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Equilibrium Structures and Absorption Spectra for Si_xO_y Molecular Clusters using Density Functional Theory

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14. ABSTRACT Calculations are presented of vibrational and electronic excited-state absorption spectra for equilibrium structures of Si _x O _y molecular clusters using density function theory (DFT) and time-dependent density functional theory (TD-DFT). The size of the clusters considered is relatively large compared to those considered in previous studies. DFT and TD-DFT can provide interpretation of absorption spectra with respect to molecular structure for excitation by electromagnetic waves at frequencies within the IR and UV-visible ranges. The absorption spectrum corresponding to excitation states of Si _x O _y -nH ₂ O molecular clusters consisting of relatively small numbers of atoms should be associated with response features that are intermediate between that of isolated molecules and that of a bulk system. DFT and TD-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

Understanding the nature of silicon oxide clusters is of major importance to nanoscience and technology. This follows in that silicon oxide clusters are characterized by many different geometries, which potentially can be optimized with respect to specific materials design criteria, i.e., molecular structures and properties, for systems consisting of nano-scale molecular clusters. Previous studies [1-9] have investigated structures and properties of small to medium-sized Si_xO_y molecular clusters. The present study presents further investigation of structures and properties of medium-sized Si_xO_y molecular clusters using density functional theory (DFT). The size of the clusters considered, however, is relatively large compared to those considered in previous studies.

Density functional theory (DFT) is applied to determine equilibrium structures and absorption spectra for Si_xO_y molecular clusters. DFT applied for the determination of equilibrium molecular structures and absorption spectra provides information complementary to that of experimental results, e.g., reference [10]. Significantly, DFT calculation of absorption spectra can adopt the perspective of computational physics, which is that numerical simulations may be viewed as "experimental" data. Here DFT calculations of vibrational modes are associated with different molecular structures. 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) [11]. The present study also considers calculation of approximate UV-Vis absorption spectra for Si_xO_y molecular clusters, which uses time-dependent density functional theory (TD-DFT) as implemented in GAUSSIAN [11].

The remainder of the paper is organized as follows. First, a general review of vibrational analysis needed for calculation of absorption spectra is presented. Second, DFT calculations of equilibrium energies for Si_xO_y molecular structures are presented. Third, DFT calculations are presented of vibration resonance structure of the Si_xO_y structures considered, which provide estimates of their IR spectra and interpretation of spectral features with respect to molecular structure. Fourth, TD-DFT calculations of UV-Vis spectra are presented. Finally, a conclusion is given.

Calculation of Absorption Spectra using DFT

In this section are presented the formal mathematical structure underlying DFT calculations, as well as the procedure for calculation of absorption spectra corresponding to

vibrational states. The present study considers DFT calculation of absorption spectra of vibrational states.

The DFT software GAUSSIAN09 (G09) can be used to compute an approximation of the IR absorption spectrum of a molecule or molecules [12]. 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 [13-18]. 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 followed in GAUSSIAN is that described in Ref [12]. Reference [18] presents a relatively detailed review of this procedure. A brief description of this procedure is as follows.

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_{n0} . The absorption intensity corresponding to a particular eigenmode n whose eigenfrequency is ν_{n0} is given by

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

where $\mathbf{l}_{\text{CART}}$ is the matrix whose elements are the displacements of the atoms in Cartesian coordinates. The matrix $\mathbf{l}_{\text{CART}}$ is determined by the following procedure. 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

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

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

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

where Λ 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

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

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

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

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. In principle, however, these spectral components must be broadened and shifted to account for anharmonic effects such as finite mode lifetimes and inter-mode couplings.

DFT Calculation of Equilibrium Energies and IR Spectra

Results of a computational investigation using DFT concerning Si_xO_y molecular structures are presented. These results include the relaxed or equilibrium configuration of these molecular structures, ground-state oscillation frequencies and IR intensities for molecular geometries having stable structures, which are calculated by DFT. For these calculations geometry optimization and vibrational analysis was effected using the DFT model B3LYP [19,20] and basis function 6-311+G(d) [21,22]. These basis functions designate the 6-311G basis set

supplemented by diffuse function: +, and polarization function: (d), having one set of d functions on heavy atoms [23]. Graphical representations of molecular geometries for a set of Si_xO_y molecular structures at equilibrium are shown in Fig. (1). The equilibrium, or ground-state energies, of these structures are given in Table 1. IR intensities as a function of frequency for these molecular structures are shown in Figs. (2) through (5), and given in Tables 2 through 8.

DFT Calculation of UV-Vis Spectra

Results of a computational investigation using TD-DFT concerning Si_xO_y molecular structures are presented. The extension of DFT for the calculation of absorption spectra corresponding to electronic excitation states, which is the formalism of time-dependent density functional theory (TD-DFT) is described in references [24,25]. The results presented include the oscillator strength as a function of excitation energy (within the UV range) for different geometries of the interacting systems associated with stable structures, which are calculated by DFT as described above. The oscillator strengths (UV-Vis intensity) as a function of excitation energy for these molecular structures are given in Table 9.

Conclusion

The DFT and TD-DFT calculated absorption spectra given here provide information concerning molecular level dielectric response structure. The calculations of vibrational and excited state resonance structure associated with Si_xO_y molecular structures using DFT and TD-DFT, respectively, are meant to serve as reasonable estimates of molecular level response characteristics, providing interpretation of dielectric response features with respect to molecular structure, for subsequent adjustment relative to experimental measurements. We have in this paper studied Si_xO_y molecular structures in order to quantify interpretation of their absorption spectra.

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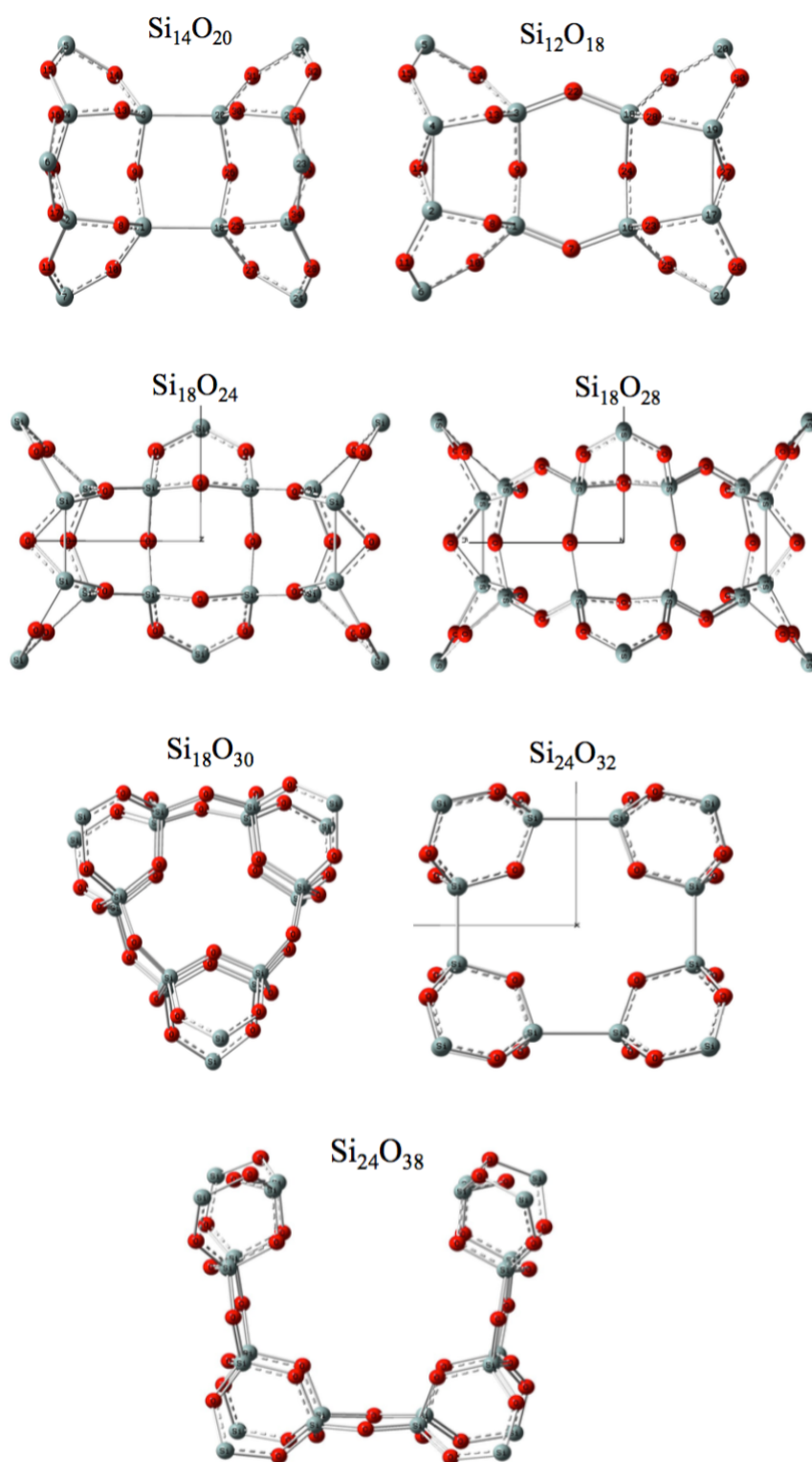


Figure 1. Molecular geometries of equilibrium structures for $\text{Si}_{14}\text{O}_{20}$, $\text{Si}_{12}\text{O}_{18}$, $\text{Si}_{18}\text{O}_{24}$, $\text{Si}_{18}\text{O}_{28}$, $\text{Si}_{18}\text{O}_{30}$, $\text{Si}_{24}\text{O}_{32}$ and $\text{Si}_{24}\text{O}_{38}$.

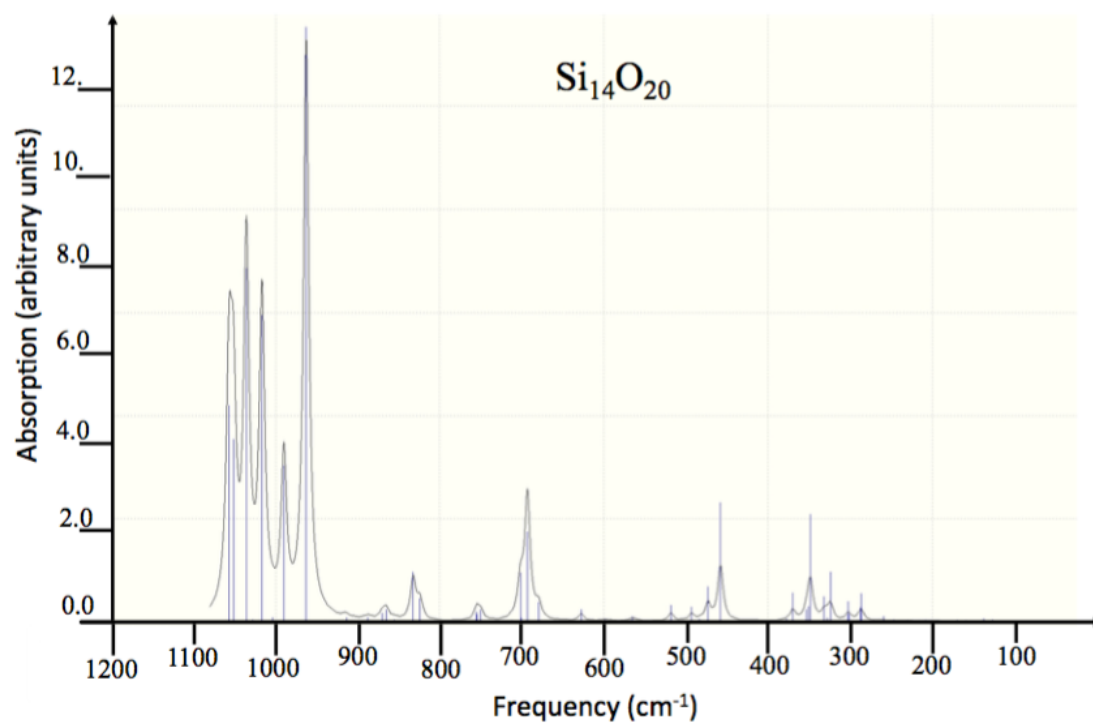


Figure 2. DFT calculated IR spectra for $\text{Si}_{14}\text{O}_{20}$.

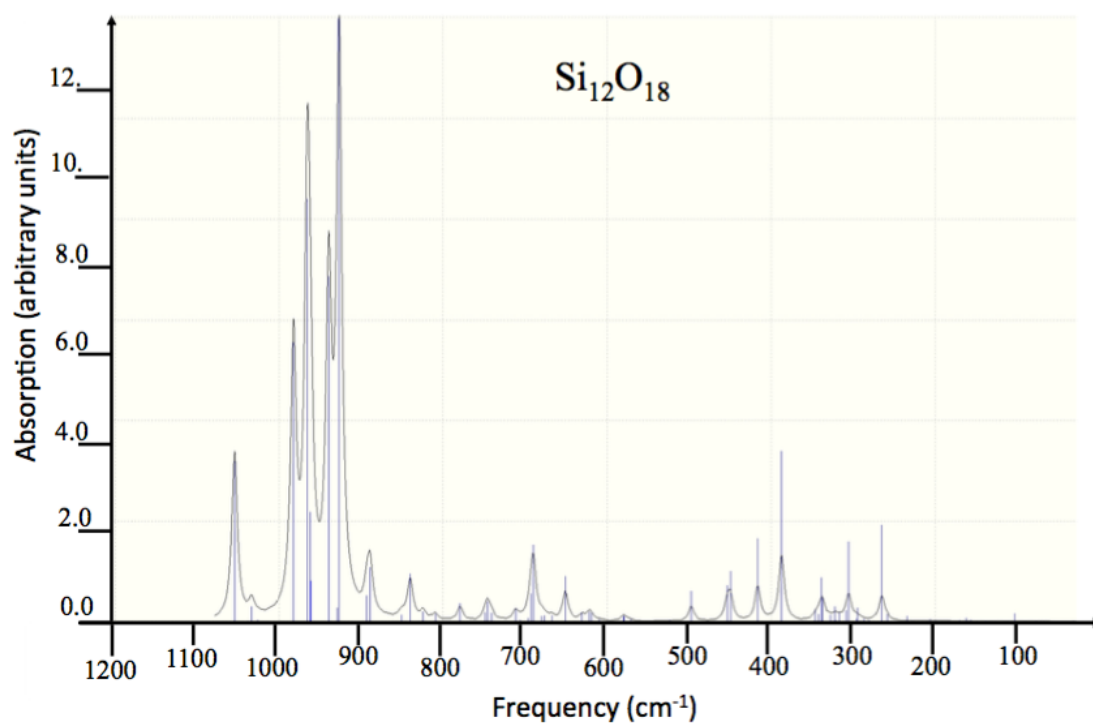


Figure 3. DFT calculated IR spectra for $\text{Si}_{12}\text{O}_{18}$.

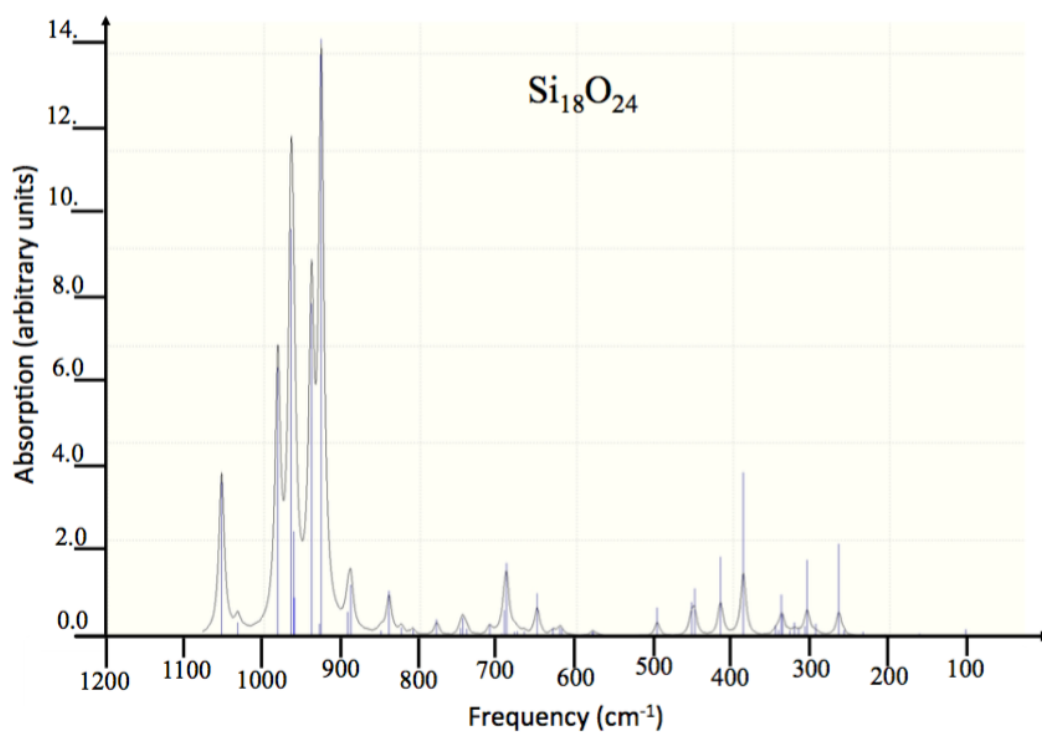


Figure 4. DFT calculated IR spectra for $\text{Si}_{18}\text{O}_{24}$.

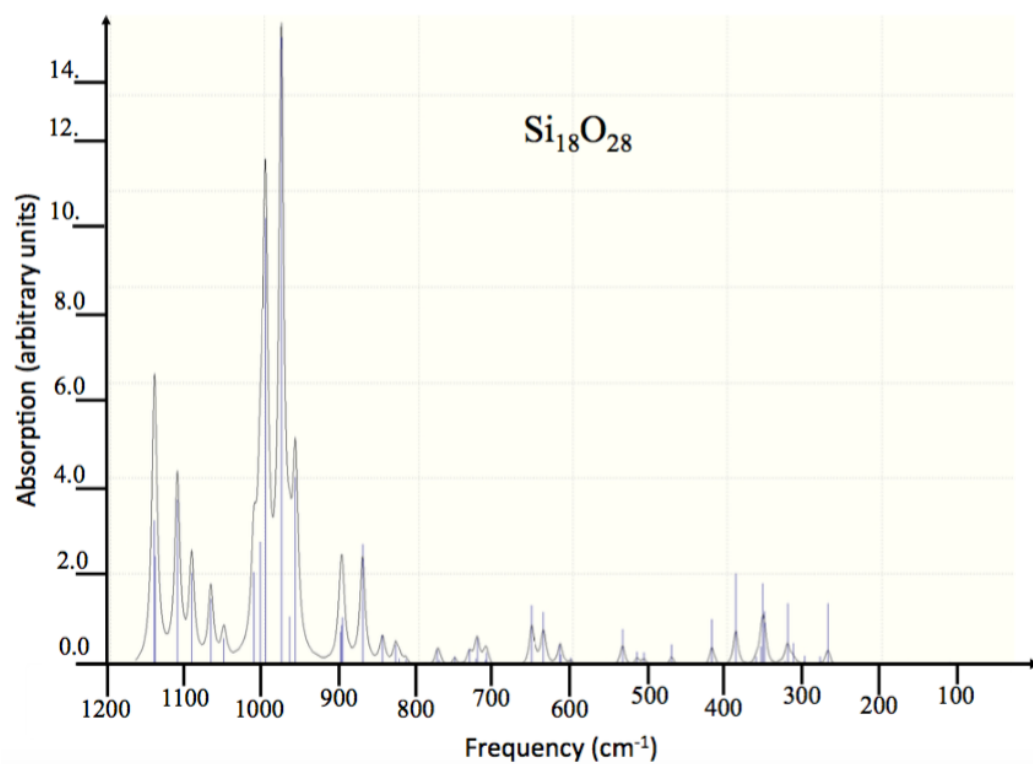


Figure 5. DFT calculated IR spectra for $\text{Si}_{18}\text{O}_{28}$.

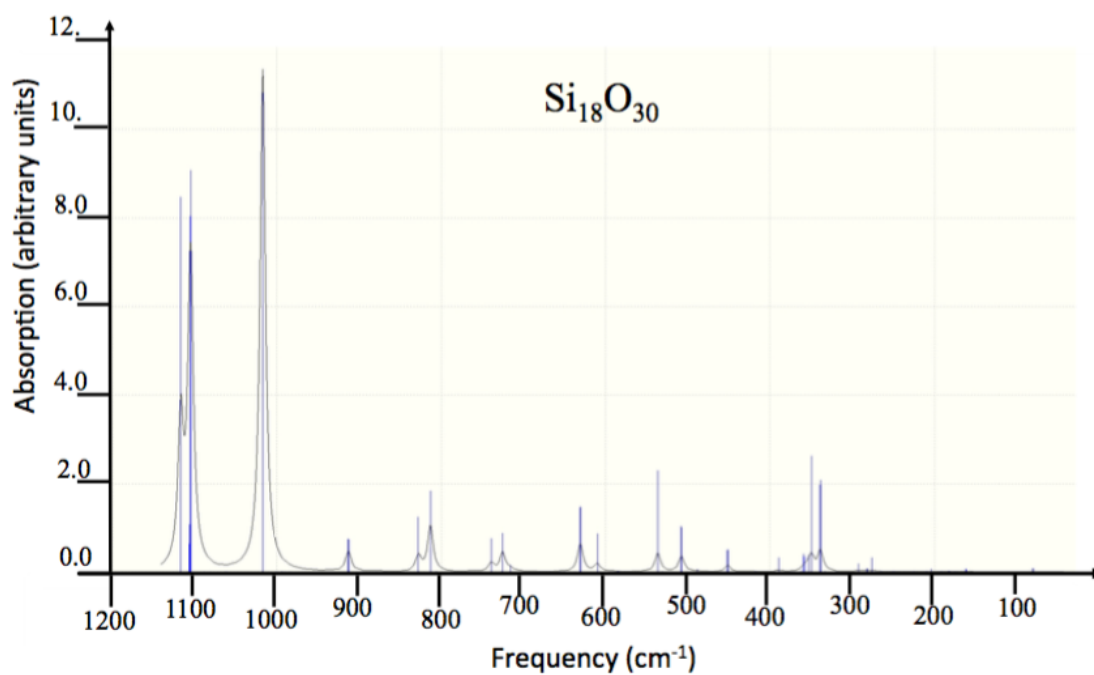


Figure 6. DFT calculated IR spectra for $\text{Si}_{18}\text{O}_{30}$.

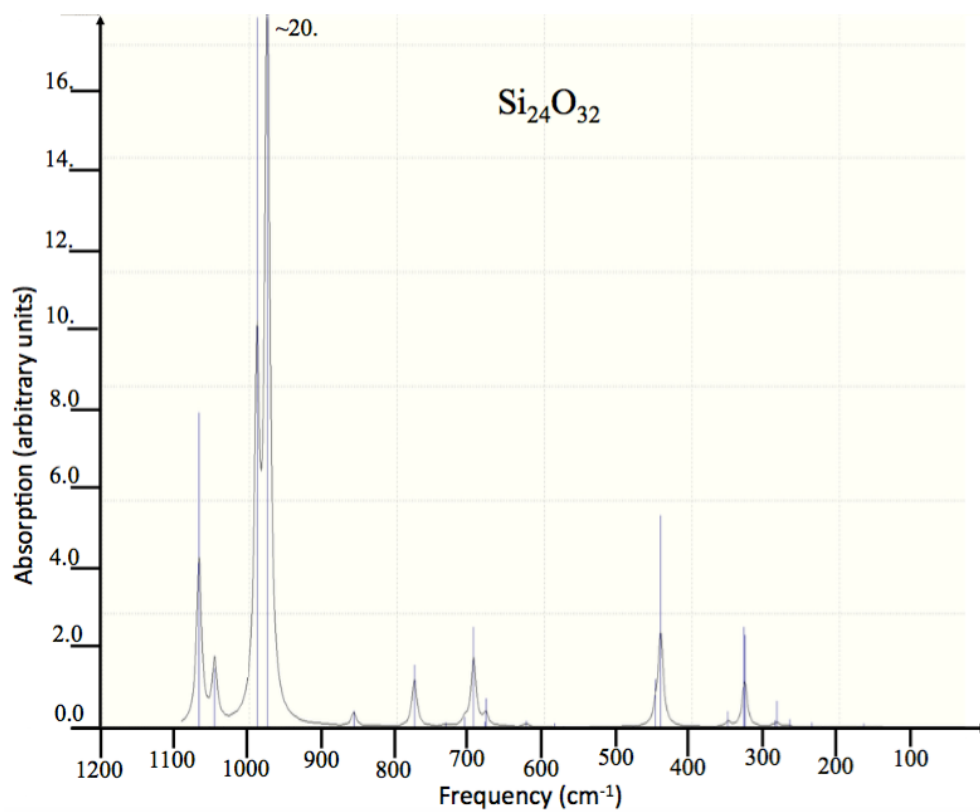


Figure 7. DFT calculated IR spectra for $\text{Si}_{24}\text{O}_{32}$.

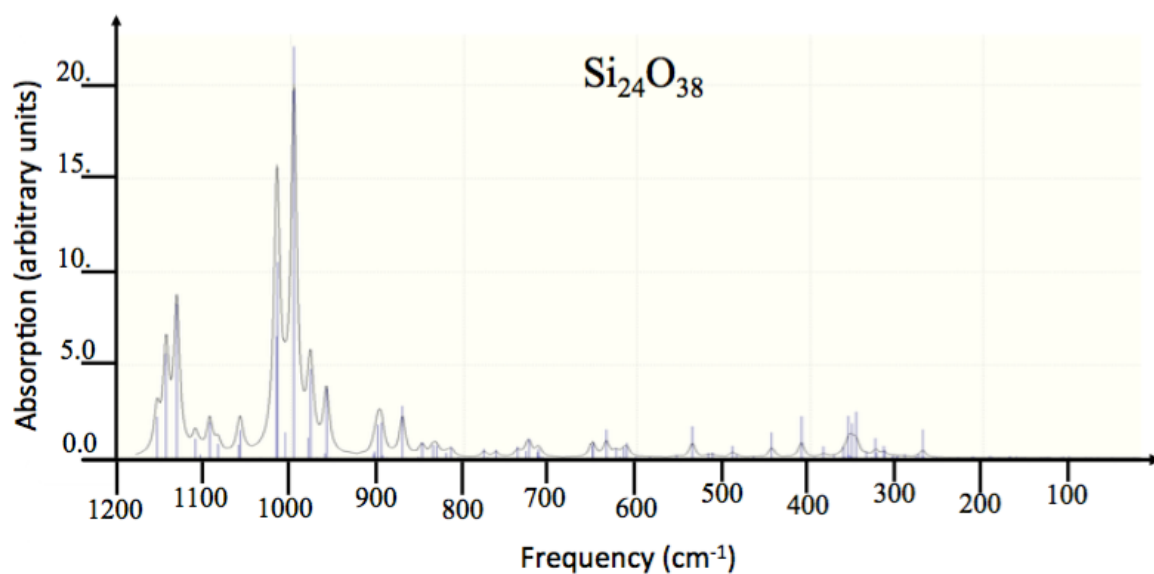


Figure 8. DFT calculated IR spectra for $\text{Si}_{24}\text{O}_{38}$.

Table 1

	Ground State Energy
$\text{Si}_{14}\text{O}_{20}$	-5559.94 a.u.
$\text{Si}_{12}\text{O}_{18}$	-4830.05 a.u.
$\text{Si}_{18}\text{O}_{24}$	-7019.11 a.u.
$\text{Si}_{18}\text{O}_{28}$	-7320.58 a.u.
$\text{Si}_{18}\text{O}_{30}$	-7471.57 a.u.
$\text{Si}_{24}\text{O}_{32}$	-9359.19 a.u.
$\text{Si}_{24}\text{O}_{38}$	-9811.12 a.u.

Table 2 ($\text{Si}_{14}\text{O}_{20}$) Freq (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity
1	22.06170	0.0000	33	301.29900	14.0086	65	679.74530	0.0000
2	27.52880	0.0127	34	302.06620	34.3556	66	693.05400	345.9265
3	54.15480	0.0068	35	321.16200	0.0000	67	693.12710	355.8343
4	69.40670	0.0033	36	323.88090	91.9909	68	700.61010	13.8734
5	70.57000	0.0047	37	327.56580	7.2588	69	701.67740	196.8550
6	77.80290	0.0040	38	331.14350	0.0000	70	712.47200	1.8588
7	86.22620	0.0094	39	331.67880	47.3215	71	748.53500	0.0000

8	91.68840	0.0000	40	348.43280	213.0488	72	750.22340	52.1549
9	102.50760	0.0000	41	349.55310	0.0043	73	754.79040	31.2962
10	105.68020	0.0083	42	350.52470	29.8979	74	755.24170	42.4713
11	126.87980	1.2892	43	353.53680	25.1054	75	824.16130	109.0397
12	135.29620	0.0000	44	367.26980	0.0000	76	832.26160	233.7261
13	137.17890	2.2022	45	369.74250	59.8899	77	848.94630	0.0000
14	139.33250	0.0013	46	377.41860	5.9524	78	855.30920	8.9385
15	159.29200	0.7200	47	392.44020	0.0000	79	864.92690	60.6102
16	166.33390	0.0269	48	458.04410	309.8548	80	869.89040	43.5494
17	169.24980	0.8884	49	473.47700	94.7430	81	886.47020	0.0000
18	174.72850	0.0000	50	483.74170	6.0708	82	887.61550	22.5721
19	201.14850	0.0000	51	493.14930	42.0140	83	906.37180	0.0000
20	202.47400	0.0373	52	518.43910	48.7707	84	913.71690	21.7066
21	208.45110	1.6991	53	524.45570	0.0000	85	938.68650	0.0000
22	222.50720	0.8457	54	564.80320	15.4181	86	962.79600	3245.6177
23	230.19010	0.4403	55	566.65700	6.2627	87	984.61880	0.0000
24	230.25330	1.7892	56	574.40130	0.0924	88	989.97710	877.8588
25	247.18280	2.8461	57	598.50090	8.8160	89	1000.07760	0.0010
26	259.22780	7.9385	58	608.25810	0.2502	90	1003.97570	24.3952
27	271.95790	0.4840	59	617.74730	0.0000	91	1012.50310	0.0000
28	272.16580	0.0000	60	627.27940	43.1179	92	1016.74510	1769.1036
29	286.24780	45.6003	61	641.43050	1.5830	93	1027.79440	8.9610
30	287.25180	22.6076	62	649.41130	0.0000	94	1035.72280	2077.7290
31	289.81290	1.3466	63	662.59030	0.7069	95	1051.73140	1088.1270
32	297.14770	0.0000	64	679.48680	76.6410	96	1056.80930	1297.3389

Table 3 ($\text{Si}_{12}\text{O}_{18}$) Freq (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity
1	28.3170	0.1900	29	311.0140	3.1530	57	707.4650	12.9420
2	32.8500	0.0000	30	320.0110	103.8510	58	711.8580	0.0000
3	62.5450	0.4280	31	321.2720	19.7580	59	712.4560	40.4570
4	73.4160	0.0940	32	330.2720	11.0510	60	722.0080	64.6230

5	78.0530	0.5890	33	331.1080	0.0000	61	726.0100	23.8010
6	103.1550	3.8790	34	335.5520	12.8690	62	750.9460	0.0000
7	104.3210	0.0000	35	341.3720	0.0000	63	765.8610	90.6290
8	111.2600	0.0000	36	351.3150	37.0160	64	778.3380	96.6890
9	129.3580	0.0200	37	353.3550	56.4110	65	784.4430	2.7910
10	133.8510	0.0110	38	363.3620	1.0830	66	805.8420	2.2280
11	138.8440	2.8440	39	392.2660	178.1600	67	826.3010	0.0000
12	139.6830	0.0000	40	393.4860	1.1590	68	831.0800	90.3550
13	159.9100	0.0000	41	396.0460	0.0000	69	844.6960	76.1300
14	164.6020	4.3320	42	443.7220	29.3700	70	851.2050	54.0220
15	198.8730	1.9000	43	469.3480	2.8110	71	851.8760	0.0000
16	207.6940	0.0100	44	497.0300	39.0140	72	881.7880	653.1660
17	215.6890	3.2980	45	513.2100	0.0000	73	896.4650	19.8590
18	217.1950	0.0190	46	522.5430	90.8390	74	903.1780	580.6260
19	220.5580	0.0000	47	535.4180	36.7000	75	951.0380	0.0000
20	228.8950	0.9240	48	562.8660	0.9240	76	961.5350	443.6140
21	266.5380	2.6050	49	599.5380	6.3970	77	969.6230	1560.2770
22	268.4810	0.0000	50	604.0180	43.8970	78	969.8460	448.5820
23	269.6890	63.9460	51	618.3510	6.6440	79	975.7000	2811.4890
24	277.8240	0.0000	52	622.9880	0.0000	80	987.4680	0.0000
25	279.9730	11.0320	53	636.6270	0.0000	81	1040.4590	43.3850
26	280.4160	67.5220	54	639.6210	192.2460	82	1073.6720	707.9010
27	301.0310	7.8850	55	653.9790	89.1140	83	1089.0950	0.0000
28	305.2020	20.6650	56	655.6590	165.7200	84	1113.2000	1285.0601

Table 4 ($\text{Si}_{18}\text{O}_{24}$) Freq (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity
1	14.1310	0.0000	41	294.5130	23.4360	81	661.1490	0.0000
2	16.3780	0.0200	42	295.8670	5.0560	82	667.3640	23.8540
3	30.7780	0.1240	43	305.1290	138.9640	83	676.3970	23.8440
4	48.7110	0.0000	44	307.9470	19.9630	84	679.6080	21.7040

5	57.8010	0.0000	45	311.3540	0.0000	85	689.7380	301.0610
6	67.2390	0.0060	46	316.3850	15.7630	86	692.4140	110.9760
7	71.3280	0.0590	47	321.1020	2.6700	87	696.2000	14.1790
8	76.7170	0.2090	48	322.0370	27.6970	88	705.7310	0.0000
9	77.1440	0.0740	49	325.1230	0.0000	89	705.9230	6.8980
10	90.3840	0.0000	50	327.5420	12.3230	90	711.5190	54.3100
11	102.4440	4.6510	51	336.7090	45.5280	91	732.3080	0.5770
12	106.5640	0.0000	52	338.4170	84.5890	92	736.8740	0.0000
13	111.5030	0.1840	53	342.0010	15.0620	93	740.8400	38.3720
14	114.9160	0.3820	54	342.8820	0.0000	94	745.7070	85.9430
15	126.8990	0.0000	55	346.1020	23.7300	95	748.4200	40.1450
16	132.3510	0.0000	56	347.5840	0.1420	96	779.3840	80.9060
17	135.6520	0.0070	57	361.7320	0.0000	97	808.2210	0.0000
18	138.5480	0.0010	58	387.1370	376.4880	98	809.3760	38.8310
19	139.2080	0.0000	59	394.1890	0.1210	99	824.2860	48.1770
20	148.6290	0.0400	60	416.2630	197.9570	100	825.1190	0.4630
21	156.3190	1.8460	61	449.7210	128.9040	101	829.9840	0.0000
22	157.8880	0.2760	62	453.6400	94.7180	102	840.1860	229.8800
23	162.0600	3.2080	63	468.9940	0.0000	103	845.7160	0.0000
24	170.3880	1.3310	64	477.3230	1.0680	104	850.8470	33.3590
25	183.1100	0.0000	65	497.4580	87.4010	105	889.1380	274.4880
26	199.3310	1.2270	66	502.4860	0.0520	106	890.7240	0.0000
27	206.1490	2.8540	67	523.6120	4.9350	107	893.0040	131.8560
28	210.5060	0.0180	68	546.3120	0.0000	108	926.8220	3264.5630
29	226.6430	0.0220	69	570.9130	7.2680	109	929.2940	75.4450
30	227.8710	0.0000	70	578.8580	17.5790	110	929.4540	0.0000
31	234.4230	0.4760	71	578.9880	3.4690	111	937.6970	0.0000
32	234.5670	7.3500	72	579.8940	19.3020	112	939.5470	1846.1100
33	254.1170	0.0000	73	608.9910	9.4010	113	961.8120	224.2890
34	258.3020	11.4020	74	619.1640	31.8600	114	962.3270	600.4500
35	262.6830	0.0000	75	621.8140	0.0000	115	965.5940	2321.1130
36	265.1410	145.9260	76	621.9820	36.7400	116	982.6410	1561.6670
37	279.6600	0.0000	77	630.4220	34.3840	117	1026.1030	11.2550

38	280.7100	2.8460	78	639.3880	0.0000	118	1033.7419	91.1170
39	286.5040	5.0130	79	650.7140	0.6440	119	1037.8960	0.0000
40	290.6830	0.6960	80	650.7910	167.4980	120	1054.5341	962.3990

Table 5 (Si₁₈O₂₈) Freq (cm⁻¹), Intensity (km/mol)

	Freq	intensity		Freq	intensity		Freq	intensity		Freq	intensity
1	9.001	0.008	41	280.642	21.151	81	617.059	90.132	121	999.141	2701.189
2	11.320	0.000	42	290.452	1.302	82	618.291	0.000	122	1005.837	766.591
3	24.548	0.210	43	296.904	0.000	83	622.141	1.170	123	1008.793	0.000
4	31.157	0.149	44	299.176	0.244	84	635.408	0.000	124	1014.016	590.031
5	55.305	0.000	45	299.546	23.902	85	638.435	219.938	125	1052.952	192.564
6	65.461	0.017	46	306.911	8.050	86	652.951	0.000	126	1069.840	452.550
7	75.429	0.509	47	314.537	48.905	87	653.051	0.099	127	1092.477	0.000
8	76.773	0.002	48	314.793	2.165	88	653.525	249.145	128	1094.663	634.193
9	81.202	0.003	49	322.019	126.424	89	708.964	0.000	129	1099.050	0.000
10	95.277	0.000	50	324.934	15.953	90	710.139	10.712	130	1113.306	1131.422
11	95.286	0.502	51	326.300	0.000	91	712.615	69.707	131	1142.442	775.077
12	103.692	1.716	52	328.338	4.568	92	713.919	40.887	132	1143.449	1018.825
13	110.324	0.000	53	334.189	10.438	93	724.245	131.798			
14	111.860	4.253	54	344.812	0.000	94	724.591	0.000			
15	122.592	0.000	55	350.408	0.000	95	726.137	44.985			
16	123.975	0.035	56	352.215	121.453	96	734.470	85.115			
17	133.991	0.000	57	354.206	182.170	97	753.932	57.550			
18	135.624	0.241	58	356.287	48.264	98	765.090	0.000			
19	136.132	0.029	59	361.561	4.394	99	773.410	41.985			
20	147.959	0.000	60	362.919	27.327	100	776.182	89.681			
21	157.409	0.022	61	375.971	0.000	101	794.152	22.167			
22	160.615	1.154	62	380.276	0.620	102	796.652	1.177			
23	166.373	2.698	63	389.323	223.329	103	816.319	48.662			
24	168.715	2.645	64	405.672	0.000	104	825.640	52.897			
25	176.362	2.744	65	408.696	1.139	105	828.605	0.000			
26	191.149	0.000	66	420.234	125.503	106	830.178	121.123			

27	196.539	2.036	67	461.999	0.719	107	847.161	167.301		
28	198.582	1.059	68	463.795	8.695	108	850.138	9.043		
29	209.646	0.336	69	472.444	69.723	109	862.908	0.000		
30	215.323	2.057	70	482.822	1.747	110	873.077	653.939		
31	224.064	1.521	71	508.392	50.831	111	891.763	0.000		
32	233.339	0.095	72	517.246	0.000	112	898.888	280.104		
33	233.624	0.000	73	517.308	54.258	113	900.373	235.643		
34	258.985	2.244	74	536.114	127.798	114	901.901	202.333		
35	268.133	1.194	75	538.407	13.107	115	953.726	0.000		
36	268.195	4.787	76	558.077	12.711	116	960.061	1104.118		
37	270.167	0.000	77	584.845	3.272	117	964.134	39.051		
38	270.287	106.889	78	597.410	0.000	118	967.731	304.184		
39	275.888	0.000	79	602.759	39.662	119	973.427	0.000		
40	277.021	0.077	80	615.858	52.866	120	978.423	3705.466		

Table 6 (Si₁₈O₃₀) Freq (cm⁻¹), Intensity (km/mol)

	Freq	intensity		Freq	intensity		Freq	intensity		Freq	intensity
1	66.3819	0.0006	41	276.4160	22.3233	81	586.4453	0.5426	121	994.3964	0.0112
2	67.6149	0.0000	42	277.9501	0.0298	82	606.6077	0.0001	122	1000.6305	0.0830
3	68.3294	0.0002	43	281.5696	5.6708	83	606.8124	0.2695	123	1000.8123	0.0371
4	74.1346	0.0666	44	282.6904	5.4811	84	609.8784	132.6477	124	1017.2802	2688.8464
5	74.4044	0.0947	45	292.2101	14.3226	85	630.2562	233.4227	125	1017.3584	2759.2964
6	79.4317	1.7553	46	318.7674	0.0012	86	631.1117	231.9293	126	1017.6141	2753.7007
7	80.7633	1.6724	47	319.4492	0.0144	87	637.1528	0.1513	127	1061.3789	0.0201
8	81.5376	0.0000	48	332.6689	0.6285	88	649.7414	0.0001	128	1062.6156	0.0412
9	84.7812	0.0000	49	333.5683	0.0070	89	655.3752	0.0045	129	1081.4360	0.6613
10	109.2111	0.0001	50	338.4559	176.2411	90	656.0884	0.0003	130	1088.4995	0.3258
11	109.4415	0.0002	51	338.7692	167.2670	91	715.5999	25.9411	131	1088.5817	0.1075
12	119.2291	0.0000	52	349.4345	229.4130	92	716.0419	28.0977	132	1104.9258	2513.8311
13	119.3273	0.0001	53	352.8460	31.4248	93	717.4545	0.0838	133	1105.3353	2227.0020
14	125.1155	0.0404	54	353.0418	34.5897	94	725.2108	157.3638	134	1106.2513	298.5966
15	125.2443	0.0000	55	355.1395	0.0002	95	725.5082	161.4826	135	1106.8257	176.4332

16	126.5282	0.0480	56	357.8951	31.7174	96	726.9264	0.0038	136	1108.2264	1.2299
17	130.7625	0.0026	57	358.9819	36.9365	97	727.5907	0.1968	137	1108.8643	0.6806
18	142.3471	0.0152	58	361.9966	1.8243	98	727.6027	0.0074	138	1117.2260	2371.6284
19	160.9953	2.6046	59	371.5903	0.0153	99	739.2004	141.2619			
20	162.0732	2.7934	60	373.4731	0.0105	100	765.0904	0.0043			
21	173.2735	0.0081	61	374.4251	0.0147	101	765.1634	0.0255			
22	176.0890	0.0000	62	389.2608	31.9043	102	805.8980	1.2464			
23	176.2523	0.0009	63	393.4240	0.0006	103	806.1957	0.0618			
24	181.5269	1.2859	64	394.5064	0.0095	104	812.9886	375.6451			
25	182.2235	1.1624	65	394.8993	0.0052	105	813.1940	373.4433			
26	191.1495	0.0000	66	417.6004	0.0017	106	826.7315	0.0226			
27	191.9546	0.0023	67	417.8479	0.0003	107	827.7051	259.2890			
28	203.9154	3.4379	68	451.2894	56.9175	108	867.7774	0.0026			
29	209.7375	0.0034	69	451.7680	56.1843	109	879.0213	0.0011			
30	210.0160	0.0020	70	455.8906	0.3836	110	896.2188	0.0067			
31	224.4568	0.2836	71	488.2256	7.9626	111	896.3728	0.0057			
32	226.2180	0.1581	72	488.4628	7.5468	112	897.1318	0.0142			
33	248.6458	0.0000	73	501.1363	0.0933	113	912.9714	169.9527			
34	249.1351	0.0025	74	507.4075	128.3534	114	913.1331	172.7865			
35	251.1763	0.2564	75	508.2856	132.5928	115	984.3954	0.0055			
36	251.4666	0.2367	76	530.9533	0.0180	116	989.6347	0.0428			
37	264.4611	0.0230	77	531.3804	0.8898	117	990.1022	0.0072			
38	264.9611	0.0002	78	536.6717	309.8163	118	992.4414	0.4727			
39	272.3941	0.0145	79	584.1747	2.4289	119	993.8059	0.1200			
40	272.7088	0.0141	80	584.9207	1.8230	120	994.0230	0.0093			

Table 7 ($\text{Si}_{24}\text{O}_{32}$) Freq (cm^{-1}), Intensity (km/mol)

	Freq	intensity		Freq	intensity		Freq	intensity		Freq	intensity
1	44.2719	0.0000	42	236.3130	0.0167	83	464.2906	0.0001	124	722.9717	0.0000
2	54.4114	0.0000	43	236.8996	6.8949	84	464.2919	0.0000	125	723.9980	0.0000
3	64.0641	0.0000	44	236.9403	6.8675	85	478.7087	0.0037	126	733.6636	23.9371
4	64.9552	0.0000	45	237.9077	0.0004	86	479.1269	0.7282	127	775.5402	0.0924

5	65.3328	0.0000	46	245.5383	0.0000	87	479.1328	0.7455	128	776.5042	305.8548
6	69.7070	0.0742	47	263.5136	0.0006	88	480.0792	0.0014	129	776.5065	306.0707
7	69.7101	0.0744	48	267.5384	13.0195	89	492.1025	0.0002	130	788.5773	0.0003
8	72.2293	0.0001	49	267.5901	13.0778	90	508.8338	0.0000	131	835.3433	0.0000
9	72.2542	0.0000	50	273.9393	0.0006	91	540.0084	0.0000	132	846.4611	0.0001
10	72.3195	0.0036	51	275.5489	0.0000	92	568.9313	0.0000	133	846.4894	0.0000
11	75.3348	0.0000	52	278.4555	0.0000	93	573.8291	2.9746	134	849.6096	0.0016
12	80.7387	0.0000	53	278.4562	0.0008	94	573.8313	2.9721	135	854.0394	0.0006
13	105.5585	0.0000	54	283.9183	0.0001	95	575.4390	0.0000	136	858.5468	88.4348
14	105.5655	0.0000	55	284.1817	47.4318	96	575.4396	0.0000	137	858.5687	87.5051
15	124.0616	0.0000	56	287.4833	13.1500	97	576.1168	0.0000	138	863.8500	0.0071
16	128.3599	0.2142	57	287.5118	13.0984	98	586.3090	14.2404	139	905.0593	0.0000
17	128.3600	0.2147	58	289.8841	0.0045	99	597.7870	0.0000	140	914.4905	0.0000
18	129.0579	0.0000	59	309.5635	0.0000	100	618.5651	0.0000	141	914.4981	0.0006
19	129.0715	0.0000	60	316.0519	0.0000	101	624.6681	24.0854	142	918.9409	0.0005
20	134.9431	0.0000	61	320.2215	0.0002	102	624.6686	23.9160	143	927.3412	0.0004
21	135.1840	0.0000	62	320.2284	0.0000	103	636.4020	0.0000	144	939.4439	0.0000
22	136.0739	0.0000	63	321.1964	0.0000	104	636.4728	0.0000	145	946.6762	0.0032
23	136.0916	0.0533	64	327.8784	190.0884	105	641.4292	0.0000	146	946.7142	0.0000
24	136.1028	0.0534	65	327.8944	190.2959	106	651.0972	0.0000	147	950.9491	0.0000
25	136.8539	0.0000	66	329.0698	208.2505	107	666.6426	0.0034	148	971.9412	0.0000
26	137.5793	0.0000	67	331.0371	0.0009	108	669.9044	0.0000	149	974.9575	1.9529
27	147.4563	0.0000	68	331.0469	0.0000	109	670.0140	0.0000	150	976.0249	4869.1626
28	155.1216	0.0000	69	331.3164	0.0018	110	679.2836	124.5355	151	976.0901	4867.7007
29	155.1407	0.0000	70	338.2622	0.0001	111	680.3802	0.0313	152	979.2794	0.0000
30	166.8812	3.9238	71	339.8687	0.0000	112	680.6977	23.8661	153	979.2978	0.0203
31	166.8938	3.9309	72	348.0604	0.0000	113	680.7921	22.9261	154	990.1533	4423.7441
32	169.0778	0.0000	73	350.2821	0.0312	114	683.1031	0.0001	155	1035.2412	0.0040
33	173.4535	0.0000	74	351.2873	36.1070	115	689.3824	0.0081	156	1047.6090	392.2287
34	173.5715	0.0773	75	351.2902	36.0582	116	692.7854	0.0311	157	1047.6885	390.5079
35	174.6679	0.0000	76	358.5202	0.0001	117	696.1019	438.9428	158	1054.1342	0.0023
36	215.1346	0.0000	77	369.5646	0.0000	118	696.1501	436.8067	159	1054.5319	0.0000
37	215.1403	0.0000	78	369.5887	0.0000	119	701.5880	0.0087	160	1054.5833	0.1345

38	218.2047	0.0000	79	400.2259	0.0000	120	708.0805	44.7842	161	1067.4734	0.0027
39	222.0724	0.9825	80	442.2666	589.4054	121	708.0983	44.6330	162	1068.8065	2116.7712
40	222.1083	0.9694	81	442.2842	588.9546	122	722.0870	0.0000			
41	222.2803	0.0089	82	449.1438	136.3743	123	722.9519	0.0001			

Table 8 (Si₂₄O₃₈) Freq (cm⁻¹), Intensity (km/mol)

	Freq	intensity		Freq	intensity		Freq	intensity		Freq	intensity
1	4.5267	0.0000	46	239.0640	0.0000	91	444.7188	152.7163	136	779.6540	0.0000
2	7.2322	0.0044	47	253.9829	1.0543	92	455.9531	0.0162	137	793.6786	0.9377
3	10.6242	0.1235	48	257.6790	0.8336	93	465.3211	0.3775	138	804.4168	0.4105
4	16.4407	0.0533	49	269.2794	0.9464	94	465.5581	7.1176	139	806.7766	2.0936
5	26.0338	0.0680	50	269.6027	4.7900	95	479.9685	0.2886	140	814.6233	122.9089
6	32.5825	0.0000	51	269.9976	103.6938	96	485.2312	20.6035	141	820.7336	56.6811
7	52.0488	0.2506	52	270.0396	0.0000	97	489.9057	80.2918	142	830.0517	0.0000
8	64.3855	0.0234	53	275.3014	15.7214	98	512.6250	38.8105	143	831.2428	143.6781
9	67.7099	0.1010	54	275.5518	0.0000	99	517.2167	0.0000	144	835.9210	146.0566
10	74.6769	0.0000	55	278.0763	0.0000	100	517.5768	35.7091	145	848.3909	174.5991
11	75.9372	0.5032	56	278.3182	5.3944	101	533.6249	0.0000	146	852.0802	8.0593
12	76.3188	0.2624	57	288.7882	0.2179	102	536.2955	226.5583	147	866.8177	0.0000
13	81.2720	0.0175	58	290.9709	0.0800	103	543.2874	0.0024	148	871.0209	605.5433
14	81.6106	0.4463	59	291.1473	15.5875	104	554.0205	22.6361	149	888.9835	0.0000
15	93.3229	0.0000	60	299.5108	8.8914	105	584.7253	3.0107	150	893.8770	27.4249
16	101.4837	2.2517	61	300.0533	4.1225	106	585.4070	2.6117	151	895.3559	424.3452
17	104.1329	0.0000	62	303.9858	0.0000	107	596.7203	0.0301	152	899.2026	400.5056
18	108.4234	1.9027	63	304.4068	10.8852	108	601.4657	10.4567	153	902.8217	79.7240
19	110.5308	0.6954	64	305.4673	4.5270	109	611.7564	122.8466	154	903.9889	48.0695
20	114.5566	0.0000	65	314.1998	32.3702	110	613.7821	0.0000	155	954.6870	0.0000
21	122.8653	0.0711	66	315.1374	51.4203	111	615.2458	86.3290	156	958.6767	907.2460
22	125.4259	1.2123	67	322.1617	0.0000	112	619.7348	8.2330	157	960.1454	62.8917
23	125.6036	0.0000	68	323.5071	24.7825	113	621.1351	0.0000	158	968.8403	0.0000
24	128.2131	0.0003	69	324.9281	86.3018	114	624.5280	83.0702	159	970.8028	0.1354
25	129.4027	0.0000	70	328.5177	0.9585	115	634.9495	0.0000	160	976.8528	1169.4301
26	133.0215	0.4545	71	330.1739	0.0000	116	635.4719	244.0928	161	979.5729	265.1758
27	134.2937	0.0000	72	335.6162	28.1499	117	650.7478	4.4431	162	996.3300	5509.6074
28	151.4851	0.0130	73	346.1808	0.0000	118	650.8148	131.8195	163	1003.2801	0.0000
29	153.0546	0.0212	74	346.8293	214.9199	119	652.5775	109.8833	164	1006.5722	346.5929

30	155.7250	0.1960	75	348.6846	0.0000	120	656.8099	0.0000	165	1009.6583	0.0000
31	157.9478	0.0000	76	351.8264	163.7585	121	709.7041	0.0000	166	1015.4174	2676.9431
32	161.9719	2.8038	77	352.7833	6.5217	122	709.9298	10.0133	167	1016.6618	1664.2430
33	168.7591	3.2591	78	355.6002	14.0228	123	712.8675	17.3818	168	1034.8029	0.0000
34	170.7401	1.4073	79	355.9556	200.4248	124	713.6085	86.6166	169	1058.0756	400.7080
35	171.3049	0.0359	80	360.6295	3.1156	125	715.0244	59.2417	170	1059.9792	187.5740
36	182.4356	0.2012	81	361.5595	58.2535	126	724.7386	4.3856	171	1084.0123	209.2796
37	189.8830	1.4345	82	363.3171	0.0178	127	724.9959	182.8292	172	1091.2065	0.0000
38	192.3508	5.7595	83	365.3573	0.0000	128	725.1458	32.1457	173	1093.6262	529.6157
39	193.9635	0.0000	84	372.8627	15.8913	129	728.3573	68.5378	174	1096.2823	0.0000
40	209.9752	0.1299	85	384.9734	59.6366	130	728.8752	0.0000	175	1104.8136	52.1242
41	211.8566	2.8184	86	393.3084	0.0000	131	738.2219	110.5214	176	1110.1714	292.5683
42	213.2027	2.1238	87	395.3449	3.3070	132	753.5160	0.0000	177	1131.5959	2347.4250
43	214.4584	0.4579	88	409.8740	1.2874	133	762.8925	85.5429	178	1143.8398	0.0000
44	228.6229	0.6971	89	410.5334	229.1532	134	772.9570	1.3848	179	1143.9194	1607.5699
45	229.7484	0.0832	90	413.0194	0.0000	135	776.8416	92.5735	180	1154.5291	637.2892

Table 9

Wavelength	Oscillator Strength (arb. units)
Si ₁₄ O ₂₀	
256.66 nm	0.019
255.63 nm	0.001
251.67 nm	0.028
251.45 nm	0.063
Si ₁₂ O ₁₈	
373.39 nm	0.002
360.61 nm	0.571
311.60 nm	0.003
311.06 nm	0.112
Si ₁₈ O ₂₄	
378.69 nm	0.475
349.65 nm	0.029

Si ₁₈ O ₂₈	
361.55 nm	0.562
312.23 nm	0.032
312.12 nm	0.007
Si ₁₈ O ₃₀	
243.60 nm	0.001
243.42 nm	0.061
Si ₂₄ O ₃₂	
259.11 nm	0.018
254.33 nm	0.004
253.21 nm	0.002
252.86 nm	0.029
252.85 nm	0.003
Si ₂₄ O ₃₈	
392.38 nm	0.014
358.44 nm	0.510
318.45 nm	0.012
317.30 nm	0.001

