

Reduced Partition Function Ratio in the Frequency Complex Plane: A Mathematical Approach

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Abstract

This paper gives a mathematical approach to calculate the fractionation factor of isotopes in a general cluster (also known as super-molecule), which composes of necessary chemical effect within three bonds outside the interested atom(s). The cluster might have imaginary frequencies after being optimized in quantum softwares. The approach includes the contribution of the difference, which is resulted from the substitution of heavy and light isotopes in the cluster, of vibrations of imaginary frequencies to give precise prediction of isotope fractionation factor. We call the new mathematical approximation “reduced partition function ratio in the frequency complex plane (RPFR_c)”. If there is no imaginary frequency for a cluster, RPFR_c is simplified to be Urey (1947) or Bigeleisen and Mayer (1947) formula. Final results of this new algorithm are in good agreement with those in earlier studies.

Keywords

Isotope Fractionation, Cluster, Reduced Partition Function Ratio, Frequency Complex Plane

1. Introduction

In 1933, Urey and Rittenberg [1] pointed out that the isotopic fractionation factor in different systems could be calculated from spectroscopic data. A more convenient method for the calculation is known as Urey (1947) [2] or Bigeleisen and Mayer (1947) [3] model. This model needs only frequencies to calculate the factor by an equation namely “reduced isotopic partition function ratio (RPFR or β factor)”. However, a practical problem arises, when a cluster (cut from a big system; see details in Section 2.1) has some imaginary frequencies in the sets of

vibrational frequencies [4], RPFRC cannot evaluate the isotope fractionation factor since it does not deal with imaginary frequencies (see details in Section 2.2).

To overcome this difficulty, Rustad *et al.* (2008) [4] applied the partial Hessian vibrational analysis (PHVA) [5] in the carbonate (e.g., calcite, aragonite and magnesite) clusters to predict the distributions of isotopes in these minerals; this operation neglects all imaginary frequencies (as well as some real ones) and then the remainder of real frequencies in the sets are used in RPFRC, giving the carbon isotope fractionation factors in these minerals. But when using PHVA, also neglected is the contribution of the differences (due to the substitution of heavy and light isotopes in clusters) of imaginary frequencies to the isotope fractionation effect [6]. Therefore, previous problem is still under debate.

This study gives a new approach, *i.e.* reduced partition function ratio in the frequency complex plane (RPFRC_C), to the calculation of isotope fractionations in general clusters. This new approach involves a more detailed physical figure of atom vibrations for the calculation than PHVA did; that is, the vibrations of all atoms due to the substitution of heavy and light isotopes in clusters are included to predict the isotope fractionations. This new approach is finally tested by studying isotope fractionation factors in liquid and mineral phases.

2. Theory

2.1. General Cluster for Isotope Research

We firstly give the theoretical background on building a general cluster for isotope research. The general cluster (Figure 1) includes three parts: A) interested isotopic atom(s) of an element at specific position; B) atoms linking three chemical bonds outside the interested atom(s). Stern and Wolfsberg (1966) [7] had theoretically proved that the biggest necessary influence of chemical effects on an interested isotope is within three bonds; and C) atoms to make the system to be converged in softwares. This kind of cluster could model isotope fractionations in both liquid and solid phases. In practical, researchers cut off atoms from a large periodical system to form solid-phase (e.g., calcite and aragonite in Ref. [4]) clusters, and terminate the outside-broken bonds in part B with some hydrogen atoms in part C. For liquid phase, one adds few water molecules (and sometimes few ions [8]) around the interested isotope to simulate its water environments; this technique is also called as “water-droplet” method [4] [9] [10]. For convenience, we represent the general cluster as a super-molecule XA_p , where A and X represent the interested atom and all atoms in parts of both B and C respectively and the subscript p the number of interested atoms of the same element in the center of the cluster (Figure 1(b)).

2.2. Harmonic Frequencies in Complex Plane

As discussed above, the super-molecule is sufficient to describe the chemical influence on isotopes at interested position; then one can use *ab initio* molecular orbital theory to get the frequencies. In Ref. [11], mass-weighted

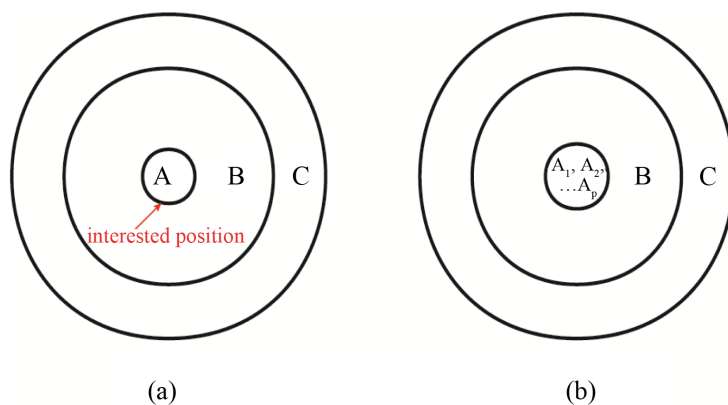


Figure 1. (a) 2-D schematic diagram of general cluster/super-molecule XA for isotope research. A represents the isotope locates at the interested position, *i.e.* the center of the cluster; X represents all atoms in B and C. (b) One more general cluster XA_p , with p interested atoms (A_1, A_2, \dots, A_p) in the center. See details in the text.

force constants are defined by

$$f'_{jk} = f_{jk} m_j^{-1/2} m_k^{-1/2} \tag{1}$$

where m_k is the mass of the k th atom in the molecule, and the force-constant f_{jk} is the second energy derivatives for coordinates R_j and R_k . And the k th normal-mode displacements has the form

$$r_k = a_k \exp(2\pi i \nu t) \tag{2}$$

where

$$\sum_j f'_{jk} a_j = 4\pi^2 \omega^2 a_k \tag{3}$$

in which $4\pi^2 \nu^2$ are the eigenvalues of the matrix f'_{jk} , and ω are the harmonic frequencies (Hz). This equation gives one set of frequencies for the heavy-isotope system and another for the light-isotope system; these two sets of frequencies are used to calculate the isotope fractionation factor.

The two sets of harmonic frequencies for a super-molecule would, however, sometimes have imaginary frequencies [12]. This is due to the fact that one cannot find a local minimal on the potential energy surface for all atoms of the cluster. And there will be some minus force constants in Equation (1). Upon taking the square root of the left hand side of Equation (3) for a minus mass-weighted force constant, a factor of complex unit i will emerge, and there will be some imaginary frequencies for the molecule. Under this case, one cannot use RPFR to calculate the distribution of isotopes in the super-molecule, because only real frequencies are suitable for RPFR.

For a super-molecule, we suggest that all frequencies, *especially the imaginary ones*, should be included in the calculation of isotope fractionation. The reasons come from the following facts [11]: for a random frequency ω_k , Equations (2) and (3) give the displacement (a_k and a_j) of each and every atom in the cluster. In other words, it gives a very important physical figure: all atoms in cluster will have a motion (with amplitude a_j) for frequency ω_k . From this point of view, even an imaginary frequency has motions of all atoms in the molecule, and it will affect the difference of the isotope fractionation as vibrational contribution (see the next subsection).

In mathematics [13], each set of frequencies has characteristic properties. The frequencies can be plotted on the complex plane (Figure 2), which is a geometric representation of the complex numbers established by the real axis and the orthogonal imaginary axis. For a general super-molecule, the eigenvalues of the mass-weighted matrix will have $3N$ frequencies, which might include n imaginary ones, 6 (5) (6, for nonlinear molecular, 5, for linear and diatom molecular) zeros (corresponding to translations and rotations), and $3N - n - 6(5)$ real ones. All non-zero frequencies locate on those two axes, and the zeros at the origin. A real frequency equals its own modulus, *i.e.* $\omega_{\text{real}} = |\omega_{\text{real}}|$; and an imaginary one equals its own modulus multiplying the unit of complex number, *i.e.* $\omega_{\text{imaginary}} = |\omega_{\text{imaginary}}| i$.

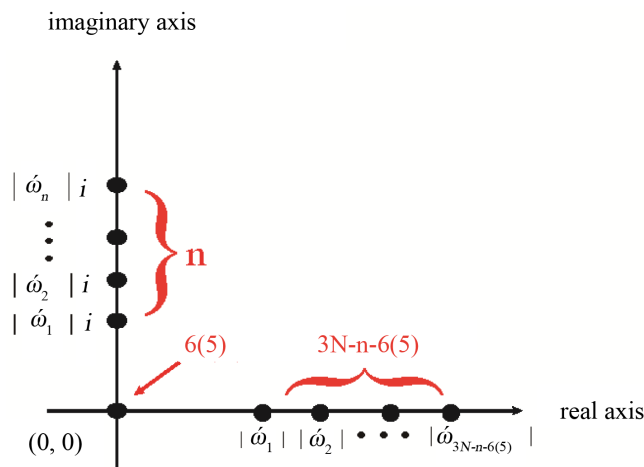


Figure 2. Plots of frequencies for one cluster/super-molecule on the complex plane.

2.3. Evaluation of Partition Function and Free Energy of the Super-Molecule

Based on the *Born-Oppenheimer* approximation (*i.e.* nearly harmonic approximation) [14], the translational and rotational, and vibrational energies are the main contribution to the difference of isotope exchange reactions [2] [3]. The followings discuss the partition functions of these three kinds of energies and give the total free energy for the super-molecule.

The translational and rotational energies are in the form of $E_{trans} = \frac{h^2}{8M} \left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right)$ ($n_{x,y,z} = 1, 2, \dots$) and $E_{rot} = \frac{h^2 J(J+1)}{8\pi^2 I}$ ($J = 0, 1, 2, \dots$) [15], which are all real numbers. So the translational partition function for the super-molecule is

$$Q_{trans} = V \left(\frac{2\pi M k_b T}{h^2} \right)^{3/2} \quad (4)$$

where V is the volume of the cluster, M is the mass of the cluster, k_b is the Boltzmann constant, T is the absolute temperature, h is the Plank constant. And the rotational partition function is

$$Q_{rot} = \frac{8\pi^2 I k_b T}{\sigma h^2} \quad (5)$$

for diatomic and linear molecules

$$Q_{rot} = \frac{\pi^{1/2} (8\pi^2 k_b T)^{3/2} (I_A I_B I_C)^{1/2}}{\sigma h^3} \quad (6)$$

for nonlinear molecules, where σ is the symmetry number of the molecule, and I_A is the moment of inertia with respect to the appropriate principal axis.

The vibrational energy is in the form of $E_{vib} = \sum_{k=1}^n h\omega_k \left(\nu_i + \frac{1}{2} \right)$ (each $\nu_i = 0, 1, 2, \dots$); but the imaginary frequencies cannot be included in this expression and the partition function in the classical mechanism [15]. However, as shown in previous subsection, this study needs to introduce the contribution of all imaginary frequencies into the partition function and free energy to calculate the isotope fractionation factor. Thus, *only for isotope research in ab initio studies*, we suggest the vibrational partition function of the super-molecule to be

$$Q_{vib}^* = \prod_{k=1}^{3N-6(5)} \frac{e^{-\frac{hc|\dot{\omega}_k|}{2k_b T}}}{1 - e^{-\frac{hc|\dot{\omega}_k|}{k_b T}}} \quad (7)$$

where $|\dot{\omega}_k|$ is the modulus of the k th frequency from Equation (3). If $\dot{\omega}_k$ is real, $Q_{vib\ k}^*$ is the vibrational partition function; and if $\dot{\omega}_k$ is imaginary, $Q_{vib\ k}^*$ is defined as imaginary-frequency correction to the vibrational partition function. Thus we call Q_{vib}^* the imaginary-frequency-corrected vibrational partition function. Furthermore, the imaginary-frequency-corrected *Helmholtz* free energy of this super-molecule is given by

$$F^* = -RT \ln(Q^*) \quad (8)$$

where R is gas constant and

$$Q^* = Q_{trans} Q_{rot} Q_{vib}^* \quad (9)$$

2.4. Teller-Redlich Product Rule in the Frequency Complex Plane

In Ref. [16], Equation (3) can also be expressed as

$$[FG] = [F]^* \mu_1 \mu_2 \cdots \mu_N = \lambda_1 \lambda_2 \cdots \lambda_N \quad (10)$$

where $[G]$ is the kinetic energy matrix, μ_k is the reciprocal mass of the k th atom in the molecule, $[F]$ is the force-constant matrix, and

$$\lambda_k = 4\pi^2 \nu_k^2 = 4\pi^2 c^2 \dot{\omega}'_k{}^2 \quad (11)$$

Since $[F]$ will be identical for the molecule of different isotopes with the same method (*i.e.* the same exchange-correlation functional/basis set), now taking Equation (11) into Equation (10) gives

$$\frac{\dot{\omega}'_1 \cdots \dot{\omega}'_{3N}}{\dot{\omega}_1 \cdots \dot{\omega}_{3N}} = \left(\frac{m_1 m_2 \cdots m_{3N}}{m'_1 m'_2 \cdots m'_{3N}} \right)^{1/2} \quad (12)$$

where the superscript “'” denotes the molecule with heavy isotopes.

Let us submit the frequencies with complex form. The number n of complex unit i is dependent on left hand side of Equation (3) and right hand side of Equation (1). Because m_k , m'_k are real and nearly the same for one element, and the force constant matrix f_{ij} is identical for a cluster with given method, n are the same in the numerator and denominator of Equation (12). We get

$$\frac{|\dot{\omega}'_1| \cdots |\dot{\omega}'_k| |\dot{\omega}'_{k+1}| \cdots |\dot{\omega}'_{3N}| i}{|\dot{\omega}_1| \cdots |\dot{\omega}_k| |\dot{\omega}_{k+1}| \cdots |\dot{\omega}_{3N}| i} = \left(\frac{m_1 m_2 \cdots m_{3N}}{m'_1 m'_2 \cdots m'_{3N}} \right)^{1/2} \quad (13)$$

After the cancellation of i , we have

$$\frac{|\dot{\omega}'_1| \cdots |\dot{\omega}'_k| |\dot{\omega}'_{k+1}| \cdots |\dot{\omega}'_{3N}|}{|\dot{\omega}_1| \cdots |\dot{\omega}_k| |\dot{\omega}_{k+1}| \cdots |\dot{\omega}_{3N}|} = \left(\frac{m_1 m_2 \cdots m_{3N}}{m'_1 m'_2 \cdots m'_{3N}} \right)^{1/2} \quad (14)$$

Equation (14) is valid only when $3N$ motions are vibrational normal modes. We consider those 6 (5) motions, corresponding to translational and rotational motions, convert of low frequency corresponding to weak forces. Then the ratio for the translational frequencies and rotation frequencies can be written as:

$$\frac{|\dot{\omega}'_T|}{|\dot{\omega}_T|} = \left(\frac{M}{M'} \right)^{1/2} \quad (15)$$

$$\frac{|\dot{\omega}'_R|}{|\dot{\omega}_R|} = \left(\frac{I}{I'} \right)^{1/2} \quad (16)$$

Submitting Equations (15) and (16) into Equation (14), we obtain the Teller-Redlich product rule in the frequency complex plane:

$$\prod_{k=1}^{3N-5} \frac{|\dot{\omega}'_k|}{|\dot{\omega}_k|} = \prod_{i=1}^{3N} \left(\frac{m_i}{m'_i} \right)^{1/2} \left(\frac{M'}{M} \right)^{3/2} \left(\frac{I'}{I} \right) \quad (17a)$$

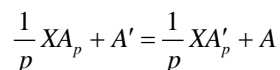
for diatom and linear molecules and

$$\prod_{k=1}^{3N-6} \frac{|\dot{\omega}'_k|}{|\dot{\omega}_k|} = \prod_{i=1}^{3N} \left(\frac{m_i}{m'_i} \right)^{1/2} \left(\frac{M'}{M} \right)^{3/2} \left(\frac{I'_A I'_B I'_C}{I_A I_B I_C} \right)^{1/2} \quad (17b)$$

for nonlinear molecules.

3. Reduced Partition Function Ratio in Frequency Complex Plane

The differences for the isotopes in the super-molecule can be written as a typical chemical exchange reaction [2] [3]:



where A and A' represent light and heavy isotope respectively, and p is the number of interested atoms in the molecule.

The equilibrium constant for this reaction is given by

$$K = \exp(-\Delta G/RT) \quad (18)$$

Because different isotopes have negligible difference of volume, isotope exchange reactions do not involve significant pressure-volume work [15]. The *Gibbs* free energy is equivalent to the *Helmholtz* free energy and we take Equation (8) into Equation (18), K can be written as partition function ratio:

$$K = \left(\frac{Q^*(XA'_p)}{Q^*(XA_p)} \right)^{1/p} \bigg/ \frac{Q(A')}{Q(A)} \quad (19)$$

Let us substitute Equations (5)-(8) into Equation (19). For diatom and linear molecules, we have

$$K = \left(\frac{m(A)}{m(A')} \right)^{3/2} \left(\frac{M(XA'_p)}{M(XA_p)} \right)^{3/2} \frac{\sigma_{XA_p}}{\sigma_{XA'_p}} \frac{I(XA'_p)}{I(XA_p)} \prod_k^{3N-5} \left(\frac{e^{-u_k(XA'_p)/2}}{1 - e^{-u_k(XA'_p)}} \right) \times \left(\frac{e^{-u_k(XA_p)/2}}{1 - e^{-u_k(XA_p)}} \right)^{-1} \bigg)^{1/p} \quad (20a)$$

and for nonlinear molecules,

$$K = \left(\frac{m(A)}{m(A')} \right)^{3/2} \left(\frac{M(XA'_p)}{M(XA_p)} \right)^{3/2} \frac{\sigma_{XA_p}}{\sigma_{XA'_p}} \frac{I_A(XA'_p)I_B(XA'_p)I_C(XA'_p)}{I_A(XA_p)I_B(XA_p)I_C(XA_p)} \prod_k^{3N-6} \left(\frac{e^{-u_k(XA'_p)/2}}{1 - e^{-u_k(XA'_p)}} \right) \times \left(\frac{e^{-u_k(XA_p)/2}}{1 - e^{-u_k(XA_p)}} \right)^{-1} \bigg)^{1/p} \quad (20b)$$

where $u_k = hc|\dot{\omega}_k|/k_bT$.

Equation (20) can be reduced to a more general expression by using Equation (17):

$$\text{RPFR}_C[XA_p] = \left(\frac{\sigma_{XA_p}}{\sigma_{XA'_p}} \prod_k^{3N-6(5)} \frac{u_k(XA'_p) \exp[-u_k(XA'_p)/2] \{1 - \exp[-u_k(XA_p)]\}}{u_k(XA_p) \exp[-u_k(XA_p)/2] \{1 - \exp[-u_k(XA'_p)]\}} \right)^{1/p} \quad (21)$$

where RPFR_C is short for reduced partition function ratio in the frequency complex plane.

Obviously, one can see that if the super-molecule is at a local minimal on the potential energy surface (*i.e.* $n = 0$), all frequencies locate on the real-axis in the frequency complex plane (Figure 2). In such case, RPFR_C becomes Urey (1947) or Bigeleisen and Mayer (1947) formula. Due to the fact that the set of real numbers (*i.e.* frequencies here) is the subset of the set of the complex numbers [13], the set of fractionation factors given by Urey (1947) or Bigeleisen and Mayer (1947) formula (*i.e.* RPFR) is the subset of the set of fractionation factors given by Equation (21) (*i.e.* RPFR_C) (Figure 3). In other words, this work extends Urey and Rittenberg's (1933) idea [1] to focus on isotope fractionation research in the frequency complex plane.

The fractionation factor between two clusters can be written as:

$$\alpha = \text{RPFR}_{C1}/\text{RPFR}_{C2} \quad (22)$$

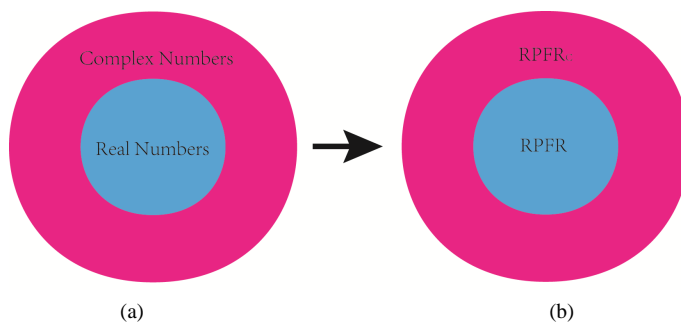


Figure 3. (a) The set of real numbers (*i.e.* frequencies here) is a subset of the set of the complex numbers; (b) The set of RPFR is a subset of the set of RPFR_C . The arrow indicates the process of the calculation of the isotope fractionation factors. Using real frequencies and imaginary ones in the calculations give RPFR and RPFR_C , respectively.

4. Tests of Present Approach

To understand the new algorithm, we compute RPFR_C and/or α in typical isotope systems. Two examples are depicted below not for the accuracy prediction of experimental data, but for the abilities of our algorithm. All frequencies needed in RPFR_C are implemented in Gaussian09 [12]. The optimized geometries and frequencies for all examples are presented in the “Electronic supplementary materials”. Present RPFR_C and α results are compared with corresponding references, *i.e.* those previously calculated from all real frequencies in published literatures. The difference ε (in %) between present result and the reference is in the form of $\varepsilon = (\text{RPFR}_C/\text{RPFR}_{ref} - 1) * 1000$ or $\varepsilon = (\alpha/\alpha_{ref} - 1) * 1000$.

1) The germanium isotope fractionation factor α between $\text{GeO}(\text{OH})_3^{-1}-(\text{H}_2\text{O})_{30}$ (Figure 4(a)) and $\text{Ge}(\text{OH})_4-(\text{H}_2\text{O})_{30}$ (Figure 4(b)) (corresponding to $\text{GeO}(\text{OH})_3^{-1}-(\text{H}_2\text{O})_{30_B}$ and $\text{Ge}(\text{OH})_4-(\text{H}_2\text{O})_{30_D}$ in Ref. [10] respectively) is a good example of study of isotopes in liquid phase. After optimized, each cluster has an imaginary frequency (Table 1). When calculating α , Li *et al.* (2009) neglected the imaginary frequencies because 1) the main vibration vector of this imaginary frequency belongs to a water molecule located at outside of the super-molecule; 2) it is less than 50 cm^{-1} ; and 3) RPFR is the same if they neglected it. The values of Li *et al.*'s α s at different temperatures are taken as references. As shown in Figure 5, the maximum difference ε_{\max} be-

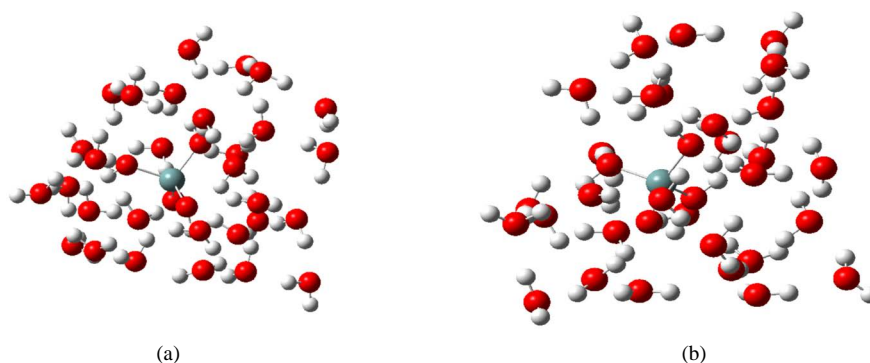


Figure 4. Water-droplets for a) $\text{GeO}(\text{OH})_3^{-1}-(\text{H}_2\text{O})_{30}$, and b) $\text{Ge}(\text{OH})_4-(\text{H}_2\text{O})_{30}$ (cyan germanium, gray hydrogen, red oxygen). The optimized structures and frequencies are taken from Li *et al.* (2009).

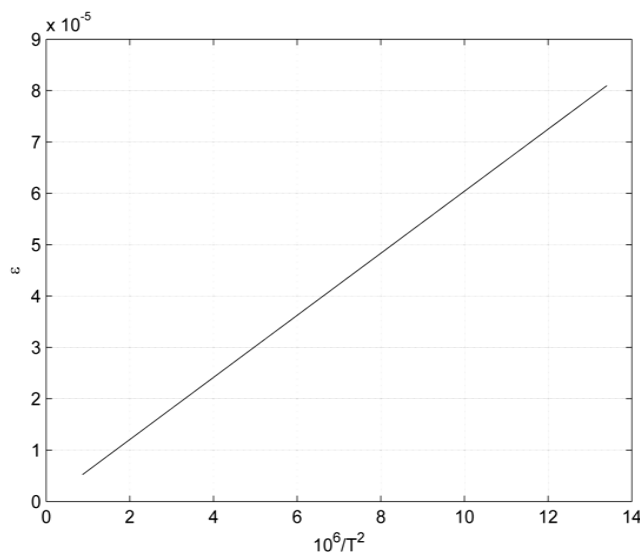


Figure 5. ε α $\text{Ge}(\text{OH})_4-(\text{H}_2\text{O})_{30}-\text{GeO}(\text{OH})_3^{-1}-(\text{H}_2\text{O})_{30}$ versus $T(\text{K})$. The corresponding reference α s are from Li *et al.* (2009).

tween Li *et al.*'s and present results is $8.2 \times 10^{-5}\text{‰}$ (273.15 K); this shows that present approach is very efficient to study isotope fractionation in liquids.

2) The carbon and ^{13}C - ^{18}O clumped isotope fractionations in inner body of calcite are good examples of study of isotopes in solid phase. We cut a cluster (**Figure 6**) from the periodical calcite, of which the primitive cell parameters (**Table 2**) are calculated in CRYSTAL06 [17], by the way published in Rustad *et al.* (2008). The fitted polynomials of $\alpha_{\text{CaCO}_3\text{-C}}$ and K3866 in Ref. [18] are taken as references.

Results shown in **Figures 7-9** indicate that our new algorithm have high accuracy. For $\alpha_{\text{CaCO}_3\text{-C}}$ in **Figure 7**, ε_{max} s are -10.2‰ (273.15 K) and -4.8‰ (273.15 K) for HF/3-21G/0.91 (the scaling factor) and B3LYP/6-31G/0.97 [19]-[21] levels, respectively; and the difference of ε_{max} s between present results and data given by PHVA in Rustad *et al.* (2008) are -0.1‰ ($=-4.1\text{‰} - (-4\text{‰})$, 298.15 K) and -3‰ ($=-7\text{‰} - (-4\text{‰})$, 298.15 K) for HF/3-21G/0.91 and B3LYP/6-31G/0.97 levels, respectively. For K3866 in **Figure 8** and **Figure 9**, ε_{max} s between present result and data given by Schauble *et al.* (2006) are 0.015‰ (273.15K) and -0.031‰ (273.15K) for HF/3-21G/0.91 and B3LYP/6-31G/0.97 levels, respectively. It seems clear that K3866 is not sensitive to the exchange-correlation functional/basis set/scaling factor, the number of imaginary frequency n and the magnitude of the frequencies (shown in **Table 1** and the "Electronic supplementary materials").

Table 1. Methods/basis_sets/scaling factors¹ used in Gaussian09 and the results of super-molecules.

Super-molecule	Method/Basis_set/Scaling factor	Imaginary Frequency (cm^{-1}) [*]		
		n	Minimal	Maximal
$\text{GeO}(\text{OH})_3^{-1} - (\text{H}_2\text{O})_{30}$	B3LYP/6-311+G**/1.05 ²	1	-5.07	-5.07
$\text{Ge}(\text{OH})_4 - (\text{H}_2\text{O})_{30}$	B3LYP/6-311+G**/1.05 ²	1	-22.23	-22.23
Calcite cluster	HF/3-21G/0.91	76	-7119.47	-11.93
Calcite cluster	B3LYP/6-31G/0.97	151	-3321.80	-69.95

¹<http://cccbdb.nist.gov/>. ²See Ref. [10]. n is the number of imaginary frequency. ^{*}The frequencies correspond to molecules with ^{70}Ge , $^{12}\text{C}^{16}\text{O}$.

Table 2. Primitive cell parameter of calcite from CRYSTAL06, with B3LYP/(Ca_86-511d3G, C_6-21Gd, O_8-411d1)¹.

$a = b = c$ (Å)	$\alpha = \beta = \gamma$ (°)	Volume (Å ³)
6.47	45.90	127.64

¹<http://www.crystal.unito.it>.

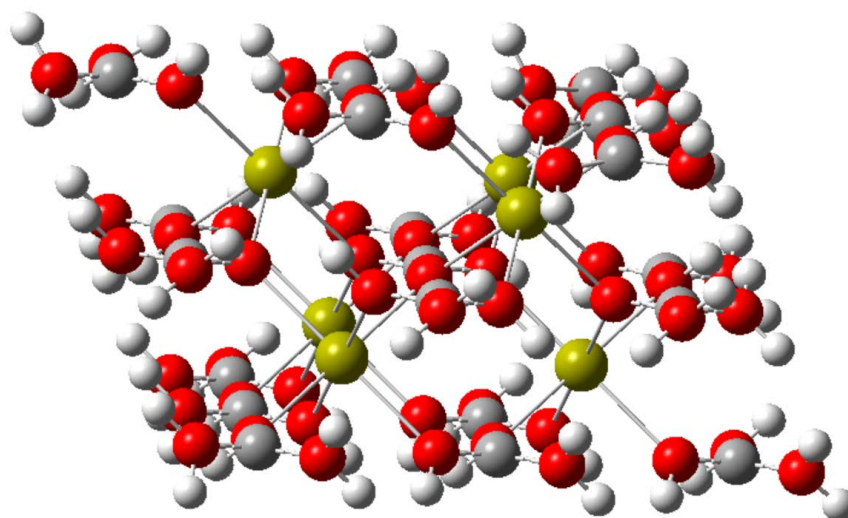


Figure 6. Cluster for calcite (dark gray—carbon, gray—hydrogen, red—oxygen, and yellow—calcium) extracted by the way in Rustad *et al.* (2008). The length of each O-H bond is 0.96 Å, and the charge of H is 0.333.

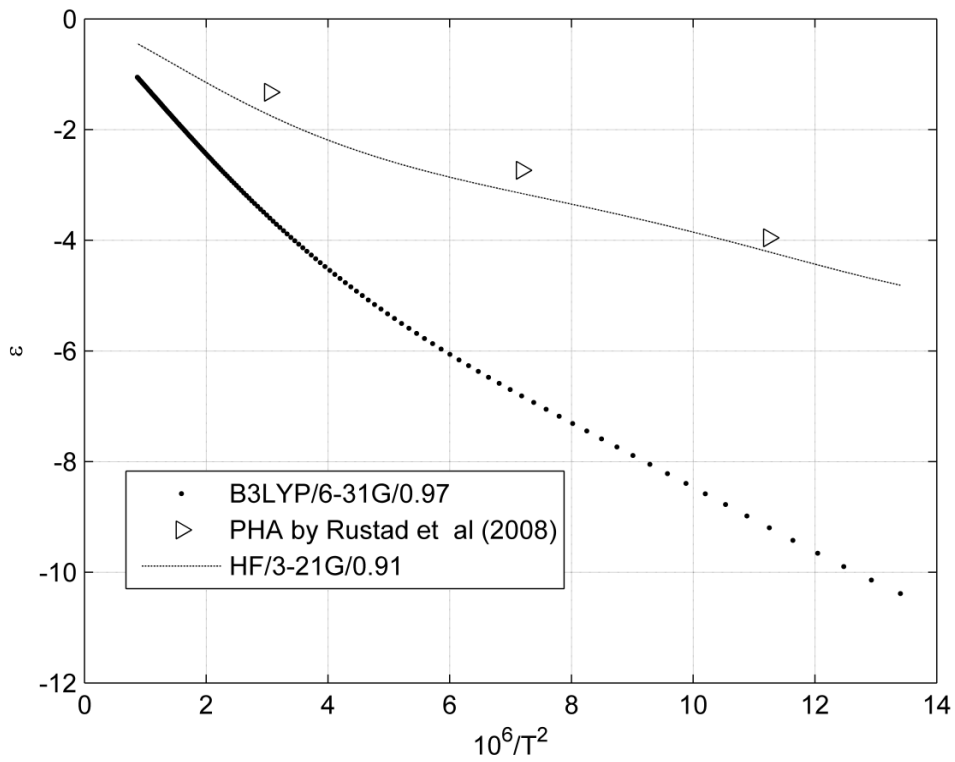


Figure 7. ϵ $\alpha_{\text{CaCO}_3\text{-C}}$ versus T(K). The reference $\alpha_{\text{CaCO}_3\text{-C}}$ s are from Schauble *et al.* (2006).

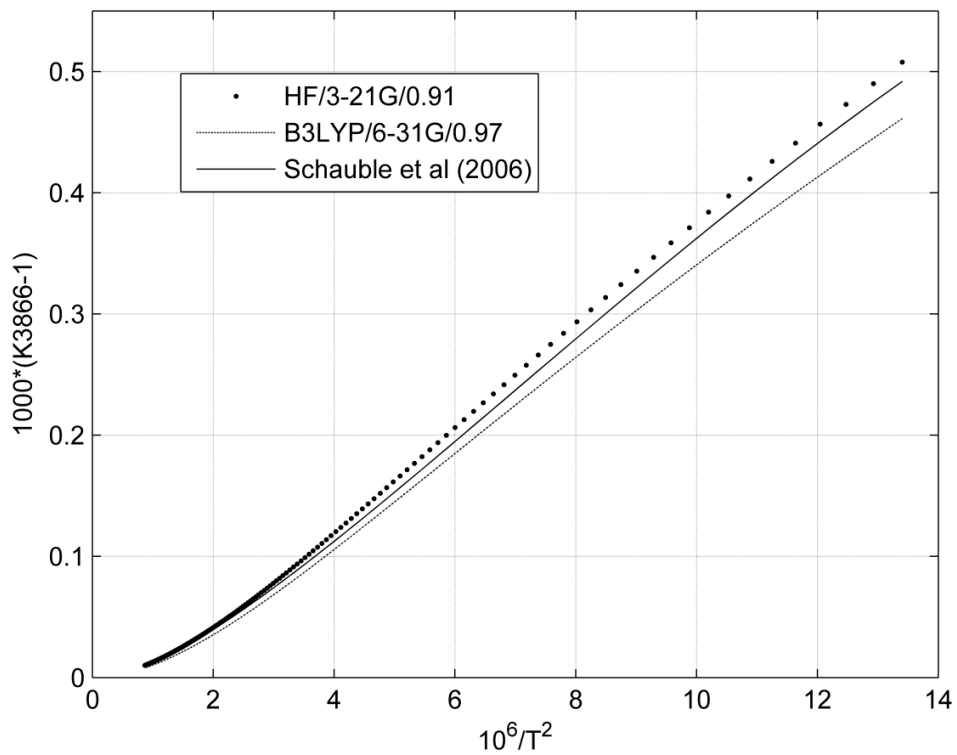


Figure 8. Comparison of K3866s versus T(K). Present K3866s are given by Equation (21) at HF/321G/0.91 (dots) and B3LYP/631G/0.97 (solid) levels. Schauble *et al.*'s (2006) K3866s (bold solid) are given by lattice dynamics.

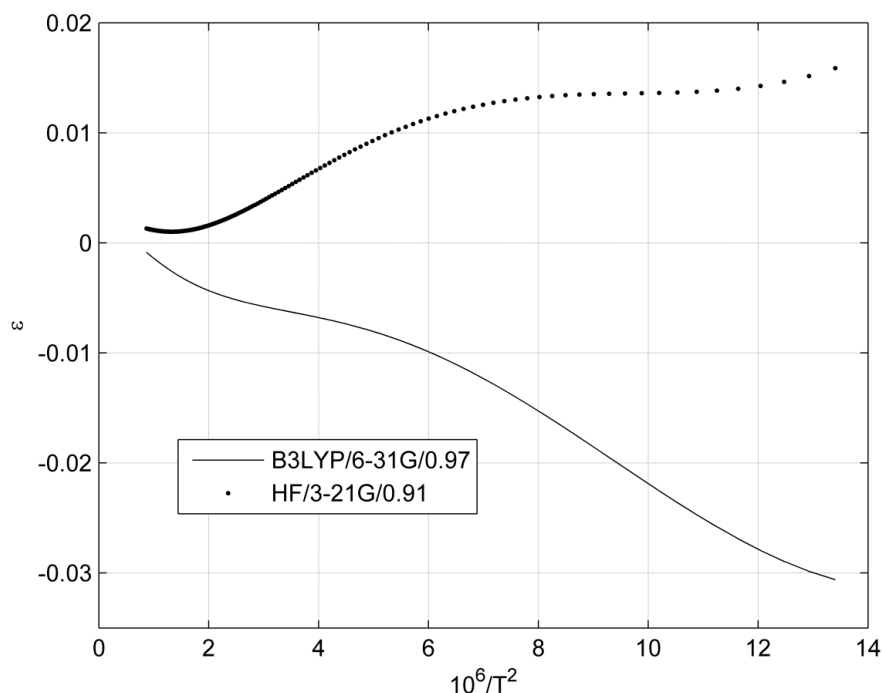


Figure 9. ϵ K3866 versus T(K). The reference K3866 is from Schauble *et al.* (2006).

5. Conclusion

For a general cluster for isotope research (defined in Section 2.1), we have a new Equation (21) to calculate the isotope fractionation factor in the cluster. The calculation based on this equation has a clearer background of physical mechanism, which includes the contribution of vibrations of all atoms to the factor, than that based on PHVA. If there is no imaginary frequencies for the cluster, Equation (21) is simplified to be the Urey (1947) or Bigeleisen and Mayer (1947) formula. The examples show that our new algorithm is valid and efficient with high accuracy. Although the accuracy is mathematically high, we again address that present approach should be only used to calculate the isotope fractionation factor.

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Electronic Supplementary Materials**Optimized Geometries and Frequencies (cm⁻¹) of All Clusters in the Text****1. GeO(OH)₃⁻-(H₂O)₃₀, Optimized Geometry (B3LYP/6-311+G(d,p))**

32	-0.596615	-0.016176	0.000428
8	-1.344083	-1.535373	-0.256154
8	0.759944	0.495686	-1.052984
1	0.443163	0.681858	-1.974307
8	-1.786742	1.350206	-0.118265
1	-2.720088	1.028346	-0.088157
8	0.191339	0.087024	1.623802
1	0.004685	-0.737764	2.138406
8	-0.250691	-2.287403	2.973304
1	0.019361	-2.930021	2.282848
1	-1.228588	-2.307321	2.948463
8	2.953986	-0.371657	1.902444
1	2.050203	-0.124577	1.629309
1	3.137374	-1.223120	1.446393
8	0.060105	4.615808	-0.759392
1	0.739234	3.964630	-0.477242
1	0.599742	5.282466	-1.211689
8	-0.289293	0.876900	-3.531483
1	-0.901161	0.113044	-3.510001
1	-0.824485	1.685431	-3.374504
8	-1.755047	3.706872	1.253116
1	-1.690600	2.869490	0.738934
1	-1.265590	4.352361	0.712271
8	3.389510	2.367456	2.131182
1	3.576766	1.417751	2.025324
1	2.924444	2.401424	2.990733
8	-1.670071	3.015607	-2.456210
1	-1.074243	3.692920	-2.086833
1	-1.856875	2.457840	-1.680515
8	2.162197	2.813700	-0.259564
1	2.575669	2.715749	0.637460
1	1.738555	1.956790	-0.475235
8	-4.377005	2.993431	1.696156
1	-3.523570	3.461707	1.550722
1	-4.983659	3.636559	2.074156
8	-3.181781	0.706008	3.265501
1	-2.343752	1.159156	3.480253
1	-3.719911	1.386249	2.832853
8	-2.911860	-1.838524	2.088474
1	-2.443170	-1.743903	1.226000
1	-3.001797	-0.937950	2.469805
8	-0.658478	2.071125	3.370753
1	-0.302726	1.433256	2.715372
1	-0.905982	2.848861	2.839829
8	2.137763	-1.312646	4.387196
1	1.247248	-1.616254	4.140448
1	2.495543	-0.920032	3.560275
8	0.393874	-3.491482	0.549170

1	0.284286	-4.281461	-0.021179
1	-0.227554	-2.821388	0.163978
8	-1.940404	-1.379942	-2.887707
1	-1.782683	-1.515882	-1.912623
1	-2.859030	-1.073731	-2.957104
8	1.934450	1.952057	4.580577
1	2.013396	1.014557	4.808848
1	0.997211	2.080198	4.346005
8	2.685883	5.221302	-1.833844
1	3.157977	5.016948	-2.647923
1	2.762427	4.407197	-1.310465
8	-4.483698	0.827015	-0.170051
1	-4.866731	0.023592	0.283481
1	-4.729783	1.607381	0.356255
8	3.523484	-3.658566	3.670302
1	3.192271	-4.436502	4.127411
1	3.082582	-2.889803	4.092676
8	3.144140	-2.957518	0.949211
1	2.213532	-3.187023	0.738114
1	3.337150	-3.377177	1.810134
8	4.597973	-2.272653	-1.443332
1	4.249163	-2.608847	-0.599296
1	3.805391	-2.173335	-2.005481
8	3.971820	2.066121	-2.562518
1	3.474098	2.275912	-1.757844
1	4.672941	1.448873	-2.261045
8	-4.622492	-0.191863	-2.707139
1	-4.613120	0.336281	-1.875300
1	-4.945259	0.393223	-3.399227
8	0.094938	-5.351034	-1.479023
1	0.066776	-4.701081	-2.224952
1	-0.605132	-5.985306	-1.651906
8	2.154240	-1.645105	-2.764170
1	1.787052	-1.130723	-2.027964
1	2.341278	-0.952721	-3.448065
8	0.062239	-3.445681	-3.426849
1	-0.699771	-2.843083	-3.412012
1	0.839447	-2.866540	-3.286664
8	-5.565204	-2.680908	-1.715460
1	-5.326260	-1.869024	-2.200186
1	-4.867932	-3.311400	-1.922399
8	5.794520	0.199586	-1.553250
1	6.163317	0.385340	-0.685046
1	5.406249	-0.706661	-1.488260
8	-5.418074	-1.452748	0.853642
1	-5.538109	-2.031146	0.077259
1	-4.657728	-1.812485	1.353188
8	2.453482	0.523722	-4.378814
1	2.977952	1.141617	-3.826756
1	1.532754	0.824715	-4.319686
Frequencies (not scaled) Ge-70:			
	-5.0668	25.2219	26.4774
	29.6821	31.2812	36.9882

39.3241	41.7256	44.9236
45.8672	46.9418	52.7282
53.8094	55.8579	60.1392
61.7466	63.3261	65.0698
66.5297	67.7003	70.2875
72.7825	75.2523	78.5047
79.7737	80.2059	82.0553
85.3947	86.1371	87.8570
90.6197	92.3606	94.4506
100.3336	102.2077	104.4558
107.0900	113.0834	115.4630
117.7642	122.6070	124.1292
128.0350	133.3625	133.7584
142.5061	147.1630	149.0385
151.7565	154.9620	156.6984
158.3733	161.3337	164.5697
168.2300	170.2515	175.2665
177.5458	181.9390	183.0915
184.4559	187.1509	188.6533
193.3047	194.7912	196.8093
200.1663	201.7391	205.8319
209.1525	212.5839	215.3375
217.8708	221.6336	225.1870
226.7962	229.8237	232.5719
237.8976	241.9078	245.5392
246.6430	247.8012	252.8295
255.7949	261.4463	263.6154
268.0495	269.9882	274.9185
277.9186	282.2063	290.5162
294.0692	298.1378	299.3166
306.5849	313.3274	322.4475
331.3289	349.5706	360.9171
364.6439	403.6281	420.6451
427.5643	450.2329	459.3963
463.4651	464.3607	468.8695
476.1623	481.2151	492.9559
503.9212	509.8416	511.5846
516.0270	541.6527	542.9077
547.7866	556.6044	560.3100
563.3569	571.6951	583.1350
584.8075	592.2609	594.9964
600.0935	604.5080	610.8354
613.1408	621.1667	625.4198
627.5091	634.5696	636.6863
643.2582	646.4700	653.2778
658.0664	659.8531	667.8292
669.0935	680.9367	681.8844
686.4149	692.3493	698.5058
699.4740	707.6462	719.1321
723.1163	729.0044	733.3574
738.8622	747.3382	761.4976
766.9444	770.3838	775.3964
782.0801	784.6794	794.8085

807.3475	812.2181	816.9983
821.4843	836.5895	840.7348
854.0293	855.9679	863.1113
871.5906	881.6800	892.9068
908.1346	911.2110	919.8440
921.6876	929.5758	935.3924
953.3906	982.5497	1005.9739
1010.4208	1023.2002	1033.2698
1035.8893	1059.6119	1096.4750
1217.8723	1243.5883	1252.8465
1647.3773	1649.8385	1654.6022
1664.2926	1666.0608	1670.3453
1672.3593	1673.5404	1681.0771
1683.2199	1684.8552	1688.1825
1690.5686	1693.9056	1697.0781
1700.2305	1702.3239	1703.2890
1704.0138	1705.4095	1707.3200
1710.0453	1713.1124	1719.9819
1722.3737	1725.2227	1727.4139
1734.4425	1738.0789	1740.3854
3139.4735	3173.1036	3264.0573
3276.2085	3279.2707	3307.9602
3312.4005	3332.1576	3350.8184
3366.9917	3393.3387	3405.0437
3409.5885	3449.8980	3463.4164
3466.6185	3473.8176	3476.9342
3485.1213	3496.5444	3498.2129
3505.5025	3509.8664	3515.0034
3530.9420	3544.1369	3546.2703
3548.3123	3561.4907	3562.9984
3580.5408	3588.5519	3596.5550
3598.1483	3606.7150	3608.6345
3611.0240	3631.4225	3639.9418
3644.3322	3655.3541	3669.7740
3675.5280	3677.9754	3682.0254
3685.9738	3695.0533	3695.5546
3699.0678	3720.0607	3724.2312
3736.9712	3743.2078	3748.3595
3764.0547	3778.6409	3871.2555
3873.3062	3880.5070	3882.0263
3885.7924	3888.5458	3895.7477
Frequencies (not scaled) Ge-74:		
-5.0643	25.2133	26.4674
29.6708	31.2793	36.9845
39.2968	41.6789	44.9075
45.8075	46.9055	52.7095
53.7415	55.7294	60.1157
61.7143	63.2936	64.9343
66.5190	67.6923	70.2713
79.7200	80.0094	81.9800
85.3455	86.1141	87.8169
90.6059	92.3203	94.3766
100.3308	102.1357	104.4006

107.0656	113.0744	115.4538
117.6493	122.5855	124.1085
127.9737	133.3224	133.7436
142.4367	147.0887	148.8962
151.5739	154.9430	156.6208
158.3356	161.1584	164.5454
168.1628	170.1113	175.1637
176.8799	181.8885	182.9734
184.3915	187.1507	188.6341
193.2785	194.7849	196.7696
200.1267	201.5844	205.7502
208.7339	212.4106	215.2986
217.8011	221.5395	225.1432
226.6914	229.7992	232.5563
237.7252	241.8830	245.5309
246.6399	247.7760	252.8223
255.6675	261.4198	263.5830
267.9678	269.9575	274.7377
277.8046	282.2005	290.5083
293.9856	298.0922	299.2603
306.4116	313.2903	322.0383
330.7451	348.8647	360.6636
364.1913	403.6273	420.6422
427.5643	450.2132	459.3936
463.4534	464.3587	468.8661
476.1612	481.2143	492.9507
503.9182	509.8331	511.5522
516.0053	541.6493	542.9005
547.7711	556.5982	560.3098
563.3369	571.6622	583.1215
584.7932	592.1727	594.9515
600.0891	604.4338	610.7464
612.8143	621.0248	625.2868
627.3615	634.2759	634.9881
642.8499	646.1902	652.9881
657.9451	659.5618	666.9272
668.8740	679.2008	681.5888
686.2180	692.3272	698.3964
699.4308	707.6221	719.0922
722.9846	728.9587	733.3143
738.7843	747.3133	761.4888
766.9324	770.3400	775.3799
781.9760	784.6409	794.7308
804.4872	812.1692	816.8852
820.7164	836.5632	840.7292
854.0113	855.9532	863.0288
871.5387	881.6729	892.8805
908.1313	911.1394	919.8339
921.6810	929.5656	935.3104
953.3631	982.5350	1005.9565
1010.4001	1023.1979	1033.2637
1035.8835	1059.6006	1096.4746
1217.7390	1243.5246	1252.7315

1647.3771	1649.8385	1654.6021
1664.2922	1666.0583	1670.3450
1672.3591	1673.5403	1681.0762
1683.2195	1684.8550	1688.1822
1690.5684	1693.9055	1697.0776
1700.2301	1702.3236	1703.2876
1704.0127	1705.4093	1707.3197
1710.0450	1713.1124	1719.9809
1722.3735	1725.2223	1727.4132
1734.4419	1738.0774	1740.3852
3139.4729	3173.0991	3264.0540
3276.2045	3279.2696	3307.9592
3312.4002	3332.1575	3350.8181
3366.9916	3393.3342	3405.0437
3409.5862	3449.8969	3463.4157
3466.6183	3473.8166	3476.9331
3485.1202	3496.5443	3498.2128
3505.5018	3509.8663	3515.0034
3530.9411	3544.1367	3546.2701
3548.3123	3561.4907	3562.9981
3580.5407	3588.5518	3596.5547
3598.1481	3606.7150	3608.6331
3611.0237	3631.4224	3639.9416
3644.3322	3655.3538	3669.7739
3675.5276	3677.9754	3682.0254
3685.9734	3695.0532	3695.5546
3699.0677	3720.0605	3724.2312
3736.9709	3743.2077	3748.3594
3764.0546	3778.6409	3871.2555
3873.3062	3880.5070	3882.0263
3885.7924	3888.5458	3895.7477

2. $\text{Ge}(\text{OH})_4\text{-(H}_2\text{O)}_{30}$, Optimized Geometry (B3LYP/6-311+G(d,p))

32	-0.169708	0.490256	-0.101782
8	-0.891759	-1.088721	0.147186
1	-0.372608	-1.885699	-0.162666
8	1.563547	0.206411	-0.387786
1	2.063147	0.960311	-0.808992
8	-0.843853	1.361120	-1.507174
1	-1.554320	2.028714	-1.273462
8	-0.489885	1.547516	1.283691
1	0.015041	1.305742	2.137938
8	0.308410	-3.380269	-0.467372
1	1.219966	-3.308631	-0.801008
1	-0.264685	-3.749271	-1.197788
8	0.843576	0.998221	3.424687
1	1.658254	0.535809	3.134690
1	0.336770	0.344851	3.969448
8	2.981069	-0.077766	2.059751
1	3.151125	-1.039648	2.230560
1	2.488563	-0.081917	1.218333
8	3.161997	2.022119	-1.466740

1	2.756477	2.798762	-1.869894
1	3.541823	1.478845	-2.215991
8	2.597711	3.593111	2.536002
1	2.205636	2.942842	3.135257
1	3.410980	3.185959	2.195100
8	0.555272	4.122492	0.693978
1	0.160803	3.257350	0.908568
1	1.317435	4.179168	1.305192
8	-2.157525	-2.072939	2.387490
1	-2.663451	-2.855404	2.073979
1	-1.791689	-1.663488	1.576744
8	0.309696	-3.699087	2.355611
1	0.305094	-3.871802	1.395106
1	-0.458359	-3.114863	2.491605
8	-2.831201	3.053244	-0.950664
1	-3.131604	2.773035	-0.052546
1	-2.527179	3.970516	-0.814692
8	2.903877	-2.346783	-0.757707
1	3.788198	-2.234659	-1.154105
1	2.496107	-1.463748	-0.780180
8	3.080141	-2.764213	2.083892
1	2.197744	-3.079709	2.347050
1	3.091488	-2.834408	1.112308
8	-0.646410	-0.941581	4.626691
1	-1.312208	-1.289875	4.010787
1	-0.186013	-1.732287	4.963951
8	-4.355576	-0.273205	1.473923
1	-4.105236	0.647956	1.669969
1	-3.781285	-0.827826	2.024977
8	-3.197368	2.293213	1.651360
1	-3.319966	3.153361	2.106303
1	-2.253459	2.065901	1.744417
8	-1.333635	-4.117032	-2.416626
1	-2.260963	-3.942573	-2.183054
1	-1.120241	-3.511123	-3.159592
8	-4.458870	-0.889447	-1.182750
1	-4.909196	-0.131558	-1.602610
1	-4.406493	-0.673995	-0.218965
8	-2.505783	-0.252533	-3.167352
1	-3.049982	-0.655888	-2.463048
1	-1.876769	0.298868	-2.670384
8	-4.810617	1.526105	-2.654827
1	-4.351449	2.217416	-2.152734
1	-4.118511	1.148010	-3.218839
8	5.447310	-1.532561	-1.753408
1	6.128468	-2.095815	-2.134663
1	5.900085	-0.966610	-1.078679
8	4.049087	0.365921	-3.328389
1	4.570174	-0.352873	-2.926085
1	3.305140	-0.038327	-3.811975
8	-1.659830	5.475752	0.118574
1	-0.757352	5.122410	0.340934
1	-1.532212	6.333522	-0.298467

8	4.647910	1.885172	1.028067
1	4.148960	1.160779	1.463045
1	4.175263	2.067773	0.195242
8	6.594152	0.156687	0.039851
1	7.179097	-0.109557	0.755298
1	6.005328	0.852023	0.412059
8	-4.064501	-3.553669	-1.440730
1	-4.805431	-4.007242	-1.856060
1	-4.310997	-2.596506	-1.416687
8	1.621749	-0.315308	-4.666636
1	1.695099	-0.327285	-5.627085
1	1.243127	0.561545	-4.434560
8	-0.766575	-2.156433	-4.306221
1	0.083617	-1.693766	-4.357868
1	-1.416104	-1.476753	-4.038728
8	-3.433825	-4.229589	1.223869
1	-2.992468	-5.084296	1.224070
1	-3.690367	-4.054711	0.295513
8	0.684981	2.104095	-3.701568
1	0.195863	2.743542	-4.228966
1	0.125078	1.910628	-2.920334
8	-3.260165	4.939510	2.377751
1	-2.708552	5.307102	1.660372
1	-3.014833	5.399151	3.185657
8	0.654477	-3.424814	5.128548
1	0.467173	-4.116740	5.768920
1	0.666824	-3.849176	4.254563

Frequencies (not scaled) Ge-70:

-22.2257	19.6523	28.3783
33.0113	33.5203	35.2689
37.7866	44.6476	44.9917
46.0637	48.5373	49.8224
50.8145	53.3679	55.7730
56.8876	59.0893	60.5302
61.0407	64.9039	67.2880
69.3018	69.6522	70.4868
73.5490	75.2931	76.7631
77.1337	80.3302	81.3045
84.0066	87.7519	90.8378
92.1415	94.6306	104.2453
106.0577	108.7853	109.2310
111.6486	115.2207	115.9120
120.4108	124.2837	125.5232
135.3280	139.2283	144.0345
144.6376	149.4271	153.5566
156.2225	158.3019	158.8944
162.4860	165.5643	168.5052
172.6976	173.7904	178.2958
178.4836	181.8807	186.2633
190.2791	192.8613	196.3889
198.7425	202.0265	204.6728
207.8245	213.7474	214.0551
218.7214	219.5876	226.0944

231.1274	235.5255	242.1860
244.5260	248.6356	254.5778
256.3999	256.7121	258.7711
266.7019	269.7869	278.6038
281.6766	286.6844	289.6794
289.9550	308.0023	311.6381
315.1413	318.5303	323.3357
328.2466	328.7730	338.7565
342.2524	346.9835	349.1994
354.0360	361.1901	374.1939
385.5776	412.1751	421.1706
427.6115	438.1148	439.4553
447.6792	451.3011	467.0777
473.4897	477.8566	479.7783
482.3430	497.1452	508.0102
512.1131	522.5043	527.1514
529.5171	535.5315	537.1088
545.0029	546.8211	551.9551
559.4088	566.4328	571.6828
576.8908	584.8178	591.8511
594.7960	598.8018	609.7641
629.8630	630.7873	641.8239
648.4057	658.9653	665.6999
672.4113	676.6044	679.5191
684.5625	687.2885	690.8769
703.8074	708.1784	708.8463
714.7296	723.0098	724.6398
729.1566	736.3073	740.1334
747.0604	750.1703	751.9887
761.3937	762.2208	770.3300
772.0863	777.9889	781.4050
792.8682	798.1769	802.4982
813.1956	827.7274	833.9391
853.4112	861.4767	862.9729
870.8832	889.5086	910.0778
916.2186	919.5493	923.8791
934.5573	942.7036	946.6920
961.6640	968.9220	1026.8224
1032.2364	1058.7412	1070.9684
1162.9268	1264.8927	1273.6644
1293.0930	1347.7565	1623.7113
1631.9879	1654.9239	1655.5733
1656.4717	1664.4790	1666.6971
1667.3911	1668.4594	1669.5516
1671.9284	1676.5365	1677.1699
1679.1071	1684.7503	1688.8095
1691.5839	1692.8089	1696.3112
1697.7049	1703.1011	1703.7148
1708.9120	1716.4307	1720.9780
1724.9416	1725.8472	1734.4971
1735.7154	1738.6210	2731.2509
3066.2107	3074.8076	3100.3878
3199.0762	3215.3294	3249.9866

3301.5269	3318.1188	3329.5014
3350.0309	3377.9426	3391.6679
3436.8102	3454.5668	3461.0578
3483.2468	3493.2054	3516.6984
3524.6411	3525.8713	3533.1320
3559.0827	3561.4088	3573.0608
3585.5851	3585.8865	3587.3008
3593.4910	3601.2218	3609.0311
3618.0837	3624.1737	3625.5726
3630.7311	3631.9500	3639.1683
3646.9939	3650.3645	3653.2042
3655.8800	3668.5314	3670.0370
3683.3482	3692.1045	3693.8278
3694.6933	3707.5970	3708.1947
3711.3797	3741.2914	3745.0075
3773.4150	3806.2244	3847.1549
3861.3956	3866.8538	3871.4351
3873.8987	3874.6260	3881.0434
3882.3324	3890.9624	3896.6846
Frequencies (not scaled) Ge-74:		
-22.2237	19.6322	28.3402
32.9965	33.4966	35.2481
37.7513	44.6305	44.9851
46.0075	48.5024	49.7140
50.7903	53.3426	55.7118
56.8450	59.0707	60.4978
60.9914	64.8902	67.1390
69.2678	69.6257	70.4493
73.5027	75.2538	76.7376
77.1179	80.3198	81.2788
83.9661	87.7067	90.8316
92.1249	94.6054	104.1907
106.0269	108.7266	109.1997
111.6414	115.1702	115.8895
120.3945	124.2661	125.3959
135.3008	139.1899	143.8901
144.5662	149.3522	153.4793
156.0744	158.2597	158.8255
162.2922	165.4776	168.1795
172.5521	173.7275	178.2323
178.4647	181.7611	186.0975
190.2630	192.7086	196.3613
198.6994	201.9084	204.4793
207.6189	213.5306	214.0274
218.6539	219.5302	226.0359
230.7868	235.5030	242.0604
244.5111	248.6188	254.5094
256.3645	256.6485	258.6888
266.6742	269.6732	278.4016
281.6238	286.6697	288.9836
289.9138	307.7967	311.6085
314.9870	318.5170	323.2948
328.1536	328.7159	338.7140

342.2270	346.6134	349.1069
353.7036	361.1077	373.9345
385.5225	412.0475	421.1137
427.6095	438.1024	439.4527
447.6759	451.2947	467.0742
473.4884	477.8425	479.7754
482.3408	497.1383	508.0059
512.0945	522.4937	527.1491
529.5158	535.5285	537.0927
545.0008	546.8127	551.9513
559.3948	566.4112	571.6719
576.8404	584.7931	591.7557
594.7726	598.7675	609.7118
629.8092	630.7388	641.8199
648.3971	658.8952	665.6062
672.2364	676.3110	679.2894
684.4763	687.1394	690.4605
701.9472	707.9999	708.7813
713.9555	720.5437	724.3569
728.9098	735.7393	739.9583
746.8926	749.8506	751.8794
759.0488	761.5189	770.1465
772.0450	777.9309	781.3433
792.8279	798.0131	802.3845
813.1654	827.7209	833.8570
853.4097	861.4500	862.9442
870.8681	889.5063	910.0642
916.2125	919.5240	923.8621
934.5115	942.7035	946.6814
961.6587	968.9178	1026.8091
1032.2337	1058.7378	1070.9655
1162.9195	1264.8202	1273.5781
1292.9971	1347.6915	1623.7112
1631.9877	1654.9237	1655.5733
1656.4716	1664.4784	1666.6966
1667.3909	1668.4592	1669.5511
1671.9283	1676.5360	1677.1698
1679.1068	1684.7500	1688.8092
1691.5836	1692.8087	1696.3109
1697.7049	1703.1004	1703.7142
1708.9110	1716.4304	1720.9780
1724.9415	1725.8466	1734.4967
1735.7149	1738.6206	2731.2403
3066.2058	3074.8041	3100.3870
3199.0756	3215.3283	3249.9864
3301.5269	3318.1188	3329.5014
3350.0306	3377.9426	3391.6677
3436.8101	3454.5657	3461.0578
3483.2468	3493.2053	3516.6983
3524.6401	3525.8697	3533.1306
3559.0824	3561.4084	3573.0608
3585.5850	3585.8864	3587.3006
3593.4910	3601.2218	3609.0310

3618.0829	3624.1734	3625.5726
3630.7299	3631.9499	3639.1674
3646.9933	3650.3640	3653.2041
3655.8795	3668.5300	3670.0370
3683.3477	3692.1042	3693.8277
3694.6931	3707.5970	3708.1947
3711.3797	3741.2914	3745.0075
3773.4150	3806.2244	3847.1549
3861.3956	3866.8538	3871.4351
3873.8987	3874.6260	3881.0434
3882.3324	3890.9624	3896.6846

3. Calcite-Super-Molecule

3.1. Calcite-Super-Molecule, Optimized Geometry (HF/3-21G)

C	0.0239840	-0.0040300	-0.0029460
O	-0.0248470	-1.2906920	-0.0035470
O	1.1506510	0.6172630	-0.0479880
O	-1.0825580	0.6700020	0.0345690
Ca	-1.3311480	2.4749540	-1.3933670
Ca	2.9310750	-0.1844980	-1.5050480
Ca	1.5327760	2.4766970	1.4785120
Ca	-1.5657850	-2.4071340	-1.4575210
Ca	-2.8626270	0.0518850	1.4429340
Ca	1.3565060	-2.5183300	1.4685980
O	-0.4582430	-3.1458930	2.8871250
O	3.8217330	-5.8371680	2.8973710
O	6.9069400	-0.9507460	-2.8665030
O	-4.3551710	-5.5032730	-2.9388640
O	-2.6794680	6.3935740	-2.7262000
C	-0.1892950	-5.0396830	0.0003550
O	0.2212940	-3.1816370	-2.8929640
O	-2.0322030	-5.6225170	-2.6372350
O	-0.2381390	-6.3334450	0.0026130
O	1.5752710	-5.7490540	2.8943680
C	-4.4636720	-2.3519290	-0.0098780
O	-4.0530820	-0.4938830	-2.9031970
O	-3.0498720	-3.6411350	-2.8962820
C	-3.0987150	-4.9348970	-2.8940240
O	-1.2853050	-4.3505050	-0.0022690
O	-4.5125150	-3.6456910	-0.0076190
O	-2.6991060	-3.0613000	2.8841360
O	-5.5596820	-1.6627510	-0.0125020
O	-6.9734820	-0.3735450	2.8739030
C	4.2755660	-2.6818390	0.0017800
O	4.6861560	-0.8237930	-2.8915390
O	2.4621570	-3.2662310	-2.8899750
O	4.2267230	-3.9756010	0.0040380
O	0.4117800	1.8639610	-2.9017720
O	-1.8122190	-0.5784760	-2.9002080
O	1.4149900	-1.2832910	-2.8948570
C	1.3661470	-2.5770530	-2.8925990
O	0.9555580	-4.4350990	0.0007200

O	3.1795570	-1.9926620	-0.0008440
O	1.7657560	-0.7034560	2.8855610
O	2.7689670	-3.8507080	2.8924750
C	2.7201240	-5.1444700	2.8947340
C	-4.2731860	2.6936690	-0.0186850
O	-3.8625970	4.5517150	-2.9120040
O	-2.8593860	1.4044630	-2.9050900
C	-2.9082290	0.1107010	-2.9028320
O	-3.3188190	-1.7473450	-0.0095120
O	-4.3220290	1.3999070	-0.0164270
O	-2.5086200	1.9842980	2.8753280
O	-4.7326190	-0.4581390	2.8768920
O	-1.5054090	-1.1629530	2.8822430
C	-1.5542520	-2.4567150	2.8845010
O	-5.3691960	3.3828470	-0.0213090
O	-5.7797860	1.5248010	2.8720100
C	-5.8286290	0.2310390	2.8742690
C	4.4660520	2.3637590	-0.0070270
O	2.6526430	1.7793670	-2.8987820
O	5.8798520	1.0745530	-2.8934320
C	5.8310090	-0.2192090	-2.8911740
O	5.4204200	-2.0772550	0.0021460
O	4.4172090	1.0699970	-0.0047690
O	4.0066190	-0.7880490	2.8885500
C	0.1916760	5.0515130	-0.0172600
O	-1.6217340	4.4671210	-2.9090150
O	1.6054760	3.7623070	-2.9036650
C	1.5566330	2.4685450	-2.9014060
O	3.3700420	3.0529360	-0.0096510
O	0.1428330	3.7577510	-0.0150020
O	1.9562420	4.3421420	2.8767540
O	-0.2677570	1.8997050	2.8783180
O	2.9594530	1.1948900	2.8836680
C	2.9106090	-0.0988720	2.8859270
C	-2.7177440	5.1562990	-2.9116390
O	-3.1283330	3.2982530	-0.0183200
O	-0.9043340	5.7406910	-0.0198840
O	-1.3149240	3.8826440	2.8734360
C	-1.3637670	2.5888830	2.8756940
O	5.6109050	2.9683430	-0.0066620
O	4.1971050	4.2575480	2.8797430
O	1.3365290	5.6560970	-0.0168940
O	3.1499380	6.2404880	2.8748610
C	3.1010950	4.9467260	2.8771190
H	0.1307550	0.5696050	-3.9024060
H	-0.5504140	-0.1784670	-3.9019270
H	0.4380190	-0.3943390	-3.9002880
H	4.4051310	-2.1181490	-3.8921730
H	3.7239620	-2.8662210	-3.8916940
H	-0.0597310	-4.4759930	-3.8935990
H	-0.6020950	-5.1854550	-3.3579080
H	-4.3341070	-1.7882380	-3.9038310
H	-4.0268430	-2.7521820	-3.9017130

H	-4.1436220	3.2573600	-3.9126380
H	-3.8363570	2.2934160	-3.9105210
H	-3.9270270	-2.5638020	3.8842880
H	-4.5498540	-1.7665030	3.8820700
H	-3.7365410	2.4817960	3.8754810
H	-4.7384380	2.3410610	3.8744650
H	0.7283200	4.8396400	3.8769060
H	-0.2735760	4.6989040	3.8758900
H	0.5378350	-0.2059580	3.8857130
H	-0.4640620	-0.3466940	3.8846970
H	-0.0849920	0.5913410	3.8834950
H	0.3473490	-5.2515560	3.8945210
H	-0.2754780	-4.4542570	3.8923020
H	4.0008000	2.0111500	3.8861220
H	4.3798700	2.9491850	3.8849200
H	3.8103150	-3.0344480	3.8949300
H	4.1893840	-2.0964130	3.8937280
H	-2.0826890	-6.9220290	-1.6055760
H	-1.2794860	-7.1497050	-0.9998410
H	-5.5538630	-4.4619510	-1.0100740
H	-5.7424470	-0.3543870	-1.0176790
H	-5.3633770	0.5836470	-1.0188810
H	-5.2810040	0.0036150	-1.9030450
H	3.1872770	4.3613000	-1.0148280
H	2.5644500	5.1585990	-1.0170470
H	2.6468240	4.5785670	-1.9012100
H	-1.0870990	7.0490540	-1.0250610
H	-5.5519610	4.6912110	-1.0264860
H	-5.0905180	5.0492130	-1.9118520
H	6.6483410	-2.5747530	-0.9980070
H	6.8388270	2.4708450	-1.0068140
H	6.9212000	1.8908130	-1.8909780
H	5.8919300	4.2626980	0.9939720
H	5.4589100	4.6575580	1.8780240
H	1.6175540	6.9504520	0.9837400
H	2.1729670	7.1294400	1.8694300
H	5.7014450	-0.7829000	1.0027800
H	5.3941800	0.1810440	1.0006620
H	5.2684240	-0.3880400	1.8868310
H	5.2036940	-4.8645540	1.0094690
H	0.7388330	-7.2223970	1.0080440
H	1.2942460	-7.0434090	1.8937340
H	-2.5471100	-4.7505150	0.9994500
H	-3.5355440	-4.5346430	0.9978110
H	-2.9801310	-4.3556550	1.8835020
H	-6.8214870	-2.0627600	0.9892180
H	-7.2545070	-1.6679010	1.8732690
H	-6.6310010	2.9828380	0.9804100
H	-6.7567570	2.4137530	1.8665790
H	-2.8473080	4.5926090	0.9823140
H	-2.1661390	5.3406810	0.9818350
H	-2.2918950	4.7715970	1.8680050
H	3.1853760	-4.7918610	-0.9984160

H	2.1834790	-4.9325970	-0.9994320
H	2.6449220	-4.5745940	-1.8847980
H	-3.5598700	7.4207260	-3.6882040
H	-2.0666420	7.0252400	-1.3187040
H	-0.7380330	4.5140220	-4.3207500
H	0.7988680	4.8466880	-3.8675640
H	3.8820690	2.0193680	-3.9880530
H	4.6796960	1.8724560	-3.7171890
H	-8.2224940	0.1725250	3.8212030
H	-4.4260650	-6.8549250	-3.8844530
H	-5.5666300	-4.9485040	-1.8635230
H	7.8699580	-0.5637470	-4.1620440
H	7.3005350	-2.2340590	-1.8898810
H	3.8656570	-6.8031440	4.2466530
H	4.2902070	6.9574440	3.8450990
H	5.0862830	-6.1608230	1.8475000

Frequencies (not scaled) C-12(1st atom)O16(2nd atom):

-7119.4749	-6335.0897	-4612.2910
-4099.4411	-3290.1844	-3113.3856
-2910.7267	-2797.2946	-2584.6316
-2484.6773	-2274.1030	-2195.4768
-1875.5031	-1802.0149	-1706.2285
-1616.6087	-1609.3139	-1579.0980
-1564.7671	-1462.3237	-1436.6981
-1405.6596	-1389.4577	-1374.7159
-1356.0239	-1318.7415	-1282.2220
-1271.2282	-1250.8088	-1239.5103
-1212.0734	-1207.5609	-1153.3111
-1133.4841	-1104.2644	-1096.1428
-1083.8243	-1001.2616	-932.2509
-917.0034	-883.2829	-705.0557
-693.0334	-629.6991	-540.6487
-481.7557	-420.8576	-409.8951
-367.1602	-359.8938	-354.5024
-343.9913	-333.1626	-321.0211
-305.7551	-272.5993	-266.8181
-239.9516	-168.5247	-154.4909
-147.5029	-135.1016	-118.5407
-114.3244	-103.5198	-98.6072
-95.8262	-84.8528	-76.3946
-74.2211	-62.3723	-58.4392
-50.8934	-47.9879	-39.9054
-11.9347	11.1668	33.4928
41.8830	50.9704	55.9996
57.6356	64.4449	67.2111
69.2846	69.7560	72.6742
76.5225	82.8870	87.2375
88.9387	91.9419	94.3886
94.7105	99.7505	103.9816
105.5742	108.6130	109.9995
111.4996	113.5123	115.1019
116.1726	119.6297	121.0665
123.3851	126.3002	126.8384

128.0487	130.7127	132.5017
133.9287	136.4166	138.5402
142.0015	142.6964	145.8531
146.7540	150.0127	151.5218
153.8898	155.6530	158.9060
160.9770	162.1721	162.3163
163.6868	167.1066	168.7441
172.1182	174.0056	175.3668
176.8814	178.0641	180.8901
184.2982	185.1016	185.8089
190.6645	191.0948	193.2214
195.8195	197.9006	201.8410
204.0788	204.1655	211.3876
212.8605	214.8272	217.0039
222.4640	224.7333	228.1320
232.6073	238.3250	242.3994
242.8380	246.6923	252.1570
253.7437	258.9818	262.0937
265.7659	268.8332	272.6238
273.4682	275.1360	278.3844
280.4970	283.5381	287.0417
288.0843	289.7196	296.5390
300.0978	303.9137	305.9763
313.3582	315.8797	321.9167
323.3901	328.0783	329.3704
331.6238	334.1869	340.3055
346.7872	355.3688	359.8604
361.4690	371.6188	386.3572
388.6562	398.0802	411.4954
442.4663	443.8085	465.8282
476.9125	485.8491	493.8297
499.2372	511.9038	520.3760
548.2306	553.0542	554.6815
557.7454	566.0371	571.6724
584.8839	591.0712	594.7122
598.5219	601.2440	604.0671
605.2453	612.8377	623.5147
629.3572	638.1712	638.9903
641.0493	653.0980	656.8783
659.6635	672.6584	676.5017
680.2590	682.7856	686.3596
689.9051	691.7900	693.8527
700.5945	703.4392	704.6559
708.7670	710.3649	711.9666
712.6669	714.3897	715.7365
716.9028	717.2845	721.0527
726.1001	726.5409	732.1504
732.5116	737.9164	739.5158
744.4629	749.1055	752.1170
754.9941	758.7997	761.6198
769.2202	771.5518	783.6097
787.4632	799.6283	804.7830
813.2503	828.0115	856.6427

861.5665	861.8345	866.6248
868.0142	873.0571	876.8846
878.6489	886.9339	891.1910
897.9691	899.0272	908.0479
911.0700	911.9038	916.0802
916.9843	921.9695	924.3112
925.6484	926.1968	930.2577
933.0948	937.1478	940.2654
950.3734	957.6485	963.9143
968.2567	974.3212	975.6495
980.6748	983.5239	989.4668
991.5716	992.3817	994.2718
998.2363	1000.0858	1002.7877
1007.4140	1008.7540	1010.8813
1013.8884	1016.4884	1020.4653
1023.0620	1024.4193	1026.1171
1028.3381	1030.0443	1030.4639
1034.7184	1040.5377	1042.7378
1044.9224	1046.8032	1052.7064
1055.5189	1058.5221	1065.5885
1073.7381	1076.4502	1078.5662
1087.3704	1087.7600	1088.5296
1094.6638	1096.7953	1101.2188
1107.5242	1115.2578	1117.6842
1120.9879	1122.4232	1125.1344
1134.2680	1135.8969	1138.3060
1141.3521	1147.9411	1151.5340
1156.8247	1167.1337	1167.9730
1173.9209	1174.3200	1177.8211
1178.5978	1179.1401	1183.0835
1188.5607	1193.9000	1199.6728
1207.5973	1217.6884	1222.7309
1241.7807	1244.2048	1251.4307
1267.4445	1270.8208	1277.3226
1284.6786	1289.2501	1318.6103
1322.4921	1330.1683	1330.9363
1334.3701	1347.2255	1349.8706
1361.5645	1374.5999	1384.6346
1389.0825	1394.4690	1396.5802
1401.5948	1402.7298	1405.9033
1414.5654	1420.5968	1420.8648
1428.0645	1429.1456	1439.6258
1444.1272	1446.7907	1451.3411
1459.3400	1463.9360	1468.1330
1474.8899	1478.8954	1482.5172
1482.8801	1484.2882	1488.9261
1492.6853	1497.0152	1499.5205
1504.0920	1508.2490	1512.0709
1513.5367	1516.1709	1522.1745
1523.5889	1524.1515	1525.1282
1528.3091	1528.5434	1534.7197
1536.7372	1542.6257	1546.7982
1549.2404	1551.4928	1554.6807

1557.0856	1561.7647	1564.2617
1567.2605	1568.5578	1571.6594
1579.6686	1580.1270	1582.2919
1585.2333	1586.2137	1592.0404
1600.4244	1603.1718	1604.8824
1615.5937	1617.8312	1628.1017
1643.7996	1649.8148	1651.1021
1655.7770	1659.6966	1661.6017
1672.2366	1673.7823	1678.9429
1690.7486	1695.1116	1702.7114
1707.2381	1717.6136	1721.6222
1724.5166	1726.1274	1728.2765
1752.3313	1778.0554	1802.7602
1809.1477	1811.5290	1831.2270
1834.3375	1873.7979	1894.9971
1900.4094	2856.4555	9814.0644

Frequencies (not scaled) C-12(1st atom)O18(2nd atom):

-7119.4675	-6335.0834	-4612.2766
-4099.4395	-3290.1774	-3113.3827
-2910.7144	-2797.2937	-2584.6287
-2484.6708	-2274.1009	-2195.4739
-1875.4973	-1802.0112	-1706.2283
-1616.6087	-1609.3134	-1579.0975
-1564.7669	-1462.3236	-1436.6975
-1405.6559	-1389.4543	-1374.7112
-1356.0233	-1318.7400	-1282.2202
-1271.2282	-1250.8072	-1239.5079
-1212.0706	-1207.5587	-1153.3084
-1133.4834	-1104.2521	-1096.1420
-1083.8150	-1001.2536	-932.2492
-916.9973	-883.2709	-705.0464
-693.0287	-629.6941	-540.6485
-481.7555	-420.8570	-409.8927
-367.1548	-359.8937	-354.5023
-343.9905	-333.1622	-321.0190
-305.7536	-272.5975	-266.8177
-239.9504	-168.5222	-154.4908
-147.5006	-135.1013	-118.5407
-114.3220	-103.5188	-98.6028
-95.8239	-84.8506	-76.3895
-74.2201	-62.3594	-58.4319
-50.8912	-47.9814	-39.9041
-11.9367	11.1706	33.4903
41.8760	50.9606	55.9893
57.6044	64.4431	67.1915
69.1739	69.7433	72.6700
76.4957	82.8712	87.2238
88.9199	91.8774	94.3467
94.7004	99.7346	103.8974
105.5537	108.5944	109.8949
111.4339	113.4856	115.0420
115.9141	119.5844	121.0510
123.3743	126.0615	126.8009

127.9900	130.6174	132.3509
133.9064	136.3686	138.5015
141.9952	142.6625	145.7082
146.5172	149.9133	151.5013
153.7571	155.5805	158.8475
160.7318	162.0555	162.2700
163.6742	166.9213	168.6382
172.0868	173.8865	175.3203
176.8591	178.0276	180.8683
184.1107	185.0505	185.7222
190.1964	190.9692	193.1843
195.2653	197.7547	201.7520
203.2376	204.0839	209.9418
212.6798	214.3797	216.9661
222.3600	224.6632	227.9746
232.3882	237.6534	242.1943
242.3971	246.2716	251.9593
253.7302	258.9185	262.0834
265.6888	268.6562	272.5822
273.1908	275.0953	278.3099
280.4589	283.0670	286.8094
287.9538	289.6662	296.5255
300.0285	303.8226	305.9629
313.2741	315.8073	321.8848
323.3075	327.9395	329.0168
331.3637	333.9400	340.0470
344.8204	351.2311	357.8586
360.8405	371.4742	386.1873
386.9928	398.0743	411.1600
442.4611	443.7893	465.8202
476.8992	485.8389	493.8115
499.1891	511.9024	520.3721
548.2299	553.0511	554.6773
557.7442	566.0370	571.6720
584.8788	591.0666	594.7117
598.5218	601.2389	604.0655
605.2450	612.8374	623.5134
629.3565	638.1681	638.9887
641.0467	653.0898	656.8780
659.6621	672.6556	676.5017
680.2580	682.7834	686.3588
689.8786	691.7871	693.8510
700.5652	703.4192	704.5951
708.7627	710.3550	711.9068
712.6604	714.3749	715.7303
716.8987	717.2716	720.9279
726.0578	726.5265	731.9791
732.4748	737.7241	739.5119
744.3129	746.5112	749.1401
752.2938	755.3755	756.2884
760.6260	771.3569	783.5829
787.4104	799.6245	804.7807
813.2366	828.0112	856.6410

861.5652	861.8327	866.6171
868.0115	873.0558	876.8712
878.6484	886.9335	891.1887
897.9653	899.0215	908.0415
911.0203	911.8761	916.0710
916.9714	921.9381	924.3092
925.5603	926.1826	930.1696
933.0587	937.1434	940.2649
950.3727	954.0178	963.9115
968.2231	974.3208	975.6488
980.6732	983.4225	989.4443
991.5665	992.3644	994.2702
998.2337	1000.0838	1002.7784
1007.4127	1008.7536	1010.8807
1013.8832	1016.4879	1020.4626
1023.0563	1024.4183	1026.1152
1028.3310	1030.0407	1030.4623
1034.7159	1040.5346	1042.7373
1044.9223	1046.8027	1052.7026
1055.5180	1058.5178	1065.5871
1073.7357	1076.4480	1078.5544
1087.3547	1087.7569	1088.5285
1094.6593	1096.7869	1101.2186
1107.4929	1112.8235	1115.2712
1117.7016	1121.0661	1122.5695
1125.1465	1135.8843	1138.2869
1141.3427	1147.9410	1151.5181
1156.8165	1167.1293	1167.9698
1173.9175	1174.3195	1177.8202
1178.5960	1179.1390	1183.0827
1188.5603	1193.8998	1199.6708
1207.5934	1217.6869	1222.7304
1241.7803	1244.1943	1251.4281
1267.4352	1270.8189	1277.3221
1284.6779	1289.2396	1318.6060
1322.4892	1330.1662	1330.9354
1334.3693	1347.2252	1349.8705
1361.5478	1374.5985	1384.6300
1389.0806	1394.4504	1396.5720
1401.5923	1402.7271	1405.9028
1414.5568	1420.5723	1420.8639
1428.0591	1429.1188	1439.6194
1444.0904	1446.7613	1451.3411
1459.3385	1463.9320	1468.1021
1474.8595	1478.8931	1482.5152
1482.8738	1484.2757	1488.9218
1492.6050	1496.9771	1499.5194
1504.0867	1508.1791	1512.0707
1513.5310	1515.9426	1522.1673
1523.5817	1524.1020	1525.1272
1528.2746	1528.4827	1534.7137
1536.7259	1542.5853	1546.7870
1549.2382	1551.1014	1554.4409

1556.9701	1561.3978	1563.7261
1567.0709	1568.3140	1571.1583
1579.6360	1580.0139	1581.7254
1585.1009	1586.1972	1591.9971
1598.7239	1600.8220	1604.3641
1615.4694	1617.5474	1622.7576
1643.5101	1649.8140	1651.1011
1655.7739	1659.6885	1661.2582
1672.2338	1673.7792	1678.9350
1690.7191	1695.1106	1702.7111
1707.2236	1717.6134	1721.6171
1724.5154	1726.1274	1728.2765
1752.3254	1778.0523	1802.7579
1809.1453	1811.5094	1831.2256
1834.3337	1873.7938	1894.9964
1900.4051	2856.4555	9814.0477

Frequencies (not scaled) C-13(1st atom)O16(2nd atom):

-7119.4628	-6335.0656	-4612.2624
-4099.4388	-3290.1757	-3113.3853
-2910.7102	-2797.2936	-2584.6264
-2484.6670	-2274.0967	-2195.4712
-1875.5012	-1802.0113	-1706.2278
-1616.6085	-1609.3136	-1579.0978
-1564.7669	-1462.3236	-1436.6973
-1405.6578	-1389.4560	-1374.7132
-1356.0237	-1318.7398	-1282.2212
-1271.2281	-1250.8081	-1239.5097
-1212.0729	-1207.5594	-1153.3103
-1133.4834	-1104.2619	-1096.1386
-1083.8215	-1001.2507	-932.2504
-917.0016	-883.2812	-705.0552
-693.0329	-629.6988	-540.6487
-481.7557	-420.8576	-409.8951
-367.1601	-359.8938	-354.5024
-343.9913	-333.1625	-321.0208
-305.7548	-272.5989	-266.8180
-239.9511	-168.5236	-154.4894
-147.5016	-135.1015	-118.5403
-114.3240	-103.5197	-98.6069
-95.8236	-84.8491	-76.3932
-74.2209	-62.3709	-58.4345
-50.8924	-47.9852	-39.9035
-11.9346	11.1666	33.4898
41.8798	50.9614	55.9969
57.6324	64.4408	67.2048
69.2765	69.7536	72.6717
76.5025	82.8778	87.2314
88.9359	91.9361	94.3854
94.7074	99.7433	103.9623
105.5526	108.6048	109.9886
111.4886	113.5031	115.0817
116.1564	119.6164	121.0634
123.3825	126.2723	126.8227

128.0412	130.6948	132.4531
133.9250	136.4137	138.5301
141.9978	142.6911	145.8375
146.7099	150.0049	151.5082
153.8591	155.6425	158.8875
160.9633	162.1565	162.2926
163.6799	167.0293	168.6748
172.0995	173.9685	175.3486
176.8669	177.9576	180.8729
184.2322	185.0751	185.7419
190.5616	191.0550	193.1990
195.7017	197.8322	201.8199
203.7409	204.0926	210.9501
212.7436	214.5902	216.8611
222.4535	224.7234	228.0543
232.5996	238.2482	242.3819
242.8198	246.6883	252.1106
253.7401	258.9647	262.0842
265.7548	268.8135	272.5983
273.4566	275.1203	278.3625
280.4870	283.5256	286.8972
288.0839	289.7060	296.5289
300.0599	303.8918	305.9674
313.3041	315.8628	321.9045
323.3100	327.9953	329.3115
331.4595	334.1391	340.2813
346.7136	355.1816	359.6508
361.3110	371.5874	386.3217
387.7672	398.0722	411.3252
442.4553	443.7862	465.8262
476.8957	485.8416	493.8288
499.2199	511.9007	520.3707
548.2292	553.0512	554.6781
557.7447	566.0357	571.6720
584.8810	591.0642	594.7078
598.5039	601.2375	604.0628
605.2444	612.8110	623.5102
629.3566	638.1654	638.9887
641.0418	653.0957	656.8716
659.6618	672.6549	676.5010
680.2590	682.7808	686.3592
689.9006	691.7850	693.8501
700.5917	703.4366	704.6491
708.7603	710.3632	711.9578
712.6635	714.3854	715.7310
716.8981	717.2839	721.0439
726.0965	726.5341	732.1440
732.5101	737.9164	739.5092
744.4561	749.0914	752.0765
754.8604	758.2492	760.3063
767.5304	771.4549	783.6011
787.4482	799.6185	804.7809
813.2363	828.0109	856.6426

861.5656	861.8266	866.6074
868.0104	873.0401	876.8828
878.6457	886.9334	891.1678
897.9593	898.9545	907.9506
909.8517	911.7339	915.8194
916.7634	920.9165	923.2725
924.3456	926.1810	928.8924
932.5599	937.0136	937.9916
940.2679	950.3742	963.9094
968.1686	974.3186	975.6471
980.6672	983.1538	989.3916
991.5607	992.3288	994.2684
998.2226	1000.0789	1002.7604
1007.4123	1008.7523	1010.8804
1013.8636	1016.4879	1020.4542
1023.0386	1024.4182	1026.1101
1028.3139	1030.0395	1030.4594
1034.7128	1040.5290	1042.7373
1044.9207	1046.8013	1052.6944
1055.5152	1058.5122	1065.5807
1073.7311	1076.4402	1078.5599
1087.3687	1087.7549	1088.5244
1094.6564	1096.7832	1101.2138
1107.5233	1115.2562	1117.6789
1120.9741	1122.4223	1125.1305
1134.2573	1135.8965	1138.2965
1141.3414	1147.9401	1151.5176
1156.8208	1167.1272	1167.9708
1173.9088	1174.3176	1177.8181
1178.5954	1179.1397	1183.0814
1188.5582	1193.8968	1199.6660
1207.5877	1217.6858	1222.7286
1241.7694	1244.1924	1251.4196
1267.4264	1270.8082	1277.3212
1284.6770	1289.2225	1318.5955
1322.4791	1330.1616	1330.9328
1334.3432	1347.2194	1349.8697
1361.4710	1374.5975	1384.6220
1389.0244	1394.4090	1396.5139
1401.5418	1402.7066	1405.8972
1414.2782	1420.4768	1420.8497
1427.9756	1429.0141	1439.5971
1443.5894	1446.6799	1451.3177
1459.0368	1463.7190	1467.9827
1474.6396	1478.7697	1482.3066
1482.6715	1484.2275	1488.8487
1492.1685	1496.8479	1499.4883
1503.3364	1507.8473	1511.6273
1513.3841	1515.0728	1520.1465
1523.4057	1523.8871	1525.0903
1527.4834	1528.0867	1533.9383
1535.6261	1541.2587	1542.1561
1547.1003	1549.2258	1551.2700

1555.4910	1558.2101	1562.3738
1565.8758	1567.9335	1569.8729
1575.1994	1579.6584	1580.2550
1584.6306	1584.9052	1586.2304
1591.6147	1592.4390	1602.5165
1610.9930	1615.9651	1618.6408
1643.2853	1649.8117	1651.0875
1655.7658	1659.6764	1660.8878
1672.2295	1673.7734	1678.9065
1690.6567	1695.0944	1702.7064
1707.2054	1717.6130	1721.6090
1724.5153	1726.1269	1728.2765
1752.3038	1778.0472	1802.7473
1809.1146	1811.4886	1831.2221
1834.3072	1873.7838	1894.9912
1900.3940	2856.4553	9814.0150

Frequencies (not scaled) C-13(1st atom)O18(2nd atom):

-7119.4554	-6335.0592	-4612.2478
-4099.4372	-3290.1687	-3113.3824
-2910.6977	-2797.2927	-2584.6235
-2484.6604	-2274.0945	-2195.4683
-1875.4954	-1802.0075	-1706.2275
-1616.6085	-1609.3130	-1579.0973
-1564.7668	-1462.3235	-1436.6967
-1405.6540	-1389.4526	-1374.7084
-1356.0231	-1318.7383	-1282.2193
-1271.2281	-1250.8064	-1239.5072
-1212.0700	-1207.5571	-1153.3075
-1133.4827	-1104.2496	-1096.1377
-1083.8120	-1001.2425	-932.2486
-916.9955	-883.2691	-705.0459
-693.0281	-629.6938	-540.6485
-481.7555	-420.8570	-409.8927
-367.1548	-359.8937	-354.5023
-343.9905	-333.1621	-321.0187
-305.7533	-272.5971	-266.8176
-239.9499	-168.5210	-154.4892
-147.4994	-135.1012	-118.5403
-114.3216	-103.5188	-98.6025
-95.8213	-84.8469	-76.3881
-74.2199	-62.3580	-58.4272
-50.8901	-47.9786	-39.9022
-11.9367	11.1704	33.4874
41.8728	50.9514	55.9866
57.6011	64.4390	67.1851
69.1658	69.7407	72.6675
76.4757	82.8618	87.2175
88.9170	91.8715	94.3432
94.6975	99.7272	103.8774
105.5315	108.5856	109.8832
111.4224	113.4762	115.0202
115.8994	119.5711	121.0479
123.3716	126.0236	126.7893

127.9839	130.5987	132.3067
133.9036	136.3661	138.4913
141.9916	142.6569	145.6882
146.4756	149.9062	151.4886
153.7238	155.5705	158.8263
160.7151	162.0379	162.2540
163.6665	166.8394	168.5717
172.0664	173.8506	175.3017
176.8453	177.9176	180.8512
184.0389	185.0156	185.6553
190.0841	190.9398	193.1633
195.1529	197.6853	201.7248
202.9084	204.0146	209.5604
212.5861	214.1557	216.8360
222.3516	224.6545	227.9083
232.3815	237.5767	242.1871
242.3799	246.2619	251.9035
253.7269	258.9026	262.0744
265.6786	268.6359	272.5556
273.1776	275.0809	278.2885
280.4501	283.0607	286.6671
287.9525	289.6535	296.5162
299.9887	303.8032	305.9540
313.2217	315.7881	321.8714
323.2267	327.8328	328.9494
331.2253	333.9069	339.9871
344.6321	351.0011	357.7868
360.8333	371.4433	385.7135
386.5711	398.0669	411.0275
442.4506	443.7680	465.8184
476.8829	485.8319	493.8106
499.1725	511.8995	520.3667
548.2285	553.0482	554.6740
557.7435	566.0357	571.6716
584.8754	591.0599	594.7072
598.5038	601.2328	604.0612
605.2442	612.8107	623.5086
629.3558	638.1621	638.9870
641.0391	653.0870	656.8713
659.6602	672.6519	676.5009
680.2579	682.7789	686.3583
689.8721	691.7823	693.8482
700.5601	703.4161	704.5847
708.7552	710.3523	711.8953
712.6567	714.3714	715.7242
716.8932	717.2708	720.9018
726.0485	726.5178	731.9378
732.4702	737.6995	739.4989
744.1043	744.8617	749.1230
752.2612	754.8276	755.5084
760.3261	771.3497	783.5776
787.4039	799.6142	804.7781
813.2226	828.0106	856.6408

861.5644	861.8239	866.5971
868.0072	873.0374	876.8685
878.6452	886.9329	891.1598
897.9523	898.9260	907.8667
909.2802	911.7023	915.6693
916.6891	920.1156	922.8976
924.3361	926.1648	928.4787
932.3762	936.1712	937.2590
940.2663	950.3740	963.9071
968.1625	974.3181	975.6468
980.6665	983.1229	989.3831
991.5578	992.3217	994.2674
998.2213	1000.0778	1002.7554
1007.4112	1008.7520	1010.8799
1013.8609	1016.4875	1020.4524
1023.0354	1024.4173	1026.1089
1028.3093	1030.0361	1030.4584
1034.7110	1040.5265	1042.7369
1044.9206	1046.8009	1052.6914
1055.5143	1058.5087	1065.5798
1073.7279	1076.4384	1078.5464
1087.3529	1087.7521	1088.5235
1094.6527	1096.7756	1101.2136
1107.4906	1112.7471	1115.2679
1117.6974	1121.0508	1122.5665
1125.1424	1135.8839	1138.2778
1141.3316	1147.9399	1151.5017
1156.8125	1167.1226	1167.9680
1173.9059	1174.3171	1177.8173
1178.5933	1179.1387	1183.0807
1188.5578	1193.8965	1199.6642
1207.5836	1217.6841	1222.7281
1241.7689	1244.1798	1251.4171
1267.4155	1270.8064	1277.3206
1284.6762	1289.2081	1318.5891
1322.4746	1330.1589	1330.9316
1334.3425	1347.2192	1349.8695
1361.4408	1374.5962	1384.6154
1389.0220	1394.3757	1396.4975
1401.5376	1402.7020	1405.8966
1414.2594	1420.4295	1420.8478
1427.9645	1428.9602	1439.5826
1443.5016	1446.6242	1451.3175
1459.0318	1463.7091	1467.8996
1474.5611	1478.7566	1482.2786
1482.6654	1484.1870	1488.8259
1491.8468	1496.7367	1499.4866
1503.3153	1507.5683	1511.5955
1513.2395	1514.2255	1520.1018
1523.3699	1523.6380	1525.0880
1527.3014	1527.7959	1533.5602
1535.6099	1537.9731	1541.9603
1546.7924	1549.0831	1550.9397

1554.4780	1557.5790	1561.8507
1565.8289	1567.8725	1568.9236
1573.9972	1579.5881	1580.2376
1584.0476	1584.8522	1586.2247
1589.9893	1592.3546	1602.4736
1610.0989	1615.9111	1618.5214
1643.2350	1649.8115	1651.0870
1655.7649	1659.6714	1660.7950
1672.2286	1673.7724	1678.9036
1690.6448	1695.0939	1702.7062
1707.1976	1717.6129	1721.6064
1724.5142	1726.1268	1728.2765
1752.3000	1778.0450	1802.7458
1809.1126	1811.4742	1831.2211
1834.3043	1873.7807	1894.9906
1900.3907	2856.4553	9813.9982

3.2 Calcite-Super-Molecule, Optimized Geometry (B3LYP/6-31G)

C	-0.0010620	-0.0345180	-0.0213170
O	0.6341650	1.1120080	-0.0415350
O	0.6778980	-1.1520560	-0.0105030
O	-1.3112390	-0.0488020	-0.0024910
O	1.8742720	2.7655380	2.6816240
Ca	0.0666880	-2.9601890	-1.4212820
Ca	-2.6012710	1.4206200	-1.4117340
Ca	-2.5088370	-1.5779770	1.4098120
Ca	2.5194490	1.5405110	-1.4163470
Ca	2.6070620	-1.3779700	1.4125080
Ca	-0.0684220	2.8427010	1.3890420
O	-0.8743090	6.9317120	2.8999830
O	-5.7901390	3.8923940	-2.8632660
O	6.3273920	3.0400760	-2.9331610
O	-0.3998110	-6.9141250	-2.7168560
C	2.3802290	4.4533240	0.0047090
O	1.1963000	2.9626160	-2.8880950
O	4.2924020	4.1669090	-2.6324190
O	2.9919440	5.5943810	0.0065230
O	1.1055490	5.8665720	2.8978280
C	5.0412730	0.1622620	-0.0030110
O	3.8573440	-1.3284460	-2.8958150
O	4.3372380	1.9397870	-2.8903890
C	4.9489520	3.0808450	-2.8885750
O	3.0625580	3.3530350	0.0027300
O	5.6529870	1.3033200	-0.0011970
O	3.7665930	1.5755110	2.8901080
O	5.7236020	-0.9380260	-0.0049900
O	6.4276370	-2.7155510	2.8823890
C	-2.6664670	4.2943250	0.0053550
O	-3.8503960	2.8036170	-2.8874500
O	-0.7800730	4.0221340	-2.8859500
O	-2.0547520	5.4353820	0.0071680
O	-1.1893520	-1.4874440	-2.8951690
O	1.8809710	-0.2689270	-2.8936700

O	-0.7094580	1.7807880	-2.8897440
C	-0.0977440	2.9218460	-2.8879300
O	1.0861850	4.4125540	0.0048750
O	-1.9841380	3.1940370	0.0033750
O	-1.2801030	1.4165120	2.8907540
O	-0.8002090	4.6847450	2.8961790
C	-0.1884940	5.8258020	2.8979930
C	2.6556210	-4.2877980	-0.0100850
O	1.4716920	-5.7785060	-2.9028890
O	1.9515860	-2.5102730	-2.8974630
C	2.5633000	-1.3692150	-2.8956490
O	3.7472290	0.1214930	-0.0028450
O	3.2673350	-3.1467400	-0.0082710
O	1.3809410	-2.8745500	2.8830340
O	4.4512640	-1.6560320	2.8845330
O	1.8608350	0.3936830	2.8884600
C	2.4725490	1.5347410	2.8902740
O	3.3379500	-5.3880860	-0.0120640
O	4.5218790	-3.8973780	2.8807400
C	5.1335930	-2.7563200	2.8825540
C	-5.0521190	-0.1557350	-0.0017200
O	-3.1657250	-0.4279260	-2.8930240
O	-5.7561540	1.6217900	-2.8890980
C	-5.1444400	2.7628470	-2.8872840
O	-3.9605100	4.2535550	0.0055200
O	-4.4404040	0.9853220	0.0000940
O	-3.2564750	2.4760300	2.8928990
C	-2.3910750	-4.4467970	-0.0094390
O	-0.5046810	-4.7189870	-2.9007440
O	-3.0951100	-2.6692720	-2.8968180
C	-2.4833960	-1.5282140	-2.8950040
O	-4.3697900	-1.2560230	-0.0036990
O	-1.7793610	-3.3057390	-0.0076250
O	-3.6657550	-3.0335480	2.8836790
O	-0.5954310	-1.8150310	2.8851790
O	-3.1858610	0.2346840	2.8891050
C	-2.5741460	1.3757420	2.8909190
C	0.1776480	-5.8192750	-2.9027230
O	1.3615770	-4.3285670	-0.0099190
O	-1.7087460	-5.5470850	-0.0114190
O	-0.5248170	-4.0563770	2.8813860
C	0.0868970	-2.9153190	2.8832000
O	-6.3461630	-0.1965050	-0.0015540
O	-5.6421270	-1.9740300	2.8858240
O	-3.6851190	-4.4875660	-0.0092740
O	-5.5715130	-4.2153760	2.8820310
C	-4.9597980	-3.0743180	2.8838450
H	-0.7146900	-0.8864580	-3.4740580
H	1.1238600	-0.1567940	-3.4731600
H	-0.4273240	1.0706030	-3.4708090
H	-3.3757340	3.4046030	-3.4663380
H	-1.5371840	4.1342670	-3.4654400
H	1.6709620	3.5636020	-3.4669830

H	3.4384020	4.3025850	-3.0494040
H	4.3320050	-0.7274590	-3.4747030
H	4.6193720	1.2296020	-3.4714540
H	1.9463530	-5.1775190	-3.4817770
H	2.2337200	-3.2204580	-3.4785280
H	4.2782930	1.0056000	3.4688700
H	4.6882830	-0.9294900	3.4655320
H	1.8926410	-3.4444600	3.4617960
H	3.7734760	-4.0569430	3.4604220
H	-3.1540550	-3.6034590	3.4624420
H	-1.2732200	-4.2159420	3.4610680
H	-0.7684030	0.8466010	3.4695160
H	1.1124320	0.2341180	3.4681420
H	-0.3584130	-1.0884890	3.4661780
H	1.6172490	5.2966610	3.4765900
H	2.0272390	3.3615710	3.4732520
H	-3.9342640	0.0751190	3.4687880
H	-5.4051090	-1.2474880	3.4668230
H	-1.5486120	4.5251790	3.4758620
H	-3.0194570	3.2025720	3.4738970
H	4.6483770	4.8296550	-2.0360550
H	3.7403470	5.7539470	-0.5731590
H	6.4013910	1.4628850	-0.5808790
H	5.4865830	-1.6645680	-0.5859890
H	4.0157380	-2.9871750	-0.5879530
H	4.3690430	-1.8983560	-2.3170530
H	-4.6068090	-1.9825650	-0.5846980
H	-4.1968180	-3.9176560	-0.5880360
H	-3.8435140	-2.8288370	-2.3171350
H	-1.9457650	-6.2736260	-0.5924170
H	3.1009310	-6.1146280	-0.5930630
H	1.9833910	-6.3484160	-2.3241270
H	-4.4722100	4.8234660	-0.5732420
H	-6.8578620	0.3734060	-0.5803160
H	-6.5045570	1.4622240	-2.3094160
H	-6.8208240	-0.7974910	0.5773340
H	-6.3992390	-1.8618970	2.3063350
H	-4.1597810	-5.0885520	0.5696150
H	-5.2893780	-4.9255610	2.3009660
H	-4.4351720	3.6525690	0.5844080
H	-4.7225390	1.6955080	0.5811590
H	-4.0135870	2.5881640	2.3134090
H	-2.3368870	6.1455680	0.5882330
H	2.7098090	6.3045670	0.5875880
H	1.5802110	6.4675580	2.3189390
H	3.8196690	3.2409020	0.5822190
H	5.3708530	2.0135060	0.5798680
H	4.2412550	2.1764970	2.3112200
H	6.4807130	-1.0501590	0.5745000
H	6.9022990	-2.1145640	2.3035000
H	4.0950610	-5.5002190	0.5674260
H	4.8040130	-4.6075640	2.2996750
H	0.8869150	-4.9295540	0.5689690

H	-0.9516350	-5.6592180	0.5680710
H	-0.2426820	-4.7665620	2.3003210
H	-1.3063490	5.5949480	-0.5725140
H	0.5744860	4.9824650	-0.5738880
H	-0.5430540	4.7486760	-2.3049520
H	-0.2029390	-7.6716010	-3.2727990
H	-0.8787250	-7.0864230	-1.9028810
H	-0.9739050	-4.5201890	-3.7143210
H	-2.9511100	-3.4377560	-3.4538600
H	-3.8653890	-0.2408890	-3.5231730
H	-5.3349520	0.9023180	-3.3650710
H	6.9379720	-3.3160690	3.4306000
H	6.7094480	3.7278750	-3.4832220
H	6.8010860	2.4627720	-2.3298920
H	-6.3886590	3.9353690	-3.6126170
H	-5.6690310	4.6594240	-2.2988200
H	-0.6520820	7.4451910	3.6800810
H	-6.3461110	-4.2982400	3.4430410
H	-1.4439690	7.4161540	2.2979840

Frequencies (not scaled) C-12(1st atom)O16(2nd atom):

-3321.7981	-1602.5775	-1352.7928
-1226.6252	-1204.1930	-1166.5604
-1136.7778	-1106.1921	-1100.8697
-1098.7335	-1093.7919	-1091.7590
-1081.8757	-1079.4406	-1071.7077
-1069.1894	-1063.0607	-1060.7296
-1056.8575	-1055.5293	-1053.9390
-1052.0844	-1045.6011	-1042.9137
-1040.7907	-1035.6329	-1035.0568
-1031.2455	-1028.8806	-1025.1590
-1020.7188	-1019.5218	-1012.4688
-1006.5072	-1005.3708	-1000.5926
-999.7570	-995.7027	-992.3508
-989.6121	-985.1151	-979.5400
-974.7300	-971.5528	-969.1526
-964.2749	-961.3124	-958.3096
-952.9169	-949.6574	-945.4404
-941.4647	-933.6505	-931.0706
-929.5400	-923.3223	-918.9698
-917.3621	-913.4966	-910.1091
-907.5373	-904.2211	-897.7662
-896.0079	-891.9802	-890.3001
-885.3306	-879.1031	-876.0451
-869.7339	-865.3447	-858.4852
-851.2349	-849.1834	-846.6720
-842.2338	-840.4016	-838.0143
-830.3399	-827.3898	-823.9854
-817.2012	-815.7150	-810.9299
-805.8690	-803.7283	-798.9532
-795.8511	-793.2904	-779.8742
-774.0226	-756.5746	-748.7377
-716.1114	-545.3387	-497.2548
-458.8176	-449.8208	-442.4416

-439.2412	-431.7137	-424.5649
-422.3336	-419.0236	-412.0560
-411.0587	-400.3035	-391.4256
-384.7515	-381.5476	-374.6206
-373.6481	-360.7179	-355.4887
-349.9711	-347.8635	-346.8953
-343.8749	-335.4791	-327.8971
-318.9477	-311.9006	-288.5289
-263.9737	-255.8104	-253.6853
-249.4138	-248.1895	-244.8034
-242.5575	-240.1254	-234.6246
-231.7996	-222.6442	-221.2681
-209.5141	-208.2501	-201.5911
-195.6224	-193.7509	-188.2179
-184.6079	-179.8252	-165.0619
-159.5234	-148.4687	-138.4023
-131.3963	-120.5305	-108.7541
-69.9491	25.4616	42.1790
48.5633	51.8386	56.3258
59.4821	62.9190	63.9809
68.2523	71.3371	74.0961
77.1275	80.4135	81.6972
84.3243	85.5870	87.8438
90.4406	91.0501	93.5600
95.2779	98.2202	100.6320
103.0211	106.4775	107.8649
108.8046	111.0974	111.9197
115.7353	117.7640	118.6368
122.7985	126.0074	128.7813
132.1446	134.1036	136.4970
139.4374	142.2917	153.1528
157.5177	158.5537	162.6642
163.4989	166.0476	170.0474
172.6546	175.5307	176.0059
178.7284	182.5771	185.9566
188.6307	189.3238	194.3494
200.8869	215.3192	216.7253
222.3991	226.6671	231.6342
234.8286	239.4254	244.1828
247.5278	255.6333	257.2524
260.3205	260.9646	264.2550
267.6146	279.9726	295.3382
296.3675	300.5932	302.8462
305.5315	310.2740	314.5210
318.6319	319.7185	324.2256
337.8686	342.2271	342.6678
349.3961	357.6020	362.3435
364.0540	370.4161	371.6702
378.2354	402.5655	414.8030
419.5829	424.4624	427.9865
430.6962	436.6242	437.8133
442.7379	447.7770	452.6603
455.3237	465.4020	470.7657

484.7722	563.8819	628.6801
663.9733	671.8361	684.5855
689.6440	693.7125	697.7559
700.6274	704.0314	714.1949
716.7313	744.0702	752.9625
756.8960	767.7440	770.0629
777.8317	784.3216	788.2642
795.8568	798.2599	806.0026
812.7866	813.7266	819.5918
833.3534	840.3056	844.6999
875.2967	889.0791	898.5207
907.4872	921.2449	928.7319
942.3337	948.1960	952.8356
958.4759	964.3750	967.7808
973.1892	984.7151	989.1694
993.4569	995.5236	996.1605
999.9932	1006.6296	1009.9217
1011.3158	1013.0661	1021.7786
1024.4843	1035.2010	1040.8590
1043.3146	1046.4110	1047.1505
1048.6717	1058.7031	1059.5836
1062.4299	1065.3535	1073.1516
1074.5830	1079.7370	1083.7990
1095.8316	1107.8786	1127.3569
1137.6551	1172.2620	1175.7260
1197.5397	1205.1112	1214.3377
1218.9298	1219.4882	1232.6001
1245.5102	1251.1327	1253.9105
1258.0257	1262.3654	1273.0381
1280.3512	1284.2864	1289.9420
1293.8011	1298.4657	1303.7511
1307.7004	1318.2124	1354.5140
1376.4093	1387.3236	1442.4731
1453.3676	1476.2010	1483.6373
1489.6288	1517.8164	1548.9343
1563.1894	1592.4113	1596.6582
1624.0599	1640.5034	1641.9212
1657.8908	1664.5168	1674.8514
1676.4961	1679.3358	1692.0463
1692.6146	1700.1386	1707.9762
1717.4968	1735.3633	1739.1869
1740.8271	1744.1306	1748.1217
1749.3857	1756.0504	1763.1437
1767.2306	1769.3772	1775.1741
1787.5207	1788.5219	1791.3144
1802.8350	1804.6541	1863.9249
1895.7743	2320.9356	2618.0299
2717.3327	2731.5892	2790.0171
2894.3691	2926.2515	2937.3797
2964.3831	2995.4997	3001.5027
3029.5976	3041.7402	3067.4680
3078.5990	3081.5578	3094.8743
3097.5822	3106.5933	3112.2715

3124.1373	3139.4996	3143.8235
3156.5196	3170.4048	3181.6290
3190.5344	3208.8917	3211.7270
3220.6028	3221.9582	3230.6192
3237.4886	3248.4949	3249.2595
3255.5952	3256.6788	3264.3165
3269.0521	3276.8967	3278.8036
3281.4508	3284.8670	3292.7586
3296.8925	3301.8276	3306.2414
3314.0576	3317.8605	3322.7167
3325.8866	3326.5315	3329.3634
3332.9838	3337.2468	3339.5104
3342.8975	3346.6696	3350.7381
3360.4953	3377.5613	3382.6810
3386.7782	3399.1933	3399.5642
3408.2199	3410.7488	3419.6224
3423.2761	3436.3044	3459.9827
3469.1146	3473.6331	3494.5962
3507.4135	3512.0593	3561.4252

Frequencies (not scaled) C-12(1st atom)O18(2nd atom):

-3321.7957	-1602.5741	-1352.7868
-1226.6245	-1204.1908	-1166.5596
-1136.7773	-1106.1916	-1100.8695
-1098.7332	-1093.7918	-1091.7590
-1081.8757	-1079.4402	-1071.7076
-1069.1893	-1063.0606	-1060.7295
-1056.8574	-1055.5292	-1053.9387
-1052.0834	-1045.6010	-1042.9132
-1040.7902	-1035.6329	-1035.0565
-1031.2453	-1028.8804	-1025.1589
-1020.7179	-1019.5211	-1012.4686
-1006.5069	-1005.3706	-1000.5924
-999.7567	-995.7023	-992.3505
-989.6120	-985.1151	-979.5398
-974.7294	-971.5524	-969.1522
-964.2747	-961.3123	-958.3095
-952.9161	-949.6572	-945.4404
-941.4644	-933.6501	-931.0704
-929.5398	-923.3216	-918.9695
-917.3621	-913.4962	-910.1078
-907.5367	-904.2208	-897.7661
-896.0071	-891.9800	-890.3000
-885.3274	-879.0970	-876.0449
-869.7328	-865.3413	-858.4848
-851.2338	-849.1825	-846.6714
-842.2331	-840.4007	-838.0143
-830.3398	-827.3894	-823.9853
-817.2001	-815.7140	-810.9298
-805.8684	-803.7278	-798.9528
-795.8510	-793.2902	-779.8742
-774.0226	-756.5621	-748.7376
-716.1113	-545.3386	-497.2542
-458.8174	-449.8200	-442.4406

-439.2411	-431.7129	-424.5647
-422.3336	-419.0230	-412.0560
-411.0584	-400.3031	-391.4246
-384.7508	-381.5474	-374.6189
-373.6475	-360.7160	-355.4885
-349.9692	-347.8621	-346.8953
-343.8746	-335.4790	-327.8962
-318.9474	-311.9006	-288.5280
-263.9728	-255.8093	-253.6838
-249.4069	-248.1887	-244.8031
-242.5529	-240.1089	-234.6215
-231.7947	-222.6396	-221.2676
-209.5139	-208.2485	-201.5891
-195.6190	-193.7479	-188.2069
-184.6042	-179.8217	-165.0567
-159.5190	-148.4684	-138.4007
-131.3910	-120.5271	-108.7515
-69.9374	25.4607	42.1788
48.5619	51.8308	56.3238
59.4737	62.8885	63.9117
68.2379	71.3258	74.0582
77.1203	80.3942	81.6377
84.2848	85.5621	87.8182
90.3677	91.0055	93.5581
95.2582	98.2036	100.6220
102.9421	106.4539	107.8457
108.7767	111.0645	111.8200
115.7314	117.7114	118.6200
122.7977	125.7520	128.5926
132.0836	133.7806	135.6468
139.2032	142.1997	153.0352
157.3905	158.2521	162.6231
163.0614	165.6626	169.9807
172.6271	175.1981	175.7857
177.9870	182.1700	185.5230
188.6126	189.1757	192.9495
200.3944	214.0832	216.6096
222.1073	226.5529	231.5741
234.7845	239.3993	244.1112
247.5021	255.5832	257.2368
260.2135	260.6141	264.2478
267.5951	279.8508	295.2704
296.3308	300.3672	302.5703
305.1930	309.9956	314.0445
318.1653	319.5229	324.0170
335.4258	341.2471	342.4388
349.2450	357.2644	361.9057
363.8756	369.6360	370.6129
375.3425	402.4782	414.6997
419.5748	424.4481	427.9798
430.6889	436.6149	437.8040
442.7305	447.7718	452.6484
455.3091	465.4007	470.7640

484.7671	563.8722	628.6764
663.9311	671.8254	679.7676
683.4722	684.9556	694.1118
700.4850	702.7159	714.1360
716.7286	744.0684	752.9593
756.8943	767.7408	770.0594
777.8261	784.3134	788.2634
795.8562	798.2598	805.9832
810.9502	813.6984	818.0083
833.3223	840.2996	844.6993
875.2940	889.0735	898.5186
907.4758	921.2317	928.7099
942.3181	948.1671	952.8121
958.4694	964.3659	967.7725
973.1819	984.7130	989.1611
993.4536	995.5233	996.1601
999.9931	1006.6291	1009.9215
1011.3157	1013.0658	1021.7745
1024.4830	1035.0618	1038.3481
1040.8661	1043.3978	1046.4146
1047.1503	1048.6915	1059.5502
1062.4096	1065.3521	1073.1441
1074.5811	1079.7369	1083.7990
1095.8316	1107.8785	1127.3565
1137.6549	1172.2616	1175.7245
1197.5382	1205.1100	1214.3377
1218.9297	1219.4882	1232.5995
1245.5098	1251.1326	1253.9105
1258.0256	1262.3647	1273.0372
1280.3506	1284.2863	1289.9409
1293.8010	1298.4656	1303.7511
1307.7003	1318.2121	1354.5124
1376.4088	1387.3234	1442.4730
1453.3386	1464.0417	1483.5509
1487.8969	1517.7991	1548.8397
1563.1848	1592.4095	1596.6579
1624.0439	1640.4925	1641.8920
1657.8900	1664.5081	1674.8413
1676.4943	1679.3344	1692.0301
1692.5957	1700.1367	1707.9675
1717.4959	1735.3631	1739.1864
1740.8261	1744.1293	1748.1213
1749.3853	1756.0447	1763.1393
1767.2290	1769.3771	1775.1737
1787.5204	1788.5214	1791.3140
1802.8348	1804.6536	1863.9248
1895.7707	2320.9329	2618.0292
2717.3318	2731.5889	2790.0166
2894.3680	2926.2506	2937.3795
2964.3831	2995.4988	3001.5026
3029.5973	3041.7401	3067.4680
3078.5988	3081.5577	3094.8742
3097.5822	3106.5932	3112.2715

3124.1371	3139.4995	3143.8234
3156.5195	3170.4047	3181.6284
3190.5343	3208.8915	3211.7270
3220.6027	3221.9582	3230.6192
3237.4886	3248.4949	3249.2594
3255.5951	3256.6788	3264.3164
3269.0520	3276.8966	3278.8036
3281.4508	3284.8669	3292.7586
3296.8925	3301.8274	3306.2412
3314.0575	3317.8605	3322.7167
3325.8866	3326.5315	3329.3633
3332.9837	3337.2467	3339.5104
3342.8974	3346.6695	3350.7381
3360.4952	3377.5613	3382.6809
3386.7781	3399.1932	3399.5642
3408.2199	3410.7488	3419.6224
3423.2761	3436.3044	3459.9827
3469.1145	3473.6331	3494.5962
3507.4135	3512.0593	3561.4252

Frequencies (not scaled) C-13(1st atom)O16(2nd atom):

-3321.7963	-1602.5771	-1352.7870
-1226.6242	-1204.1899	-1166.5599
-1136.7769	-1106.1913	-1100.8692
-1098.7331	-1093.7919	-1091.7590
-1081.8757	-1079.4403	-1071.7077
-1069.1893	-1063.0606	-1060.7295
-1056.8575	-1055.5292	-1053.9388
-1052.0842	-1045.6011	-1042.9134
-1040.7906	-1035.6328	-1035.0566
-1031.2454	-1028.8803	-1025.1589
-1020.7186	-1019.5217	-1012.4682
-1006.5066	-1005.3707	-1000.5922
-999.7568	-995.7022	-992.3506
-989.6120	-985.1147	-979.5398
-974.7298	-971.5528	-969.1524
-964.2748	-961.3123	-958.3096
-952.9169	-949.6573	-945.4404
-941.4645	-933.6504	-931.0705
-929.5399	-923.3223	-918.9698
-917.3620	-913.4966	-910.1085
-907.5372	-904.2210	-897.7661
-896.0077	-891.9801	-890.2998
-885.3304	-879.1021	-876.0450
-869.7330	-865.3445	-858.4846
-851.2341	-849.1831	-846.6715
-842.2333	-840.4011	-838.0140
-830.3399	-827.3893	-823.9854
-817.2011	-815.7148	-810.9297
-805.8683	-803.7282	-798.9531
-795.8510	-793.2901	-779.8742
-774.0226	-756.5729	-748.7377
-716.1114	-545.3387	-497.2548
-458.8176	-449.8208	-442.4416

-439.2412	-431.7137	-424.5649
-422.3336	-419.0236	-412.0560
-411.0587	-400.3035	-391.4256
-384.7515	-381.5475	-374.6204
-373.6481	-360.7178	-355.4885
-349.9709	-347.8634	-346.8953
-343.8748	-335.4791	-327.8969
-318.9476	-311.9006	-288.5288
-263.9734	-255.8099	-253.6848
-249.4112	-248.1882	-244.8020
-242.5559	-240.1231	-234.6231
-231.7986	-222.6435	-221.2679
-209.5141	-208.2497	-201.5903
-195.6214	-193.7501	-188.2146
-184.6062	-179.8248	-165.0612
-159.5229	-148.4685	-138.4017
-131.3954	-120.5298	-108.7541
-69.9485	25.4609	42.1786
48.5631	51.8358	56.3233
59.4803	62.9135	63.9693
68.2427	71.3309	74.0798
77.1231	80.4033	81.6883
84.3086	85.5773	87.8417
90.4262	91.0498	93.5578
95.2734	98.2189	100.6317
103.0117	106.4676	107.8644
108.8041	111.0932	111.9134
115.7344	117.7518	118.6316
122.7976	125.9754	128.7601
132.1350	134.0472	136.2854
139.3889	142.2612	153.0857
157.4557	158.4196	162.6563
163.3487	165.9553	170.0170
172.6398	175.4178	175.9339
178.6141	182.5467	185.9454
188.6084	189.2293	193.9456
200.6379	215.1736	216.5707
222.3359	226.6329	231.6231
234.8190	239.4193	244.1807
247.5187	255.6237	257.2522
260.3061	260.9171	264.2503
267.6059	279.8069	295.3221
296.3412	300.5302	302.7627
305.2594	310.0764	314.4810
318.5869	319.6539	324.1741
337.6478	342.0435	342.6073
349.2406	357.4101	362.2449
364.0119	370.3219	371.5535
377.6483	402.5485	414.7694
419.5798	424.4603	427.9834
430.6935	436.6240	437.8079
442.7354	447.7715	452.6567
455.3216	465.4010	470.7641

484.7719	563.8720	628.6479
663.8964	671.8291	684.4130
687.7523	693.5615	696.2729
700.5724	703.6917	714.1844
716.7141	744.0575	752.9619
756.8914	767.7182	770.0547
777.8273	784.3203	788.2628
792.1750	795.8580	798.2635
806.0660	813.6827	816.1314
833.2854	840.2927	844.6993
875.2703	889.0433	898.5051
907.4643	921.2311	928.6713
942.3301	948.1802	952.8259
958.4746	964.3728	967.7746
973.1873	984.7119	989.1598
993.4529	995.5210	996.1536
999.9928	1006.6273	1009.9213
1011.3158	1013.0656	1021.7783
1024.4831	1035.1949	1040.8523
1043.3095	1046.4099	1047.1466
1048.6681	1058.6995	1059.5809
1062.4289	1065.3531	1073.1496
1074.5788	1079.7369	1083.7989
1095.8314	1107.8781	1127.3551
1137.6547	1172.2593	1175.7228
1197.5372	1205.1072	1214.3377
1218.9293	1219.4882	1232.5969
1245.5078	1251.1316	1253.9095
1258.0254	1262.3630	1273.0341
1280.3482	1284.2858	1289.9325
1293.7961	1298.4646	1303.7510
1307.7001	1318.2112	1354.5072
1376.4058	1387.3227	1435.0493
1442.4721	1446.8014	1453.4289
1484.5336	1517.7850	1548.7448
1563.1764	1592.4065	1596.6572
1623.9547	1640.4483	1641.8248
1657.8894	1664.3841	1674.8287
1676.4920	1679.3327	1691.9893
1692.5110	1700.1230	1707.9476
1717.4938	1735.3629	1739.1857
1740.8237	1744.1197	1748.1209
1749.3837	1756.0317	1763.1278
1767.2214	1769.3760	1775.1726
1787.5194	1788.5190	1791.3133
1802.8333	1804.6530	1863.9247
1895.7634	2320.9296	2618.0257
2717.3310	2731.5887	2790.0143
2894.3641	2926.2492	2937.3791
2964.3828	2995.4980	3001.5022
3029.5969	3041.7400	3067.4680
3078.5978	3081.5576	3094.8741
3097.5821	3106.5931	3112.2715

3124.1367	3139.4989	3143.8231
3156.5194	3170.4034	3181.6274
3190.5342	3208.8914	3211.7270
3220.6025	3221.9581	3230.6190
3237.4885	3248.4948	3249.2594
3255.5951	3256.6788	3264.3164
3269.0520	3276.8967	3278.8036
3281.4507	3284.8669	3292.7586
3296.8924	3301.8274	3306.2411
3314.0575	3317.8604	3322.7167
3325.8866	3326.5315	3329.3632
3332.9837	3337.2467	3339.5102
3342.8974	3346.6696	3350.7381
3360.4952	3377.5613	3382.6809
3386.7781	3399.1932	3399.5642
3408.2199	3410.7488	3419.6224
3423.2761	3436.3044	3459.9827
3469.1145	3473.6331	3494.5962
3507.4135	3512.0593	3561.4252

Frequencies (not scaled) C-13(1st atom)O18(2nd atom):

-3321.7938	-1602.5736	-1352.7809
-1226.6234	-1204.1878	-1166.5591
-1136.7764	-1106.1909	-1100.8690
-1098.7328	-1093.7918	-1091.7590
-1081.8756	-1079.4400	-1071.7076
-1069.1892	-1063.0606	-1060.7294
-1056.8573	-1055.5292	-1053.9385
-1052.0832	-1045.6009	-1042.9129
-1040.7900	-1035.6328	-1035.0563
-1031.2452	-1028.8801	-1025.1588
-1020.7177	-1019.5210	-1012.4680
-1006.5063	-1005.3706	-1000.5920
-999.7565	-995.7019	-992.3502
-989.6119	-985.1147	-979.5396
-974.7292	-971.5524	-969.1520
-964.2746	-961.3122	-958.3095
-952.9161	-949.6572	-945.4404
-941.4643	-933.6500	-931.0704
-929.5397	-923.3216	-918.9695
-917.3620	-913.4962	-910.1071
-907.5366	-904.2206	-897.7660
-896.0069	-891.9799	-890.2997
-885.3272	-879.0960	-876.0448
-869.7319	-865.3411	-858.4843
-851.2330	-849.1822	-846.6709
-842.2326	-840.4001	-838.0139
-830.3398	-827.3889	-823.9852
-817.2000	-815.7139	-810.9296
-805.8677	-803.7276	-798.9527
-795.8509	-793.2899	-779.8742
-774.0226	-756.5602	-748.7376
-716.1113	-545.3386	-497.2541
-458.8174	-449.8199	-442.4406

-439.2411	-431.7129	-424.5647
-422.3336	-419.0230	-412.0560
-411.0584	-400.3031	-391.4246
-384.7508	-381.5473	-374.6187
-373.6475	-360.7159	-355.4883
-349.9691	-347.8621	-346.8953
-343.8744	-335.4790	-327.8961
-318.9473	-311.9006	-288.5280
-263.9725	-255.8087	-253.6833
-249.4043	-248.1875	-244.8018
-242.5513	-240.1067	-234.6201
-231.7937	-222.6390	-221.2674
-209.5139	-208.2482	-201.5883
-195.6181	-193.7471	-188.2037
-184.6025	-179.8213	-165.0561
-159.5186	-148.4682	-138.4002
-131.3901	-120.5264	-108.7515
-69.9368	25.4599	42.1784
48.5617	51.8280	56.3213
59.4718	62.8833	63.8997
68.2281	71.3196	74.0416
77.1158	80.3838	81.6289
84.2689	85.5523	87.8162
90.3528	91.0053	93.5559
95.2537	98.2024	100.6217
102.9325	106.4438	107.8452
108.7762	111.0601	111.8132
115.7303	117.6989	118.6149
122.7968	125.7039	128.5643
132.0715	133.6676	135.4958
139.1799	142.1769	152.9718
157.3032	158.1266	162.5917
162.9276	165.5784	169.9484
172.6094	175.0708	175.7332
177.8653	182.1490	185.5146
188.5904	189.0821	192.6284
200.1685	213.9516	216.4235
222.0398	226.5221	231.5629
234.7752	239.3940	244.1100
247.4928	255.5718	257.2366
260.1805	260.5881	264.2434
267.5870	279.6836	295.2527
296.3055	300.2905	302.4757
304.9282	309.8087	313.9808
318.0978	319.4625	323.9661
335.1939	341.0469	342.4220
349.0798	357.0571	361.8086
363.8422	369.5156	370.4760
375.0400	402.4664	414.6712
419.5719	424.4464	427.9765
430.6858	436.6147	437.7988
442.7282	447.7666	452.6454
455.3075	465.3999	470.7626

484.7669	563.8630	628.6434
663.8365	671.8117	677.9925
681.5538	684.8509	694.0754
700.4660	702.6978	714.1325
716.7108	744.0554	752.9587
756.8886	767.7086	770.0484
777.8197	784.3103	788.2501
788.6228	795.8572	798.2623
806.0594	813.6817	816.0651
833.2750	840.2900	844.6989
875.2670	889.0368	898.5024
907.4545	921.2182	928.6538
942.3141	948.1511	952.8002
958.4678	964.3633	967.7660
973.1802	984.7098	989.1505
993.4491	995.5207	996.1533
999.9927	1006.6268	1009.9210
1011.3157	1013.0652	1021.7738
1024.4816	1035.0374	1038.2458
1040.8586	1043.3879	1046.4132
1047.1464	1048.6891	1059.5481
1062.4085	1065.3516	1073.1425
1074.5770	1079.7368	1083.7988
1095.8314	1107.8781	1127.3547
1137.6546	1172.2588	1175.7209
1197.5355	1205.1055	1214.3377
1218.9292	1219.4882	1232.5960
1245.5072	1251.1313	1253.9094
1258.0252	1262.3619	1273.0326
1280.3471	1284.2857	1289.9307
1293.7958	1298.4645	1303.7509
1307.7000	1318.2108	1354.5034
1376.4038	1387.3220	1422.2058
1442.4713	1445.0873	1453.4117
1484.5021	1517.7798	1548.6999
1563.1740	1592.4053	1596.6569
1623.9442	1640.4397	1641.8053
1657.8887	1664.3780	1674.8213
1676.4905	1679.3317	1691.9771
1692.4968	1700.1214	1707.9411
1717.4931	1735.3628	1739.1852
1740.8229	1744.1187	1748.1205
1749.3833	1756.0271	1763.1244
1767.2200	1769.3759	1775.1723
1787.5192	1788.5186	1791.3130
1802.8330	1804.6527	1863.9247
1895.7603	2320.9271	2618.0250
2717.3301	2731.5884	2790.0138
2894.3630	2926.2484	2937.3790
2964.3828	2995.4972	3001.5021
3029.5966	3041.7399	3067.4680
3078.5976	3081.5575	3094.8741
3097.5821	3106.5930	3112.2715

3124.1365	3139.4988	3143.8230
3156.5194	3170.4033	3181.6268
3190.5342	3208.8912	3211.7270
3220.6024	3221.9581	3230.6190
3237.4885	3248.4948	3249.2593
3255.5951	3256.6787	3264.3163
3269.0520	3276.8966	3278.8036
3281.4507	3284.8669	3292.7586
3296.8924	3301.8272	3306.2410
3314.0574	3317.8604	3322.7167
3325.8866	3326.5314	3329.3631
3332.9836	3337.2466	3339.5102
3342.8974	3346.6695	3350.7381
3360.4951	3377.5613	3382.6809
3386.7781	3399.1932	3399.5641
3408.2199	3410.7488	3419.6224
3423.2761	3436.3044	3459.9827
3469.1145	3473.6331	3494.5962
3507.4135	3512.0593	3561.4252

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