17.1307	109	1650.4768	39.0013	148	3780.7903	186.5165
32	152.6137	5.8436	71	477.2608	19.1736	110	1650.8488	47.3163	149	3807.8325	168.3941
33	160.6048	4.7033	72	500.1076	32.9328	111	1655.2323	173.7800	150	3835.3459	207.7699
34	165.5665	6.1559	73	506.8448	47.9450	112	1661.1082	47.2414	151	3877.9221	67.0289
35	168.8222	40.5939	74	512.7886	31.3729	113	1669.7130	49.2653	152	3879.1299	87.5277
36	176.1778	59.5555	75	525.3718	93.6886	114	1673.1985	46.4295	153	3879.8982	77.7006
37	179.7311	4.6811	76	534.6659	92.8233	115	1679.2938	14.8184	154	3883.3169	87.5604
38	181.5732	4.3587	77	545.0127	120.0074	116	1684.2332	54.5513	155	3885.9827	102.3529
39	192.0652	0.4599	78	554.6502	1.2922	117	1690.7787	81.3654	156	3889.6191	65.3065

PCE-24H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	8.0916	0.2091	58	213.3909	61.4017	115	582.9199	21.0963	172	1710.0153	12.6596
2	11.2160	0.1355	59	214.8804	11.2800	116	602.7831	85.4199	173	1712.0701	44.9328
3	13.9606	0.8137	60	216.0390	26.0163	117	609.9191	118.8753	174	1712.9976	36.6454
4	15.9610	0.6945	61	224.9022	28.8288	118	622.0255	19.5945	175	1718.4596	72.5391
5	19.9038	0.3634	62	230.0983	134.6476	119	628.6315	107.3442	176	1728.9377	3.9028
6	23.0255	1.9072	63	232.7806	23.7211	120	635.3889	45.7896	177	1733.3032	46.9592
7	25.1837	0.3876	64	234.0489	40.3899	121	645.0648	105.6544	178	1737.3597	18.0384
8	27.1683	1.0585	65	236.2888	11.2451	122	657.7390	229.2986	179	1747.7972	78.7708
9	31.4310	3.4461	66	239.2175	1.9565	123	676.8140	26.3321	180	1750.2374	21.3749
10	34.9808	1.3269	67	244.0051	9.0088	124	681.9767	26.6622	181	3242.6975	1190.2388
11	39.3937	1.6021	68	252.2011	9.1610	125	692.5789	577.3634	182	3275.6716	1257.0272
12	42.3053	2.9322	69	255.0347	64.8106	126	697.8294	49.7409	183	3293.1672	1669.8444
13	45.1463	1.7746	70	259.0510	13.9413	127	702.4611	102.1421	184	3312.9346	714.9397
14	45.7743	0.7365	71	260.2390	12.5821	128	717.8702	167.9936	185	3319.8796	13.7764
15	48.5271	0.5906	72	266.5919	65.5976	129	721.1001	82.7780	186	3356.8171	1068.1649
16	51.3270	1.0499	73	271.8785	68.3869	130	744.1634	97.7786	187	3388.4626	1035.7927
17	52.1635	0.5431	74	279.5064	47.0941	131	746.9255	450.5439	188	3407.8401	1278.8185
18	56.8662	2.1716	75	283.4023	5.8092	132	762.8915	73.1140	189	3412.7825	302.0772
19	58.4296	1.3614	76	285.9465	4.5651	133	772.8815	467.8011	190	3435.6213	1148.2603
20	62.3591	0.7563	77	292.2829	17.7072	134	780.9737	53.3978	191	3452.6873	124.7998
21	63.5677	1.2258	78	293.3544	20.7092	135	788.3895	140.3340	192	3456.2996	356.2387
22	64.5072	0.6967	79	299.6625	56.3761	136	794.2964	66.4582	193	3475.6360	291.3351
23	67.2018	0.7663	80	304.8076	14.0681	137	812.5827	87.8078	194	3504.6116	575.0024
24	69.1896	1.6962	81	309.1510	48.1821	138	822.8191	109.9419	195	3510.7402	1038.3851
25	70.8326	1.5648	82	313.3127	0.1986	139	830.0347	26.4498	196	3539.8191	18.1447
26	73.8382	0.1959	83	319.8265	16.8267	140	839.5984	81.6475	197	3550.6870	234.1120
27	75.5509	0.6624	84	323.6705	22.3348	141	847.9600	76.5050	198	3553.8894	831.4195
28	76.8668	1.7979	85	345.0512	1.6242	142	859.4931	173.1638	199	3555.9634	463.7961
29	80.1115	0.4973	86	346.7263	8.6119	143	861.9088	57.9137	200	3569.4336	583.5479
30	83.4276	2.2998	87	351.3907	8.1270	144	872.0728	153.7626	201	3587.9583	865.4857
31	86.7061	0.2178	88	357.0444	77.3864	145	902.2698	77.1961	202	3604.0969	250.9747
32	89.2234	2.3247	89	367.7116	33.5485	146	917.3043	32.3812	203	3610.3845	109.4583
33	94.1370	0.4489	90	400.9302	50.5553	147	929.3137	182.0564	204	3621.1567	318.1346
34	97.5348	0.8771	91	414.8259	69.6564	148	930.7038	23.7659	205	3625.4800	680.3745
35	101.9931	0.5600	92	421.8514	29.7648	149	938.6262	27.8250	206	3642.3123	395.7008
36	104.0078	1.5209	93	425.8469	41.1421	150	947.4681	255.8020	207	3643.2405	260.3053
37	106.6205	3.5282	94	438.2359	10.0461	151	960.5904	11.3270	208	3655.3599	637.6733
38	112.3496	1.6803	95	442.0648	0.1377	152	966.3242	50.5536	209	3663.9319	350.0124
39	115.7880	2.7977	96	448.8459	10.9205	153	975.3607	9.3357	210	3672.5066	167.2137
40	119.1954	1.1644	97	452.6497	29.7282	154	984.3539	58.4785	211	3676.8208	499.7396
41	132.7783	15.7806	98	456.0718	4.2339	155	1024.2871	134.0901	212	3705.5984	320.2934
42	133.3303	4.4588	99	463.4490	59.7352	156	1613.6124	0.0285	213	3712.5891	108.4774
43	136.0226	2.6839	100	477.1580	47.3346	157	1652.2042	126.4780	214	3718.7373	684.0207

44	138.9294	3.5031	101	480.2601	29.2075	158	1655.0293	85.5164	215	3740.9688	216.9694
45	144.8210	8.9431	102	481.3071	42.9498	159	1656.8297	54.6882	216	3761.1948	262.1964
46	155.7154	13.7395	103	495.2224	22.7065	160	1660.3596	118.2102	217	3777.6682	354.5198
47	160.3547	8.5557	104	500.2774	9.2441	161	1665.5880	159.6340	218	3833.8525	150.5165
48	168.0628	10.8557	105	502.2400	71.3844	162	1670.8048	126.2334	219	3836.5991	148.4113
49	171.5054	7.7721	106	507.3474	1.4657	163	1678.8236	37.6722	220	3858.3689	61.9395
50	178.2037	6.7816	107	529.5221	73.4732	164	1680.5282	128.5817	221	3868.7554	72.3287
51	178.3752	4.7352	108	536.2709	5.6974	165	1681.5272	71.3464	222	3874.6306	87.3458
52	182.8462	6.6038	109	540.6840	28.5219	166	1687.1356	31.6874	223	3874.8843	59.6223
53	184.1895	2.4591	110	543.3529	0.0167	167	1688.4132	3.3716	224	3875.7546	58.0213
54	189.7059	10.8169	111	552.8929	79.1734	168	1691.4547	3.7439	225	3876.3108	107.3189
55	192.9388	9.6942	112	561.0010	57.0394	169	1701.5424	14.5652	226	3884.7939	44.9952
56	197.9023	12.0959	113	569.8229	164.8516	170	1703.3326	96.3154	227	3885.6003	68.1419
57	209.0404	36.8442	114	570.8369	74.3488	171	1706.8596	127.1839	228	3892.4465	71.7722

PCE-39H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	3.8835	0.0074	92	218.7239	17.3526	183	653.5753	65.9490	274	1712.9885	16.0417
2	7.8351	0.1950	93	220.3452	49.8119	184	656.2538	51.0284	275	1715.7113	124.9504
3	9.9163	0.0465	94	226.1831	17.5815	185	660.4777	112.2728	276	1718.1527	39.3102
4	14.2325	0.0222	95	227.0820	21.8286	186	663.8357	17.3375	277	1720.7664	3.0265
5	19.2022	1.1009	96	229.5206	74.7368	187	670.6823	97.6790	278	1725.9685	5.2880
6	20.9817	1.4799	97	230.4917	50.2048	188	672.9632	186.0035	279	1733.6694	63.3764
7	22.4619	0.7665	98	233.7477	58.3984	189	679.6130	121.1763	280	1737.2312	67.4396
8	23.2557	1.1889	99	235.7429	89.6437	190	684.8030	90.9778	281	1737.7889	93.8799
9	24.4990	1.0456	100	237.2593	0.1237	191	689.9091	43.8232	282	1742.0619	89.6017
10	26.4043	1.4897	101	243.0879	26.6460	192	690.6916	70.0762	283	1745.5813	111.3801
11	27.2347	1.7355	102	244.3894	35.1060	193	699.9634	94.0351	284	1747.7723	27.6004
12	29.1222	0.7739	103	246.7123	57.6736	194	715.5342	66.9576	285	1758.9639	71.4785
13	31.2771	1.4457	104	248.9636	4.5983	195	724.0790	212.9072	286	3160.6458	1753.7562
14	34.9716	0.2760	105	251.6320	34.1886	196	726.5616	209.5351	287	3170.9202	905.8451
15	36.0725	0.3358	106	255.0895	84.3941	197	739.5959	168.6944	288	3227.7661	1282.4742
16	38.6818	0.3547	107	258.7109	54.0755	198	742.9046	65.8569	289	3280.8545	348.0664
17	39.0386	0.6311	108	259.1237	76.7809	199	747.2936	20.3614	290	3292.2615	387.2240
18	41.4007	0.1435	109	263.8151	25.6026	200	751.1995	290.0377	291	3301.1536	532.7189
19	42.5234	0.0390	110	267.0738	10.0517	201	760.5612	23.9555	292	3304.7070	507.9453
20	43.6484	1.4339	111	267.5800	7.3488	202	762.6466	43.7773	293	3311.2744	377.9583
21	46.2711	0.5382	112	269.8327	16.7988	203	766.2303	189.0123	294	3335.3618	1357.6143
22	48.2105	1.0288	113	271.7732	28.9267	204	773.1008	42.8146	295	3341.8350	1727.2615
23	50.0204	0.5662	114	275.3577	44.3127	205	780.0007	74.2544	296	3352.1487	388.4852
24	51.5173	0.9903	115	276.0956	66.4378	206	781.9701	27.3697	297	3358.8899	725.0396
25	54.7120	0.7185	116	276.9272	22.0871	207	786.4932	419.7122	298	3365.3269	210.0538
26	56.1922	0.4352	117	279.2745	48.2460	208	788.9239	172.7757	299	3376.0515	1192.9189
27	57.8255	0.8034	118	281.7298	38.0417	209	794.9281	207.3326	300	3383.9482	819.2775
28	59.4369	0.5715	119	284.4010	31.5585	210	800.1116	178.0725	301	3390.6580	1346.1718
29	60.8748	1.7987	120	290.1422	2.4143	211	804.9807	50.4364	302	3398.6943	228.8055

30	61.8699	3.8110	121	291.3045	25.9342	212	809.9663	282.1800	303	3404.3904	1079.6569
31	62.6167	1.4325	122	295.4883	9.4054	213	814.3855	6.8080	304	3407.4236	1266.9202
32	62.8764	0.8600	123	302.3642	52.8265	214	827.3341	139.0766	305	3432.1641	1446.0654
33	66.2581	1.5895	124	307.6090	22.0118	215	835.9336	39.0486	306	3439.4700	1061.3798
34	68.0035	1.6282	125	310.5196	1.9545	216	840.5041	54.7205	307	3444.2363	341.1739
35	68.5691	1.5823	126	313.2705	0.0717	217	849.8626	84.7651	308	3451.1736	626.0359
36	69.4837	0.8653	127	317.2997	0.8211	218	859.1917	190.2699	309	3469.1780	2545.6042
37	71.6791	0.0925	128	319.6042	22.4973	219	869.1222	86.6588	310	3470.9250	93.8890
38	73.2397	0.1235	129	322.0547	28.0708	220	869.2170	23.5473	311	3490.0481	416.3356
39	75.6646	1.4666	130	323.7088	120.5788	221	872.9363	185.4477	312	3503.0745	1187.4810
40	76.4809	1.8695	131	327.5316	34.3278	222	886.0019	8.6917	313	3506.0933	720.2669
41	77.0146	0.9139	132	330.9821	32.0438	223	890.7569	99.3258	314	3511.4407	324.2613
42	78.3018	2.4061	133	333.5509	38.2537	224	895.5443	65.2563	315	3516.3269	450.2725
43	79.2093	8.8421	134	344.2230	0.1497	225	897.8084	20.7577	316	3521.5176	316.6932
44	82.7884	0.6680	135	344.7434	69.9707	226	904.4778	118.9312	317	3522.4021	476.8131
45	84.6671	2.8403	136	371.0857	35.6519	227	905.6906	352.2169	318	3524.3933	243.8165
46	86.3418	2.1107	137	371.3381	123.3396	228	909.1958	38.8985	319	3529.7246	326.6828
47	87.9455	1.7169	138	391.2156	28.9106	229	929.7121	154.8504	320	3553.1831	529.5285
48	90.7656	6.9778	139	408.6139	53.7251	230	938.2486	239.1361	321	3558.7251	795.5456
49	92.1877	3.3511	140	410.2696	63.9284	231	952.7194	55.1318	322	3564.6824	406.0486
50	93.0948	4.1128	141	413.6930	71.7411	232	957.2387	28.1953	323	3567.9958	345.6859
51	95.5067	0.0533	142	420.5870	29.6943	233	958.7000	65.5866	324	3568.8267	363.3691
52	98.2949	1.6042	143	433.9039	40.5372	234	961.5717	46.3428	325	3570.4846	177.3365
53	99.6470	0.3086	144	435.6239	26.5801	235	967.4666	34.6349	326	3574.8894	355.4636
54	102.8103	3.3485	145	442.5909	0.2393	236	982.8072	153.9850	327	3576.0708	679.0726
55	106.8322	0.5862	146	455.8344	9.2416	237	1003.2278	18.6289	328	3593.3113	61.6044
56	111.1246	4.3218	147	458.2174	39.7608	238	1005.7724	176.2843	329	3593.7056	210.8442
57	115.0605	4.4502	148	458.7431	29.7251	239	1012.0060	9.5395	330	3598.1306	434.1019
58	116.2456	21.9189	149	465.3586	20.4365	240	1019.2889	22.1470	331	3602.1987	265.3904
59	122.4638	4.5817	150	482.7452	65.5466	241	1021.1606	68.0437	332	3605.8479	607.4217
60	125.4105	4.2887	151	483.4583	40.9256	242	1048.3949	66.1087	333	3613.2673	1262.2198
61	130.2364	9.7610	152	494.1063	166.7444	243	1058.4478	121.2716	334	3622.5791	398.3068
62	131.4647	7.0931	153	500.6387	76.4916	244	1081.6637	64.0242	335	3623.3245	798.7147
63	134.8138	2.0694	154	502.9139	135.0802	245	1085.1418	46.5811	336	3632.0210	115.6765
64	136.2613	1.3225	155	508.6892	32.1935	246	1614.1074	0.4502	337	3647.8362	570.8704
65	142.5223	1.8871	156	516.6867	13.5997	247	1647.0015	74.1914	338	3672.9243	162.8588
66	145.2428	7.2448	157	524.4658	8.1629	248	1650.1689	53.9678	339	3697.9067	765.0175
67	153.3034	11.8823	158	526.1588	26.2704	249	1652.0850	135.6887	340	3701.4602	624.2443
68	158.4251	6.2692	159	530.4195	109.2723	250	1654.8568	48.4065	341	3703.6980	190.4297
69	160.2435	21.7436	160	536.6256	197.2382	251	1657.0544	68.2493	342	3704.9023	433.3600
70	163.7352	3.9595	161	538.3318	26.3830	252	1657.9443	91.9020	343	3706.4478	459.5886
71	167.6377	9.7248	162	542.3421	0.5938	253	1659.8763	82.4992	344	3719.9902	256.4404
72	169.3306	1.4164	163	546.9906	5.0881	254	1668.3278	85.5885	345	3724.2488	365.9355
73	170.1751	27.0547	164	552.5098	7.0207	255	1671.6427	72.0053	346	3728.0801	250.3617
74	173.5691	6.3032	165	561.6425	15.3591	256	1672.0758	22.3281	347	3753.4036	472.4510
75	174.5748	10.9174	166	570.8162	10.1242	257	1675.4625	100.6347	348	3754.6882	226.1561
76	176.0853	14.7355	167	571.2233	45.4167	258	1679.2953	48.9814	349	3761.7385	228.5702

77	176.6311	1.2942	168	574.7550	22.3125	259	1681.3492	74.2185	350	3832.8896	125.0629
78	184.6440	7.1480	169	586.1883	66.4734	260	1681.8182	21.5683	351	3856.0459	91.7314
79	186.8107	1.1700	170	591.3142	74.8213	261	1686.2542	33.5774	352	3867.7161	61.6238
80	187.9206	8.4837	171	595.8356	176.5645	262	1688.6768	38.4702	353	3868.8354	82.8715
81	189.4075	17.3487	172	598.1662	12.4922	263	1689.0522	1.8589	354	3869.9316	63.7569
82	193.5414	0.5416	173	602.4854	54.5546	264	1691.1832	60.4990	355	3872.3835	75.1456
83	196.6864	21.8827	174	604.1874	113.2527	265	1691.5941	36.2436	356	3873.2283	73.3207
84	198.6511	32.8032	175	608.0824	119.3711	266	1696.5017	76.8552	357	3879.9546	59.9298
85	202.0499	57.5452	176	615.2370	53.4972	267	1697.9800	9.3896	358	3880.1560	67.3860
86	203.4571	28.6254	177	619.1646	3.2640	268	1698.5912	5.7743	359	3880.4646	75.6380
87	206.2747	21.9248	178	633.9437	83.7914	269	1700.4327	43.2451	360	3881.1707	85.5876
88	208.2020	14.3173	179	640.5972	44.4094	270	1703.4742	14.1228	361	3884.6636	85.3149
89	209.6384	18.8240	180	643.3869	61.7605	271	1705.2338	78.7132	362	3887.8547	59.4039
90	210.7944	16.8839	181	644.3651	41.4658	272	1706.0044	23.5725	363	3890.6521	100.3129
91	217.4469	33.9672	182	647.9058	54.2149	273	1709.3302	18.3441			

Appendix 2

Table 3. IR Intensity as a function of frequency (TCE-nH₂O)

Freq (1/cm) IR Intensity (KM/Mol)

TCE

	Freq	Intensity
1	170.6727	0.7883
2	203.4142	0.3379
3	275.1784	0.2439
4	382.9169	0.1403
5	476.7353	4.3174
6	623.4844	14.1402
7	816.7475	23.0903
8	821.6689	122.5342
9	908.3589	98.6496
10	1274.2227	9.7056
11	1637.4661	11.3984
12	3238.0959	14.5033

TCE-2H₂O

	Freq	Intensity		Freq	Intensity
1	18.8058	1.0441	16	471.7999	3.4215
2	33.6127	0.5066	17	617.8306	19.0629
3	37.7048	1.1780	18	683.3344	155.3695
4	61.5939	9.7118	19	826.2874	102.3681
5	66.5555	0.7008	20	826.8470	21.8688
6	135.7406	28.7650	21	905.6402	100.9330
7	177.2793	7.2834	22	1273.5229	7.5191
8	182.9382	3.1585	23	1637.9386	8.1487
9	186.8034	163.6868	24	1644.0795	73.2862
10	202.2489	88.5920	25	1658.4174	30.4059
11	214.6494	7.9256	26	3229.5991	13.7730
12	267.8217	122.9480	27	3672.0698	289.6667
13	276.7334	20.3631	28	3788.3750	80.0960
14	384.7781	0.4875	29	3891.6006	80.6586
15	420.2590	48.3516	30	3894.1194	149.5370

TCE-5H₂O

	Freq	Intensity		Freq	Intensity
1	5.4729	0.7010	30	582.3647	41.4511
2	8.8769	0.0695	31	622.0677	25.1228
3	17.2488	2.0413	32	660.4985	129.6881

4	20.2755	4.1525	33	685.5278	98.6434
5	27.5838	1.2500	34	793.5627	161.8847
6	35.2275	3.1161	35	811.8128	120.7253
7	43.4658	0.6228	36	824.2706	250.4842
8	54.6769	2.4123	37	863.9985	22.5170
9	78.3675	2.0595	38	904.6797	96.1796
10	84.6966	0.7106	39	985.3914	21.7452
11	146.4729	3.3838	40	1300.7933	11.0877
12	172.2253	1.6889	41	1639.8578	5.2346
13	184.9507	15.7087	42	1641.5925	100.8463
14	203.3062	0.0820	43	1668.3677	61.5052
15	211.5935	11.3559	44	1688.7349	44.3736
16	215.7630	66.6951	45	1696.7913	56.7101
17	221.7435	74.6312	46	1709.1825	43.1584
18	230.8087	18.1117	47	3219.2285	88.1483
19	248.9233	46.1800	48	3363.8545	188.0218
20	256.4990	16.5476	49	3447.1570	1247.8722
21	274.1841	76.2292	50	3473.0947	940.0100
22	276.8299	31.9083	51	3545.0310	504.7721
23	300.8223	185.2178	52	3753.5417	382.1690
24	315.0450	35.7195	53	3808.6460	19.4632
25	381.3057	0.2405	54	3858.4873	123.1604
26	423.8433	41.9832	55	3879.4888	65.2532
27	443.7695	11.9695	56	3886.7888	62.2495
28	483.0284	6.4355	57	3905.7893	86.5177
29	541.3463	84.4664			

TCE-7H₂O

	Freq	Intensity		Freq	Intensity
1	5.3331	0.0265	39	598.2691	200.7602
2	15.1402	0.0968	40	622.2501	30.3103
3	25.9980	0.6174	41	661.3830	95.4214
4	30.1912	0.7261	42	723.6514	84.3820
5	36.4889	0.9320	43	756.7881	291.7054
6	39.9868	0.6110	44	783.4116	86.7196
7	56.4182	1.0332	45	803.0895	87.7886
8	57.3297	3.3690	46	806.5598	298.8978
9	62.3474	0.9990	47	874.0392	23.4576
10	73.2511	1.1413	48	891.6973	24.6958
11	96.0434	1.2082	49	903.9023	99.6826
12	101.4801	2.0710	50	958.4495	81.3724
13	106.8060	11.3154	51	1065.6595	59.9784
14	157.3581	7.2540	52	1309.7725	8.0030
15	172.4585	9.3595	53	1639.7208	66.7747
16	179.1041	5.7414	54	1641.2979	9.2902
17	191.6748	6.2396	55	1658.7919	98.0316

18	207.0176	30.3275	56	1662.9095	57.9819
19	213.1670	4.6451	57	1674.4467	58.0014
20	216.8632	55.2320	58	1686.1414	20.6975
21	232.0288	147.3943	59	1700.7352	26.0611
22	235.9900	49.7485	60	1712.2161	63.0507
23	249.2656	20.1031	61	3179.8496	194.2329
24	263.0646	14.5099	62	3244.5706	710.1458
25	272.6250	37.8111	63	3370.6245	713.3592
26	276.0782	9.3359	64	3472.2957	360.4057
27	280.8241	85.7139	65	3523.5776	1284.8682
28	320.7590	98.6318	66	3548.0493	814.6366
29	372.3169	69.5176	67	3571.1482	235.4518
30	380.9438	1.4885	68	3597.7483	355.9054
31	396.6452	60.3010	69	3683.5588	494.3890
32	415.8463	40.0426	70	3783.2449	265.7836
33	424.1791	21.1501	71	3791.0364	193.8938
34	459.4669	89.1757	72	3876.8079	60.8848
35	488.3182	31.0497	73	3881.9065	76.4405
36	504.8112	66.9749	74	3884.6111	108.4904
37	519.8221	52.6490	75	3886.6294	54.3476
38	587.4424	18.2155			

TCE-10H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity
1	4.7206	0.2708	35	265.4152	13.0824	69	1084.8011	36.2858
2	8.2085	0.2381	36	273.2783	39.8421	70	1272.0721	7.7816
3	9.6160	0.5245	37	277.1118	16.2671	71	1636.8324	14.6294
4	14.8835	0.1125	38	282.7802	20.0600	72	1651.6279	34.9656
5	19.0404	0.5986	39	290.1611	76.1465	73	1652.3940	43.7709
6	25.6008	0.2177	40	297.1155	69.4396	74	1654.5438	91.5654
7	26.4420	0.3216	41	328.2642	77.7257	75	1657.5736	128.9907
8	31.7325	0.6515	42	350.5589	34.1329	76	1657.7784	133.1387
9	32.5000	0.0118	43	366.5347	21.3789	77	1663.9524	10.4330
10	35.5940	0.3931	44	368.5348	77.2977	78	1665.9091	21.1769
11	38.7686	1.9189	45	384.6181	1.8339	79	1676.4672	1.7225
12	42.3006	1.2310	46	390.0868	85.4564	80	1677.7931	59.7956
13	44.5400	0.5635	47	410.4756	29.7763	81	1688.8777	12.0463
14	48.8741	0.3291	48	414.0151	122.5427	82	3195.9707	894.9674
15	51.8972	0.4073	49	435.4773	37.1024	83	3234.0337	12.7082
16	56.6477	2.2354	50	470.9550	150.7334	84	3475.6775	370.2433
17	62.2932	0.8297	51	478.5295	10.8992	85	3529.9067	232.2785
18	89.4770	1.6629	52	531.5005	60.4755	86	3531.4763	864.9122
19	117.4011	5.9138	53	562.0235	167.9262	87	3562.3154	170.8146
20	130.4414	5.4867	54	582.2162	270.8316	88	3569.0222	435.2474
21	159.8429	20.7503	55	608.0668	145.3933	89	3606.8423	650.5472
22	170.4738	44.5343	56	618.5947	53.2839	90	3623.6099	151.9791

23	176.6703	4.2116	57	631.5714	248.6687	91	3632.7917	596.7001
24	187.7614	14.3914	58	654.3980	257.5791	92	3660.7771	651.9901
25	190.6369	18.7549	59	662.4558	199.0366	93	3701.2190	167.4106
26	198.0889	2.1704	60	737.2538	306.3891	94	3750.5632	372.8897
27	200.4990	64.0842	61	740.5522	133.7806	95	3863.2971	137.9299
28	202.1390	16.8779	62	796.4941	186.3709	96	3871.3560	69.1179
29	212.0917	33.9567	63	818.2602	22.5956	97	3878.5459	77.7471
30	216.4887	32.6029	64	824.2509	105.6762	98	3880.3789	75.2822
31	216.9940	100.9752	65	904.3177	15.5137	99	3884.3232	64.6078
32	223.5692	50.3269	66	906.7054	121.0016	100	3886.0991	80.1157
33	238.7055	144.2749	67	914.6911	44.3343	101	3886.9829	74.0407
34	246.4633	162.0121	68	935.3569	15.7048	102	3892.8218	93.5099

TCE-12H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	6.1830	0.4305	31	195.3010	29.5547	61	543.3746	43.5188	91	1670.6449	26.6248
2	7.7422	0.3304	32	200.3182	56.1232	62	565.7736	70.0232	92	1683.5271	41.9550
3	8.2404	0.6263	33	201.1250	68.2894	63	577.9956	137.8055	93	1685.0490	5.2082
4	13.9834	0.8315	34	211.5544	61.9337	64	578.3690	46.0005	94	1692.6000	18.3789
5	16.0871	1.5601	35	212.0935	61.2890	65	606.6917	248.2274	95	1732.7848	38.0199
6	17.8878	1.3092	36	213.2540	64.6073	66	616.9501	29.4622	96	3233.2668	14.4174
7	21.3892	1.4930	37	225.5356	56.9232	67	647.4547	69.1768	97	3277.2412	191.5164
8	23.3061	0.6890	38	230.1684	146.1817	68	658.5111	210.6302	98	3355.5171	2053.8591
9	28.6496	1.8598	39	242.3352	2.0209	69	692.5464	55.9719	99	3418.8774	628.3118
10	30.7179	1.3132	40	250.1704	26.8665	70	702.8943	242.2698	100	3485.7798	548.0365
11	34.1708	0.7933	41	259.7826	108.1580	71	776.5787	324.3796	101	3498.1279	327.0552
12	35.6309	0.1339	42	261.6435	9.0428	72	782.1954	193.4251	102	3511.9697	223.0123
13	39.5777	2.0822	43	274.0897	47.9347	73	820.0095	23.0893	103	3560.8713	817.6588
14	42.9716	1.5250	44	276.8143	12.3017	74	824.9602	97.9402	104	3576.5691	441.8436
15	44.2432	1.2230	45	282.8960	65.6604	75	844.6609	52.7065	105	3580.0366	345.5290
16	47.6522	1.2027	46	286.1039	76.0986	76	853.5235	239.1866	106	3614.1436	440.6516
17	50.3574	0.5200	47	289.8611	57.1558	77	909.6330	84.3892	107	3669.0703	331.6720
18	57.7522	7.1757	48	299.6440	169.7657	78	917.6694	171.2978	108	3673.6335	524.7653
19	60.6331	0.7458	49	320.0398	108.2248	79	933.6400	23.3730	109	3683.1975	659.8476
20	63.4821	4.6488	50	357.0945	43.2544	80	957.5934	24.9892	110	3744.7073	529.8757
21	71.8139	29.9938	51	376.4331	43.0126	81	1047.0604	16.5583	111	3816.2795	7.6841
22	77.7630	0.3078	52	385.3109	2.0186	82	1270.9076	8.9305	112	3839.5305	214.4345
23	99.7361	2.1945	53	392.5300	77.8273	83	1636.1504	12.6449	113	3875.2524	66.5765
24	105.6530	10.2743	54	401.6052	51.7989	84	1639.3300	78.6684	114	3878.1641	53.2962
25	149.6851	9.9570	55	410.0099	94.5029	85	1654.9735	56.8189	115	3879.4043	68.0156
26	167.7541	0.2714	56	432.7016	61.4268	86	1659.2712	77.1962	116	3881.6313	67.7633
27	170.7386	42.8146	57	459.0206	57.6967	87	1661.7072	114.4768	117	3882.3904	63.0247
28	179.0687	0.6736	58	479.1184	0.2418	88	1663.4965	81.5036	118	3885.9907	66.7959
29	184.1186	4.7300	59	479.9719	29.4713	89	1663.7419	38.3934	119	3888.7546	85.1626
30	189.7731	29.2137	60	503.9214	65.7858	90	1670.3063	73.5248	120	3915.4541	86.2485

TCE-16H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	7.6246	0.0507	40	201.2618	50.0488	79	595.9023	3.0379	118	1699.658	90.9518
2	11.3038	0.0400	41	205.0270	3.0617	80	608.5495	130.9499	119	1710.3954	24.3239
3	15.8487	0.4088	42	209.7100	2.4283	81	618.8683	121.0486	120	1713.6852	118.0895
4	25.8070	0.6612	43	211.6088	120.3232	82	623.4044	29.7419	121	1716.1272	43.5010
5	27.7837	2.0863	44	221.0523	67.4498	83	636.3000	57.3882	122	1724.2091	82.3521
6	30.3350	0.2909	45	224.3865	41.3366	84	646.1940	98.9885	123	1733.3591	49.9474
7	31.8149	0.4625	46	232.8282	48.6230	85	668.4221	141.2001	124	3241.9695	14.2491
8	35.9891	0.2293	47	238.7089	36.9088	86	679.5001	66.3936	125	3371.5522	700.8492
9	41.2146	0.6146	48	244.0907	9.7930	87	703.2079	425.1243	126	3382.0952	636.7804
10	46.8105	2.5846	49	249.4785	39.4552	88	719.6911	295.4751	127	3462.1658	178.6387
11	47.9965	3.9420	50	261.6052	28.3870	89	720.4832	78.6946	128	3481.3484	443.6514
12	51.5550	3.1272	51	264.5009	80.6606	90	740.5844	51.0845	129	3483.7585	309.8090
13	57.1868	2.2722	52	268.0136	67.8198	91	746.9561	401.3469	130	3488.5603	1454.4041
14	61.2504	2.5539	53	271.0682	15.3369	92	764.4399	119.7255	131	3496.5186	672.1242
15	63.1932	0.7397	54	275.9816	4.6238	93	788.7223	11.8563	132	3502.6917	11.3172
16	69.6368	3.4832	55	278.2037	8.3261	94	810.6235	21.9631	133	3529.8118	1322.2430
17	71.7249	2.1938	56	284.7023	6.5509	95	815.7231	50.9546	134	3540.6838	70.3503
18	77.0059	3.6593	57	288.4700	55.1846	96	816.5758	248.3305	135	3548.7332	922.5378
19	80.6305	1.3553	58	337.4214	61.5810	97	832.0256	102.2118	136	3563.8003	745.2013
20	83.9182	1.3072	59	383.2041	3.7418	98	851.5544	81.5350	137	3590.9661	27.8744
21	86.8503	3.6373	60	389.8807	17.9078	99	862.3648	91.4996	138	3602.3303	477.2499
22	90.4794	1.3418	61	399.6923	19.3636	100	893.9075	134.3975	139	3612.6482	198.9719
23	95.2342	0.9229	62	402.2941	84.8657	101	909.4550	121.3625	140	3623.7627	205.5390
24	98.7664	1.3720	63	417.2998	98.9953	102	919.8671	96.3986	141	3654.1594	304.6422
25	107.5394	1.6849	64	424.8160	45.8399	103	944.5199	61.3918	142	3658.9348	796.2105
26	114.6514	19.4431	65	437.8037	4.0957	104	961.8390	8.6907	143	3677.0117	856.9096
27	119.1945	0.7591	66	442.8405	77.3960	105	1056.0541	35.3401	144	3686.2659	603.4561
28	135.2110	11.2698	67	452.9006	30.4824	106	1274.0781	7.5383	145	3696.7788	234.9633
29	138.4700	13.4184	68	478.9246	18.7872	107	1638.1827	12.8525	146	3702.8096	112.0769
30	150.8219	23.3822	69	482.1710	4.4490	108	1647.1102	45.4725	147	3721.9172	411.2306
31	153.2164	1.1666	70	499.6025	29.6347	109	1651.4636	39.8431	148	3779.7556	191.2199
32	160.8226	5.3421	71	509.4558	58.4848	110	1655.0950	159.2791	149	3811.0215	155.4690
33	166.8963	7.9747	72	515.6915	54.1202	111	1661.3429	49.9716	150	3825.1111	234.2795
34	169.7894	32.9987	73	524.1333	75.2145	112	1667.7208	54.8745	151	3878.2983	61.5225
35	177.1952	65.0209	74	534.9135	100.6173	113	1673.2382	43.6791	152	3878.8367	86.0803
36	178.0893	7.1901	75	547.1490	88.6630	114	1678.2418	15.9213	153	3879.5764	83.1848
37	182.0975	8.3119	76	558.3803	63.6812	115	1683.8835	49.6782	154	3883.3699	86.7917
38	193.7905	1.0575	77	571.6182	109.1700	116	1690.8325	67.5365	155	3886.3708	98.2560
39	196.5104	3.5698	78	584.8848	128.7522	117	1694.4155	43.9518	156	3889.9419	65.0710

TCE-24H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	10.2678	0.2923	58	212.2634	27.2371	115	626.2123	43.4734	172	1710.6002	26.4617
2	17.1312	0.7152	59	214.4097	14.7753	116	626.5805	25.1886	173	1713.2686	70.0255
3	21.7851	0.7712	60	217.8370	9.5292	117	631.5348	89.1993	174	1716.6034	73.7774
4	24.7459	0.9624	61	224.2016	16.5060	118	635.6655	41.1821	175	1728.6053	5.7104
5	25.8201	0.1777	62	231.5466	18.6943	119	651.0687	138.4381	176	1733.7213	44.0924
6	28.1399	0.2023	63	234.2945	11.1806	120	655.8842	159.4441	177	1737.6324	13.5467
7	30.3553	1.8680	64	242.7941	9.1394	121	683.0638	31.8945	178	1748.0518	65.9188
8	31.4732	0.3364	65	247.3721	33.3506	122	687.4657	69.6886	179	1752.7454	31.2594
9	37.7766	1.6299	66	251.3600	8.3450	123	693.1470	516.5673	180	3241.8149	13.7069
10	39.8065	2.5530	67	258.8155	51.5524	124	698.7609	74.2611	181	3261.8848	696.4013
11	40.8954	0.7698	68	259.3012	63.8745	125	708.2264	66.7210	182	3269.0278	2521.3491
12	42.8403	2.6267	69	265.6126	1.8848	126	718.7461	219.7073	183	3274.3184	466.4310
13	46.7149	1.6075	70	272.0688	17.0165	127	730.1413	115.9304	184	3303.2937	477.7386
14	49.5935	2.1526	71	279.0216	105.0784	128	745.6771	121.5118	185	3313.0679	701.5551
15	51.8529	1.4521	72	280.1284	6.0828	129	750.3958	386.9078	186	3360.6702	992.8265
16	54.3447	1.2211	73	281.8463	2.7937	130	776.8174	475.1800	187	3383.6682	1353.6232
17	58.6876	2.1079	74	285.0840	16.1067	131	781.1284	36.9494	188	3402.2080	1134.7448
18	59.6505	1.4504	75	288.6215	14.1823	132	792.7199	46.2942	189	3409.6223	424.7014
19	62.8463	0.5065	76	296.7731	83.7985	133	806.8972	24.7979	190	3448.7654	163.3880
20	64.5289	1.9580	77	297.0963	35.3162	134	810.5868	173.0331	191	3452.2610	1126.6881
21	67.8038	0.3855	78	301.9241	22.1844	135	817.4895	69.1092	192	3462.8347	229.3583
22	68.0333	0.0450	79	307.5349	11.6694	136	820.9286	69.3399	193	3481.3613	345.1153
23	70.5470	1.6508	80	316.7607	21.1478	137	831.4768	30.6234	194	3506.6235	530.9276
24	73.8731	0.8548	81	327.0566	18.2109	138	839.2751	111.7260	195	3521.3904	772.1073
25	75.7098	0.7363	82	339.8169	38.4723	139	843.1847	13.8677	196	3526.1023	337.6614
26	76.9331	0.4235	83	348.2718	47.4305	140	852.8967	210.0987	197	3540.3313	487.2262
27	77.3607	0.8940	84	356.3652	28.4654	141	857.0868	28.8634	198	3549.5310	39.3336
28	79.3272	0.3664	85	357.8981	46.5076	142	861.0475	166.5884	199	3557.0544	120.5119
29	83.6544	2.5938	86	368.1864	115.4036	143	905.0887	97.7857	200	3558.1426	820.8866
30	84.9316	1.0707	87	381.2470	0.3858	144	908.9535	70.6696	201	3564.5442	1980.8109
31	90.1172	2.1666	88	407.6945	33.2381	145	916.0666	116.2775	202	3597.3706	61.1113
32	90.8848	0.1765	89	416.7185	60.1697	146	927.0251	181.9430	203	3611.8208	69.1879
33	94.7836	0.8593	90	422.2974	9.3885	147	932.3712	12.0411	204	3617.3958	241.1401
34	97.1044	0.7316	91	428.0783	49.7166	148	935.6380	32.6565	205	3626.9250	714.8526
35	103.3468	2.4002	92	440.9630	4.3284	149	956.8630	114.3594	206	3632.6702	389.0952
36	104.6571	2.1203	93	449.8569	9.3065	150	970.4881	72.1753	207	3636.9846	206.2660
37	106.2280	2.0372	94	451.1988	12.6543	151	983.1876	26.5587	208	3646.1416	339.3804
38	114.2101	1.7971	95	456.6777	27.1929	152	987.6170	68.0088	209	3660.4375	598.0594
39	120.7263	1.8622	96	465.8134	46.7677	153	1030.9098	161.6809	210	3672.5945	156.2110
40	129.3752	7.9005	97	470.6510	59.9919	154	1274.3282	8.5064	211	3677.5564	537.5309
41	132.7698	12.4981	98	481.3311	33.1748	155	1634.8918	9.6840	212	3709.1118	315.1664
42	136.8343	3.2324	99	483.7206	36.9302	156	1653.5082	75.8288	213	3712.2600	126.2697
43	139.1202	4.1120	100	487.5205	42.3463	157	1657.4021	61.7952	214	3715.4573	649.2834
44	149.2936	10.5085	101	494.3243	33.6634	158	1659.2596	145.6718	215	3742.1965	240.8248
45	158.4047	4.1009	102	499.3476	19.7989	159	1664.0955	110.1705	216	3769.4434	224.3720

46	161.8604	17.6592	103	504.6190	17.4772	160	1665.6993	206.9260	217	3778.9863	326.6033
47	168.3146	8.7588	104	515.4679	5.8257	161	1668.8385	49.2054	218	3829.8667	198.6944
48	171.4212	6.6198	105	521.3047	99.6834	162	1679.0453	32.2314	219	3840.6162	221.0525
49	175.4795	2.7936	106	535.6200	2.3465	163	1680.3938	135.3959	220	3857.9070	79.3002
50	177.4676	6.9370	107	541.7755	75.9720	164	1681.4031	49.4010	221	3859.4063	57.1492
51	182.8424	3.6929	108	554.8016	50.0475	165	1686.4875	13.9974	222	3867.9280	72.4001
52	184.8671	1.0396	109	561.7143	19.0366	166	1687.0377	20.1976	223	3874.8613	61.9297
53	189.0776	24.9284	110	571.0829	79.1737	167	1691.7671	3.2149	224	3875.3550	84.1937
54	190.6261	66.2832	111	573.5738	160.8673	168	1699.7018	28.0959	225	3876.3555	53.6866
55	198.1125	8.4472	112	590.2202	19.1168	169	1701.6310	78.4727	226	3876.5598	92.5784
56	200.5970	10.8250	113	603.8211	94.3250	170	1706.7126	144.8831	227	3880.8462	53.9203
57	211.6067	3.3278	114	613.3244	118.9806	171	1708.6410	8.2417	228	3892.3206	75.2060

TCE-39H₂O

	Freq	Intensity		Freq	Intensity		Freq	intensity		Freq	Intensity
1	6.3268	0.0567	92	218.5218	5.5035	183	659.5153	46.2163	274	1714.4846	131.3451
2	10.4414	0.1754	93	220.8941	62.1141	184	661.9030	13.8888	275	1717.5229	41.9089
3	13.6603	0.0532	94	223.9258	74.2581	185	670.3019	189.5925	276	1720.2839	6.9938
4	20.1695	0.3503	95	226.5502	15.2469	186	672.8439	144.2347	277	1725.9200	5.2667
5	20.3621	0.5514	96	228.1465	46.5479	187	677.8375	52.4333	278	1732.9933	57.8430
6	23.8653	1.8667	97	229.9388	25.5705	188	682.8225	121.0232	279	1735.3033	75.7564
7	26.0649	1.6728	98	231.6924	94.4184	189	688.5772	8.8139	280	1736.6589	84.6282
8	26.1597	0.9122	99	235.0924	68.8232	190	689.8905	116.0767	281	1740.4114	72.7675
9	27.0929	0.0717	100	239.6694	56.8920	191	698.5211	83.9925	282	1744.1915	132.1040
10	27.6483	1.2110	101	242.5595	6.0400	192	713.3157	68.6236	283	1746.3840	25.5302
11	28.5225	2.6506	102	245.3876	65.3097	193	725.8506	340.0200	284	1758.8601	72.8325
12	31.4033	0.9017	103	249.2190	13.9833	194	728.3352	100.0756	285	3141.7937	1158.4274
13	34.1508	0.3667	104	251.2814	41.1210	195	739.0853	201.4012	286	3186.1626	1325.1013
14	35.4929	0.6862	105	252.2775	55.1636	196	743.0108	55.4177	287	3232.5190	1312.0978
15	38.1655	1.3576	106	256.0907	42.5605	197	750.5789	18.4108	288	3237.3938	12.6708
16	39.4557	0.1063	107	260.0109	94.5731	198	753.1351	309.9836	289	3289.7961	312.7198
17	39.8640	0.1814	108	262.7154	23.6860	199	763.3582	51.6744	290	3293.9995	474.7441
18	42.0553	0.4208	109	264.1802	0.9245	200	765.6841	137.2700	291	3298.7139	637.8306
19	43.7394	1.0881	110	268.4720	4.3866	201	773.8977	39.8140	292	3306.7803	439.6125
20	44.8420	0.0496	111	269.8947	27.2399	202	781.2984	83.0389	293	3311.2312	314.5314
21	45.9867	1.3704	112	271.6044	28.6166	203	781.9598	31.2743	294	3335.0220	1328.7949
22	48.2621	1.6400	113	273.1692	21.1438	204	787.5283	336.0635	295	3340.3477	1846.2198
23	50.6490	0.9051	114	275.1915	28.3755	205	787.9405	211.8714	296	3351.3362	394.7395
24	52.5489	0.4219	115	277.4213	36.7406	206	796.3756	186.1386	297	3354.5020	749.4915
25	55.2601	0.5718	116	278.6205	61.2373	207	802.3160	178.6862	298	3365.3157	245.2428
26	55.4367	1.9812	117	280.3190	1.4979	208	805.5633	27.2930	299	3379.4055	1116.8726
27	58.0719	0.8410	118	281.3887	33.7438	209	812.1835	293.4040	300	3382.9861	965.0654
28	58.5482	0.7076	119	285.0542	39.9801	210	812.7417	20.6149	301	3390.2463	1300.0325
29	59.6825	1.6826	120	292.1692	43.0651	211	814.5814	57.1653	302	3402.5173	535.3145
30	61.5327	2.6133	121	296.4066	19.1602	212	816.3625	104.7592	303	3413.6851	915.9203
31	62.1729	2.0158	122	303.2119	24.7593	213	827.8626	165.2653	304	3423.6523	495.0104

32	62.9739	0.3651	123	309.8797	8.7442	214	837.3192	47.5528	305	3431.1238	1404.9438
33	64.8088	2.5309	124	314.3349	21.5077	215	841.4080	90.5652	306	3440.5244	1334.9821
34	67.8842	1.8808	125	317.2825	7.0315	216	854.1420	87.2070	307	3444.8503	452.3205
35	68.4839	0.4668	126	317.7901	9.8410	217	862.0148	240.0243	308	3452.9878	597.1762
36	69.6123	1.8132	127	320.2622	68.2682	218	869.4737	50.4176	309	3469.3550	1843.0568
37	71.9519	0.1426	128	321.7821	41.4203	219	871.8437	45.2642	310	3470.0984	734.4600
38	73.0776	0.4477	129	323.6574	19.7929	220	885.0329	17.2278	311	3492.5029	389.7551
39	75.0461	1.9033	130	329.3177	25.2228	221	891.4051	129.8968	312	3504.7246	1072.5293
40	75.9649	1.7001	131	331.9684	49.8818	222	894.5858	53.6297	313	3507.7761	847.6452
41	77.0400	1.7230	132	341.1032	137.7391	223	896.3393	21.9953	314	3510.0740	328.7100
42	78.3243	7.6295	133	343.6660	54.9173	224	903.9513	77.3310	315	3515.2449	538.1415
43	79.5813	2.3299	134	367.7555	102.4200	225	905.0840	287.0391	316	3522.6021	381.7902
44	82.8133	1.8678	135	381.6641	0.2339	226	907.5091	145.0416	317	3523.5278	124.0887
45	84.7950	1.0412	136	397.0483	29.0978	227	908.8915	62.1192	318	3526.7769	512.2667
46	87.3147	3.7267	137	408.8566	106.7719	228	925.9292	115.7855	319	3530.8052	301.4741
47	89.3567	3.3299	138	412.0198	40.8088	229	937.8027	289.5069	320	3545.4854	696.9530
48	90.5639	7.6909	139	413.2711	35.0947	230	953.7208	69.9155	321	3557.8081	760.5049
49	91.1939	1.7230	140	417.2646	33.3769	231	960.6839	21.9017	322	3563.4646	422.0537
50	94.9969	0.6231	141	433.6979	44.3750	232	962.6502	52.2134	323	3565.9756	300.7025
51	97.3660	2.9021	142	436.9126	24.4914	233	966.5861	48.2855	324	3569.9546	63.9413
52	100.7043	0.8539	143	448.9202	9.6953	234	983.5169	152.8881	325	3570.9209	516.5867
53	102.3234	1.9183	144	457.7460	15.9298	235	1002.0527	16.4853	326	3572.5703	791.3948
54	107.9522	1.4517	145	458.8682	67.0464	236	1004.7057	197.4166	327	3574.5020	407.2921
55	111.4215	7.7173	146	459.2399	17.4642	237	1011.5511	17.9332	328	3588.4026	89.5028
56	114.1991	4.2480	147	479.0517	51.0260	238	1017.1050	10.1344	329	3591.2178	212.6210
57	114.5989	16.8527	148	479.7155	32.5506	239	1022.1410	78.5833	330	3597.6858	432.3276
58	122.0276	7.2302	149	481.9421	2.1495	240	1044.2712	54.4383	331	3600.4622	254.0020
59	123.8750	7.4859	150	489.5881	184.6179	241	1057.6760	118.4514	332	3605.3362	602.9752
60	127.1928	7.6615	151	506.2943	35.4408	242	1082.9181	67.8169	333	3611.6985	1277.0262
61	129.9260	8.9382	152	508.1922	72.4136	243	1085.3400	45.8650	334	3615.9951	278.9485
62	135.5473	0.9173	153	511.4577	36.9633	244	1275.5498	13.2402	335	3622.1350	724.2344
63	135.8561	1.1861	154	516.2063	27.2203	245	1638.0719	13.9129	336	3623.5747	465.4320
64	144.7981	5.6790	155	520.3112	31.2231	246	1643.7878	81.1478	337	3647.3020	575.3650
65	145.3595	3.8743	156	526.1703	16.7879	247	1649.0006	59.0931	338	3672.9360	165.8653
66	151.3267	10.2726	157	530.6105	138.9484	248	1651.8319	134.5412	339	3684.5220	736.5510
67	158.7885	3.1546	158	534.2081	180.8358	249	1653.7823	51.9503	340	3697.5935	544.8382
68	160.5882	26.8517	159	537.8012	19.7227	250	1656.3270	71.1928	341	3704.8684	528.7012
69	163.1043	3.4294	160	544.5294	13.3457	251	1656.9014	92.5805	342	3706.3794	228.3825
70	167.1102	13.5583	161	551.8969	13.5526	252	1659.5697	78.7678	343	3710.7834	383.3365
71	169.4069	4.4930	162	558.4679	13.6932	253	1669.0381	96.2290	344	3725.5078	256.7076
72	170.8506	17.2733	163	566.5345	70.5876	254	1671.1777	44.8638	345	3726.4221	403.7668
73	173.1104	4.4282	164	573.3625	13.3140	255	1671.9487	33.0403	346	3728.6155	263.3279
74	173.8771	14.2914	165	579.6164	57.8381	256	1674.3853	90.3085	347	3754.5349	396.8749
75	176.0905	11.5330	166	587.0562	26.5326	257	1680.2097	49.1088	348	3757.8389	288.9115
76	176.8476	9.8254	167	593.8389	70.9163	258	1681.9543	25.1799	349	3763.3486	245.0559
77	185.5329	1.4643	168	594.7440	135.7024	259	1682.1771	81.4094	350	3833.6555	152.3179
78	186.7745	3.9644	169	597.5336	84.8450	260	1685.6279	35.0018	351	3866.6111	50.8206

79	187.4458	7.7559	170	602.0062	159.3231	261	1688.0198	4.6176	352	3868.9905	140.8725
80	189.8630	21.4851	171	605.7581	1.7415	262	1689.4941	21.2259	353	3869.1506	34.4157
81	194.4676	2.9054	172	607.7768	96.6147	263	1690.6910	66.2358	354	3869.2058	41.4210
82	196.5630	23.5680	173	618.7216	7.2798	264	1691.2086	33.3671	355	3873.0103	77.0160
83	199.1339	64.8502	174	619.7459	12.2807	265	1695.2059	72.9957	356	3874.0046	73.0321
84	201.3230	30.5016	175	625.0492	12.5367	266	1697.5806	9.8422	357	3879.6985	67.6239
85	203.1574	13.5532	176	633.2221	51.6104	267	1697.9264	7.1393	358	3880.0693	55.1985
86	204.7329	5.1438	177	640.1019	42.4556	268	1698.6794	52.0672	359	3880.7444	120.3071
87	205.5270	22.8772	178	641.6888	78.4016	269	1703.0352	12.9306	360	3880.7766	49.1735
88	206.7779	16.5485	179	642.0019	53.4862	270	1704.2299	61.5722	361	3883.9902	85.2545
89	209.1592	16.0050	180	650.9407	26.6346	271	1706.2941	18.3803	362	3887.9946	58.3338
90	210.8997	13.3679	181	654.3340	23.5578	272	1707.9916	19.5774	363	3890.0105	101.1970
91	217.1488	51.0020	182	656.5472	197.5752	273	1712.9036	13.2990			

Appendix 3

Table 4. IR Intensity as a function of frequency (DCE1-nH₂O)

Freq (1/cm) IR Intensity (KM/Mol)

DCE1

	Freq	Intensity
1	166.0909	0.2356
2	421.4800	0.0000
3	569.5776	7.5562
4	701.6504	20.0725
5	710.9440	57.5055
6	844.2749	88.1058
7	913.2452	0.0000
8	1218.7231	0.0213
9	1324.5959	29.2871
10	1644.8334	39.7615
11	3210.8660	16.0437
12	3230.9395	0.6739

DCE1-2H₂O

	Freq	Intensity		Freq	Intensity
1	19.3054	3.3157	16	696.6648	24.7880
2	37.2992	0.3669	17	711.1461	60.2003
3	45.3847	3.5696	18	842.1796	77.9919
4	59.0225	8.3690	19	915.0080	0.0566
5	72.4706	1.4036	20	1217.0175	0.1363
6	132.5689	45.7763	21	1323.1564	24.9665
7	173.4429	5.5928	22	1644.9508	59.8951
8	183.3816	43.0559	23	1646.5575	59.9894
9	186.5420	109.0302	24	1662.0856	28.7560
10	206.7350	62.5944	25	3209.1128	14.4894

11	279.5154	152.7638	26	3233.3081	1.6549
12	417.5722	45.0746	27	3665.8335	313.7713
13	424.5319	6.2105	28	3780.4246	96.8950
14	572.2601	10.4746	29	3891.1233	79.2118
15	691.1682	132.4379	30	3891.4868	131.5371

DCE1-5H₂O

	Freq	Intensity		Freq	Intensity
1	10.1445	0.3240	30	602.5369	115.5702
2	17.3103	1.1140	31	667.8615	386.2846
3	21.4719	0.1830	32	690.2690	17.5388
4	24.4908	1.1436	33	691.1445	110.9383
5	33.5486	0.4316	34	765.2320	55.5819
6	46.0803	3.9709	35	832.3319	74.5139
7	53.9203	0.6942	36	875.9394	31.2774
8	60.6397	0.5798	37	955.2108	0.2264
9	68.7276	6.2725	38	1238.1539	3.1560
10	81.0284	0.8401	39	1338.0636	29.6342
11	89.3933	0.7748	40	1644.0537	83.1876
12	120.6021	59.4855	41	1647.2557	74.0653
13	172.7386	7.7205	42	1648.3296	72.7760
14	174.6771	15.5161	43	1648.9456	61.3953
15	179.4752	84.9729	44	1663.9507	30.1313
16	187.2297	58.7078	45	1669.2124	7.6238
17	192.5087	14.9649	46	3199.8120	27.8193
18	213.1990	61.2195	47	3219.5999	50.6673
19	222.9926	9.0786	48	3543.5930	199.7982
20	238.2855	107.1685	49	3622.9956	356.1891
21	249.9171	112.5340	50	3654.2212	386.1676
22	279.2201	44.2140	51	3661.3203	347.5730

23	301.4247	128.2968	52	3775.0117	122.1595
24	360.7932	26.3731	53	3882.5125	113.5920
25	381.1700	139.8070	54	3883.4209	105.7647
26	428.1872	39.4643	55	3885.2966	43.2804
27	432.1244	21.4623	56	3889.5564	134.5603
28	459.7756	131.4996	57	3891.7815	73.6157
29	567.3994	8.4546			

DCE1-7H₂O

	Freq	Intensity		Freq	Intensity
1	5.7952	0.0510	39	590.8360	206.6695
2	7.9533	0.0242	40	674.9911	7.9643
3	8.4590	0.1904	41	690.5292	36.3461
4	10.3914	0.2216	42	693.0129	276.5206
5	18.7361	0.2076	43	746.2060	78.2924
6	21.4217	0.1144	44	790.0140	162.5840
7	25.7552	0.3442	45	820.9170	263.6816
8	30.4579	2.6119	46	833.3994	104.4878
9	46.2070	0.2491	47	910.9344	10.1769
10	52.2467	0.7386	48	949.3079	3.3957
11	55.7314	0.9303	49	973.5878	9.7876
12	63.2456	2.7985	50	1228.7760	2.7944
13	90.0609	0.1779	51	1333.6672	19.1902
14	91.9837	2.0867	52	1649.2250	41.7505
15	172.9946	16.1852	53	1654.8727	66.4415
16	175.0887	1.2513	54	1657.8638	75.1629
17	189.8015	23.5150	55	1667.0107	40.9638
18	197.2015	0.8072	56	1672.8324	144.4893
19	219.4792	123.2706	57	1677.0846	11.8002
20	223.0339	2.3881	58	1690.0774	68.2911
21	223.9264	57.2614	59	1699.9269	3.2588

22	229.3057	6.9533	60	3194.5244	137.6919
23	244.9649	23.4944	61	3226.9993	4.0188
24	253.2421	105.8541	62	3358.6177	254.4616
25	259.3115	19.7353	63	3442.5847	1192.9867
26	266.5024	216.1578	64	3479.7625	885.1559
27	287.4168	98.9158	65	3539.7769	156.3339
28	288.6931	47.3173	66	3557.1284	408.6266
29	334.1591	14.6519	67	3606.5867	583.4682
30	372.7259	73.2427	68	3646.4043	448.5586
31	388.1164	6.2641	69	3850.3872	241.7086
32	408.1134	78.3313	70	3860.0017	75.5085
33	422.3688	5.3406	71	3878.0295	64.6233
34	428.3866	24.0658	72	3882.9854	96.9063
35	467.7499	137.5010	73	3883.4490	91.5288
36	519.7934	8.1830	74	3883.8560	42.6439
37	566.6648	142.4387	75	3887.0020	60.6390
38	567.7261	17.9198			

DCE1-10H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity
1	9.0778	0.2842	35	299.4963	9.9043	69	1335.2317	34.6306
2	11.9697	0.4486	36	321.4129	62.6835	70	1646.2727	17.3725
3	20.3542	0.5070	37	336.7994	48.2870	71	1648.9711	99.8542
4	27.4963	0.3418	38	391.3218	66.0943	72	1652.9595	51.5859
5	33.0294	0.2430	39	398.1541	27.3958	73	1658.5157	43.9942
6	34.3195	3.6302	40	403.3686	58.1874	74	1663.9298	86.2947
7	39.7129	1.9778	41	424.9942	18.4388	75	1667.0405	28.8743
8	44.1777	1.6875	42	430.4039	35.9224	76	1669.4642	17.7141
9	45.7156	2.4202	43	440.1323	39.5775	77	1682.3699	86.2750
10	52.6031	0.5733	44	469.0174	92.1409	78	1689.3529	67.0491
11	61.4836	1.5382	45	490.1231	73.2545	79	1694.9089	17.9746

12	62.8698	1.6061	46	514.6929	245.5301	80	1705.0378	26.9988
13	68.1688	4.6458	47	561.3083	112.5841	81	3191.0232	118.0235
14	74.1369	0.8063	48	564.5468	41.3857	82	3224.6619	4.2554
15	84.1111	3.5897	49	570.6707	22.0489	83	3250.8545	360.0149
16	91.0093	2.3041	50	594.5053	513.4065	84	3298.6528	1277.0201
17	101.4937	2.3702	51	599.2648	59.2647	85	3407.9707	490.5129
18	122.9010	3.8553	52	616.8794	70.9484	86	3412.7446	996.7635
19	130.0611	8.6676	53	638.4865	149.5156	87	3534.3440	443.3255
20	149.0084	5.3803	54	655.7064	47.4832	88	3544.1946	658.5954
21	159.9827	53.0867	55	691.1984	30.9763	89	3595.2153	592.3261
22	168.3893	0.5183	56	714.2182	238.3060	90	3596.5857	383.0241
23	173.9824	59.8224	57	730.0139	92.3722	91	3655.9080	659.0337
24	177.4677	27.4337	58	754.0879	70.4443	92	3671.3313	478.8955
25	192.4656	14.9315	59	768.1071	55.7470	93	3688.1335	142.3278
26	209.6861	19.8705	60	801.7253	227.1752	94	3692.5254	212.0041
27	211.1613	45.9296	61	832.5244	95.1855	95	3709.1709	381.0673
28	215.8907	10.5397	62	852.6443	10.2340	96	3801.1194	25.6838
29	225.4701	45.5052	63	921.9069	104.8909	97	3805.6238	390.3515
30	230.7667	6.8016	64	951.3939	3.8963	98	3867.7725	78.1201
31	235.0965	118.2479	65	975.5230	69.8555	99	3881.5510	73.6260
32	246.0280	112.0101	66	1055.1724	74.8476	100	3885.5437	70.8393
33	260.5654	40.0345	67	1083.8918	27.4269	101	3887.6968	86.7675
34	279.5637	39.2515	68	1229.2201	0.5003	102	3893.2502	103.4408

DCE1-12H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	15.9406	0.1354	31	227.1185	6.8681	61	653.1711	58.6109	91	1696.8530	7.1005
2	18.3010	0.0508	32	228.1743	168.5627	62	687.3758	36.8879	92	1715.2258	56.4013
3	24.2826	0.3152	33	237.7995	56.0253	63	713.1638	18.8336	93	1718.5656	32.1052
4	25.7370	0.0104	34	249.6954	100.7291	64	742.1762	360.2139	94	1729.3215	53.0118
5	29.5805	0.0829	35	251.9094	55.9221	65	747.0740	13.6303	95	3200.9912	30.8818
6	34.1941	0.1722	36	256.1246	50.4186	66	764.7076	108.2705	96	3218.9602	47.8366
7	37.8035	1.1217	37	267.4229	14.9972	67	810.5545	124.6774	97	3271.1331	655.6666
8	41.4476	2.1394	38	272.7007	68.0353	68	826.4159	18.4143	98	3328.3008	713.1563
9	47.0670	0.4069	39	281.4829	51.5720	69	829.6874	421.0343	99	3350.6790	995.6200
10	50.0917	1.4558	40	286.0800	37.8308	70	837.5241	178.0311	100	3365.6860	1384.3324
11	56.3098	0.4263	41	290.3834	83.0616	71	848.5011	163.1916	101	3394.4238	981.9328
12	60.9480	1.9557	42	306.0916	16.9634	72	874.7611	57.4517	102	3447.1130	1559.9481
13	65.2557	0.0283	43	313.2216	86.6873	73	890.6744	141.0921	103	3455.4717	867.4876
14	71.7169	2.2918	44	327.7917	105.3253	74	910.6861	88.8937	104	3461.1321	585.6563
15	75.7424	0.4626	45	408.1001	25.9510	75	943.3878	48.0597	105	3484.5168	739.5124
16	77.2191	2.1012	46	415.1642	44.8374	76	953.1375	9.9744	106	3509.1511	692.2309
17	80.7875	2.1353	47	428.1281	24.8025	77	978.8089	26.3469	107	3533.4014	172.1103
18	86.9952	2.5013	48	433.7935	64.1157	78	1014.6282	14.6020	108	3544.5056	503.1139
19	94.2176	3.0639	49	442.5748	32.7610	79	1049.5313	105.6533	109	3588.2063	215.6851
20	104.3578	1.6255	50	448.8356	49.6141	80	1235.7406	2.2889	110	3639.4897	406.8118
21	134.3566	1.0847	51	461.5867	84.2883	81	1331.9623	34.7119	111	3654.6599	415.8561
22	151.7758	7.6461	52	473.5610	49.7316	82	1647.0814	30.1492	112	3739.1838	421.6824
23	161.6307	5.2499	53	490.2705	52.4391	83	1655.4014	90.7156	113	3788.9297	284.4457
24	168.0080	0.9135	54	515.1119	19.7981	84	1659.6635	30.7390	114	3873.6204	74.0268
25	177.0529	10.7245	55	549.8530	22.4102	85	1664.1434	69.4239	115	3877.2646	73.5598
26	180.7055	5.2263	56	555.4237	46.6792	86	1669.9198	85.4292	116	3881.2151	72.5893
27	195.0543	42.3587	57	562.2937	7.0334	87	1672.5754	41.7048	117	3882.5315	37.8348
28	205.9303	57.7893	58	609.7254	24.7029	88	1683.8582	70.2060	118	3883.2390	117.8515
29	218.3679	2.2454	59	619.9096	59.2040	89	1689.7480	27.2891	119	3886.9841	59.9901

30	221.4297	47.0204	60	632.5233	11.4118	90	1694.4836	25.3560	120	3887.7090	60.7701
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DCE1-16H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	7.4660	0.1260	40	201.4270	54.3060	79	618.3620	116.0640	118	1709.4880	25.4150
2	7.7720	0.3240	41	209.6430	3.4240	80	638.0540	33.6790	119	1714.1801	130.4910
3	16.6100	0.1160	42	214.8380	79.8960	81	644.8100	154.3030	120	1716.9150	44.2510
4	27.2650	0.6480	43	222.7230	25.4120	82	669.0280	126.1230	121	1724.8910	75.0100
5	29.1350	1.3910	44	233.1610	50.8520	83	676.7730	69.9580	122	1733.7980	49.6630
6	34.3880	0.4850	45	237.5870	5.5400	84	697.3080	27.1460	123	3211.1470	14.9050
7	35.0110	0.5580	46	238.9100	92.4550	85	704.8890	458.6210	124	3231.9771	0.7000
8	39.6160	1.7430	47	246.2570	18.0920	86	711.1250	53.6360	125	3376.8000	683.7550
9	41.8260	0.5860	48	248.5890	79.0540	87	714.5710	205.3530	126	3391.8149	571.8480
10	46.4560	2.3230	49	253.6960	139.9570	88	720.0150	124.9460	127	3464.7070	166.5960
11	48.2510	4.8370	50	262.9770	60.3040	89	740.4390	68.7020	128	3479.8391	407.7540
12	51.8980	2.3050	51	266.3480	35.1440	90	745.4230	394.4240	129	3486.2361	320.4590
13	57.1310	2.5970	52	269.8430	8.3240	91	766.0450	129.1080	130	3491.5110	2101.4910
14	61.7970	0.4080	53	276.4410	12.7870	92	789.6930	5.2370	131	3496.3740	101.9100
15	62.3580	1.0660	54	280.3870	6.0340	93	816.7550	167.7870	132	3505.8440	14.3350
16	68.5550	3.5380	55	283.7090	3.2280	94	829.1160	103.6420	133	3531.5161	1321.9280
17	71.8370	1.3680	56	341.9550	47.4020	95	841.9360	79.3350	134	3542.6890	215.1380
18	75.8140	5.1950	57	386.2360	21.0940	96	849.7260	73.4390	135	3555.5969	868.7230
19	79.5290	1.0220	58	395.7420	60.8640	97	859.8150	92.1860	136	3565.8521	582.7940
20	83.1290	2.5400	59	399.3700	52.6420	98	891.8390	138.0500	137	3586.8770	24.5680
21	87.1360	3.5670	60	415.6560	83.8830	99	913.4350	0.0050	138	3602.6790	517.9440
22	92.0090	0.8740	61	422.5120	0.8730	100	917.9770	118.0470	139	3610.7190	151.1060
23	95.8180	1.3900	62	430.2080	67.4810	101	942.9390	60.1360	140	3623.1389	195.2720
24	98.8830	0.9930	63	438.3390	16.1530	102	962.0010	10.0010	141	3652.2241	141.0500
25	107.8290	1.6490	64	445.3730	63.0270	103	1055.0540	36.4340	142	3658.0740	992.6710
26	115.0060	18.9940	65	453.6950	27.0290	104	1217.9990	0.1400	143	3673.4519	854.7860
27	119.0770	0.6860	66	475.0900	17.4880	105	1322.8879	22.6730	144	3687.9629	645.8610

28	134.9580	9.3400	67	500.9850	32.7470	106	1645.0760	51.3600	145	3691.4561	208.8980
29	141.3030	18.0310	68	508.1040	47.7330	107	1646.4080	39.8440	146	3704.2881	76.0380
30	149.9500	22.4000	69	515.2280	29.7370	108	1652.7820	34.9930	147	3718.9751	440.0270
31	152.6800	5.4110	70	527.6330	82.2130	109	1655.1840	153.3550	148	3780.3240	185.3670
32	161.0290	2.5480	71	536.8100	119.3350	110	1660.9800	59.2930	149	3806.7881	168.5460
33	166.4030	10.3180	72	548.1630	90.9990	111	1667.8060	53.5130	150	3816.6780	238.9420
34	168.0650	48.1550	73	560.4680	83.2090	112	1673.2371	42.0720	151	3878.7151	49.3860
35	174.8690	5.2930	74	571.8430	7.7880	113	1678.4230	18.2780	152	3878.8950	102.4630
36	175.7220	50.1850	75	575.0450	76.0540	114	1684.2159	46.0250	153	3882.4141	79.4510
37	182.4140	9.3240	76	586.3890	144.6320	115	1690.5540	67.8040	154	3884.0330	89.4860
38	193.7970	0.9890	77	597.2030	2.2630	116	1694.6379	49.6290	155	3885.9070	93.8760
39	196.5070	5.9430	78	610.0270	116.3100	117	1702.0341	77.9460	156	3889.3169	64.6480

DCE1-24H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	14.8749	0.9155	58	216.4849	9.4965	115	637.9186	84.3544	172	1716.8629	47.5763
2	20.1014	0.5812	59	221.5897	16.5402	116	647.5026	158.7922	173	1719.7667	83.9011
3	23.5850	0.9746	60	226.7175	32.7592	117	660.3136	174.4936	174	1732.4866	30.3447
4	24.9153	0.6474	61	235.9280	14.6305	118	675.9109	38.6358	175	1738.2262	22.9000
5	29.6891	0.6244	62	239.4232	58.2294	119	679.2567	25.1698	176	1741.8094	15.5919
6	34.0792	2.5190	63	245.2048	6.7391	120	686.0337	74.1773	177	1747.2417	60.7782
7	35.0725	2.9978	64	247.9791	15.7906	121	688.2540	319.5672	178	1751.3215	18.1194
8	40.3937	0.1462	65	251.7988	79.8280	122	693.8285	51.0104	179	3193.1699	76.9799
9	41.5792	0.1979	66	256.4523	36.1746	123	699.0741	45.8094	180	3214.3379	98.9965
10	44.2760	0.7619	67	259.3169	13.8829	124	706.2889	594.8960	181	3246.2268	797.3286
11	48.4571	1.5263	68	259.9420	1.1311	125	720.8372	19.6880	182	3263.2527	1843.3376
12	49.7802	0.3277	69	264.8512	10.7051	126	739.8593	349.0167	183	3282.2268	620.9446
13	50.4750	1.8419	70	274.9132	104.3371	127	750.9003	94.0760	184	3313.2078	669.2698
14	51.4086	3.0238	71	276.2102	28.2904	128	770.4634	662.1374	185	3370.6440	592.4689
15	55.1753	1.9043	72	281.1091	21.2543	129	774.6677	56.4173	186	3384.4102	935.6686
16	59.5213	1.6143	73	286.8068	122.3391	130	783.5421	70.0548	187	3398.2300	1452.8575

17	61.8501	2.4151	74	287.9013	23.9780	131	795.8916	20.7568	188	3404.2737	536.3565
18	62.4255	1.0898	75	297.2328	13.1322	132	806.7561	165.7690	189	3430.0952	1130.0753
19	64.8688	1.5627	76	302.9185	119.5527	133	810.4031	51.9423	190	3433.9998	320.6174
20	66.4799	0.0424	77	304.3969	1.8835	134	820.1752	99.7774	191	3457.2227	589.5859
21	68.7944	0.8857	78	309.6810	7.5081	135	824.9351	101.1147	192	3466.5254	490.5731
22	70.0152	0.8487	79	315.4772	28.3671	136	832.4712	48.1407	193	3484.7871	941.6662
23	73.7499	1.0822	80	321.9501	19.8350	137	842.8759	57.5795	194	3503.0632	413.3633
24	75.3130	0.5036	81	355.4109	13.5118	138	846.1148	68.3966	195	3513.3828	556.2141
25	76.1723	0.5544	82	359.0027	20.0317	139	858.2774	150.4001	196	3534.9922	346.0802
26	77.6983	0.9210	83	385.1331	52.4803	140	875.3917	32.2908	197	3538.6885	24.9104
27	81.8009	1.9989	84	391.8437	9.5566	141	884.2069	84.3774	198	3553.0364	746.0296
28	83.6848	2.5312	85	394.6644	72.2622	142	910.6161	20.0844	199	3562.6875	417.1185
29	88.1984	1.3090	86	426.0822	16.5366	143	918.6217	129.7366	200	3569.7561	403.2038
30	89.8799	2.3652	87	427.9883	14.5354	144	921.4600	208.5868	201	3582.3718	623.8218
31	94.9490	1.0899	88	435.2422	12.5274	145	934.8409	48.2750	202	3594.9197	585.6189
32	97.5814	1.4826	89	438.3025	12.4201	146	938.4128	60.5851	203	3611.3997	318.3913
33	101.5302	2.3613	90	443.1017	41.8742	147	962.4255	13.5614	204	3612.5425	603.3889
34	102.9158	1.1673	91	450.0584	14.5000	148	972.2287	99.6420	205	3637.4253	254.4646
35	104.7872	0.8368	92	458.3513	6.8069	149	975.7772	71.6965	206	3639.7852	149.8813
36	111.1440	3.5526	93	465.4689	52.3987	150	981.9432	29.6357	207	3642.4470	346.0860
37	113.9626	0.1173	94	479.3112	43.3931	151	1027.6307	119.1984	208	3656.6533	511.6493
38	116.5689	7.6023	95	482.0011	9.3221	152	1246.6976	0.6451	209	3667.0879	523.3572
39	122.4405	2.1300	96	491.7763	46.4108	153	1343.8466	30.2602	210	3679.2466	248.6816
40	133.1836	13.6992	97	498.0651	9.5498	154	1648.9104	16.7191	211	3692.2542	312.7586
41	135.4658	1.0063	98	504.4683	83.8529	155	1653.4395	86.1795	212	3708.8708	474.3451
42	135.6564	2.1290	99	510.3910	15.0644	156	1659.0669	48.2098	213	3712.4653	542.8649
43	138.7951	5.5678	100	519.1168	50.0421	157	1660.4740	286.6406	214	3714.0935	138.6107
44	147.8091	2.2865	101	524.5191	15.3354	158	1661.6719	26.5094	215	3733.6123	175.0086
45	156.5107	10.4426	102	529.0688	44.1680	159	1664.5071	199.7162	216	3757.0298	273.3468
46	159.4668	15.1697	103	536.6472	15.8348	160	1666.7181	42.8108	217	3779.0068	383.0251
47	166.3992	14.9483	104	546.7603	11.4126	161	1680.0286	20.9662	218	3790.3250	226.7530
48	170.6452	1.5056	105	552.4704	53.2333	162	1681.8362	148.5192	219	3798.5264	165.4354

49	176.4292	4.1053	106	561.1337	10.4402	163	1682.3075	53.5339	220	3857.5078	67.9331
50	179.7938	1.0675	107	564.4063	78.6386	164	1688.0244	40.5770	221	3869.2615	68.6813
51	181.6632	5.9818	108	568.0030	45.0238	165	1689.0642	5.4376	222	3872.7952	63.0368
52	183.4978	11.7728	109	575.1536	21.9367	166	1691.8073	4.6079	223	3875.2097	128.0688
53	191.9235	11.5840	110	580.9849	184.7144	167	1698.6379	65.8148	224	3875.8452	84.6586
54	196.4772	12.1262	111	606.6508	123.4413	168	1703.9023	68.9568	225	3877.0691	63.1845
55	197.6294	5.8861	112	613.7080	18.8585	169	1707.8864	120.9440	226	3877.2463	41.0219
56	210.1822	15.1218	113	620.7108	55.1492	170	1710.7423	22.9518	227	3878.1321	54.6160
57	213.5517	25.9419	114	625.5299	50.4861	171	1713.4711	34.8797	228	3889.7639	76.1493

DCE1-39H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	11.8337	0.0358	92	222.0377	33.8869	183	674.0942	183.8787	274	1718.0800	33.3456
2	16.5804	0.2850	93	226.8342	89.1929	184	678.3138	91.2539	275	1720.4719	0.7295
3	18.0145	0.1092	94	228.1586	14.0676	185	684.0189	116.8156	276	1726.1752	3.2585
4	21.4154	0.2528	95	228.8585	33.6734	186	688.9544	9.3018	277	1734.6378	64.6521
5	23.7278	0.9593	96	230.5586	12.1904	187	690.1321	48.1710	278	1736.9783	115.7237
6	26.4166	1.2232	97	233.3725	75.5588	188	693.0622	31.4777	279	1739.3260	122.3156
7	28.0520	3.5245	98	235.7494	99.5046	189	699.6702	90.9902	280	1739.8430	41.7457
8	28.5945	0.1111	99	241.8658	53.3740	190	715.2722	68.3595	281	1743.5049	102.8598
9	30.0137	1.1022	100	244.5527	6.1081	191	719.5046	81.4422	282	1747.1788	19.7137
10	30.4305	0.8745	101	246.9843	79.3776	192	726.1039	128.0826	283	1759.0043	73.2544
11	32.2439	1.9422	102	249.1902	5.8306	193	728.6797	336.0505	284	3172.1389	1582.3656
12	35.1663	0.8434	103	251.4509	38.5008	194	741.0626	205.2761	285	3217.2026	700.7086
13	36.0844	0.7060	104	254.5193	87.9707	195	745.9095	51.0675	286	3219.2954	152.8535
14	38.0443	0.1763	105	256.4889	17.5905	196	748.5526	6.8995	287	3232.2798	1180.4097
15	39.4450	0.8778	106	259.3138	115.2623	197	757.1469	290.1707	288	3237.7520	0.3107
16	42.0481	0.2839	107	263.9561	15.2307	198	760.7572	35.3881	289	3279.1167	536.8096
17	42.9248	0.4962	108	265.4696	0.0849	199	766.8414	178.8406	290	3284.8770	805.7739
18	44.1787	0.0980	109	267.8547	6.6340	200	771.9090	64.2154	291	3294.2024	262.5833
19	44.4446	1.7013	110	270.3504	27.0292	201	781.9062	41.4462	292	3307.1548	222.3780

20	46.8838	0.6094	111	272.1149	21.7596	202	782.9916	2.6529	293	3309.4407	539.2101
21	49.0675	0.6999	112	275.9332	15.9897	203	786.7807	436.1487	294	3333.2673	1093.8026
22	49.9529	0.0747	113	276.4795	36.1323	204	791.3364	174.1834	295	3335.2786	2046.1803
23	52.2126	2.0413	114	278.7976	31.3046	205	795.3261	191.6196	296	3352.3848	417.9642
24	54.0718	2.5992	115	280.8588	65.4861	206	801.0296	196.1582	297	3357.0154	712.1573
25	54.9393	1.8083	116	283.4782	9.0886	207	807.3990	85.6733	298	3362.6768	277.4223
26	57.1179	0.0803	117	287.3232	39.3488	208	808.3893	242.9593	299	3377.6812	1118.0562
27	59.6851	2.0461	118	293.2098	74.4574	209	815.8558	5.8516	300	3383.2119	792.7919
28	60.1191	7.1113	119	296.8766	7.3936	210	827.3567	118.0308	301	3385.5593	1371.3250
29	61.5758	3.6165	120	299.6372	24.2938	211	833.0331	60.1440	302	3398.5664	17.6249
30	62.1830	0.9846	121	307.9036	5.1530	212	837.8231	47.6494	303	3402.6926	1320.4274
31	63.4743	0.6924	122	311.2340	35.9839	213	840.3373	40.2275	304	3412.9321	808.3471
32	63.8067	0.7356	123	318.0342	19.4259	214	852.2448	67.5467	305	3429.5168	1182.0353
33	67.7128	2.0004	124	320.7681	17.8895	215	859.4783	263.7779	306	3435.7080	1545.1084
34	68.4748	1.6670	125	323.4751	13.5163	216	869.7243	22.7837	307	3443.6575	458.6131
35	69.8702	1.2385	126	324.5460	52.6325	217	871.4370	76.3784	308	3450.2432	531.2973
36	70.7772	0.3402	127	329.1389	79.0884	218	883.2570	1.8352	309	3467.9749	2232.6709
37	72.3067	0.4271	128	329.5169	52.4348	219	889.9777	94.6576	310	3473.6797	611.6980
38	73.3446	0.5454	129	331.7043	38.9835	220	894.0693	28.0925	311	3490.3264	392.5005
39	76.0392	2.1138	130	347.4943	74.8454	221	897.2246	84.3208	312	3502.6523	959.3089
40	76.9881	1.4647	131	367.6959	115.3068	222	903.2189	96.8920	313	3507.2417	1071.2819
41	78.2954	1.1180	132	406.7783	31.0948	223	906.5677	357.2162	314	3512.4326	137.3958
42	79.3166	6.6641	133	409.4895	58.7651	224	909.1794	56.6566	315	3518.4307	814.5009
43	80.1382	3.6586	134	412.9104	109.6325	225	917.0562	11.8859	316	3521.4851	56.9251
44	83.5858	1.8504	135	416.4159	6.0928	226	927.0355	121.9916	317	3524.7927	516.4087
45	86.2254	1.7885	136	416.5419	20.5628	227	937.8681	243.3589	318	3525.1362	168.8604
46	87.7265	2.4198	137	424.6116	2.7141	228	957.0009	44.4907	319	3530.6416	278.9845
47	88.3258	2.4326	138	425.9327	43.4198	229	959.1710	138.0351	320	3541.1838	664.1215
48	91.0376	5.7720	139	433.8711	35.9624	230	963.7961	19.3401	321	3555.0278	558.1460
49	92.2087	2.8500	140	435.2797	40.1334	231	967.2947	38.7343	322	3563.2053	634.5837
50	94.4057	7.1517	141	460.2359	10.7275	232	982.1654	141.3017	323	3564.7451	279.4163
51	95.9471	0.1047	142	461.9315	33.8018	233	996.6509	43.3596	324	3566.8762	399.0096

52	98.6216	1.9984	143	463.8876	38.2040	234	1003.7896	148.1852	325	3569.0991	40.0737
53	103.8452	5.0039	144	465.0306	13.4098	235	1011.9778	18.2666	326	3574.9209	412.4430
54	109.1729	0.6805	145	483.6893	53.5708	236	1017.0237	17.4009	327	3575.9272	795.4157
55	111.7632	3.9683	146	483.9155	79.4263	237	1020.1357	64.6157	328	3585.7710	95.5973
56	115.4493	5.1040	147	494.0612	173.7931	238	1046.4078	86.7179	329	3589.2112	254.5191
57	117.1394	20.0809	148	496.1324	128.7466	239	1060.2373	132.5814	330	3597.4360	558.0984
58	122.6496	4.9446	149	502.9194	71.3555	240	1083.0168	58.1001	331	3602.4319	271.7180
59	126.2991	4.9359	150	510.0530	13.1334	241	1086.3439	48.1973	332	3607.6965	392.6609
60	130.3600	10.7049	151	519.9152	22.1516	242	1218.1586	0.0833	333	3611.2761	1340.7233
61	131.6996	6.1402	152	525.6525	1.4678	243	1319.5778	26.9418	334	3621.3193	314.9114
62	135.3470	2.6048	153	527.4697	11.4047	244	1643.5280	73.4299	335	3622.7571	864.5549
63	136.5050	1.2166	154	531.1344	118.0323	245	1646.9233	55.6046	336	3633.7134	134.9222
64	142.4639	1.4932	155	536.1328	220.2219	246	1648.9028	23.9705	337	3643.8999	580.2131
65	146.3429	7.4815	156	540.1762	19.6084	247	1651.4476	126.7686	338	3671.5471	167.0478
66	154.5612	10.0071	157	546.4515	5.7660	248	1655.9585	93.3309	339	3695.8047	690.5574
67	159.6297	5.6316	158	552.0095	5.2857	249	1656.1764	21.1080	340	3697.1035	224.5880
68	161.1412	25.5698	159	560.9979	16.7573	250	1657.5909	101.3207	341	3703.9570	347.3789
69	164.3831	2.1627	160	563.4804	11.8274	251	1660.8777	82.0629	342	3707.0713	243.8015
70	166.6808	2.2248	161	565.8939	8.6980	252	1669.6576	94.5137	343	3708.4265	975.5240
71	167.9815	12.9787	162	571.2201	49.2246	253	1671.6558	41.4055	344	3719.5093	260.8156
72	170.8651	21.0390	163	575.6559	29.7727	254	1673.1255	51.9434	345	3721.3313	356.0089
73	171.6060	3.4109	164	585.7263	53.2674	255	1675.3278	102.8731	346	3726.4358	269.5445
74	174.5785	14.3786	165	591.1041	89.0350	256	1680.7565	65.0219	347	3752.1592	389.5995
75	176.8977	8.6961	166	598.0817	44.2241	257	1681.0597	70.8528	348	3756.0654	306.4868
76	179.4125	10.8964	167	599.4819	60.6248	258	1682.3245	14.9700	349	3762.9263	224.0803
77	186.6440	1.0010	168	602.9903	65.6519	259	1685.0225	28.9792	350	3812.6809	142.5854
78	187.8193	10.0467	169	605.9561	193.2541	260	1685.4886	33.6752	351	3837.2400	133.5839
79	188.9233	4.0285	170	610.6923	78.3373	261	1687.6368	2.5882	352	3867.8035	66.4978
80	189.6309	13.8945	171	616.7674	66.4258	262	1691.1976	66.3440	353	3868.2258	78.1614
81	194.2233	5.9208	172	621.0441	7.2512	263	1693.0836	37.7451	354	3869.2080	64.7556
82	196.2939	13.4218	173	634.9508	65.9168	264	1696.6290	58.7951	355	3872.9763	77.2062
83	199.3234	30.5137	174	641.0113	60.6518	265	1697.1926	10.8893	356	3873.4529	70.5394

84	204.0871	31.8810	175	643.1512	21.2909	266	1698.4413	8.3516	357	3880.4705	54.1918
85	204.7533	30.0149	176	644.3344	135.9995	267	1700.8578	27.7966	358	3880.5542	74.9326
86	206.4277	45.8044	177	649.0654	63.3351	268	1704.4072	11.6664	359	3881.3408	125.0301
87	208.9814	5.6100	178	654.4790	53.4033	269	1706.2269	82.8152	360	3881.3691	38.3454
88	210.3146	31.0509	179	657.1220	45.8161	270	1706.4862	41.5611	361	3884.1831	86.2003
89	212.5890	14.3662	180	662.1637	123.3462	271	1710.9550	18.2815	362	3887.7180	59.8423
90	218.2678	58.3339	181	664.3650	16.7459	272	1714.1812	13.4634	363	3890.0637	100.8201
91	219.3380	15.4416	182	669.8470	76.6854	273	1715.9955	132.7328			

Appendix 4

Table 5. IR Intensity as a function of frequency (DCE2-nH₂O)

Freq (1/cm) IR Intensity (KM/Mol)

DCE2

	Freq	Intensity
1	211.6987	0.2019
2	238.0044	3.1561
3	348.3319	0.0000
4	800.1919	136.6090
5	803.9162	0.0139
6	839.6255	0.0043
7	930.2238	58.2960
8	1222.9431	21.6884
9	1303.7646	0.0000
10	1642.4180	0.0001
11	3232.4878	15.3932
12	3234.6914	0.3262

DCE2-2H₂O

	Freq	Intensity		Freq	Intensity
1	21.9095	0.8663	16	785.3579	136.3068
2	46.2210	0.2121	17	816.7534	7.3531
3	89.4747	3.7771	18	831.5364	7.1334
4	99.8972	9.7134	19	986.0871	50.5077
5	115.4738	5.5817	20	1239.7336	19.0494
6	172.4946	60.6024	21	1324.5551	2.2158
7	200.5217	12.4998	22	1638.4178	21.9180
8	211.3852	30.2939	23	1642.6887	45.3228
9	225.3381	101.5720	24	1660.5250	36.1613
10	229.8151	73.2665	25	3176.8210	114.6425

11	246.9883	22.6103	26	3238.6897	6.2951
12	342.2916	36.7473	27	3642.4392	330.4379
13	354.8585	78.4790	28	3758.3921	180.6473
14	458.2821	81.0636	29	3887.5879	144.4593
15	716.2557	120.6932	30	3890.5955	77.4832

DCE2-5H₂O

	Freq	Intensity		Freq	Intensity
1	13.0213	0.1067	30	668.6455	252.1890
2	20.7892	0.0631	31	764.3806	160.7126
3	32.8257	0.2105	32	789.3220	126.1435
4	34.5155	0.7352	33	817.3113	6.9454
5	44.2372	0.0544	34	832.9073	1.1646
6	51.1101	2.4606	35	920.4136	26.8060
7	68.0918	2.6972	36	967.6044	100.2659
8	90.2838	2.5035	37	980.9358	2.5660
9	110.9252	7.3073	38	1236.1400	21.9227
10	116.5153	2.0540	39	1315.9384	3.2010
11	173.3477	14.7426	40	1641.7108	2.3424
12	182.4344	10.0053	41	1651.7455	59.2532
13	199.8402	22.1358	42	1653.6312	71.9383
14	201.7234	48.6611	43	1657.1591	66.8063
15	217.0870	13.9310	44	1662.4478	26.4084
16	219.0124	81.6578	45	1679.1598	22.4081
17	239.9906	122.3941	46	3199.7383	76.3077
18	244.2258	13.6714	47	3236.9700	5.9053
19	271.4604	19.6357	48	3459.8643	570.3534
20	292.5032	39.0284	49	3512.1489	210.4584
21	345.7805	13.3210	50	3633.4292	279.6968
22	349.0574	57.8000	51	3639.8186	482.6107
23	374.2044	28.5801	52	3661.9736	515.4921

24	380.5335	49.5742	53	3677.2893	267.2406
25	405.8744	37.2621	54	3836.4600	249.8332
26	433.9740	236.0583	55	3878.6692	89.3292
27	565.4568	76.7835	56	3886.3506	76.9679
28	587.5634	159.2225	57	3887.7666	78.5999
29	607.9882	367.3576			

DCE2-7H₂O

	Freq	Intensity		Freq	Intensity
1	14.1574	0.1095	39	704.1639	183.4466
2	21.7193	0.4641	40	740.0667	257.6141
3	27.9150	0.7555	41	774.3752	45.8278
4	32.9882	0.1475	42	788.6621	87.0486
5	36.8077	0.5562	43	791.9170	227.7919
6	47.7330	1.2852	44	817.5435	2.6886
7	48.2853	0.9125	45	832.8410	0.1468
8	61.7890	1.8699	46	857.4606	38.2602
9	70.2373	0.6840	47	910.0332	63.6250
10	77.6676	0.5347	48	962.0359	63.3430
11	88.6060	0.6217	49	1065.8339	68.8311
12	105.6171	6.5507	50	1233.9634	22.4104
13	113.1633	10.8474	51	1311.2913	2.7460
14	161.3984	3.1553	52	1619.0465	79.5214
15	177.3663	20.7791	53	1643.1570	0.2566
16	186.8186	2.1576	54	1663.9508	58.2444
17	191.3101	2.1287	55	1666.3145	139.1810
18	214.6836	2.7833	56	1672.1993	24.1172
19	227.4811	18.3561	57	1684.4998	71.1389
20	238.3575	5.8445	58	1697.5062	30.8757
21	244.6951	12.7766	59	1709.2208	73.5017
22	247.8870	24.4522	60	3170.0928	865.5388

23	254.3087	81.4036	61	3211.2769	62.2889
24	260.0343	106.2503	62	3236.4907	6.3219
25	291.0572	66.5639	63	3465.0000	517.8580
26	312.7010	107.2875	64	3495.1470	241.6258
27	324.4688	103.0053	65	3524.5474	788.3404
28	345.7781	2.2188	66	3594.4429	797.8096
29	356.0212	53.0663	67	3596.5396	156.1916
30	379.7806	82.9703	68	3636.1084	333.9138
31	405.2707	23.1861	69	3637.1548	673.5835
32	416.4865	15.9027	70	3786.8462	140.8789
33	437.6320	61.3136	71	3853.0862	129.6635
34	486.9593	51.5620	72	3859.7146	90.5034
35	500.4074	85.5021	73	3861.9192	39.3069
36	545.9497	21.4581	74	3880.6389	84.0067
37	599.6584	283.0148	75	3888.0471	64.8563
38	675.7419	78.1845			

DCE2-10H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity
1	8.8925	0.2131	35	284.2565	20.1083	69	1318.3887	3.2076
2	10.5270	0.2939	36	292.9028	103.8454	70	1640.7515	2.6097
3	15.4777	0.7944	37	309.4369	44.9168	71	1650.3342	77.9249
4	17.9354	0.3732	38	346.5020	0.6718	72	1657.3274	106.5696
5	22.6982	0.7037	39	358.9145	147.9801	73	1657.9615	21.6032
6	27.8018	0.1942	40	360.3296	37.9716	74	1661.7426	43.4940
7	33.1784	0.2681	41	367.1773	62.5856	75	1667.3252	80.8792
8	37.8547	0.6563	42	391.4919	37.7278	76	1672.3229	33.6271
9	43.2033	1.8486	43	423.6655	39.3376	77	1677.3774	19.2953
10	45.9600	0.3129	44	430.4427	6.9673	78	1682.1285	34.3469
11	53.5182	1.3515	45	446.5444	45.8549	79	1688.4717	14.3950
12	60.0541	5.1979	46	460.6409	117.1139	80	1703.6084	15.7048

13	61.6603	1.3482	47	472.3340	186.1205	81	3189.1238	938.5688
14	76.8595	3.6665	48	485.9229	28.1856	82	3193.5637	62.6915
15	89.4455	0.6980	49	557.1381	297.7976	83	3236.5286	5.8090
16	98.0152	0.5787	50	604.8550	184.4753	84	3336.4619	360.5134
17	117.8290	1.2055	51	626.5411	96.8315	85	3425.9922	1829.3267
18	125.5398	6.1407	52	630.2196	137.7344	86	3478.2539	462.8552
19	142.1362	5.3206	53	650.6767	179.8365	87	3493.7434	161.5717
20	144.5060	64.7723	54	679.5801	97.8349	88	3521.5935	1449.7247
21	154.7150	51.3289	55	727.1451	150.8871	89	3533.6682	667.7145
22	165.6285	32.0738	56	770.5076	198.2232	90	3555.3542	613.9745
23	185.4684	10.5740	57	785.7563	79.1687	91	3576.9961	160.9886
24	197.3576	55.4879	58	791.1882	41.4681	92	3623.1770	269.4590
25	203.2376	73.6836	59	816.9060	5.2501	93	3651.7253	415.8756
26	210.4102	36.4593	60	830.7891	86.0624	94	3701.2644	187.0586
27	215.6302	38.2444	61	836.0208	140.9481	95	3763.0669	300.7106
28	218.0264	26.7708	62	870.1620	256.1780	96	3830.8936	260.3239
29	236.4774	46.9880	63	938.3135	32.1819	97	3872.1223	70.0850
30	243.1329	9.5984	64	967.1477	128.3511	98	3873.5601	73.7345
31	247.9301	24.2815	65	979.8781	12.8992	99	3881.1375	61.3697
32	256.7507	12.3657	66	1045.1478	19.1906	100	3883.5432	67.3978
33	264.1123	74.2224	67	1086.0566	38.1040	101	3887.3452	82.7031
34	276.3430	14.7464	68	1236.4423	21.2959	102	3895.6438	91.5238

DCE2-12H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	10.6088	0.6637	31	216.7021	12.2230	61	683.4055	52.0736	91	1696.2460	49.8630
2	13.1573	0.3818	32	228.3862	31.8806	62	717.4894	261.2673	92	1704.7836	2.6667
3	17.5683	0.0043	33	234.4216	34.4526	63	734.2833	137.3377	93	1718.5118	12.1266
4	20.7586	0.1072	34	242.3190	14.3112	64	752.7598	93.3773	94	1740.1425	4.7160
5	24.1924	0.2122	35	247.4730	17.8820	65	769.4861	51.4472	95	3048.7058	1144.3575
6	28.2686	1.2649	36	259.2247	13.9417	66	778.1652	34.4883	96	3192.9468	375.9319

7	34.2522	0.1234	37	259.7295	129.9493	67	786.6419	245.9109	97	3209.6799	492.9628
8	36.1412	0.0658	38	274.7648	10.6350	68	790.0121	145.1739	98	3238.7644	5.6950
9	41.8327	0.6440	39	275.9620	136.4732	69	812.5653	12.9121	99	3398.2986	948.9834
10	47.5970	0.6188	40	288.8859	39.4028	70	817.7863	241.0145	100	3418.0498	1112.0090
11	52.6317	0.5963	41	299.9110	30.8263	71	832.2181	23.1446	101	3433.6807	859.5228
12	56.0126	0.5344	42	305.0524	69.9502	72	841.3581	137.4999	102	3464.0105	1267.6835
13	60.7786	3.5459	43	312.4333	45.6874	73	877.5402	323.3102	103	3491.0615	376.4501
14	68.4960	0.9444	44	346.4131	3.5441	74	886.8675	20.5021	104	3502.8896	865.6353
15	73.3520	2.4458	45	353.4083	119.6662	75	918.6896	27.3707	105	3520.6270	797.2348
16	73.9535	0.9273	46	355.6975	69.2478	76	926.5837	90.6948	106	3529.9131	165.5679
17	85.6630	0.4391	47	396.5388	123.8099	77	963.5395	46.4550	107	3550.1257	422.6830
18	90.0066	2.3611	48	414.3060	6.8951	78	1051.8601	52.7161	108	3585.3933	531.6023
19	104.6495	0.3986	49	430.4647	49.9461	79	1127.3174	46.5420	109	3623.4312	488.7177
20	106.8183	4.0150	50	436.5864	11.5929	80	1233.3105	16.6176	110	3641.3855	570.8135
21	132.0285	14.1086	51	453.4255	25.8917	81	1320.7428	0.3356	111	3693.8301	669.8026
22	156.4572	1.9001	52	457.0042	8.8614	82	1641.0551	2.6012	112	3698.6338	338.7278
23	168.6979	5.6279	53	464.2076	93.7235	83	1651.3372	52.6692	113	3856.8242	42.5034
24	172.4508	9.1618	54	496.2828	40.4735	84	1654.8263	50.4378	114	3857.9058	145.3478
25	180.3285	2.8274	55	508.7450	20.8538	85	1659.9916	72.6861	115	3863.1504	69.7870
26	186.1897	40.1631	56	538.8864	50.8026	86	1665.2175	98.1691	116	3876.5012	77.3923
27	192.6324	12.7980	57	562.7965	62.1057	87	1671.1947	149.8210	117	3880.5918	69.5405
28	206.4561	65.0824	58	595.0851	28.7680	88	1674.5785	2.9426	118	3882.9866	61.0065
29	211.0123	113.1853	59	611.0215	1.9653	89	1682.9487	96.2591	119	3886.1006	56.8623
30	215.3448	1.4506	60	644.1751	102.1147	90	1688.8884	36.7662	120	3889.6804	93.4000

DCE2-16H₂O

	Freq	Intensiy		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	7.6240	0.1677	40	209.0179	2.8352	79	618.9819	147.0067	118	1707.2806	16.7090
2	11.3290	0.0469	41	212.4609	111.4938	80	630.0306	10.3912	119	1714.1572	150.3600
3	18.3847	0.4338	42	214.0672	4.4014	81	643.1265	158.7135	120	1715.0023	5.6951
4	27.0187	2.6550	43	223.8576	50.8245	82	666.0514	149.3122	121	1724.2429	80.1778

5	29.0962	0.2675	44	225.5988	54.2042	83	679.0785	66.6628	122	1733.1924	51.0359
6	31.6498	0.4719	45	228.5947	32.0053	84	700.1665	419.6035	123	3201.3096	81.2921
7	36.6288	0.1825	46	236.5005	42.2926	85	715.5160	241.1376	124	3238.1899	5.7936
8	41.1965	0.8245	47	244.5308	2.3465	86	719.5334	85.2054	125	3368.0659	706.7234
9	47.8866	0.9365	48	246.9913	22.7946	87	741.5277	26.4907	126	3371.3975	682.1683
10	49.7497	4.4548	49	253.3077	53.4374	88	744.6999	377.5831	127	3462.3103	159.1087
11	52.1974	3.6083	50	260.4401	41.9490	89	761.9177	78.5126	128	3476.9131	545.6214
12	58.6385	0.4460	51	264.2432	36.9176	90	786.0566	25.3882	129	3481.2139	950.1078
13	61.9885	4.0728	52	270.5237	15.6734	91	790.7531	145.3415	130	3488.8123	280.8615
14	62.4034	0.2913	53	271.1754	43.2442	92	814.5730	206.1774	131	3499.0322	910.5500
15	70.0127	2.9756	54	278.3271	13.9390	93	816.2612	5.8882	132	3504.4141	134.8776
16	72.7515	2.6857	55	285.7869	4.8651	94	834.2171	33.0008	133	3532.1582	1030.4323
17	78.2401	2.8506	56	310.7255	104.7338	95	836.4008	71.2625	134	3538.5681	410.2144
18	83.4676	1.1592	57	337.1921	64.4259	96	853.5782	100.8333	135	3545.7053	683.7471
19	87.3035	3.3892	58	347.2122	2.6542	97	863.6238	78.9907	136	3566.8452	813.0560
20	90.3149	2.3077	59	386.0590	6.4471	98	894.5560	150.4134	137	3599.1521	136.9493
21	93.7270	0.7150	60	399.6474	35.9881	99	922.1971	79.5179	138	3604.6257	396.6924
22	96.1127	0.9011	61	414.4961	33.9711	100	949.4690	64.4319	139	3614.3765	219.1702
23	100.3748	0.7568	62	417.7358	102.8276	101	963.0394	8.9729	140	3627.9209	207.3517
24	104.1902	3.9756	63	434.4897	51.0578	102	968.3386	65.7663	141	3654.4966	57.1103
25	109.1035	5.0733	64	439.6362	68.4489	103	1054.1790	41.5984	142	3660.0635	991.3134
26	116.5424	16.8236	65	447.8129	14.1554	104	1239.1014	23.6334	143	3674.2144	742.7600
27	119.0023	0.8510	66	453.7668	32.5122	105	1318.9800	4.0546	144	3687.1848	658.1985
28	134.8039	12.4547	67	475.9526	19.1895	106	1643.4218	0.6914	145	3698.3025	262.5651
29	138.3294	9.6306	68	498.4275	39.2315	107	1650.5175	20.8803	146	3705.5442	123.6876
30	152.3896	20.1784	69	506.4742	50.0298	108	1652.7019	51.2485	147	3727.8069	383.4439
31	153.9765	5.6405	70	512.0708	20.6681	109	1655.5922	192.4317	148	3778.7559	193.7305
32	160.4856	4.0434	71	526.6723	73.7334	110	1661.9073	54.7258	149	3801.4673	258.2322
33	166.7737	4.3645	72	539.4268	131.8741	111	1672.5662	55.1305	150	3809.8169	166.0251
34	171.9156	10.8828	73	549.1906	97.1445	112	1674.0461	40.1603	151	3873.6648	71.8303
35	182.5066	5.4033	74	556.4152	76.9167	113	1678.7710	22.0593	152	3877.8936	77.1283
36	190.7296	83.7964	75	569.2923	87.4666	114	1684.4113	66.2614	153	3880.2832	80.0537

37	191.9966	0.3210	76	586.6410	121.1017	115	1690.7389	96.1469	154	3882.5581	86.9381
38	197.9667	6.1268	77	597.5316	5.8999	116	1696.6759	8.5296	155	3885.9988	100.6237
39	203.0023	54.6424	78	607.5402	132.2918	117	1699.2426	81.8755	156	3889.7122	65.2149

DCE2-24H₂O

	Freq	Intensiy		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	17.9918	0.8659	58	217.7801	14.6337	115	639.3230	122.6579	172	1713.7157	97.9456
2	19.9917	0.2660	59	219.0769	3.6029	116	654.6068	38.5459	173	1715.8617	7.9303
3	22.4472	0.5754	60	225.9167	26.4045	117	669.3625	120.3981	174	1727.2723	13.6190
4	28.6360	1.1411	61	229.0579	18.9143	118	685.0441	34.5319	175	1735.9697	44.6727
5	30.9114	1.6754	62	232.6973	11.1008	119	686.8869	268.2708	176	1737.1971	6.0132
6	33.3753	0.9222	63	244.8958	16.4844	120	691.9184	331.3051	177	1746.8364	80.6318
7	35.8428	0.8191	64	246.2921	9.9837	121	699.3232	34.9253	178	1753.7015	23.3525
8	36.5907	3.6393	65	250.5986	26.0682	122	705.4128	117.5909	179	3213.2815	75.5263
9	41.3087	0.4240	66	253.2069	16.5417	123	719.6292	258.1094	180	3232.0176	11.5977
10	42.2697	1.9271	67	260.9096	13.8294	124	729.5966	117.3625	181	3236.4453	1078.4727
11	45.6956	2.9888	68	263.1639	78.3188	125	745.2071	69.8321	182	3259.3589	1052.5657
12	46.8596	3.7564	69	266.6889	8.7867	126	753.3851	367.0513	183	3267.9817	1205.7902
13	50.6584	1.4900	70	274.2779	26.3579	127	771.0008	567.8681	184	3314.6223	649.8084
14	54.7064	1.1161	71	282.9688	93.8958	128	780.0917	54.8260	185	3335.8889	931.7592
15	56.0211	0.8012	72	286.3361	4.0558	129	781.4109	89.1443	186	3343.2483	1009.5094
16	57.4801	0.5098	73	289.5870	4.7745	130	798.4287	97.3263	187	3401.3679	1181.4363
17	58.2597	0.2836	74	293.5375	16.8549	131	808.8479	21.8767	188	3405.2800	754.2186
18	60.8297	1.8987	75	295.4743	20.8886	132	817.0118	5.0247	189	3412.2390	903.0468
19	65.5131	2.1172	76	300.1854	28.3770	133	819.7114	20.5230	190	3445.4680	291.6523
20	66.7049	0.6983	77	308.9109	68.8839	134	821.8522	165.6929	191	3450.6829	509.6874
21	68.3997	0.0922	78	309.4810	31.8978	135	827.8282	40.9614	192	3466.8325	316.3496
22	70.2037	0.3156	79	311.2201	54.7016	136	830.3474	16.6318	193	3489.8022	463.8480
23	72.4957	2.5660	80	319.4559	33.2183	137	841.4761	60.7096	194	3494.1353	601.0606
24	75.5814	0.5203	81	339.7913	56.6077	138	847.0451	144.4765	195	3530.6682	789.3413
25	76.7697	0.4798	82	341.0901	45.9733	139	848.7857	74.7030	196	3535.6313	407.9621

26	79.3930	0.1120	83	345.9789	1.1356	140	859.9024	158.8105	197	3535.8733	293.1745
27	83.1101	2.2376	84	356.7902	21.0247	141	897.4286	83.2094	198	3539.6318	64.1444
28	86.1230	2.2969	85	370.0647	84.5055	142	921.8312	29.5042	199	3549.5457	504.6005
29	87.5385	0.5366	86	391.8810	39.2007	143	928.4095	85.5497	200	3560.1360	448.2096
30	89.4907	1.7894	87	401.9112	10.0027	144	936.9523	2.4262	201	3567.2109	2024.5530
31	90.7082	2.9275	88	422.9005	4.4279	145	945.7157	111.8037	202	3599.1450	153.5523
32	94.4363	0.1070	89	432.5808	29.9356	146	950.7759	30.1118	203	3610.7173	233.0703
33	96.6532	1.0117	90	437.8438	42.4929	147	954.8844	173.2231	204	3621.6692	310.4266
34	99.0482	1.5765	91	447.9946	39.7341	148	968.4277	163.9802	205	3623.7639	50.1100
35	103.7769	0.5613	92	448.4322	4.3843	149	983.0485	51.2427	206	3627.3662	318.7704
36	107.1518	2.9436	93	460.8088	50.5216	150	987.0613	23.9284	207	3631.5005	827.6700
37	113.7144	1.9041	94	466.4919	75.1472	151	1031.2174	134.9326	208	3646.9924	181.6237
38	118.2511	0.8576	95	473.7793	30.8822	152	1244.3442	28.0820	209	3661.9600	541.7635
39	123.4589	3.4007	96	478.9114	16.1747	153	1312.2579	1.1242	210	3673.1040	464.4966
40	127.7523	4.7202	97	482.1773	19.5195	154	1643.9093	0.5031	211	3674.4292	183.6829
41	134.4205	12.0801	98	489.0636	55.2627	155	1648.7715	38.8503	212	3709.1628	109.0751
42	140.2854	7.8894	99	496.7153	25.2160	156	1657.7644	83.1786	213	3717.1738	296.1339
43	142.6098	6.8654	100	502.4293	25.9076	157	1661.4957	121.6250	214	3723.2144	625.6689
44	146.6446	8.4280	101	507.6703	78.6078	158	1664.4679	99.1139	215	3743.8586	252.2918
45	158.9981	8.4158	102	509.4635	21.0397	159	1667.1771	237.1410	216	3762.6021	253.2762
46	160.3858	10.7750	103	525.8193	26.5027	160	1674.3097	75.2918	217	3771.3315	421.8182
47	166.4029	12.9782	104	534.9887	8.5607	161	1680.3348	96.7804	218	3786.1721	190.7849
48	171.2936	2.0390	105	545.2317	4.6235	162	1680.8979	64.8389	219	3821.0581	274.4444
49	178.3413	3.0858	106	552.7196	127.9860	163	1681.1173	58.6000	220	3856.1499	68.1998
50	179.2397	6.5941	107	558.2276	33.5650	164	1688.1602	25.4099	221	3868.9075	103.9685
51	184.6531	2.9576	108	567.0223	80.3983	165	1688.4871	34.7503	222	3869.1423	72.2218
52	188.3995	9.9260	109	580.6131	143.7660	166	1689.6866	1.5970	223	3871.9868	73.0792
53	194.0376	13.4596	110	582.4716	16.7408	167	1701.2605	44.2991	224	3872.8376	50.6408
54	197.4446	6.6751	111	595.5468	70.6557	168	1705.9889	91.3769	225	3874.7532	62.4233
55	204.8354	58.6449	112	610.6055	124.0408	169	1707.0031	58.4765	226	3875.5315	68.5856
56	211.7627	24.8194	113	628.6658	67.5551	170	1708.4680	69.9798	227	3877.4399	74.8218
57	213.0851	13.7495	114	632.0409	131.7784	171	1709.9193	18.6023	228	3891.2798	73.6595

DCE2-39H₂O

	Freq	Intensiy		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	8.0190	0.0233	92	222.3413	67.0050	183	674.6592	170.1528	274	1716.6259	33.1479
2	10.7029	0.0804	93	225.0881	83.3502	184	679.5391	62.8494	275	1719.7872	17.9796
3	18.9503	0.1014	94	227.2323	6.4481	185	683.1988	169.7379	276	1724.3992	5.3060
4	20.0515	0.0265	95	229.5057	24.1431	186	690.8529	12.8885	277	1733.5869	54.1202
5	22.9644	1.1553	96	230.5658	12.8880	187	693.6241	86.6204	278	1735.6157	70.1117
6	24.2488	0.6226	97	233.7917	173.4043	188	698.9685	110.4932	279	1736.0745	107.7897
7	25.6108	2.8210	98	234.9294	29.3587	189	716.7287	70.3974	280	1738.2323	75.0527
8	27.1804	0.8035	99	238.9881	60.0457	190	727.1165	370.1113	281	1744.6479	121.9702
9	28.9162	1.6179	100	244.3396	9.9738	191	729.9369	110.9859	282	1745.1793	22.6210
10	30.4025	0.3691	101	245.8604	63.9206	192	736.5613	205.2999	283	1757.5336	73.9685
11	30.9927	1.6286	102	247.5276	34.7365	193	743.1464	56.6588	284	3149.6191	1148.9927
12	32.9744	0.1675	103	248.2938	43.4774	194	753.2224	213.8613	285	3180.3982	199.1004
13	36.7141	0.8255	104	251.0021	28.5169	195	755.8774	81.5938	286	3195.1262	1351.5784
14	38.3105	1.6867	105	251.5169	24.5924	196	761.5013	91.6180	287	3232.0103	5.3236
15	38.7578	0.2015	106	256.7155	22.6415	197	766.3285	134.5993	288	3242.3538	1228.4515
16	41.5736	0.5037	107	261.3894	97.5638	198	774.9315	24.5212	289	3289.1670	290.8390
17	43.4684	1.4173	108	262.9576	20.0595	199	780.2972	58.3370	290	3298.0774	739.3415
18	44.8027	0.4838	109	265.6472	7.9815	200	783.4713	195.1213	291	3300.4087	494.6237
19	45.0216	1.4856	110	268.4246	6.8746	201	784.0407	14.3980	292	3305.4402	422.5135
20	47.3469	0.1181	111	270.5060	36.6741	202	788.3297	307.5350	293	3311.8628	350.2007
21	48.7153	1.5541	112	273.0898	30.5129	203	790.7192	248.8952	294	3335.7646	1152.1909
22	51.0589	0.3314	113	274.0877	13.6877	204	798.2999	111.7129	295	3339.7271	1887.2083
23	52.1342	1.7321	114	275.3124	17.9773	205	800.8557	179.0879	296	3350.7820	419.7302
24	54.8170	1.1045	115	278.1061	27.5713	206	807.0230	21.0138	297	3352.4409	822.0740
25	56.4777	1.6443	116	279.6650	69.7933	207	812.3852	279.4720	298	3366.2524	231.8818
26	57.4634	0.6751	117	282.9786	6.5589	208	816.3674	28.5565	299	3381.1770	1228.8976
27	58.3633	0.8635	118	286.5499	42.4058	209	821.7340	3.5585	300	3381.9590	803.9584
28	59.9682	3.5810	119	292.5252	44.5940	210	831.2988	10.0244	301	3389.9292	1364.1173

29	61.4871	1.7211	120	297.4630	67.2624	211	832.3373	216.5535	302	3402.5833	529.3865
30	62.7286	1.3890	121	303.9407	12.7432	212	837.0129	19.4941	303	3414.2676	877.8509
31	64.0960	1.3503	122	307.2539	13.3567	213	846.4656	79.5214	304	3428.3435	1154.6732
32	65.4789	2.9992	123	317.0149	11.7245	214	851.9789	74.8365	305	3435.3152	478.7889
33	68.2426	1.2926	124	318.9548	16.7259	215	865.0937	192.4604	306	3444.3835	817.9607
34	69.3743	1.5557	125	319.8326	17.9659	216	868.8496	20.3253	307	3453.1409	88.8235
35	70.1089	1.4424	126	322.4628	49.5981	217	874.1250	78.7252	308	3454.8555	1493.7899
36	72.5166	0.0831	127	323.4777	25.9319	218	884.1377	6.9195	309	3469.1990	1767.2170
37	74.5248	2.0209	128	324.2043	19.1324	219	891.5871	156.4952	310	3470.8098	994.0831
38	76.1312	0.6387	129	329.4070	20.9700	220	894.9637	58.2398	311	3493.2695	416.7042
39	76.6420	1.0140	130	334.4533	47.7253	221	898.1530	19.4872	312	3505.1177	981.9642
40	77.9720	2.8372	131	343.5643	140.4449	222	906.5565	239.3272	313	3508.3486	458.6395
41	79.9673	5.0789	132	346.5633	0.5479	223	907.2909	175.9099	314	3509.2698	720.9412
42	80.4010	1.4623	133	347.8396	74.5623	224	912.1337	62.5164	315	3514.4221	603.7788
43	84.1954	2.6170	134	367.1017	102.1485	225	924.3640	157.4694	316	3522.3423	289.2532
44	85.5666	0.8525	135	409.4763	58.1429	226	936.7554	319.2896	317	3523.4993	359.0855
45	87.2587	3.8861	136	412.8487	105.1231	227	957.1924	66.9892	318	3529.7683	479.4595
46	89.3536	2.5233	137	414.8371	20.3700	228	962.1133	14.4544	319	3532.5962	262.1052
47	91.2778	6.5120	138	418.1139	31.3040	229	964.7243	35.2141	320	3537.5559	689.5867
48	92.4230	2.2347	139	435.0757	47.4229	230	965.4668	39.8627	321	3558.4514	598.6775
49	95.2382	0.2570	140	443.6339	27.7772	231	973.5573	74.2554	322	3565.4011	478.5899
50	97.5598	3.6934	141	449.3752	6.5414	232	986.6836	139.3662	323	3566.8994	252.4436
51	102.1865	2.3875	142	458.7137	20.2643	233	1003.6878	29.1190	324	3569.3423	1024.2598
52	103.7578	3.2711	143	465.1845	29.6229	234	1006.7233	180.5451	325	3570.3467	160.6909
53	111.5061	1.0004	144	466.7173	53.1219	235	1011.2375	25.8367	326	3572.0425	271.2026
54	113.0677	10.8529	145	470.2297	7.8089	236	1015.7301	4.1243	327	3574.4155	390.8686
55	114.8271	4.7024	146	482.8555	56.6190	237	1023.0108	82.1854	328	3581.4329	54.9008
56	115.9918	4.8315	147	486.3576	27.8690	238	1040.6310	63.2955	329	3589.7292	157.9852
57	120.1435	15.0876	148	493.4156	187.4362	239	1058.8320	122.0813	330	3595.3840	223.3448
58	122.6316	3.5767	149	507.9270	1.7228	240	1084.8723	79.2756	331	3598.0908	227.2203
59	124.5179	3.8480	150	512.2339	97.9302	241	1085.3809	24.1566	332	3599.1787	667.5987
60	129.7359	10.2359	151	513.7503	14.9540	242	1241.7787	18.5765	333	3606.6394	464.2233

61	131.5117	7.2851	152	518.6543	19.2243	243	1324.5638	3.2936	334	3610.1577	1473.4279
62	135.7811	0.6114	153	522.1926	61.0011	244	1643.7701	1.5757	335	3623.1616	278.0540
63	135.9671	0.8458	154	528.5754	36.2216	245	1644.7819	87.7320	336	3624.0142	826.0512
64	145.7358	3.2815	155	534.1240	100.2742	246	1651.6674	116.7284	337	3647.0081	607.6326
65	148.5138	8.8807	156	536.3499	185.7502	247	1651.8473	83.0408	338	3655.6760	676.3283
66	154.3296	8.6029	157	540.6046	10.1311	248	1654.2747	49.7186	339	3671.9045	173.6227
67	160.0344	4.6041	158	546.0070	27.6797	249	1656.2928	67.5893	340	3696.4119	545.6717
68	161.2441	22.4442	159	552.5236	22.2918	250	1657.5653	92.5219	341	3703.8672	517.9807
69	164.4940	3.8955	160	563.3520	11.7317	251	1659.4895	84.1252	342	3705.9548	251.1700
70	166.8140	15.9101	161	565.7094	66.1807	252	1669.5200	101.7299	343	3712.9961	343.6626
71	169.9929	5.1120	162	572.1316	33.2196	253	1671.3127	39.1064	344	3724.7222	435.1627
72	171.5163	12.3649	163	578.6836	88.5374	254	1671.7697	24.6796	345	3726.2349	264.9238
73	174.4717	16.9685	164	587.2424	49.8827	255	1674.0332	89.3281	346	3729.1145	257.4992
74	176.9166	17.6896	165	592.4504	14.6492	256	1679.2769	45.7444	347	3754.7896	438.0314
75	181.3443	12.3655	166	596.5696	79.5003	257	1680.6599	79.9302	348	3756.1777	241.4674
76	185.6826	0.7142	167	597.5098	101.6554	258	1682.6605	28.2000	349	3765.4641	245.0208
77	187.4854	9.8276	168	601.0956	49.6999	259	1685.5048	37.2331	350	3792.5420	258.4954
78	189.0278	8.0625	169	602.7963	93.8762	260	1688.2302	6.4506	351	3866.3728	51.1127
79	189.8496	16.2348	170	610.0717	157.9542	261	1688.9220	34.0204	352	3868.8423	106.3700
80	194.9679	5.8454	171	618.1664	2.0932	262	1690.1923	34.3511	353	3869.4727	57.0829
81	196.5163	22.7485	172	626.1259	1.4720	263	1691.3730	63.7755	354	3870.1589	50.1922
82	198.9568	59.1745	173	633.3112	70.2901	264	1695.3898	68.7337	355	3872.8728	83.3661
83	202.1813	40.9977	174	639.8810	30.1993	265	1697.5980	8.5020	356	3873.5762	72.3603
84	202.9144	7.1725	175	641.4656	53.0976	266	1698.2163	8.8608	357	3879.4707	64.3869
85	204.8778	28.9129	176	643.6784	98.5011	267	1698.7814	50.6144	358	3879.7195	65.3036
86	207.0554	14.7600	177	648.7137	36.9862	268	1702.9315	15.3350	359	3881.2937	126.4944
87	209.8830	15.1639	178	654.3968	149.1372	269	1704.4039	58.4133	360	3881.3208	37.9522
88	211.6180	14.1460	179	657.6817	54.1788	270	1706.3167	3.1146	361	3884.6924	86.2248
89	213.7765	2.9494	180	662.9872	36.2983	271	1706.8389	25.3479	362	3887.8926	59.6681
90	216.2438	35.9427	181	663.9456	28.7147	272	1712.0118	18.0722	363	3889.6377	100.7724
91	219.4091	2.6821	182	670.4316	82.6279	273	1714.3401	119.8377			

Appendix 5

Table 6. IR Intensity as a function of frequency (DCE3-nH₂O)

Freq (1/cm) IR Intensity (KM/Mol)

DCE3

	Freq	Intensity
1	296.5063	0.0011
2	379.0503	0.2035
3	476.2627	6.8656
4	592.6356	15.4795
5	691.9037	0.0000
6	761.9635	110.1626
7	907.6060	44.5726
8	1100.1938	92.9078
9	1410.1508	0.1144
10	1659.8861	83.2797
11	3174.8557	2.1989
12	3268.7097	0.2230

DCE3-2H₂O

	Freq	Intensity		Freq	Intensity
1	20.9618	0.6442	16	705.0475	134.2980
2	41.2515	0.2445	17	734.0715	8.5104
3	59.6230	1.8594	18	753.5762	123.2287
4	86.8938	4.2835	19	970.9865	42.0223
5	99.2616	7.9702	20	1096.4196	79.8197
6	153.9663	63.6715	21	1427.9980	0.2469
7	193.4080	9.2339	22	1640.8065	66.2220
8	209.1577	158.8447	23	1660.1920	61.0168
9	223.0047	61.1788	24	1663.8666	31.9370
10	296.7551	2.8266	25	3144.2971	70.9291
11	330.8462	120.7153	26	3246.5293	28.1396

12	387.8862	0.3994	27	3650.3748	328.3481
13	444.9096	80.0811	28	3765.6675	158.7124
14	472.1271	8.5162	29	3888.8413	147.0838
15	583.0419	20.8904	30	3889.4304	75.8449

DCE3-5H₂O

	Freq	Intensity		Freq	Intensity
1	7.5807	0.1967	30	619.6753	78.6173
2	14.6911	1.0340	31	684.3114	101.1538
3	16.9819	2.8116	32	695.3359	0.0914
4	22.9235	0.4212	33	747.2053	500.7148
5	28.5688	0.6994	34	763.7930	113.3170
6	31.7755	0.0583	35	900.7889	10.4526
7	45.3769	0.5096	36	911.5248	43.9269
8	56.2408	1.8435	37	938.7484	9.4446
9	64.5184	0.2315	38	1099.4365	83.8153
10	114.9395	2.9858	39	1410.8962	0.0902
11	165.5087	77.1714	40	1652.4271	62.2697
12	191.4933	10.6810	41	1653.8086	77.9417
13	196.7049	4.5014	42	1659.5032	90.0503
14	208.7402	69.1638	43	1661.7584	72.6017
15	209.5405	24.7351	44	1668.4437	27.9102
16	233.7488	51.0321	45	1676.9844	18.3709
17	259.8254	31.7704	46	3175.0239	2.8953
18	267.8294	96.0835	47	3269.0100	0.4141
19	296.9097	13.8605	48	3532.7600	76.8567
20	320.7952	89.7531	49	3556.9580	206.5163
21	352.3417	159.7434	50	3603.8052	579.1147
22	374.3915	16.7501	51	3620.4580	750.6549
23	378.8351	14.6175	52	3646.0117	131.3911
24	425.1783	86.8089	53	3658.7534	728.9096

25	451.3228	51.1475	54	3852.5635	177.3444
26	477.3577	5.8584	55	3884.1592	74.6794
27	526.8414	195.4851	56	3888.5034	93.3416
28	573.8263	213.9235	57	3889.9556	58.6660
29	589.8407	16.4907			

DCE3-7H₂O

	Freq	Intensity		Freq	Intensity
1	5.9539	0.2513	39	541.7510	25.6642
2	8.3551	1.0921	40	579.0894	22.9245
3	10.1806	1.4833	41	597.4591	251.9208
4	13.8596	0.7369	42	616.4276	197.5387
5	16.0574	0.4052	43	666.6727	62.2831
6	23.6169	3.0405	44	670.2989	217.8705
7	26.9509	0.6661	45	731.3348	1.6873
8	32.5742	5.9797	46	750.7106	154.3333
9	42.1629	6.4763	47	767.2856	163.5755
10	47.1738	3.5624	48	937.2573	16.5751
11	51.8576	7.2746	49	967.1368	42.0478
12	58.5820	19.1628	50	1096.8346	79.7765
13	58.8253	3.5906	51	1427.6313	0.2994
14	66.8905	54.3639	52	1640.6722	37.6931
15	96.7966	1.8086	53	1643.7472	91.1238
16	102.0011	24.0280	54	1648.9382	41.3992
17	137.2801	75.9141	55	1657.0983	85.2257
18	140.9402	28.9839	56	1660.1617	24.1475
19	143.8329	3.4136	57	1661.4783	53.3638
20	149.2899	83.4797	58	1664.2373	58.8891
21	174.7442	49.4545	59	1681.3969	14.3997
22	188.6772	2.3577	60	3147.6226	63.1044
23	194.0034	14.5988	61	3247.5786	29.1737

24	219.5185	167.5267	62	3506.0801	463.8118
25	220.0033	99.7099	63	3601.3113	531.7265
26	229.1555	10.5624	64	3646.8516	147.3707
27	233.8222	67.8064	65	3692.3389	255.9573
28	248.2372	12.5976	66	3712.6311	834.7648
29	262.4767	56.9698	67	3715.5210	336.5645
30	286.0514	49.5884	68	3743.4031	99.4532
31	288.3539	273.1271	69	3801.1941	33.8124
32	304.3363	3.8745	70	3867.2427	158.7379
33	347.4041	101.6644	71	3883.1096	76.7551
34	376.4143	46.2029	72	3887.9136	65.2818
35	386.1018	2.3667	73	3891.5857	81.4067
36	408.5476	153.5608	74	3896.3982	112.0935
37	475.2887	9.1475	75	3902.9656	133.2712
38	512.0942	87.0204			

DCE3-10H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity
1	9.1468	0.0407	35	323.7641	89.7842	69	1428.4045	0.2237
2	15.1653	0.1020	36	347.3893	103.7090	70	1648.6804	104.8289
3	22.3985	0.0288	37	376.9170	48.7372	71	1652.7815	23.2092
4	34.5229	2.0666	38	382.6265	24.3492	72	1657.8763	63.3683
5	38.8429	1.5711	39	391.6736	19.7756	73	1660.6356	130.9256
6	43.1955	0.0831	40	431.8467	21.6366	74	1663.4515	37.0681
7	47.0287	1.5569	41	448.7879	144.2657	75	1666.4868	18.5401
8	54.3670	0.6461	42	456.4819	27.9543	76	1672.5353	100.0814
9	57.3587	1.2835	43	470.0636	32.3919	77	1680.3611	49.5447
10	58.7882	0.7105	44	474.2482	3.2758	78	1682.7925	20.1668
11	64.5022	3.3627	45	502.3788	53.2961	79	1688.0035	33.8994
12	67.0953	1.9409	46	517.5815	144.8348	80	1715.7579	40.9358
13	79.0911	2.2892	47	522.3034	53.9319	81	3141.6431	83.7999

14	87.4561	1.0880	48	543.2706	76.7417	82	3245.1628	32.1739
15	93.7932	2.2328	49	572.1892	33.1836	83	3293.5449	85.3567
16	106.2123	19.0735	50	583.6368	120.8789	84	3332.8474	972.6652
17	115.4921	6.4071	51	587.8847	249.4905	85	3435.8552	924.6338
18	126.3949	1.9808	52	597.6497	166.7575	86	3487.4316	464.3648
19	147.0962	5.8281	53	628.0277	88.8006	87	3553.1575	83.0306
20	156.3223	3.8982	54	640.2467	195.3129	88	3588.7874	408.5517
21	180.5442	5.1413	55	661.2744	100.0617	89	3612.6831	408.5548
22	186.8337	11.5327	56	719.6084	384.0484	90	3613.7698	827.6797
23	189.1943	63.2949	57	723.4294	183.4608	91	3642.0659	512.3957
24	193.8988	19.3671	58	733.7505	21.6803	92	3653.1992	175.3530
25	209.3369	23.4742	59	754.6978	24.8890	93	3682.2693	254.5579
26	225.4411	74.7508	60	756.2884	158.0319	94	3696.0693	568.3262
27	228.3607	21.6398	61	800.8955	191.1761	95	3718.7515	289.9749
28	237.1945	58.8465	62	889.0800	107.2764	96	3738.0867	302.6065
29	242.4429	13.3383	63	914.7719	12.0399	97	3757.8301	406.4028
30	249.7657	7.5469	64	931.7349	125.9359	98	3820.4353	326.1579
31	255.9748	24.3060	65	973.2745	40.6820	99	3868.4375	65.6314
32	266.0406	57.7116	66	1008.8809	44.9639	100	3880.1528	69.3019
33	296.0742	0.2981	67	1065.9456	16.3830	101	3886.5352	75.3549
34	316.6968	74.1121	68	1097.8915	77.8842	102	3892.1191	92.3805

DCE3-12H₂O

	Freq	Intensiy		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	9.4945	0.0144	31	232.8592	27.4897	61	629.5670	34.3410	91	1684.279	31.4046
2	16.2428	0.1432	32	239.0836	63.5830	62	635.1901	101.1268	92	1696.261	9.5674
3	21.2096	0.2381	33	240.0483	11.9412	63	669.0115	80.0027	93	1710.577	19.5114
4	24.2796	0.5903	34	250.1608	45.5630	64	685.9172	120.9254	94	1737.879	48.5083
5	29.6265	0.0941	35	256.4617	17.6592	65	693.3485	84.6211	95	3093.666	809.1234
6	34.2115	0.7896	36	259.8421	19.5645	66	727.4357	398.1325	96	3134.571	119.0631
7	38.4786	0.4684	37	263.4909	28.0780	67	736.7619	28.1277	97	3243.700	36.7880

8	42.2804	0.7767	38	280.5017	39.3622	68	754.2747	142.1116	98	3330.164	694.9378
9	43.3984	1.5878	39	295.3329	0.4639	69	759.1831	65.7726	99	3423.800	794.6427
10	49.5377	1.1218	40	296.0595	120.3176	70	781.8704	60.0073	100	3438.771	1300.5634
11	53.4459	1.4670	41	301.5302	78.2284	71	831.5930	193.2438	101	3473.609	591.5959
12	55.9842	2.3933	42	328.2170	70.7167	72	853.1309	75.8357	102	3502.759	177.3238
13	59.9631	0.6156	43	364.2058	56.3331	73	862.6811	97.1249	103	3514.406	714.8668
14	62.1381	1.0575	44	388.8630	7.8164	74	901.1040	205.6024	104	3546.925	326.5020
15	66.7385	0.1641	45	393.6354	8.5204	75	912.2628	144.7441	105	3562.980	508.7250
16	85.5004	3.0435	46	399.8289	79.5634	76	957.6990	30.3482	106	3575.697	501.9216
17	89.3363	7.4435	47	418.9732	35.6183	77	980.6107	51.0477	107	3587.604	524.2725
18	96.7143	3.2378	48	437.2518	23.8455	78	1000.6635	37.9929	108	3620.008	457.9661
19	101.4149	3.3455	49	443.4008	99.9249	79	1100.1357	80.1197	109	3642.321	510.3749
20	114.8362	2.5754	50	470.6229	7.0799	80	1131.5015	34.3295	110	3651.401	397.9384
21	141.7055	16.3599	51	482.3456	112.5876	81	1432.3879	0.0687	111	3679.465	604.7204
22	149.9543	10.5793	52	488.4903	8.4732	82	1651.6371	60.6559	112	3720.119	281.5951
23	161.9378	0.6152	53	504.3150	71.1135	83	1659.6854	23.0544	113	3743.910	449.1257
24	173.9769	11.4731	54	530.7715	15.0048	84	1661.3115	181.9385	114	3784.891	378.5466
25	180.8097	0.9594	55	541.0256	231.1122	85	1661.4343	71.0525	115	3865.955	60.3691
26	184.7542	19.3951	56	558.8835	50.7361	86	1663.5835	38.8562	116	3878.423	61.1747
27	191.7454	13.0381	57	577.5834	60.4620	87	1671.3387	57.9307	117	3879.098	80.8708
28	205.1717	38.7266	58	582.8591	41.1510	88	1671.9078	17.9197	118	3883.395	91.9991
29	209.5044	68.1982	59	594.7985	24.4383	89	1677.4600	119.1390	119	3884.502	60.6056
30	218.9593	76.1791	60	607.5010	193.6091	90	1681.7238	5.9015	120	3885.138	67.0213

DCE3-16H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	7.5382	0.1616	40	207.7714	4.3575	79	608.0788	139.8517	118	1708.3778	34.4426
2	14.1161	0.2493	41	212.4427	81.3873	80	619.7967	154.6161	119	1712.9620	149.7770
3	18.9454	0.2536	42	225.0406	28.7076	81	635.8464	39.5761	120	1714.0919	7.6187
4	26.3117	0.7269	43	228.0092	119.7071	82	645.7945	112.8187	121	1723.7004	80.6227
5	29.0081	1.6382	44	230.7283	40.5983	83	666.0840	123.8659	122	1732.7197	50.7344

6	31.1074	0.7599	45	234.2730	47.7636	84	679.9880	51.3203	123	3157.7515	34.3245
7	33.8484	0.7214	46	244.2201	11.2074	85	703.3316	452.5327	124	3256.0293	17.4008
8	41.2007	0.9091	47	248.7295	22.1334	86	716.4183	251.4389	125	3369.8491	708.8316
9	43.4375	1.3895	48	259.4335	37.8093	87	719.1521	90.5128	126	3374.6233	628.3030
10	46.7437	2.1890	49	263.4322	103.3029	88	723.4561	12.7332	127	3460.9741	169.7300
11	49.9953	4.6068	50	267.0434	61.4167	89	741.0200	16.0872	128	3476.9158	733.4326
12	52.0432	3.5212	51	270.3144	9.6692	90	745.6562	382.7442	129	3482.2375	367.5581
13	58.1342	2.6440	52	276.6578	5.8827	91	758.0786	81.5338	130	3485.3416	1138.9843
14	61.4123	1.3149	53	281.3513	24.0960	92	762.3755	179.8690	131	3501.5579	440.3885
15	63.2111	1.0346	54	285.9197	3.5134	93	782.2619	28.5119	132	3509.8425	253.5810
16	69.5480	4.5372	55	296.2382	0.2659	94	813.7382	166.0679	133	3531.0613	1228.5431
17	71.7152	3.4478	56	340.1633	73.9054	95	833.1075	111.8064	134	3539.5613	57.1371
18	76.4607	1.9536	57	383.7032	1.0068	96	854.8286	93.9235	135	3545.3044	971.0558
19	79.4460	1.6352	58	387.8911	16.6430	97	863.1603	76.2776	136	3568.8015	708.5368
20	81.9452	1.1286	59	397.0005	28.3216	98	896.2363	156.2888	137	3595.1787	30.4265
21	86.3048	3.7911	60	410.0255	28.0132	99	920.7862	89.2240	138	3603.6899	503.2300
22	92.1281	1.6701	61	416.2413	108.6447	100	947.8597	42.3057	139	3612.6838	185.5446
23	94.0907	1.0642	62	433.6966	76.3902	101	950.4993	64.3812	140	3626.2727	218.1200
24	100.3228	1.6235	63	439.3990	55.8498	102	965.7202	7.5830	141	3653.5442	68.0948
25	106.0561	2.5812	64	446.5057	6.2808	103	1054.1469	44.4745	142	3658.8369	1002.3667
26	114.1121	21.1039	65	453.1321	38.6632	104	1099.8042	84.1580	143	3673.5266	732.2760
27	118.1168	1.1285	66	475.3953	10.5881	105	1423.6923	0.0313	144	3684.1985	668.6685
28	135.3902	9.3005	67	476.5310	21.7790	106	1650.3639	16.7686	145	3697.1245	264.0013
29	139.0490	13.9095	68	496.9740	41.5340	107	1652.0782	35.8520	146	3702.1887	141.5253
30	151.9454	20.8578	69	506.8111	45.1047	108	1654.5588	212.2747	147	3725.7024	379.9340
31	153.1950	2.4162	70	516.9810	46.2710	109	1662.1840	3.6996	148	3781.2583	194.4120
32	160.6088	5.0534	71	524.5484	69.2934	110	1662.7073	123.3712	149	3805.3113	258.8992
33	166.7258	6.0917	72	537.3280	122.6631	111	1673.0887	53.5611	150	3814.7388	151.3740
34	170.4139	18.7592	73	550.4639	82.1011	112	1675.0426	27.9911	151	3876.7671	73.3987
35	181.1804	12.3165	74	556.6774	78.1284	113	1678.0696	23.1687	152	3879.2397	74.2273
36	181.3374	84.5333	75	571.8426	86.4591	114	1684.4115	56.9174	153	3879.9622	84.3359
37	192.5690	1.0803	76	586.7157	11.7567	115	1691.0872	97.2199	154	3882.8560	89.7698

38	197.7817	5.4259	77	587.7721	109.9115	116	1695.9346	11.7491	155	3886.0652	99.6842
39	202.1937	55.2798	78	596.8827	5.5272	117	1699.6606	83.5670	156	3889.2158	65.4820

DCE3-24H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	11.7913	0.6117	58	218.5661	11.8879	115	631.1448	129.2673	172	1714.6991	84.5954
2	13.6497	0.9399	59	225.1214	15.1878	116	636.7974	28.9589	173	1717.9570	32.0229
3	18.2666	0.1186	60	231.6407	16.6332	117	650.1999	127.7628	174	1729.6962	12.6252
4	21.6227	0.7873	61	234.1473	14.3248	118	658.5824	144.7746	175	1737.9960	50.4624
5	24.7476	0.5709	62	241.3126	14.3345	119	685.2564	42.8422	176	1740.8508	7.1371
6	28.4000	0.8460	63	245.6463	35.7192	120	688.8473	60.3139	177	1748.3604	66.2045
7	31.7638	2.1956	64	252.1764	3.5080	121	697.0157	475.8979	178	1754.6636	34.7528
8	32.3062	3.7872	65	253.6819	14.1307	122	698.5295	38.6878	179	3172.9998	2.8321
9	37.9369	0.7618	66	263.2698	28.4403	123	701.1191	86.0760	180	3245.4866	1044.1869
10	39.5187	1.3408	67	264.1768	59.8443	124	709.6217	60.8012	181	3266.6116	0.3412
11	42.3154	1.2695	68	271.4820	18.0445	125	719.5878	315.3238	182	3270.6272	1952.2821
12	45.3319	3.2745	69	279.1881	101.7600	126	730.5628	116.4245	183	3276.4473	694.7397
13	46.4003	1.0305	70	281.5012	7.2917	127	742.0702	155.2947	184	3312.0503	469.9745
14	47.3438	0.6038	71	287.0065	22.0073	128	749.8297	368.4292	185	3335.5864	592.6318
15	50.4831	0.9371	72	288.6769	19.6139	129	760.0056	75.8040	186	3361.1731	1006.5923
16	51.3710	0.7990	73	296.1435	36.2770	130	775.8617	528.8269	187	3389.6392	1471.7584
17	54.7779	0.2550	74	300.6464	34.8529	131	785.6012	45.2416	188	3393.6099	1298.4703
18	59.6359	0.7333	75	302.0701	55.5842	132	798.9783	34.1258	189	3398.3052	133.1840
19	59.9281	2.2202	76	304.0915	9.6934	133	823.0345	16.6104	190	3434.0957	1041.6833
20	62.1926	1.7114	77	307.6569	12.2224	134	826.4092	112.9907	191	3448.4309	338.8914
21	64.9101	0.6503	78	319.4866	16.7120	135	832.7929	69.3505	192	3453.5874	164.0828
22	65.1282	0.3756	79	325.5408	18.4109	136	833.6423	59.3996	193	3474.0137	538.2192
23	68.9142	1.2911	80	337.6497	90.9540	137	842.9668	46.5686	194	3507.9482	537.6008
24	70.4886	0.7426	81	356.1200	47.9446	138	852.2265	71.6105	195	3514.0974	940.7175
25	72.9163	3.3204	82	360.7352	19.9035	139	858.1414	68.9901	196	3530.5388	634.7401
26	75.8933	0.6428	83	363.7512	59.4277	140	863.7583	135.6422	197	3539.7073	122.4482

27	77.1522	0.3422	84	370.5683	91.4113	141	908.1644	80.4888	198	3545.2451	379.1388
28	78.8149	0.6990	85	378.0200	3.2733	142	913.5247	39.2180	199	3559.9399	487.7672
29	81.9578	0.7588	86	390.4434	9.6167	143	925.1398	113.8379	200	3561.8711	376.7936
30	83.1717	2.6289	87	413.7636	65.0223	144	928.6723	148.6952	201	3575.5984	1376.0902
31	89.2306	3.2081	88	427.6165	0.3900	145	932.3152	87.1411	202	3607.1182	69.4651
32	89.9734	0.1301	89	433.4634	31.2254	146	937.8339	40.4262	203	3609.2354	177.2370
33	93.5523	1.4638	90	436.8894	9.6271	147	952.2962	112.1861	204	3615.2991	362.6339
34	97.9609	1.3852	91	444.0209	18.5233	148	967.1094	75.4005	205	3623.2334	865.6523
35	103.0811	2.4083	92	451.6406	24.9744	149	984.5083	65.6572	206	3633.8145	275.8577
36	104.4721	1.5523	93	452.6143	5.2665	150	1002.5807	44.9185	207	3635.0037	166.5528
37	105.8725	1.9329	94	462.6473	39.7927	151	1029.2040	155.1022	208	3647.6482	339.5483
38	114.5659	1.9389	95	472.2422	83.9306	152	1099.4918	77.8431	209	3660.1704	566.7128
39	121.2757	0.9889	96	477.3897	14.7608	153	1410.7415	0.0263	210	3669.5679	166.9971
40	127.1101	6.5379	97	481.9627	59.3127	154	1654.6353	111.6532	211	3679.1052	535.4677
41	132.0941	13.7121	98	483.7107	25.4820	155	1657.4552	41.9323	212	3712.9871	128.5619
42	137.4566	3.5739	99	498.2203	13.5066	156	1659.5983	82.5742	213	3714.0718	627.5738
43	139.2837	5.1796	100	506.7571	24.8746	157	1661.1443	122.6206	214	3721.3765	314.4246
44	150.6929	4.8314	101	508.7853	13.4071	158	1667.7897	193.0842	215	3743.9768	230.6808
45	158.5602	7.8977	102	517.4789	37.6716	159	1670.0573	111.4997	216	3764.8005	237.5326
46	162.0452	13.2173	103	524.3491	96.7158	160	1678.4193	48.3697	217	3780.0811	322.1679
47	169.7084	8.8294	104	534.1991	3.3762	161	1679.0806	159.8383	218	3832.6184	160.9853
48	172.4873	8.2638	105	545.2876	16.2326	162	1679.6323	62.5565	219	3838.1541	201.7500
49	179.2371	4.2070	106	551.6253	95.3819	163	1681.8043	49.3873	220	3856.2305	82.6712
50	183.5890	7.7074	107	562.1551	39.0797	164	1687.0134	28.8999	221	3859.2522	54.6849
51	185.2880	1.3859	108	566.9208	73.2842	165	1687.5587	13.5319	222	3868.2732	71.7968
52	191.5066	9.7020	109	573.2184	162.7473	166	1692.8230	3.5843	223	3874.3599	62.9227
53	192.9611	48.0602	110	583.4018	12.1058	167	1699.1360	21.6640	224	3874.7832	79.5158
54	198.0621	22.0638	111	588.8996	12.7215	168	1701.5815	98.2778	225	3876.8882	67.0817
55	201.6273	29.8893	112	604.8765	110.8999	169	1707.1614	102.4499	226	3876.9468	82.3761
56	212.5909	33.0216	113	614.1916	109.6640	170	1709.2245	35.3474	227	3879.9272	51.6682
57	213.3215	15.3478	114	621.9592	60.9784	171	1711.3286	30.4253	228	3892.8630	74.2447

DCE3-39H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	9.9203	0.0198	92	222.7933	76.4260	183	667.3229	76.2156	274	1717.0247	42.2724
2	15.1821	0.3615	93	228.2493	22.8420	184	670.3706	198.6860	275	1719.8878	15.5254
3	20.3734	0.2678	94	229.8310	63.5077	185	675.4033	21.1483	276	1726.2780	10.8490
4	22.7234	1.4169	95	233.2831	54.9674	186	680.3749	141.0634	277	1734.0931	56.9953
5	25.3365	1.3343	96	235.6768	32.9845	187	688.3200	9.6924	278	1736.8395	74.9080
6	26.1462	3.4546	97	237.9788	69.3296	188	689.4553	173.5434	279	1737.5092	104.3501
7	27.3378	0.3900	98	238.7728	57.6106	189	695.9856	101.1967	280	1741.1025	38.6437
8	27.9277	2.6076	99	244.4720	49.1462	190	711.2131	59.0509	281	1744.5533	146.6691
9	30.1318	1.1616	100	247.3852	3.6245	191	719.9500	139.2905	282	1746.4261	36.6684
10	32.6521	0.3743	101	250.5723	31.4913	192	722.5219	213.8994	283	1759.5977	67.5681
11	34.5941	0.4837	102	250.8046	16.9799	193	725.6652	62.8519	284	3139.7998	1177.0535
12	37.1047	0.7702	103	255.9089	41.3518	194	738.9367	143.4464	285	3148.9355	31.1675
13	38.4498	0.4943	104	259.1704	69.2874	195	739.2920	77.6861	286	3195.4924	1239.2686
14	39.5223	0.0900	105	261.6831	8.0022	196	743.4784	22.6679	287	3243.1003	1297.9993
15	40.2695	0.7943	106	263.3864	5.4097	197	753.7105	226.8270	288	3252.1748	7.4764
16	42.2127	0.4884	107	269.2845	15.3186	198	758.6912	101.5449	289	3290.3269	290.9673
17	43.4772	0.4593	108	270.5005	32.3581	199	761.9810	154.1975	290	3305.1765	456.1379
18	44.5787	0.5323	109	272.6454	27.7186	200	762.8237	128.0269	291	3307.0442	525.3239
19	46.1006	1.5600	110	274.4631	86.1639	201	774.8222	310.8230	292	3309.0874	183.9514
20	47.2966	0.7456	111	274.9025	20.1651	202	776.2347	52.7208	293	3313.0776	581.5213
21	49.5184	0.7141	112	277.0470	8.3939	203	779.6534	40.9433	294	3335.9187	1173.9858
22	51.3626	1.2025	113	278.8469	33.2276	204	781.4986	248.2141	295	3344.1135	1949.9590
23	52.5957	1.2617	114	280.8321	38.3669	205	788.9577	183.1545	296	3350.4487	421.0424
24	56.3879	0.9603	115	284.2063	36.6917	206	795.2469	69.4048	297	3366.2720	246.1663
25	57.8675	2.7124	116	290.5541	25.7873	207	798.8075	171.0587	298	3375.7969	681.7705
26	58.3811	1.2577	117	293.8369	8.7232	208	805.2890	76.5833	299	3383.8679	890.5404
27	59.2033	0.4841	118	297.6487	4.3309	209	810.7459	144.4032	300	3385.9692	916.3920
28	60.3889	0.6146	119	301.2990	98.9624	210	816.0935	102.3474	301	3392.3826	937.1922
29	60.8797	2.7847	120	305.6963	7.6916	211	827.5919	166.0473	302	3401.5105	795.2829

30	62.6209	1.9799	121	311.0152	5.9926	212	836.7627	22.8972	303	3411.9619	1078.7316
31	63.2293	1.3217	122	316.7290	6.4751	213	842.3478	55.3546	304	3413.1304	1037.4230
32	65.5589	2.3618	123	318.6600	43.4246	214	858.9014	64.9001	305	3431.4524	1582.1053
33	67.8643	1.7410	124	320.1099	30.9322	215	865.8009	43.1563	306	3438.1121	808.6677
34	68.9137	0.4890	125	321.3437	54.6803	216	873.7151	98.3366	307	3444.8782	274.3397
35	70.5711	1.3401	126	325.4727	24.6069	217	875.7303	293.9303	308	3451.8899	469.2574
36	71.4953	0.2985	127	327.5700	55.5775	218	884.2306	12.0914	309	3454.5691	1515.3030
37	74.1567	0.7480	128	328.7261	19.2473	219	890.7460	142.7649	310	3467.7710	841.0200
38	74.7727	0.4642	129	331.8100	62.3958	220	893.7756	46.4722	311	3472.4890	1220.3640
39	75.9829	1.0251	130	342.8467	72.3619	221	897.1044	2.2267	312	3502.8147	1217.8114
40	76.4101	0.8193	131	349.4531	128.9087	222	901.9343	182.9968	313	3505.6943	547.6657
41	77.4329	7.7124	132	367.8577	97.9353	223	904.3044	295.7159	314	3511.0151	500.1123
42	79.3519	2.1870	133	384.7183	2.9367	224	910.2894	63.4763	315	3514.3022	467.5083
43	80.8562	2.5689	134	409.8892	103.0480	225	924.0455	78.3487	316	3519.0562	190.9964
44	82.6048	1.8495	135	411.7055	35.0034	226	935.9002	308.5950	317	3523.6328	155.7525
45	85.1112	0.5012	136	412.9862	44.2298	227	942.7121	33.9966	318	3525.2930	497.5352
46	87.4887	2.6036	137	417.9840	32.2001	228	957.7351	65.0963	319	3529.5273	82.4947
47	91.1954	6.4601	138	420.9628	23.8397	229	959.7031	51.6113	320	3547.6267	693.5625
48	92.1019	3.5477	139	434.1038	6.5513	230	965.2922	28.0144	321	3558.4773	720.4326
49	93.1859	3.3632	140	434.8032	60.6851	231	966.3891	76.8092	322	3560.4294	477.8546
50	94.8445	0.6334	141	452.4086	10.9263	232	987.5257	143.3859	323	3565.5823	345.1927
51	97.9560	2.2787	142	460.8407	38.1825	233	1003.7711	193.7985	324	3571.3315	282.6767
52	100.0340	0.5187	143	463.4586	20.5185	234	1005.5034	17.2034	325	3571.7878	254.0376
53	102.7487	4.7338	144	464.5109	34.1794	235	1010.4217	37.9504	326	3579.4895	719.7113
54	107.7898	1.8601	145	477.8451	0.9424	236	1014.7938	6.0841	327	3591.4470	190.5854
55	113.1807	2.2606	146	483.5553	26.8512	237	1024.2238	78.4428	328	3591.8979	177.8791
56	114.8617	1.7395	147	484.3712	65.1230	238	1037.3584	41.0109	329	3592.7014	122.2034
57	116.2948	25.6754	148	497.6921	167.0247	239	1056.2217	113.3318	330	3598.4802	347.3890
58	122.0517	6.3925	149	501.5432	32.3686	240	1076.4895	43.2529	331	3599.9209	577.8492
59	124.6395	5.3943	150	507.0351	175.2076	241	1087.9399	56.6368	332	3606.4983	668.0753
60	130.0741	8.2840	151	512.6168	27.2657	242	1108.1487	98.4397	333	3611.9622	1318.5083
61	134.0459	6.1068	152	515.9907	17.2398	243	1420.1891	0.7911	334	3624.4709	341.0939

62	135.5102	2.2825	153	519.0428	17.9462	244	1644.4811	76.4405	335	3624.7444	108.8955
63	136.4836	1.6640	154	524.5452	7.4052	245	1646.0122	64.0328	336	3625.2588	852.7573
64	144.7777	5.2214	155	530.5343	112.8969	246	1651.5762	128.8909	337	3648.7224	562.2271
65	148.3193	4.9057	156	535.8325	187.2016	247	1651.9489	50.0604	338	3672.3916	165.1983
66	153.9876	11.0996	157	538.9730	27.9518	248	1657.1526	99.4089	339	3694.4429	868.7468
67	160.1262	5.8959	158	544.9900	9.0831	249	1658.2690	68.4259	340	3697.5618	458.9059
68	160.5603	16.3228	159	550.9331	10.7279	250	1659.7273	86.9703	341	3702.6887	528.0683
69	164.6297	5.2634	160	562.1951	15.5032	251	1660.2279	53.7042	342	3705.8225	269.9065
70	166.9909	10.9657	161	568.6271	48.8906	252	1668.0018	80.3025	343	3712.6587	373.3031
71	169.2979	5.0766	162	572.8349	32.2146	253	1671.5952	80.4423	344	3723.5764	258.5784
72	169.7333	18.2165	163	578.7179	23.3164	254	1673.0181	58.0811	345	3724.0996	427.9402
73	174.1753	13.0910	164	583.8700	76.7135	255	1673.7496	48.1538	346	3729.1765	241.0450
74	176.0798	9.0365	165	587.3920	16.6931	256	1679.6625	50.1768	347	3749.7969	455.0653
75	177.8390	24.6685	166	593.7925	44.0997	257	1682.0114	18.8350	348	3752.4924	304.3919
76	179.6362	6.2263	167	594.7740	40.8826	258	1683.0042	85.4251	349	3763.0291	243.8485
77	184.9875	14.5487	168	596.5790	109.9118	259	1684.8184	36.3301	350	3835.9297	94.7922
78	185.2242	3.8171	169	600.5199	180.1906	260	1687.7332	29.0278	351	3866.1697	51.3108
79	189.5300	11.3419	170	605.6579	24.5310	261	1687.9893	16.8502	352	3868.7134	103.2051
80	194.8753	4.7605	171	608.6695	96.6588	262	1690.9218	36.9890	353	3869.4805	54.9222
81	195.5288	30.9258	172	616.2505	69.4687	263	1691.4320	69.2347	354	3869.7378	61.0973
82	198.0252	35.4818	173	620.7074	3.3401	264	1696.1935	11.3703	355	3870.9231	52.9580
83	199.6577	25.8155	174	633.1676	103.3040	265	1696.5981	57.5293	356	3873.1311	90.9522
84	202.4144	35.3184	175	640.7584	69.1706	266	1697.6195	18.5796	357	3873.4990	67.2080
85	206.6161	34.2669	176	641.8227	37.8344	267	1699.7671	44.3357	358	3879.3684	76.9795
86	207.4804	12.7636	177	643.7869	29.3437	268	1703.3444	13.4341	359	3879.9209	75.6743
87	208.8511	5.2369	178	649.1763	31.2018	269	1705.4222	61.5418	360	3880.3870	76.4340
88	212.4951	34.3988	179	652.7110	87.8754	270	1706.3893	8.3784	361	3885.0105	85.3243
89	216.2321	23.5166	180	654.8997	106.3613	271	1706.7596	27.4368	362	3888.6094	56.4540
90	218.5933	62.4370	181	657.6659	8.3631	272	1711.6508	27.3679	363	3890.4077	101.2942
91	221.0818	14.5442	182	662.3635	103.9946	273	1714.8469	105.2116			

Appendix 6

Table 7. IR Intensity as a function of frequency (VC-nH₂O)

Freq (1/cm) IR Intensity (KM/Mol)

VC		
	Freq	Intensity
1	398.8904	0.2318
2	634.4023	14.9054
3	698.5957	47.0773
4	935.9978	37.3290
5	975.8162	30.4232
6	1045.2053	16.7202
7	1306.9344	11.9193
8	1411.7913	10.5155
9	1662.5070	63.3659
10	3156.8633	0.0066
11	3217.4026	3.4702
12	3248.3340	1.9335

VC-2H ₂ O					
	Freq	Intensity		Freq	Intensity
1	27.8078	1.9395	16	961.2254	0.0114
2	53.8665	0.5522	17	1009.4229	59.9937
3	93.3366	6.9315	18	1044.4399	15.7014
4	105.6815	16.8662	19	1304.2761	14.6674
5	113.0928	4.7908	20	1426.5189	11.0843
6	160.8635	69.0792	21	1643.8304	63.7578
7	196.9382	12.2754	22	1661.1471	79.8550
8	207.9594	136.2970	23	1665.6317	5.7235
9	240.4490	62.8839	24	3136.8940	28.8924
10	351.0895	98.1176	25	3219.2993	12.7590

11	406.3114	3.6388	26	3234.8672	11.6766
12	469.4304	85.4723	27	3642.8633	344.1757
13	639.6852	12.7835	28	3744.3325	221.2061
14	677.8058	52.0544	29	3885.8164	133.4169
15	721.7078	132.4768	30	3889.8447	72.6158

VC-5H₂O

	Freq	Intensity		Freq	Intensity
1	16.8828	0.7647	30	683.2694	9.4990
2	21.3202	0.2775	31	716.4437	130.6119
3	22.3848	0.4466	32	724.6813	182.1596
4	33.6331	0.9554	33	828.4807	76.1629
5	37.9647	0.1961	34	987.7747	20.3393
6	49.1605	2.6238	35	1044.4918	34.6798
7	60.6740	2.6333	36	1052.2657	41.7727
8	90.4381	2.8900	37	1339.7467	11.1554
9	103.5872	21.1242	38	1423.0342	9.9286
10	113.2344	1.3957	39	1643.7451	66.2207
11	128.0098	23.9545	40	1646.4592	14.9203
12	136.1167	89.6909	41	1652.2667	117.0920
13	177.0802	42.4595	42	1662.9601	74.5864
14	183.2673	43.4024	43	1664.1278	18.0472
15	192.3511	62.8059	44	1682.1534	15.4026
16	197.4484	10.0733	45	3130.6963	44.4493
17	202.6360	48.2347	46	3178.3081	78.5071
18	216.7637	130.3959	47	3224.5994	31.7947
19	228.9653	6.3098	48	3544.7107	560.2959
20	245.0202	57.8364	49	3592.9976	572.0949
21	267.2228	140.0205	50	3638.7769	344.0896
22	285.1546	44.6557	51	3727.3430	286.7211
23	350.5630	100.9296	52	3742.4075	211.1438

24	390.1092	41.0760	53	3879.8799	133.4727
25	406.3389	5.8329	54	3883.1428	102.7359
26	419.5105	64.1243	55	3884.4065	100.7046
27	463.7964	84.8917	56	3887.8413	65.4718
28	482.3580	78.9186	57	3890.2334	73.8997
29	665.6063	59.9213			

VC-7H₂O

	Freq	Intensity		Freq	Intensity
1	8.1439	0.9276	39	684.7212	41.3014
2	17.1723	0.2561	40	733.9141	100.8309
3	21.7964	2.8673	41	790.1973	113.1550
4	26.0592	1.7762	42	865.5562	130.2320
5	35.3040	0.5390	43	889.1348	212.2836
6	39.7086	0.7459	44	940.6830	83.5311
7	46.6880	2.6754	45	946.1601	43.4423
8	49.6925	0.5608	46	1003.5384	66.5554
9	52.8363	1.9448	47	1011.7643	27.0380
10	64.9174	2.3558	48	1041.5643	18.6151
11	77.7064	7.0458	49	1317.7318	9.2470
12	80.1445	7.1848	50	1406.2375	9.3182
13	87.6523	2.9310	51	1653.4980	65.0499
14	125.9077	84.9214	52	1659.2784	40.5881
15	142.5147	11.0332	53	1660.8375	71.5869
16	156.6690	9.4489	54	1669.6333	16.8908
17	177.1179	5.7783	55	1679.8114	96.7323
18	210.1517	25.7064	56	1692.6744	57.5479
19	219.3763	80.1046	57	1704.0415	13.6851
20	239.5458	10.2421	58	1718.9860	18.8033
21	250.5680	143.3099	59	3151.9729	0.3952
22	272.3056	50.5950	60	3212.7502	19.3275

23	284.6718	8.3804	61	3244.8689	8.5003
24	286.6213	188.6929	62	3250.3384	736.1895
25	297.9461	21.6664	63	3360.1829	1010.8732
26	311.2301	141.8360	64	3400.0791	1309.3767
27	346.5495	209.1672	65	3450.4272	1459.1879
28	390.5308	52.8775	66	3485.9751	360.9905
29	397.6151	12.2949	67	3504.3599	377.7935
30	427.8570	2.3825	68	3642.4011	255.4891
31	440.3808	34.7068	69	3791.0110	172.8778
32	447.0306	44.9950	70	3832.3833	200.6948
33	466.1496	17.0241	71	3879.1853	78.9179
34	493.1740	29.1383	72	3880.9187	67.8337
35	561.7535	36.7146	73	3881.1108	66.1698
36	604.8960	49.9993	74	3884.0735	65.5489
37	653.1181	53.0712	75	3893.2976	76.5739
38	681.0603	5.2093			

VC-10H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity
1	6.3650	0.0372	35	293.4918	34.1952	69	1650.3499	92.2967
2	13.6370	0.3957	36	303.2905	12.0546	70	1651.1385	47.4581
3	16.5596	0.7611	37	355.7037	51.2366	71	1653.7954	45.6372
4	18.4077	0.2967	38	367.2906	64.9609	72	1656.2025	52.0050
5	25.4196	0.5006	39	377.8559	29.1488	73	1657.5614	54.2368
6	28.8588	4.6766	40	402.7644	41.4503	74	1660.5587	113.4725
7	30.4878	0.4908	41	404.8024	31.4065	75	1665.8792	28.8387
8	34.6443	0.6198	42	407.0579	23.1507	76	1676.9760	34.2817
9	39.4048	0.7619	43	428.7698	12.8238	77	1681.8053	45.1226
10	44.8016	1.6994	44	451.8495	185.4124	78	1684.4817	20.7303
11	47.7649	0.8643	45	466.7591	22.6997	79	1701.3059	13.6827
12	51.1318	0.1377	46	535.9644	128.0361	80	3130.8154	52.3520

13	65.5079	1.3599	47	572.2259	159.7544	81	3203.3376	870.4765
14	77.0944	7.4058	48	582.6102	142.0806	82	3207.8840	92.8922
15	89.1308	3.8923	49	587.1495	408.9212	83	3229.0271	20.1294
16	91.2852	4.7204	50	597.7765	323.5448	84	3388.3518	345.3644
17	112.4403	4.1245	51	612.6992	140.0836	85	3413.6255	1417.9703
18	128.6737	1.1150	52	639.0627	15.6705	86	3483.1499	258.5327
19	138.5453	5.1949	53	658.1164	25.6945	87	3552.7219	644.8201
20	155.1001	17.4335	54	667.7406	208.8961	88	3607.3860	299.9214
21	162.8158	41.2795	55	697.6526	70.5510	89	3629.8164	816.4884
22	167.4169	16.1497	56	701.0280	33.7958	90	3642.5618	250.9449
23	181.3598	10.5307	57	725.8607	154.7952	91	3666.4443	156.3331
24	190.9306	34.5176	58	757.0182	202.6509	92	3673.9768	953.1155
25	197.8428	64.6437	59	798.2612	156.1450	93	3694.0920	166.1734
26	204.4630	39.9883	60	931.7868	19.3081	94	3701.3628	158.2711
27	206.1605	16.6993	61	941.1091	93.0239	95	3737.7129	277.7703
28	212.7663	49.9320	62	966.7439	8.6515	96	3807.6990	371.7693
29	227.8304	91.5536	63	993.5541	43.3060	97	3873.2375	68.9149
30	236.8904	103.1490	64	1012.9697	58.5215	98	3875.7668	93.3827
31	244.2563	84.7975	65	1051.9095	22.4297	99	3884.2964	65.8462
32	254.0758	44.8777	66	1085.2606	41.3602	100	3885.3853	80.5861
33	281.3275	42.6439	67	1309.6063	11.5671	101	3887.0852	77.7660
34	289.7904	18.0296	68	1426.5168	14.4185	102	3892.4944	91.3917

VC-16H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	11.7088	0.2745	40	208.0881	3.6857	79	638.4799	18.5143	118	1712.8367	131.0833
2	18.6626	0.1043	41	213.3697	79.8632	80	646.4151	135.8282	119	1714.5874	27.9857
3	21.4397	0.4669	42	223.4639	27.4892	81	669.8126	118.9858	120	1723.6346	76.4341
4	28.2943	1.6718	43	232.2329	76.7960	82	677.7682	57.4518	121	1733.1670	54.9469
5	30.4804	0.4697	44	236.2615	49.9340	83	686.6821	54.0775	122	3144.9985	11.5600
6	35.1164	0.2253	45	237.2252	53.2444	84	701.9791	450.6993	123	3222.1555	4.7373

7	41.0535	2.1353	46	245.2432	12.1358	85	714.7890	260.6385	124	3240.3130	8.6443
8	44.2550	1.5843	47	250.0443	46.2726	86	720.5930	74.6539	125	3373.9744	689.9679
9	47.9767	2.3302	48	256.0805	77.3033	87	743.0177	42.3361	126	3383.2036	586.7544
10	52.4905	0.8035	49	261.3065	29.6236	88	746.4799	397.8150	127	3462.6409	176.9600
11	54.9031	3.4927	50	268.1213	76.4459	89	765.3102	107.6629	128	3481.5247	536.2627
12	57.2206	2.8113	51	269.9726	20.8908	90	786.6040	16.3260	129	3485.4038	451.9256
13	62.4957	0.1749	52	276.7299	12.3660	91	815.5852	171.3176	130	3489.9749	1547.7166
14	63.2478	4.5686	53	283.8729	16.3292	92	833.0524	105.3698	131	3499.1567	389.3348
15	68.8462	3.1222	54	286.0460	36.3032	93	853.4687	117.9960	132	3505.5876	29.4795
16	72.6217	3.8112	55	345.7164	72.2344	94	861.1588	61.6718	133	3532.5483	1295.4592
17	77.1591	2.2303	56	388.1989	10.3746	95	894.4707	145.3500	134	3543.1187	208.2689
18	79.8159	0.8006	57	399.4591	34.3038	96	918.4383	95.4988	135	3550.0078	674.3374
19	84.6447	1.7762	58	403.0506	0.1395	97	947.2593	55.1912	136	3567.7231	738.9573
20	85.7689	3.6679	59	414.2935	46.7009	98	955.8953	3.9762	137	3589.7900	29.2670
21	92.0331	1.0543	60	419.8452	81.2783	99	960.7454	6.8647	138	3602.6155	555.0489
22	95.5774	1.0139	61	438.3073	13.6217	100	993.1268	65.7966	139	3609.7146	130.7643
23	99.7827	2.0356	62	440.9974	127.7502	101	1046.7773	15.2138	140	3626.2136	186.3027
24	102.6738	4.1196	63	449.9340	38.7591	102	1051.9366	41.1622	141	3650.8367	102.5521
25	108.3330	1.9209	64	464.4822	8.0438	103	1305.5519	13.3540	142	3658.5737	1074.1437
26	116.7569	24.9200	65	475.2477	17.1824	104	1423.8422	12.3032	143	3669.8586	700.1353
27	119.6178	0.8716	66	499.6794	41.4651	105	1650.2657	12.5553	144	3687.6582	678.2792
28	136.3550	9.2949	67	507.4085	36.3552	106	1652.3262	24.0796	145	3691.3818	259.5964
29	141.3948	13.8590	68	516.2152	36.5005	107	1654.1000	225.7037	146	3704.3191	100.9376
30	152.2772	18.8960	69	525.8567	87.0658	108	1662.2385	44.6555	147	3722.9070	413.0677
31	153.8460	3.0979	70	535.2659	119.7417	109	1664.6248	57.8664	148	3779.6162	191.4052
32	161.1716	2.6666	71	550.6357	51.0497	110	1673.3866	45.8268	149	3784.1992	298.9432
33	166.8759	3.4563	72	557.6801	71.2016	111	1675.3119	28.0462	150	3808.2532	167.9642
34	170.6915	20.2834	73	571.1167	106.6223	112	1677.7513	25.4029	151	3877.7461	65.5193
35	178.9755	79.1057	74	586.8070	104.1930	113	1684.6501	55.4576	152	3878.6953	86.8120
36	182.1044	11.1914	75	598.6909	6.4345	114	1691.2975	105.2099	153	3880.3169	79.5994
37	192.8304	0.6791	76	609.0206	120.9329	115	1695.6697	10.4564	154	3883.6858	87.0344
38	196.7692	5.4522	77	619.8337	163.8630	116	1699.8907	81.0216	155	3885.7896	96.8434

39	201.8002	53.9963	78	634.9594	41.7627	117	1709.1654	32.9703	156	3889.6965	64.9699
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VC-24H₂O

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	11.7942	0.9626	58	214.9064	2.8939	115	652.5078	136.6562	172	1722.5192	74.9369
2	12.7834	0.8391	59	227.0460	21.2976	116	663.5469	170.8127	173	1731.3782	28.0390
3	19.9266	0.1490	60	233.0845	18.5179	117	675.2043	35.4991	174	1736.4164	30.7403
4	23.8212	0.1602	61	236.1012	25.2583	118	681.6546	33.0634	175	1738.9027	24.3751
5	27.1806	2.5443	62	242.6826	4.7515	119	686.6740	35.8345	176	1747.1825	59.5123
6	31.6925	1.9532	63	246.0291	20.4413	120	689.7541	107.5219	177	1750.2255	18.5090
7	33.9091	0.4647	64	246.9026	81.4678	121	698.7880	360.1459	178	3150.6299	20.2612
8	35.8069	2.6815	65	253.7133	35.9781	122	700.1669	48.8698	179	3222.7815	2.2768
9	42.7079	0.6619	66	256.1642	18.4802	123	713.0025	465.9693	180	3244.6204	4.4151
10	44.2936	2.3385	67	258.6849	16.5251	124	723.7920	31.3068	181	3274.0808	839.5857
11	47.0097	1.0265	68	261.3303	10.0111	125	737.2372	279.1869	182	3285.4707	2104.3167
12	47.6733	1.4754	69	267.1921	47.0148	126	744.2266	184.7313	183	3290.0198	554.2793
13	51.1721	2.7350	70	276.5842	147.2035	127	774.3334	656.8316	184	3325.9407	612.5094
14	53.1427	1.4047	71	277.9637	45.3960	128	788.8621	69.7633	185	3356.1931	505.0763
15	57.7656	2.3028	72	282.2070	24.5158	129	798.0102	34.9706	186	3381.3384	850.3704
16	59.6230	6.1840	73	286.8498	10.5417	130	813.1996	205.3867	187	3398.9536	1695.6246
17	61.5564	2.1732	74	292.1057	13.0423	131	817.6552	78.2542	188	3408.6128	588.7979
18	62.2319	0.4105	75	300.6860	92.1381	132	825.1666	68.5088	189	3416.9670	760.5367
19	65.5601	0.5263	76	304.9407	19.9736	133	835.6755	13.1005	190	3443.4128	603.0763
20	67.1552	0.4252	77	308.5229	14.1676	134	840.1131	78.3759	191	3444.8662	87.8518
21	68.3697	1.3940	78	314.9145	19.6451	135	853.4496	45.1395	192	3461.5469	382.2350
22	69.5228	0.7292	79	320.8922	26.0665	136	866.5336	134.0499	193	3474.4873	945.4470
23	74.0065	0.5950	80	355.5389	32.0541	137	879.4475	23.6052	194	3485.6907	1031.5009
24	74.8199	0.3996	81	357.1844	12.3926	138	891.3450	88.4409	195	3514.5791	471.8443
25	76.5467	0.9866	82	379.1873	65.5342	139	907.0314	91.5189	196	3534.8040	380.4181
26	77.9286	1.8840	83	388.7768	50.7015	140	919.0233	175.4523	197	3543.8767	108.8396
27	81.3244	1.5971	84	397.1518	8.6088	141	925.7115	49.4253	198	3550.2405	610.0307

28	85.7556	2.3482	85	399.7716	2.6883	142	935.7767	51.7776	199	3558.9299	486.8357
29	87.6839	1.4647	86	422.0791	12.3446	143	937.9314	71.8930	200	3571.8662	381.9863
30	89.2438	0.8386	87	435.3044	8.3820	144	958.4849	130.8235	201	3581.8457	913.1814
31	92.6238	1.3608	88	438.0245	18.8633	145	971.6567	19.0367	202	3599.0649	206.9619
32	97.2852	1.3057	89	448.1985	7.4364	146	977.4821	54.1783	203	3612.2312	333.6446
33	97.7240	1.7594	90	449.2635	58.2075	147	982.4085	13.9744	204	3612.6555	816.4170
34	103.3839	2.4608	91	462.4796	9.2046	148	997.5325	60.5718	205	3626.9470	289.3848
35	106.0994	2.1053	92	466.5386	56.5849	149	1031.8842	65.7729	206	3639.6223	363.5821
36	112.9092	2.0894	93	471.7929	26.8338	150	1034.0962	68.5087	207	3644.8918	558.4249
37	115.4542	0.4094	94	484.7546	12.7313	151	1296.6469	18.9385	208	3650.0662	175.5397
38	119.3666	4.5771	95	486.6130	11.1727	152	1421.9752	11.2257	209	3651.0610	375.8798
39	125.2534	5.6017	96	501.2156	78.1979	153	1654.1115	103.4293	210	3665.7917	377.6342
40	131.8841	13.8366	97	506.1836	89.5250	154	1659.9512	48.3226	211	3705.0913	333.0417
41	134.0664	3.1835	98	508.9848	6.4795	155	1661.8182	278.1026	212	3710.2566	139.7018
42	135.4957	3.5457	99	511.2034	39.1680	156	1663.2393	10.6782	213	3714.2615	802.1446
43	137.0230	1.1982	100	514.7163	5.0836	157	1663.4875	59.5558	214	3716.6729	75.9354
44	149.4048	2.6201	101	532.7639	58.3883	158	1665.7397	184.3929	215	3742.2910	206.1642
45	159.0904	17.8220	102	540.5072	22.6692	159	1668.4027	54.5897	216	3768.3142	229.1255
46	159.6439	3.4663	103	544.6977	30.6927	160	1679.2806	61.3874	217	3770.1731	518.3415
47	167.8284	15.1715	104	555.0079	74.5780	161	1680.9445	124.7398	218	3779.7805	91.6689
48	173.2717	8.5618	105	563.2295	15.7852	162	1682.1136	38.3507	219	3782.3438	261.5622
49	178.7499	5.1501	106	569.4322	62.7496	163	1687.3167	37.3210	220	3857.8601	67.7905
50	181.5432	3.9577	107	573.4675	154.9007	164	1689.3540	10.9905	221	3868.8391	70.5962
51	183.3804	6.7292	108	580.3479	46.3257	165	1691.9475	1.6283	222	3873.8411	113.5516
52	186.8849	14.6513	109	606.1805	128.0955	166	1699.1375	49.4448	223	3874.4277	64.7934
53	197.8815	32.6591	110	610.4611	71.9771	167	1702.2528	59.1295	224	3874.6455	76.8244
54	202.7922	17.7764	111	617.3366	42.8208	168	1706.7480	140.5169	225	3876.4900	67.2657
55	204.0776	39.2763	112	621.0556	59.4670	169	1709.7865	16.9723	226	3877.2092	59.1095
56	212.7391	13.3322	113	634.1642	130.7259	170	1712.7235	55.4486	227	3880.5225	52.6017
57	214.0245	27.9182	114	643.2327	73.7659	171	1714.3120	42.9447	228	3889.1726	74.5270

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	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	10.6161	0.1347	92	222.0738	70.0970	183	680.4835	150.8814	274	1720.8513	3.7321
2	15.3523	0.3326	93	227.0297	47.5010	184	681.7707	38.6009	275	1726.3600	4.3795
3	19.7254	0.2473	94	227.7627	16.6821	185	685.1299	42.2197	276	1734.0013	64.1411
4	22.6771	1.8098	95	230.0983	37.3589	186	687.6128	49.0872	277	1737.6940	90.7750
5	24.9448	0.4137	96	230.9251	103.5770	187	690.4943	84.3270	278	1738.6639	115.5998
6	25.7003	1.2505	97	234.9962	33.6371	188	699.1355	89.9107	279	1739.4895	56.3533
7	26.7306	0.8623	98	242.0326	56.7162	189	713.9046	47.8639	280	1744.6652	99.3614
8	28.1361	4.0392	99	244.1755	6.2499	190	724.8530	167.8592	281	1747.3325	23.3359
9	28.8809	0.6359	100	245.6258	91.1030	191	727.8705	263.7846	282	1758.0970	73.1060
10	29.8776	1.5511	101	248.1221	3.4037	192	742.8371	116.5907	283	3151.5298	1576.0745
11	33.4849	0.3607	102	250.4694	31.6170	193	745.1190	112.1499	284	3160.5408	2.8106
12	34.6108	0.3953	103	254.9841	82.4310	194	747.4357	8.9078	285	3226.0681	0.0821
13	36.3233	0.5651	104	256.7005	14.0469	195	752.2595	299.0472	286	3228.6592	1005.3063
14	38.4779	1.1649	105	259.4992	101.6280	196	760.8020	6.6243	287	3232.7278	1106.6781
15	39.6174	0.8561	106	263.3765	19.1075	197	763.8439	179.2211	288	3251.9749	1.0426
16	41.8829	0.3262	107	265.0664	1.0606	198	770.6103	77.4902	289	3276.4668	372.4189
17	42.1187	0.2324	108	267.6925	5.6142	199	779.8054	49.7780	290	3294.8157	431.9027
18	43.0455	1.1008	109	269.4970	28.3736	200	781.3043	5.7829	291	3300.7512	454.8694
19	45.2919	0.4602	110	271.7168	23.0879	201	783.4340	534.2581	292	3306.9395	504.1108
20	48.3434	0.7543	111	275.7171	24.0357	202	788.9723	130.8039	293	3310.3557	350.9077
21	49.0686	0.7177	112	276.7751	48.7370	203	792.6303	208.4366	294	3334.3323	1406.0922
22	50.1070	2.0199	113	278.4987	23.3807	204	798.6837	115.9603	295	3341.6833	1669.4502
23	52.9785	1.8351	114	279.8460	76.4110	205	805.0827	93.3258	296	3349.8423	507.8624
24	54.9237	0.4830	115	281.8074	11.1022	206	808.9769	292.1599	297	3357.9387	720.4184
25	55.7551	0.2682	116	284.9147	40.9847	207	813.9584	10.5551	298	3363.2590	258.7468
26	57.9939	2.7631	117	290.8237	45.9724	208	828.4317	135.2905	299	3377.0068	1058.5323
27	58.8236	0.5644	118	294.8966	9.2141	209	836.1287	26.6853	300	3380.4380	1139.2563
28	60.2561	2.0768	119	298.9904	30.9030	210	848.9870	83.4764	301	3383.9155	1029.6317
29	61.2014	3.1059	120	303.5664	12.2860	211	852.1695	41.3294	302	3389.9233	1070.1808

30	62.3044	2.6614	121	307.5892	35.1712	212	859.0324	251.3892	303	3399.3118	518.7938
31	62.9459	0.8122	122	315.3445	23.2863	213	868.9904	50.4598	304	3409.4348	1157.9567
32	65.7192	0.7472	123	319.1754	14.9241	214	871.3757	67.0148	305	3431.2856	1260.9113
33	67.6719	0.5302	124	323.0799	21.8168	215	884.5391	4.6340	306	3438.9780	1099.8489
34	68.3253	0.8911	125	326.7125	35.5090	216	889.1911	101.4790	307	3443.1494	263.0589
35	68.9853	1.6547	126	330.7049	18.9439	217	894.4379	35.1384	308	3447.5127	755.9120
36	70.1870	0.1885	127	332.5632	49.6749	218	896.2536	75.2242	309	3468.0371	2605.0989
37	70.6428	0.3649	128	333.6028	94.3130	219	902.6593	97.4215	310	3473.8110	164.2905
38	72.5182	0.1397	129	346.7322	74.6613	220	905.6865	357.1146	311	3489.6970	367.9361
39	75.4425	1.9672	130	358.2451	53.2708	221	909.1823	53.9098	312	3500.8037	843.1077
40	76.4113	1.4649	131	368.7963	111.3847	222	926.3620	129.7921	313	3506.5181	941.1035
41	78.0081	1.8138	132	398.4605	0.4752	223	936.9640	213.2690	314	3512.0186	406.2962
42	78.6138	6.4552	133	409.6670	69.6034	224	951.9353	123.6710	315	3517.9009	578.7689
43	79.8277	2.4581	134	411.3465	55.0789	225	955.5904	33.6947	316	3521.8962	234.4975
44	82.3908	1.5022	135	414.1876	65.5637	226	957.1777	83.0009	317	3522.5110	435.1223
45	84.9466	2.5570	136	422.3106	18.2502	227	962.9992	27.2882	318	3524.7512	205.0111
46	86.8507	2.0099	137	435.1643	14.0290	228	966.7509	28.5403	319	3529.5398	405.0054
47	88.9366	3.7333	138	435.8280	56.6677	229	972.4951	50.9339	320	3555.3352	486.3530
48	90.0570	3.5452	139	440.2861	28.2986	230	983.0454	138.6783	321	3557.3484	630.0794
49	91.7034	3.4717	140	457.8624	33.0783	231	997.8749	35.2950	322	3562.7153	31.2362
50	95.2572	0.7247	141	459.9388	15.3873	232	1005.8180	165.3976	323	3564.1880	949.4850
51	96.7318	4.9190	142	461.2572	43.7502	233	1013.0704	11.1988	324	3567.6016	349.6304
52	98.5751	1.4917	143	468.5644	14.2776	234	1018.1504	17.1011	325	3570.0225	85.9141
53	103.9474	7.3305	144	479.1746	30.6358	235	1021.1663	69.6169	326	3574.9614	467.6031
54	107.0768	1.8535	145	484.0347	73.3649	236	1037.8226	16.7095	327	3580.2502	600.6717
55	111.5167	3.7471	146	497.3429	82.2014	237	1047.3929	69.5660	328	3590.3296	113.9070
56	115.1241	4.2147	147	500.0829	176.3899	238	1057.0231	135.5840	329	3597.5713	564.8472
57	117.7107	22.5630	148	502.4665	126.8983	239	1081.6884	52.6639	330	3598.8445	229.2742
58	121.9331	5.4937	149	513.0066	13.7351	240	1086.2028	49.1808	331	3604.0300	182.3403
59	126.9458	3.4614	150	521.9610	26.4414	241	1302.0529	13.7437	332	3605.9753	555.6698
60	130.1246	9.5776	151	527.0947	25.0213	242	1414.7445	8.4306	333	3611.3469	1406.2195
61	132.3058	7.4678	152	528.7596	27.6725	243	1643.1536	80.0542	334	3621.4363	351.7968

62	134.2131	3.5641	153	531.8105	98.6281	244	1651.0590	62.6361	335	3622.1653	785.6386
63	136.5573	0.9084	154	536.0460	51.9272	245	1651.6667	120.6003	336	3635.0911	116.1181
64	142.2322	1.5061	155	537.5162	140.4424	246	1655.6787	63.4980	337	3645.7295	579.3535
65	145.9645	6.3948	156	546.4919	16.5084	247	1656.1168	56.3251	338	3672.4539	159.9300
66	155.0747	8.7718	157	552.5702	4.3146	248	1656.5673	90.2962	339	3692.0732	431.3513
67	158.9453	10.3102	158	558.7148	25.9438	249	1660.7465	83.3992	340	3697.7651	638.4365
68	160.6917	19.2144	159	565.2224	22.6580	250	1663.6738	45.6169	341	3702.6284	378.7595
69	166.1726	7.8048	160	573.0090	42.7474	251	1669.2073	92.1557	342	3704.5774	281.0217
70	167.7509	6.8791	161	574.8789	28.9441	252	1671.8456	48.9719	343	3705.9319	939.3634
71	170.0563	25.9995	162	587.0238	54.0868	253	1673.1456	46.1696	344	3714.7383	379.6465
72	171.2948	5.0245	163	591.6113	59.6125	254	1675.5653	104.0065	345	3719.0110	249.6671
73	173.9194	11.0498	164	596.9870	48.7038	255	1681.1169	59.7771	346	3728.0537	247.4400
74	175.9795	11.7674	165	599.2099	55.7002	256	1681.3215	65.6887	347	3751.7698	453.3627
75	176.7297	9.5997	166	602.3534	56.4612	257	1682.7454	20.2320	348	3753.6016	251.6962
76	184.8965	4.0470	167	606.3788	78.9363	258	1684.5228	30.2627	349	3757.5183	243.0083
77	186.8405	1.5121	168	609.2178	243.0817	259	1687.2900	2.9598	350	3778.1995	215.9363
78	187.7957	8.4427	169	615.7262	34.9784	260	1690.1940	29.9227	351	3864.0688	56.3667
79	188.9358	9.6052	170	619.4690	1.8398	261	1691.5356	64.4897	352	3868.2913	63.8085
80	192.9985	4.6965	171	632.9593	84.1317	262	1694.1136	43.4154	353	3868.7581	77.6928
81	195.9297	18.8172	172	635.6097	24.0725	263	1696.6135	64.1862	354	3869.4060	63.1591
82	198.7874	18.6544	173	640.1221	44.3605	264	1696.9646	8.3601	355	3872.7432	75.2999
83	203.0630	27.9686	174	642.1582	14.8816	265	1698.3486	8.8929	356	3873.6594	72.5020
84	204.6250	36.3325	175	644.0489	75.4360	266	1700.6105	35.0087	357	3879.7942	72.7299
85	205.5616	56.2246	176	647.5397	35.9823	267	1703.9220	19.8707	358	3880.3362	54.7981
86	208.0926	2.8456	177	653.7756	100.6525	268	1705.3232	12.7990	359	3880.5737	77.5391
87	209.5477	25.7660	178	656.7792	58.0208	269	1705.6742	106.0285	360	3881.1772	84.9941
88	212.8724	30.4755	179	660.9847	102.6047	270	1709.0071	24.8759	361	3883.4644	86.4659
89	217.2559	20.5971	180	664.4359	25.1408	271	1712.7914	16.9175	362	3888.1882	60.2368
90	218.0971	9.0329	181	670.2108	60.7131	272	1716.1058	117.1977	363	3890.2039	100.0836
91	218.9082	90.1149	182	674.8156	186.0972	273	1718.2749	40.7530			