

SUPPLEMENTARY INFORMATION for:

Solvation or not solvation: Tunneling

reactions of molecules embedded in cryogenic

matrices

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The Semiclassical Transition State Theory (SCTST)

The exact rate constant for reactions within the canonical ensemble can be characterized according to the definition provided by Miller et al.^{2,3}

$$k(T) = \frac{1}{h} \frac{1}{Q_r(T)} \int N(E) e^{-\beta E} dE \quad (\text{S1})$$

where $N(E)$ is the Cumulative Reaction Probability (CRP), $\beta = 1/(k_B T)$ where T and k_B are respectively the temperature and the Boltzman constant, $Q_r(T)$ is the reactant partition function at temperature T . In its exact Quantum Mechanical (QM) formulation, $N(E)$ can be seen as the sum of the probabilities to reach the final state α from the reactant state β at a certain energy E and over all the possible angular momenta J

$$N(E) = \sum_J (2J+1) \sum_{\alpha, \beta} |S_{\alpha, \beta}(E, J)|^2 \quad (\text{S2})$$

where $S_{\alpha, \beta}$ is the scattering matrix.

We introduce the Semiclassical (SC) approximation to the $N(E)$. We can write the semiclassical tunneling probability $P(E)$ as a function of the multidimensional generalized non-separable WKB (Wenzel, Kramer, Brillouin) barrier penetration integral Θ ⁴

$$P_{\mathbf{n}}(E) = [1 + e^{2\Theta(E, \mathbf{n})}]^{-1} \quad (\text{S3})$$

where $\mathbf{n} = (n_1, \dots, n_{N-1})$ for a system with $(N-1)$ bound degrees of freedom, for a total of N degrees of freedom with one reactive mode variable expressed as E . Maintaining the non-separability of the system's Hamiltonian by employing "effective" action-angle variables, these can be expressed for the n bound degrees of freedom and the N^{th} reactive mode as

follows

$$\begin{aligned} I_n &= (n_n + \frac{1}{2}) \\ I_N &= (n_N + \frac{1}{2}) = \frac{i\Theta}{\pi} \end{aligned} \tag{S4}$$

where for the reactive mode,⁵ using the Bohr-Sommerfeld quantization rule, the above identity holds, and we have obtained an expression for the barrier penetration integral Θ . The final semiclassical CRP can be written as

$$N_{\text{SC}}(E) = \sum_{\mathbf{n}=0}^{\infty} P_{\mathbf{n}}(E) \tag{S5}$$

In a general non-separable system, the total vibrational energy can be represented as a function of its vibrational degrees of freedom: $E(n_1, \dots, n_N)$. Reversing this relation and applying the identity mentioned in equation S4 for the reactive mode makes it possible to evaluate the barrier penetration integral, denoted as Θ . Following this, by incorporating the integral into equation S3, the SC CRP is obtained using equation S5. Miller and Hernandez tackled the challenge of inversion by exploiting the VPT2, a second-order perturbation expression, for the vibrational energy in a molecule at the Transition State (TS), as detailed in their 1993 study.⁶ The total vibrational energy is written as

$$\begin{aligned} E &= \Delta V_0 + G_0 + \sum_{k=1}^{N-1} \omega_k (n_k + \frac{1}{2}) + \sum_{k=1}^{N-1} \sum_{l=k}^{N-1} \chi_{kl} (n_k + \frac{1}{2})(n_l + \frac{1}{2}) + \\ &+ \omega_N (n_N + \frac{1}{2}) + \sum_{k=1}^{N-1} \chi_{kN} (n_k + \frac{1}{2})(n_N + \frac{1}{2}) + \chi_{NN} (n_N + \frac{1}{2})^2 \end{aligned} \tag{S6}$$

where ΔV_0 is the classical forward barrier height for the reaction, G_0 is a constant energy term coming from the VPT2 expansion, ω_k is the vibrational frequency, and χ_{kl} are the anharmonic constants involving the vibrational quantum numbers n_k and n_l . Substituting

the expression for n_N from Eq. S4, we can rewrite the energy expression S6 as

$$\begin{aligned}
E = & \Delta V_0 + G_0 + \sum_{k=1}^{N-1} \omega_k \left(n_k + \frac{1}{2}\right) + \sum_{k=1}^{N-1} \sum_{l=k}^{N-1} \chi_{kl} \left(n_k + \frac{1}{2}\right) \left(n_l + \frac{1}{2}\right) + \\
& + \frac{i\Theta}{\pi} \left[\omega_N + \sum_{k=1}^{N-1} \chi_{kN} \left(n_k + \frac{1}{2}\right) \right] - \frac{\chi_{NN}}{\pi^2} \Theta(\mathbf{n}, E)^2
\end{aligned} \tag{S7}$$

Grouping some terms and inverting the above equation, we obtain the following expression for the SC penetration integral

$$\begin{aligned}
\frac{\Theta}{\pi} = & \frac{-\Omega_N + \sqrt{\Omega_N^2 + 4\chi_{NN}\Delta E}}{2\chi_{NN}} \\
= & \frac{2\Delta E}{\Omega_N \left(1 + \frac{4\chi_{NN}\Delta E}{\Omega_N^2}\right)^{\frac{1}{2}}}
\end{aligned} \tag{S8}$$

where ΔE is the remaining unbound energy given a certain set of bound vibrational quantum numbers, and Ω_N is the effective reaction coordinate frequency that accounts for the effects of the coupled anharmonic constants χ_{kN} by modifying the magnitude of the imaginary frequency ω_N .

When considering the molecule in its center of mass, translations, and rotations can be factored out from the density of states calculation. This separability assumption allows us to write the working formula for the SCTST as

$$k_{\text{SCTST}}(T) = \frac{1}{h} \frac{Q_{\text{TS}}^{\text{tra}}(T)}{Q_{\text{R}}^{\text{tra}}(T)} \frac{Q_{\text{TS}}^{\text{rot}}(T)}{Q_{\text{R}}^{\text{rot}}(T)} \frac{\int_0^{+\infty} N^{\text{SC}}(E) e^{-\beta E} dE}{Q_{\text{R}}^{\text{vib}}(T)} \tag{S9}$$

where $Q^{\text{tra}}(T)$ and $Q^{\text{rot}}(T)$ are, respectively, the TS translational and the rotational partition functions while $Q_{\text{R}}^{\text{vib}}(T)$ is the reactant vibrational partition function.

The vibrational partition function for the reactant is computed as

$$Q_{\text{R}}^{\text{vib}}(T) = \int \rho_{\text{vib}}(E) e^{-\beta E} dE \tag{S10}$$

where $\rho_{\text{vib}}(E)$ is the VDOS, which is computed together with the SC CRP, using the Wang-Landau (WL) method implemented and parallelized in the Paradensum and Parsctst codes.⁷⁻⁹ The free-motion partition functions for rotations and translations are computed as

$$\begin{aligned} Q^{\text{rot}} &= \frac{\sqrt{\pi}}{s} \prod_{\alpha} \left(\sqrt{8\pi^2 I_{\alpha} \frac{k_b T}{h^2}} \right) \\ Q^{\text{tra}} &= \left(\frac{2\pi M k_b T}{h^2} \right)^{\frac{3}{2}} \end{aligned} \quad (\text{S11})$$

where s is the rotational symmetry number, I_{α} is the moment of inertia along the α axis and M is the mass. Hindered internal rotations were not present in this work, but extra care is necessary, as modified rotational partition functions may be necessary. Finally, the parallel efficient FDACC code, developed by us,¹⁰ is used to compute the missing terms in Eq. S7, i.e. the anharmonic constants χ_{kl} and the G_0 terms. Following the VPT2 formulation, we report here the expressions. For a molecule in its equilibrium geometry, we have

$$\begin{aligned} \chi_{kk} &= \frac{\hbar^2}{16\omega_k^2} \left[f_{kkkk} - \sum_{m=1}^N \frac{f_{kkkm}^2}{\omega_m^2} \left(2 + \frac{\omega_m}{2(2\omega_k + \omega_m)} - \frac{\omega_m}{2(2\omega_k - \omega_m)} \right) \right] \\ \chi_{kl} &= \frac{\hbar^2}{4\omega_l\omega_k} \left[f_{kkll} - \sum_{m=1}^N \frac{f_{kkm}f_{llm}}{\omega_m^2} + \sum_{m=1}^N \frac{2f_{klm}^2(\omega_k^2 + \omega_l^2 - \omega_m^2)}{[(\omega_k + \omega_l)^2 - \omega_m^2][(\omega_k - \omega_l)^2 - \omega_m^2]} \right] + \\ &+ \left(\frac{\omega_k}{\omega_l} + \frac{\omega_l}{\omega_k} \right) \sum_{\alpha} B_{\alpha}(\zeta_{kl}^{\alpha})^2 \\ &= \frac{\hbar^2}{4\omega_l\omega_k} \left[f_{kkll} - \sum_{m=1}^N \frac{f_{kkm}f_{llm}}{\omega_m^2} - \sum_{m=1}^N \frac{f_{klm}^2}{2\omega_m} \left(\frac{1}{\omega_k + \omega_l + \omega_m} - \frac{1}{\omega_k + \omega_l - \omega_m} + \right. \right. \\ &\left. \left. + \frac{1}{\omega_k - \omega_l + \omega_m} - \frac{1}{\omega_k - \omega_l - \omega_m} \right) \right] + \left(\frac{\omega_k}{\omega_l} + \frac{\omega_l}{\omega_k} \right) \sum_{\alpha} B_{\alpha}(\zeta_{kl}^{\alpha})^2 \end{aligned} \quad (\text{S12})$$

where $k, l = 1, 2, \dots, N$ since all frequencies are real. At the transition state geometries, we

have

$$\begin{aligned}
\chi_{kk} &= \frac{\hbar^2}{16\omega_k^2} \left[f_{kkkk} + \frac{f_{kkN}^2}{\tilde{\omega}_N^2} \left(\frac{8\omega_k^2 + 3\tilde{\omega}_N^2}{4\omega_k^2 + \tilde{\omega}_N^2} \right) - \sum_{m=1}^{N-1} \frac{f_{kkm}^2}{\omega_m^2} \left(2 + \frac{\omega_m}{2(2\omega_k + \omega_m)} + \right. \right. \\
&\quad \left. \left. - \frac{\omega_m}{2(2\omega_k - \omega_m)} \right) \right] \\
\chi_{kl} &= \frac{\hbar^2}{4\omega_k\omega_l} \left[f_{kkll} + \frac{f_{kkN}f_{lN}}{\tilde{\omega}_N^2} + \frac{2f_{klN}^2(\omega_k^2 + \omega_l^2 + \tilde{\omega}_N^2)}{[(\omega_k + \omega_l)^2 + \tilde{\omega}_N^2][(\omega_k - \omega_l)^2 + \tilde{\omega}_N^2]} + \right. \\
&\quad - \sum_{m=1}^{N-1} \frac{f_{kkm}f_{llm}}{\omega_m^2} - \sum_{m=1}^{N-1} \frac{f_{klm}^2}{2\omega_m} \left(\frac{1}{\omega_k + \omega_l + \omega_m} - \frac{1}{\omega_k + \omega_l - \omega_m} + \right. \\
&\quad \left. \left. + \frac{1}{\omega_k - \omega_l + \omega_m} - \frac{1}{\omega_k - \omega_l - \omega_m} \right) \right] + \left(\frac{\omega_k}{\omega_l} + \frac{\omega_l}{\omega_k} \right) \sum_{\alpha} B_{\alpha}(\zeta_{kl}^{\alpha})^2
\end{aligned} \tag{S13}$$

with $k, l = 1, 2, \dots, N-1$ and $\chi_{kN} = -i\tilde{\chi}_{kN}$. From this perturbative treatment, a constant term arises, and it must be included in the anharmonic zero point energy corrections to V_0 , the G_0 term. For a molecule in its equilibrium geometry

$$\begin{aligned}
G_0 &= \sum_i^N \hbar^2 \left(\frac{f_{iiii}}{64\omega_i^2} - \frac{7f_{iii}^2}{576\omega_i^4} \right) + \sum_{i \neq j}^N \hbar^2 \frac{3f_{ij}^2}{64\omega_i^2\omega_j} \frac{1}{2} \left(\frac{1}{2\omega_i - \omega_j} - \frac{1}{2\omega_i + \omega_j} \right) + \\
&\quad - \sum_{k > j > i}^N \hbar^2 \frac{f_{ijk}^2}{4\omega_i\omega_j\omega_k} \frac{1}{8} \left(\frac{1}{\omega_i + \omega_j + \omega_k} - \frac{1}{-\omega_i + \omega_j + \omega_k} + \right. \\
&\quad \left. - \frac{1}{\omega_i - \omega_j + \omega_k} - \frac{1}{\omega_i + \omega_j - \omega_k} \right)
\end{aligned} \tag{S14}$$

while for a TS molecule, we have

$$\begin{aligned}
G_0 = & \sum_i^{N-1} \hbar^2 \left(\frac{f_{iiii}}{64\omega_i^2} - \frac{7f_{iii}^2}{576\omega_i^4} \right) - \hbar^2 \frac{f_{NNNN}}{64\tilde{\omega}_N^2} - \hbar^2 \frac{7f_{NNN}^2}{576\tilde{\omega}_N^4} + \\
& + \sum_{ij; i \neq j}^{N-1} \hbar^2 \frac{3f_{ijj}^2}{64\omega_i^2\omega_j} \frac{1}{2} \left(\frac{1}{2\omega_i - \omega_j} - \frac{1}{2\omega_i + \omega_j} \right) + \\
& + \sum_i^{N-1} \hbar^2 \frac{3f_{iiN}^2}{64\omega_i^2} \frac{1}{4\omega_i^2 + \tilde{\omega}_N^2} + \sum_j^{N-1} \hbar^2 \frac{3f_{NNj}^2}{64\tilde{\omega}_N^2} \frac{1}{4\tilde{\omega}_N^2 + \omega_j^2} + \\
& - \sum_{k>j>i}^{N-1} \hbar^2 \frac{f_{ijk}^2}{4\omega_i\omega_j\omega_k} \frac{1}{8} \left(\frac{1}{\omega_i + \omega_j + \omega_k} - \frac{1}{-\omega_i + \omega_j + \omega_k} + \right. \\
& \left. - \frac{1}{\omega_i - \omega_j + \omega_k} - \frac{1}{\omega_i + \omega_j - \omega_k} \right) + \\
& - \sum_{j>i}^{N-1} \hbar^2 \frac{f_{ijN}^2}{4[(\omega_i^2 + \omega_j^2 + \tilde{\omega}_N^2)^2 - 4\omega_i^2\omega_j^2]}
\end{aligned} \tag{S15}$$

The ONIOM-SCTST Protocol

The employed 2-Layer ONIOM method is implemented in the Gaussian16 (Rev C02) suite of codes,^{11–13} and our FDACC code has been interfaced to the ONIOM driver to provide the required data for SCTST calculations. No link atoms are required as the environment/system division does not require them, which greatly simplifies the modeling. The ONIOM approximation uses a subtractive QM/MM scheme. This is also called "extrapolation scheme", and the total ONIOM energy for the system can be expressed as follows

$$E_{\text{high,real}} \simeq E_{\text{ONIOM2(high:low)}} = E_{\text{high,model}} + E_{\text{low,real}} - E_{\text{low,model}} \tag{S16}$$

where $E_{\text{low,model}}$ removes the double counting of the model system energy from $E_{\text{low,real}}$. *Low* refers to the low-level approach used for energy calculations, while *high* denotes the high-level approach. Extrapolative methods enable low- and high-level combinations (such as QM1/QM2). In our situation, we will utilize a classical Force Field (FF) as the *low* level component, alongside an ab initio post-HF or DFT method for the *high* level component.

The electrostatic component in the QM/MM functional of the energy can be treated using the mechanic or the more refined electrostatic embedding. In the electrostatic embedding, the QM subsystem can be polarized by the MM surrounding molecules, and the total ONIOM energy is expressed as follows

$$E_{\text{ONIOM-EE}} = E_{\text{QM,model}} + E_{\text{MM,real}} - E_{\text{MM,model}} \quad (\text{S17})$$

with

$$E_{\text{QM,model}} = H_{\text{QM,model}} + \sum_J \sum_N \frac{Z_J s_N q_N}{R_{JN}} - \sum_I \sum_N \frac{s_N q_N}{R_{IN}} \quad (\text{S18})$$

where I runs on the QM electrons, N runs on the nuclear coordinates of the MM subsystem, q_N is the embedded charge, s_N is the scale factor for the N -th MM atom, and Z_J is the nuclear charge of the J -th atom in the QM subsystem. This expression is the simplest one implemented in ONIOM schemes and employs a fixed charge approximation. For the MM component, we selected the highly versatile Universal Force Field (UFF). The ONIOM-UFF configuration has effectively addressed various chemical issues.¹² In studying cryogenic noble gas matrices, we found the Universal Force Field (UFF) effective as the primary interaction between the central molecule and the lattice is non-bonded and non-electrostatic. The UFF does an excellent job of modeling the atomic radii of noble gas atoms, often serving as a reference for other applications, such as calculations of the solvent-accessible surface area (SASA). Nonbonded interactions, including damped dispersion forces and electron-exchange repulsion, are not easily separated. Their contributions to the interaction energy are encompassed in a single term known as the van der Waals energy term, which is expressed in the UFF through a Lennard-Jones 6-12 type formula as follows:

$$E_{\text{QM/MM}}^{\text{VdW}} = \sum_{AB} \epsilon_{AB} \left\{ \left(\frac{\sigma_{AB}}{r_{AB}} \right)^{12} - \left(\frac{\sigma_{AB}}{r_{AB}} \right)^6 \right\} \quad (\text{S19})$$

In this equation, A and B denote the involved atoms, ϵ represents the suitable depth parameter, and σ is the van der Waals bond length parameter.¹⁴ For reactions occurring in monoatomic matrices, the multiscale modeling using UFF might benefit from an extrapolation method such as ONIOM, as a subtractive approach can eliminate poorly parameterized subsystems, keeping only the necessary quantum terms in the final total energy expression.

Reaction Energetics

Table S1: RMP2/aVDZ energetics (including ZPE corrections for anharmonic barriers) for glycine, formic acid, and acetic acid interconversion reactions in the gas phase and noble gas matrices.

System	Glycine	Formic Acid	Acetic Acid
<i>Classical Barrier</i> [kJ mol ⁻¹]			
Gas Phase	31.171	36.745	31.946
Ar Matrix	28.872	36.733	—
Kr Matrix	29.877	37.439	—
Xe Matrix	29.336	37.991	31.493
<i>Anharmonic Barrier</i> [kJ mol ⁻¹]			
Gas Phase	26.947	32.358	27.760
Ar Matrix	24.465	32.348	—
Kr Matrix	25.591	32.842	—
Xe Matrix	25.062	33.448	27.509
<i>-iω</i> [cm ⁻¹]			
Gas Phase	548.575	610.532	558.104
Ar Matrix	529.192	609.246	—
Kr Matrix	545.312	604.778	—
Xe Matrix	542.911	594.100	555.334

SCTST MP2 Results on Formic Acid

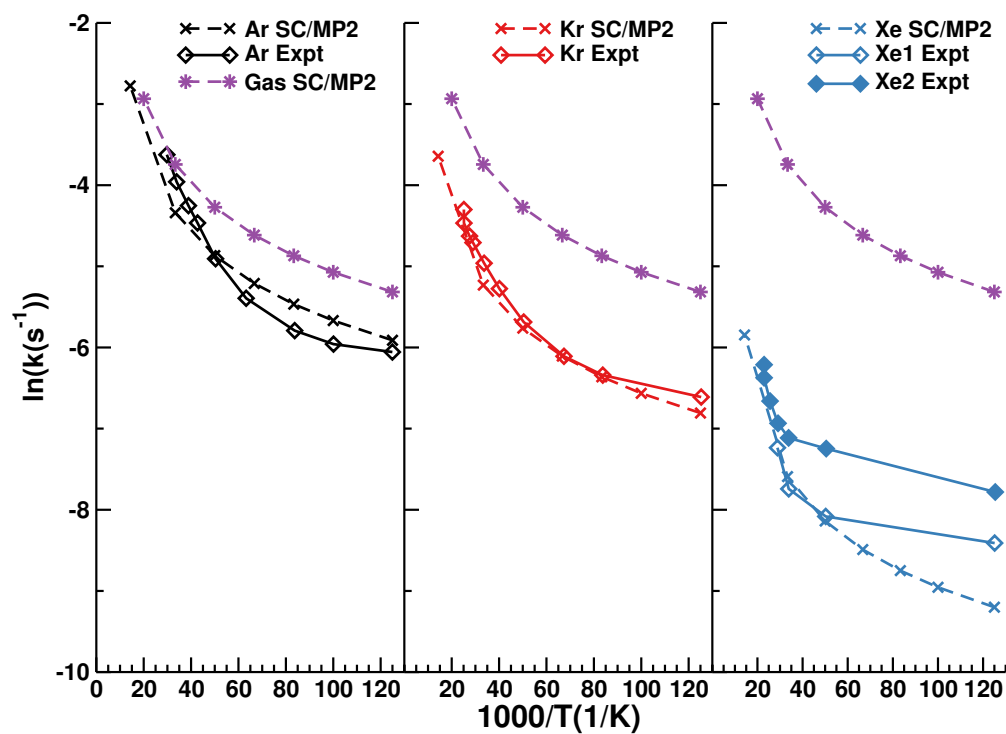


Figure S1: Formic acid interconversion rates in noble gas matrices. The continuous lines represent the experimental results at different temperatures.¹

SCTST B3LYP Results

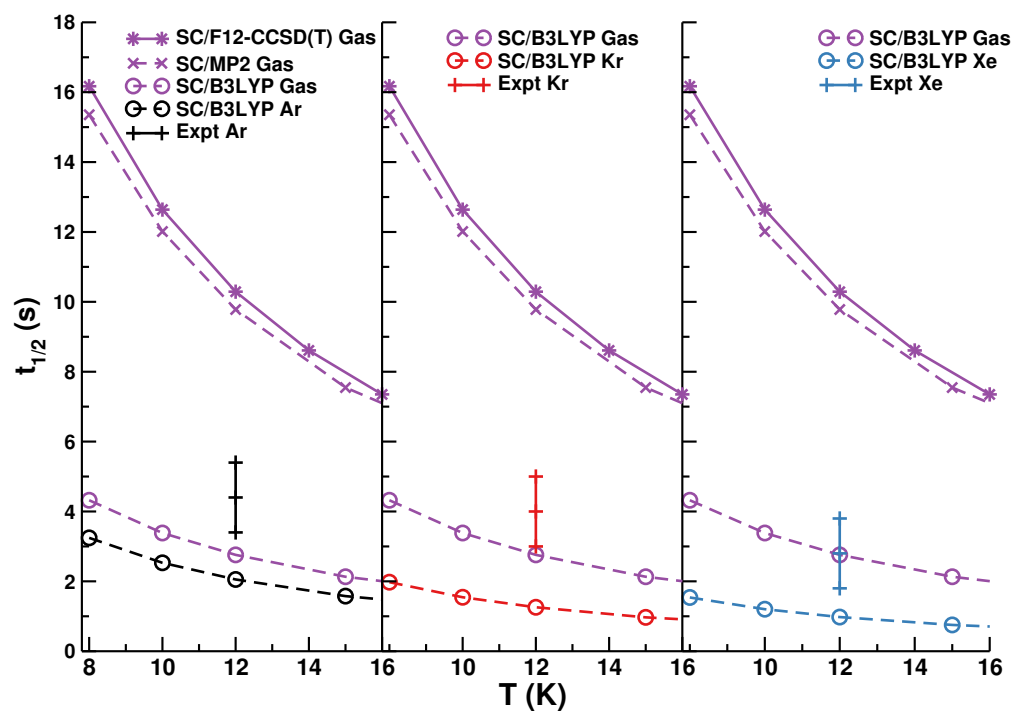


Figure S2: SCTST half-life times at the B3LYP/def2-TZVP level of theory for the interconversion of the glycine molecule in cryogenic matrices.

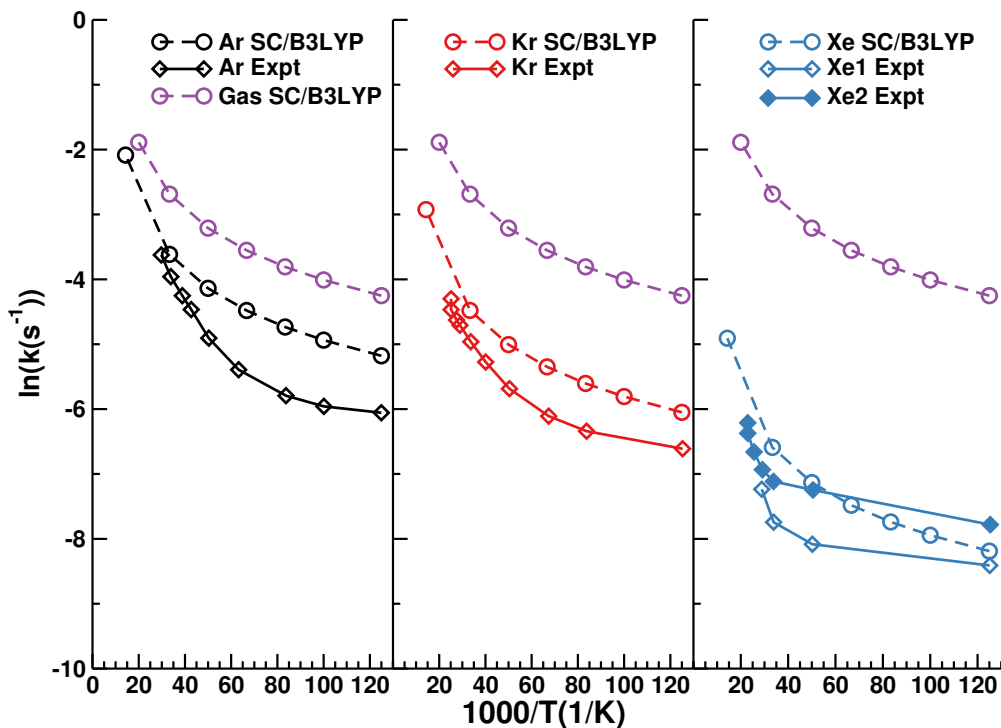


Figure S3: SCTST reaction rates at the B3LYP/def2-TZVP level of theory for the interconversion of the formic acid molecule in cryogenic matrices.

Vibrational Frequencies

In this section, we report the frequencies of the active modes for all systems considered at the ONIOM(MP2/aug-cc-pVDZ:UFF) level of theory. In Table S2 below, we report in red the mode additionally included with respect to the gas phase in the anharmonic calculation for glycine in the different matrices. In the same table, the green values indicate the low-frequency normal mode of the isolated molecule, which exhibits the most significant changes upon including the matrix effect. The primary effect can be interpreted as a compression of the normal-mode movement, mainly due to electron-cloud repulsion. This compression stiffens the bonds, resulting in higher frequencies in the matrix environment. See Figure 1 in the main text for the corresponding normal mode displacements of modes with 86.98 cm^{-1} and 158.61 cm^{-1} . Both modes involve displacements of the molecule atoms and some of the surrounding matrix atoms. A similar situation is observed for the acetic acid in Table S4.

Interestingly, we observe that this phenomenon is susceptible to substituents on the α -

carbon. Deviations from gas-phase values are more pronounced for α -substituted molecules. For instance, in the case of formic acid, the low-frequency modes are at around 600 cm^{-1} and show no interactions with the surrounding matrix, see the purple values in Table S4. The corresponding normal-mode displacements involve just the atoms of the molecule, both in the gas phase and in the matrix. In our view, the low-frequency modes that are coupled with the matrix act as a bridge, facilitating energy transfer through vibrational coupling between these low-frequency vibrations and other modes. In the case of the FA, these modes are absent, leading to less efficient energy transfer through vibrational coupling. We believe this is the primary reason for its different behavior regarding the bulkiness of the matrix. Our fully anharmonic and non-separable SCTST approach enables an accurate representation of the system, resulting in behavior that aligns well with experimental observations.

Table S2: *Glycine* Vibrational Frequencies for Gas Phase, Argon, Krypton, and Xenon Matrices at the SCTST-ONIOM MP2/aug-cc-pVDZ Level

R (Gas)	TS (Gas)	R (Ar)	TS (Ar)	R (Kr)	TS (Kr)	R (Xe)	TS (Xe)
78.593	548.576 <i>i</i>	110.525	529.192 <i>i</i>	89.351	545.312 <i>i</i>	94.951	542.911 <i>i</i>
216.238	102.796	150.234	107.922	149.138	86.980	143.085	92.855
258.661	216.734	239.001	163.118	237.338	158.607	236.010	154.915
451.968	254.131	266.274	231.953	265.751	240.879	264.617	240.523
464.342	461.497	462.393	257.861	453.289	258.533	448.240	258.068
569.001	514.474	468.710	465.882	466.285	463.817	464.984	463.055
638.069	639.240	580.990	527.349	575.910	524.267	574.945	522.511
838.833	836.177	643.886	644.116	643.855	642.321	642.847	642.035
918.944	873.680	843.059	838.651	841.868	838.968	841.858	838.883
937.697	930.260	929.426	884.318	925.388	881.820	925.141	880.127
1127.335	1075.259	939.836	930.151	939.582	931.398	939.621	931.779
1174.014	1126.957	1132.388	1083.165	1128.817	1079.584	1127.124	1078.470
1181.276	1169.761	1179.078	1132.171	1176.509	1129.773	1176.229	1128.667
1285.551	1216.119	1187.927	1175.246	1186.662	1176.141	1185.418	1175.922
1377.005	1368.809	1290.932	1224.476	1286.438	1219.648	1283.334	1217.338
1391.804	1380.399	1381.134	1370.183	1378.001	1370.671	1377.394	1369.782
1457.158	1441.946	1397.213	1387.295	1397.254	1385.726	1396.410	1384.868
1657.650	1655.474	1471.219	1454.046	1469.491	1454.237	1468.373	1452.641
1812.080	1790.134	1664.336	1662.165	1661.070	1659.428	1660.436	1658.873
3063.138	3077.043	1819.213	1796.357	1815.564	1793.966	1815.527	1793.477
3117.960	3131.303	3077.859	3091.029	3079.435	3092.793	3080.151	3094.054
3509.119	3509.950	3133.572	3147.268	3134.499	3146.352	3135.508	3148.080
3597.899	3600.116	3522.396	3526.625	3518.313	3521.568	3516.120	3518.945
3779.902	3815.950	3611.750	3617.341	3607.971	3612.679	3605.572	3609.808
		3801.805	3824.287	3795.792	3822.437	3798.307	3821.116

Table S3: *Formic Acid* Vibrational Frequencies for Gas Phase, Argon, Krypton, and Xenon Matrices at the SCTST-ONIOM MP2/aug-cc-pVDZ Level

R (Gas)	TS (Gas)	R (Ar)	TS (Ar)	R (Kr)	TS (Kr)	R (Xe)	TS (Xe)
524.562	610.532 <i>i</i>	526.346	609.246 <i>i</i>	560.005	604.778 <i>i</i>	561.998	594.100 <i>i</i>
642.510	655.258	642.722	655.608	648.109	659.884	646.612	660.149
1019.882	905.674	1020.335	905.294	1021.691	909.958	1028.238	916.508
1097.205	1064.422	1097.474	1064.794	1105.157	1071.883	1104.947	1073.518
1273.849	1192.078	1274.056	1191.502	1281.665	1196.791	1279.626	1200.553
1404.412	1381.705	1405.600	1383.258	1406.815	1383.581	1409.733	1392.703
1805.281	1767.031	1805.093	1766.802	1809.613	1771.659	1810.029	1772.722
3052.972	3086.918	3053.700	3087.599	3055.011	3087.095	3060.357	3094.268
3790.376	3812.029	3791.123	3815.191	3802.469	3830.194	3800.002	3823.882

Table S4: *Acetic Acid* Vibrational Frequencies for Gas Phase and Xenon Matrices at the SCTST-ONIOM MP2/aug-cc-pVDZ Level

R (Gas)	TS (Gas)	R (Xe)	TS (Xe)
101.068	580.706 <i>i</i>	77.353	578.186 <i>i</i>
433.951	141.969	83.817	75.907
465.069	425.063	437.787	145.751
599.477	554.140	467.199	429.334
599.820	606.218	600.946	557.941
858.066	844.014	602.706	607.623
988.811	971.628	857.385	844.148
1063.287	1011.402	988.971	972.250
1204.056	1153.400	1063.234	1011.934
1294.202	1220.401	1202.919	1153.551
1397.997	1397.484	1292.536	1220.111
1473.197	1465.291	1401.416	1400.249
1485.832	1477.828	1473.904	1467.541
1855.777	1841.418	1486.883	1479.573
3040.035	3046.791	1855.251	1840.978
3095.884	3102.599	3048.630	3053.584
3159.032	3154.598	3103.636	3108.383
3782.246	3803.093	3165.486	3160.115
		3793.031	3807.873

SCTST Results with Implicit Solvation

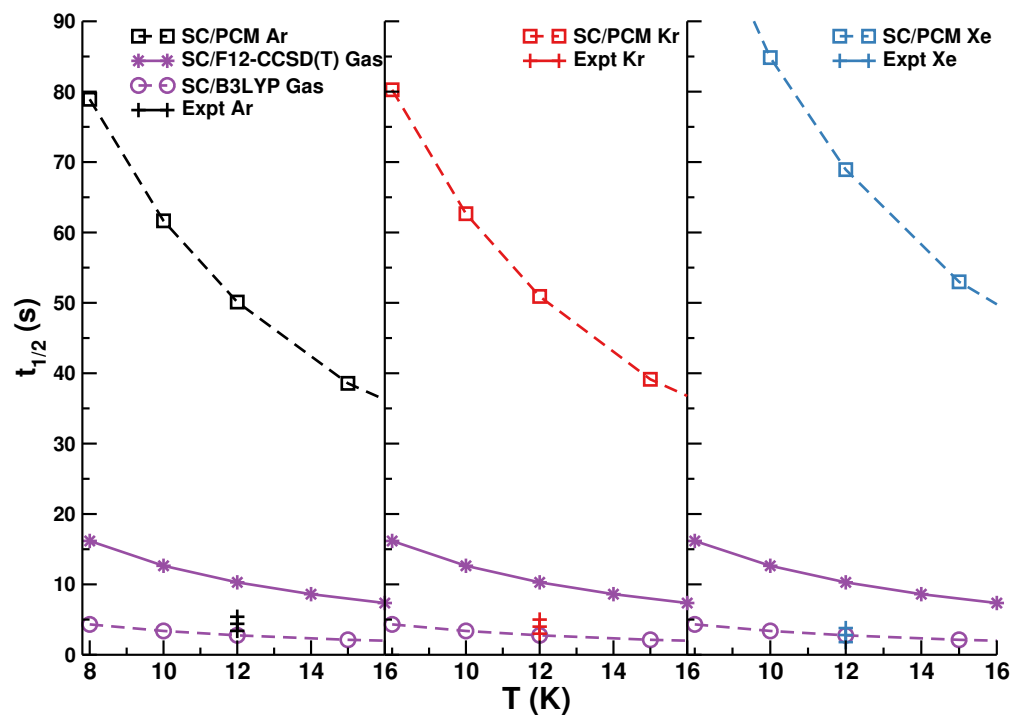


Figure S4: SCTST half-life times at the B3LYP/def2-TZVP level of theory for the interconversion of the glycine molecule in cryogenic matrices simulated using the implicit PCM method.

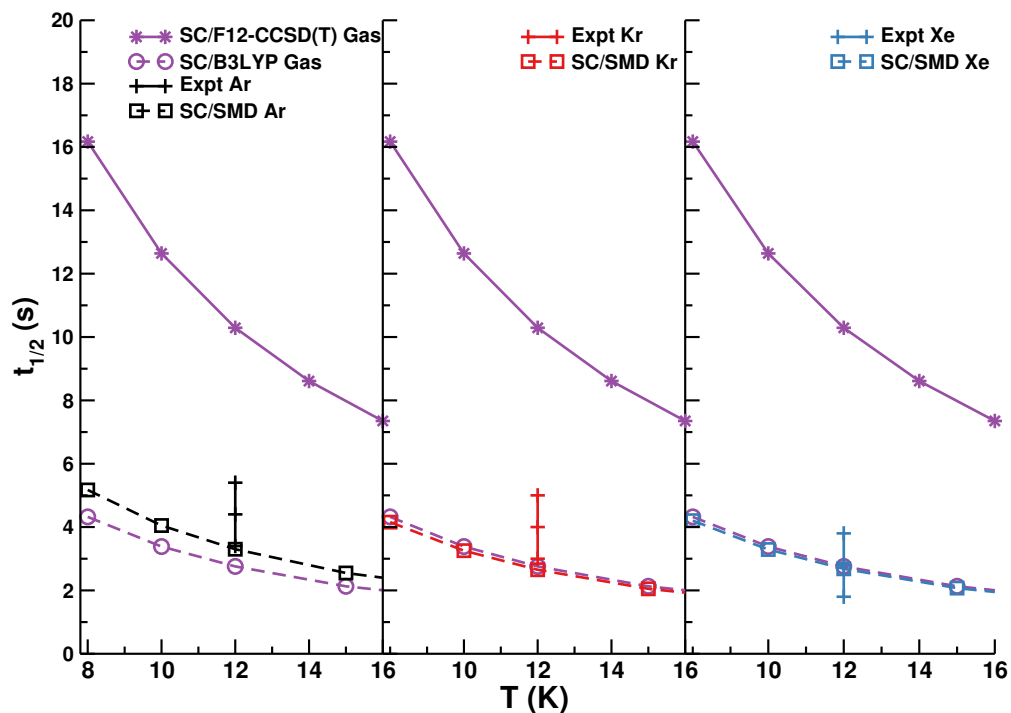


Figure S5: SCTST half-life times at the B3LYP/def2-TZVP level of theory for the interconversion of the glycine molecule in cryogenic matrices simulated using the implicit SMD method.

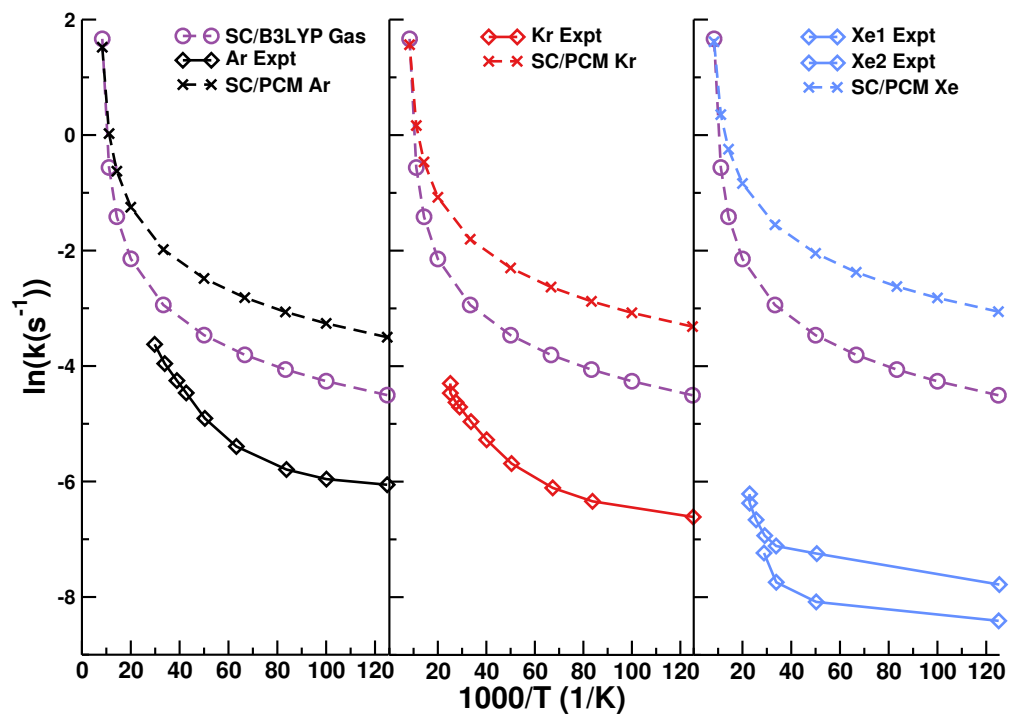


Figure S6: SCTST reaction rate constants at the B3LYP/def2-TZVP level of theory for the interconversion of the formic acid molecule in cryogenic matrices simulated using the implicit PCM method.

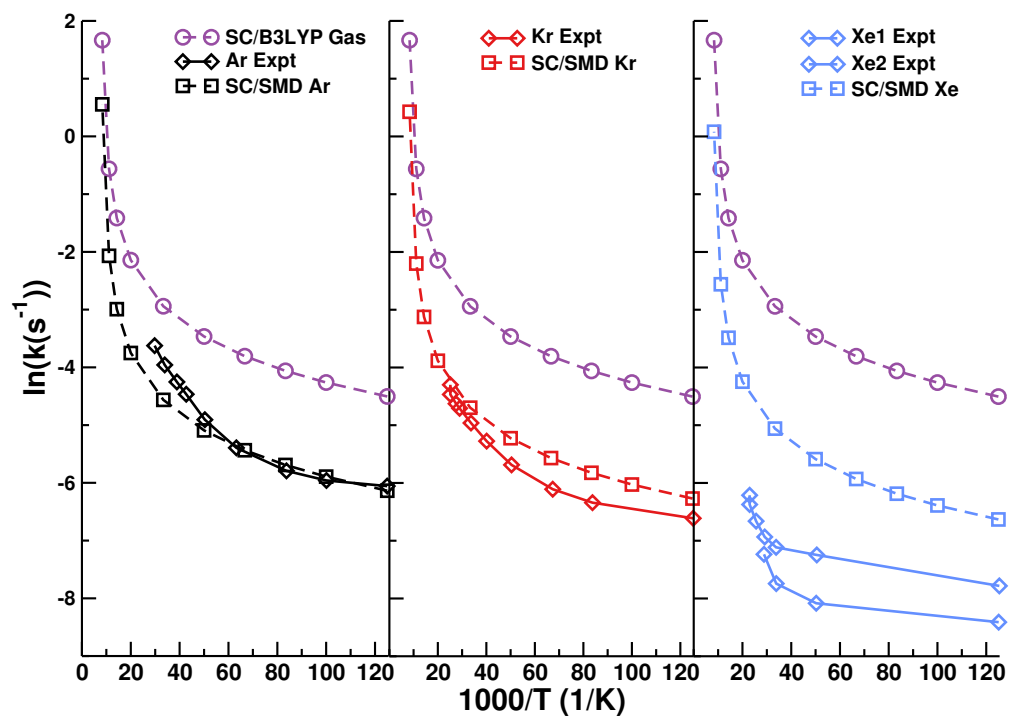


Figure S7: SCTST reaction rate constants at the B3LYP/def2-TZVP level of theory for the interconversion of the formic acid molecule in cryogenic matrices simulated using the implicit SMD method.

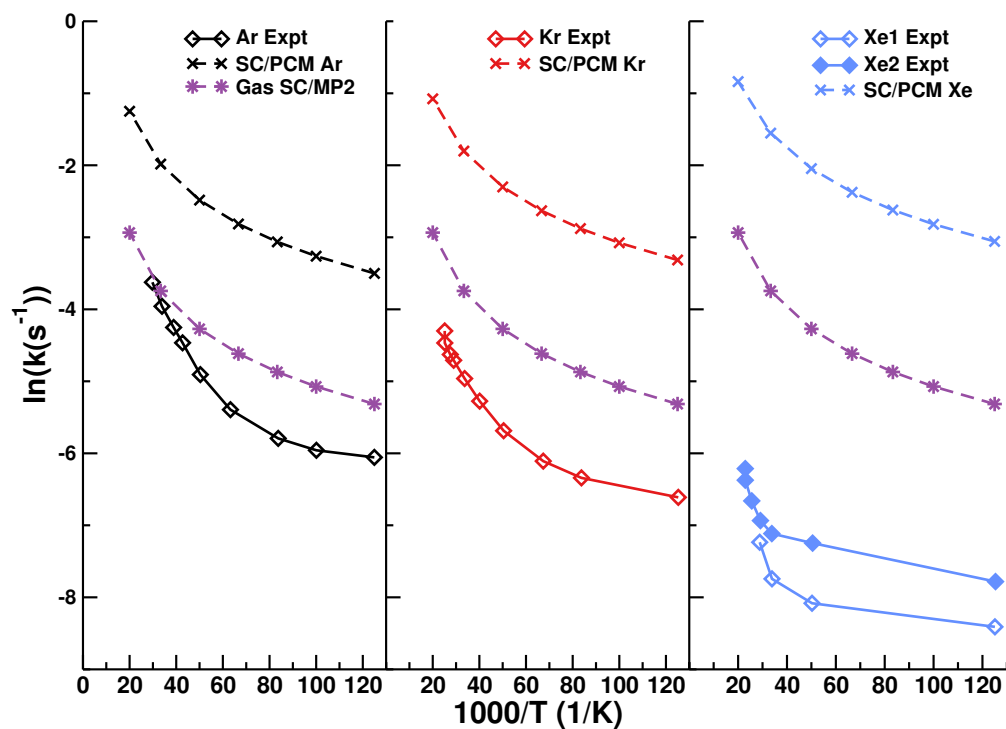


Figure S8: SCTST reaction rate constants at the MP2/aVDZ level of theory for the inter-conversion of the formic acid molecule in cryogenic matrices simulated using the implicit PCM method.

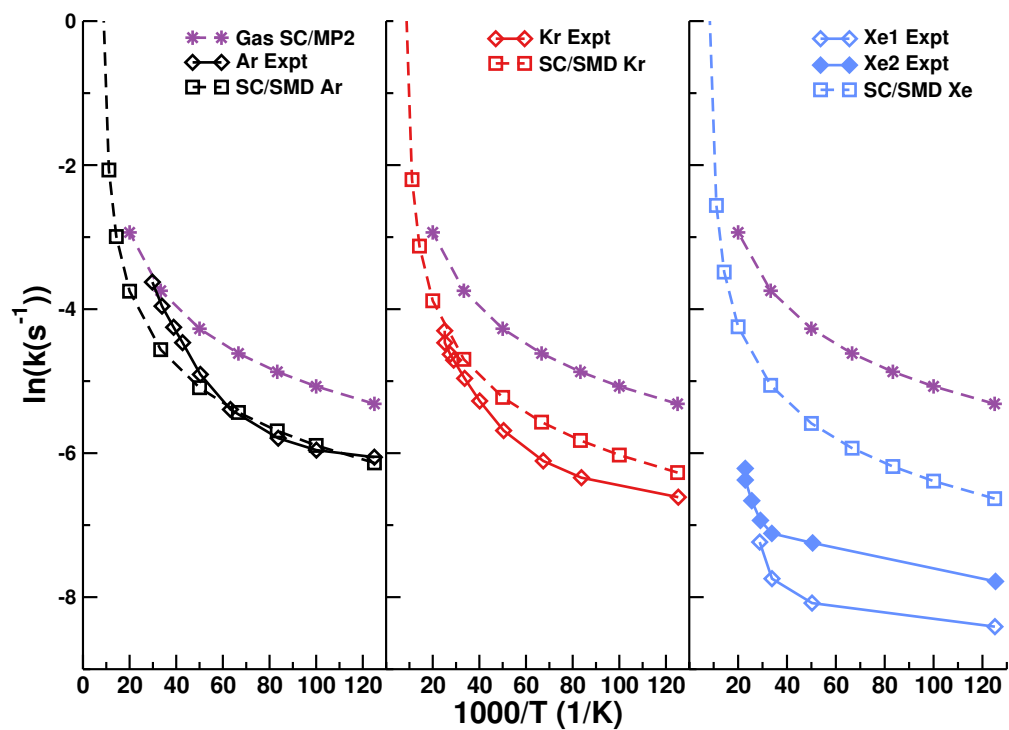


Figure S9: SCTST reaction rate constants at the MP2/aVDZ level of theory for the interconversion of the formic acid molecule in cryogenic matrices simulated using the implicit SMD method.

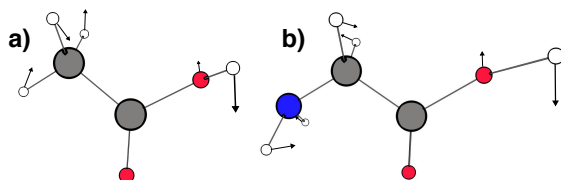


Figure S10: Pictorial representation of the reactive normal mode of vibration for Panel a) The acetic acid interconversion reaction; Panel b) The glycine molecule interconversion reaction.

Optimized Geometries

The optimization algorithm is based on micro-iterations: optimizations of QM and MM parts are done separately, keeping the other subsystem fixed until the required tight convergence of the whole system atomic forces is achieved. The initial geometry of the QM subsystem is guessed starting from the gas phase geometry at the same ab initio theory level. Then, the initial noble gas matrix conformation is guessed. The lattice parameters are taken from the Crystallography Open Database, where it is possible to find the appropriate Crystallographic Information File (CIF). Using the program cif2cell,¹⁵ we generated the structure for the lattice cell, setting the desired supercell size. The different supercell sizes and the optimized geometries for the relevant reactions TS in cryogenic matrices are shown in the listings below. The reactant coordinates will be attached at the end of the present document.

Listing 1: Glycine(TS)-Argon System

N. Ar Atoms 499

Ar (UFF)

Gly (MP2/aug-cc-pVDZ)

C	1.0458278096872313	-2.4294687832273070	-3.7691649946390369
O	1.8912244247983421	-1.8753739877360642	-4.7386217817080611
O	0.39236834960332467	-3.4243928492853306	-3.9902431571572246
H	1.4271896462486933	-1.1660056605940154	-5.2073700922437567
C	1.1366450800273420	-1.7150474401515523	-2.4274291840508249
N	0.31724088109189447	-2.2444185026992192	-1.3495117495252893
H	0.89072123690810578	-0.65259464453796623	-2.5908066705547510
H	2.1995061134937774	-1.7314329207969237	-2.1386952064353060
H	-0.66547930312303794	-2.2110131470992758	-1.6197132026020820
H	0.52339247835965863	-3.2349373063782805	-1.2175821754368774
Ar	16.150997015490045	13.155741210253833	0.26348758916504700
Ar	14.904436557014590	9.8523194452492167	-1.1630593487116083
Ar	12.473901830839978	12.794933073818607	-0.63770534296404879
Ar	13.936411854848943	10.920109174804217	2.4014511850339395
Ar	11.968692733345360	-1.4321650731847000	7.7312309331016715
Ar	7.9682916218480955	8.6824894503230396	-12.921732744293660
Ar	-2.7459358440523762	2.1278909867592146	2.5770106852985788
Ar	5.9881793243612371	-8.5964656655503333	-5.7668059398700979

Ar	11.876703162080931	3.6417357023911068	6.0972192499381723
Ar	-2.8511330106091464	7.2092125709997159	0.99096965836736017
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Ar	13.920596230355478	-8.7465332629217318	2.3246589473490809
Ar	7.4233809307380829	-0.67603076953005437	10.348281260671374
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Ar	-1.1536157307649380	10.173804037813184	-7.5791065280954584
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Ar	−4.1695368961911541	3.9494896933813131	−0.34398782611649315
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Ar	10.432105422215693	5.4536320889636976	3.0773490389717391
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Ar	−4.2802229075900700	9.0642203240529238	−1.9608047154704402
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Ar	−8.5572012585356116	−5.3565955182542933	5.5870158997810417
Ar	10.282219453819382	10.551617214679673	1.4817427375206096
Ar	12.585108947966974	−12.044223459597919	0.96847753094589839
Ar	6.0614159739606253	−3.9511368626482013	8.9552519481622781
Ar	2.0601775651106671	6.1098143265679985	−11.538996310561412
Ar	4.3467631952080996	−16.207655893618899	−11.970976732635114
Ar	−8.6660132900702322	−0.30979163517602981	3.9276394973911364
Ar	−2.3592929081063176	−8.4502470534124825	−4.0199235283006836
Ar	6.8283114048045315	0.30694282981741522	−12.621254084230841
Ar	5.9758525969058578	1.1063795673324406	7.3150019490082316
Ar	12.533094135707366	−6.9364082565248539	−0.66832922270686046
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Ar	−2.4966752185606511	−3.2597643918577166	−5.6614222949702127
Ar	4.2094522294973444	−11.152413084820815	−13.631541945152769
Ar	5.8581120381040277	6.1624548463012641	5.7015269743094050
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Ar	1.5986518058425423	−8.3052978334689076	13.232328724506257
Ar	−8.8451883138482863	9.8209408196985244	0.69804708676800387
Ar	−2.5144467966234267	1.8735423133591125	−7.3675689897550161
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Ar	5.7219878050536810	11.247000494369228	4.0865073991823531
Ar	12.446537820138063	3.2987695086215334	−3.9192624269179355
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Ar	1.5117365225691772	−3.1816137840500316	11.561919312734370
Ar	−2.4944314083646573	6.8630673761708536	−8.9028847644330948
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Ar	3.1463290529723409	−5.0248014455752168	−11.667930701499055
Ar	−7.5904964694274106	−11.670915924410389	3.8480981668295837
Ar	4.8420242361527288	12.336699894534283	7.6062072728245678
Ar	11.426225636908953	4.3881919259759208	−0.40899555325918585
Ar	7.0564605545935342	−10.205135461495873	7.1402092681278742
Ar	0.64296460676849265	−2.0472349538627514	15.084152088027329
Ar	−3.3829195364241906	7.9630762488106965	−5.4292137636582822
Ar	3.0678874276746750	−4.9218955443717280E−002	−13.390963808372655
Ar	−1.1673294291002512	−14.512790172066623	−5.8394000339256102
Ar	−7.6720854144772597	−6.5039144982733781	2.1197825155977901
Ar	11.234954703037420	9.4882991090720239	−2.0144387716099459

Ar	0.53857956456172495	2.9798965530329453	13.466078945143455
Ar	6.9760966542770815	−5.0727976917780504	5.4929302499397465
Ar	2.9418828168103026	5.0079319320024416	−15.027221521513361
Ar	−7.7663658650197940	−1.4224925794734022	0.43702976024937945
Ar	−1.3308785874594109	−9.3755363434147743	−7.4681557395610305
Ar	0.42838337581319413	7.9996135574500897	11.836762566210044
Ar	6.8956449251032259	1.0694188485210327E−002	3.8280926624623852
Ar	−3.8697862405476910	−6.3509743419225986	19.348509434327621
Ar	−7.8521320674202988	3.6570071043884571	−1.1703523352344753
Ar	−1.4684095135878230	−4.3175784690203773	−9.0859842053351354
Ar	−12.154386907270261	−10.809013650566694	6.4776385079650245
Ar	0.30652596874771904	13.047263109366913	10.192911112369957
Ar	6.7833015346078431	5.1022764429485177	2.2169632477193115
Ar	2.5034176917114048	−9.4353432836007460	9.7639539078547628
Ar	−3.9737343711453472	−1.2725492623931909	17.756479259491115
Ar	−7.9356607018838909	8.7444093897406514	−2.7778752760682566
Ar	−1.5480654055351382	0.72602388679854613	−10.786471350744026
Ar	−5.7854714567735224	−13.862782361337803	−3.2070649816903676
Ar	−12.258250800322754	−5.6895105143946223	4.7862382926359262
Ar	6.6483041615956715	10.197809853125102	0.61255728608148841
Ar	−4.9038067809519443	−5.0001992734689162	6.4328015732013473
Ar	8.8823894580816543	−12.386819601430753	0.15924296232340768
Ar	−4.0829757436465499	3.7530102361753879	16.132429587690652
Ar	2.4067064189331471	−4.2983749009308383	8.0857750860219024
Ar	−1.6056558886357737	5.7644042014945613	−12.393633971086141
Ar	−12.370599390245019	−0.63932586243451139	3.1318086105270102
Ar	−5.9837594262467864	−8.7520966668222346	−4.8695800861192335
Ar	−4.1960918762708808	8.7708324834303522	14.491320838127947
Ar	2.3216205813477075	0.74696339230253095	6.4478730124245889
Ar	8.8247111328995622	−7.2554350169400088	−1.4695984251127450
Ar	−12.464435481566666	4.4182396858427815	1.5235736557591806
Ar	−6.1075120347199503	−3.6235543725746435	−6.5271307696760683
Ar	−4.3006447101652938	13.783796413492936	12.827077480184714
Ar	2.2062171655676428	5.7774061984582978	4.8256573759668484
Ar	8.7937534434131521	−2.1531674077549532	−3.0831065747607962
Ar	−2.0502077228673925	−8.6570653946976552	12.387714078517396
Ar	−12.544664563964975	9.5074515902675270	−8.5517563423865323E−002
Ar	−6.1622504437882277	1.4969617709609904	−8.1790938693855146
Ar	−10.362370968777157	−13.091903423612512	−0.52249414712305620
Ar	2.0829789700529178	10.865147674583442	3.1966965098429236
Ar	8.7805964424440131	2.9854326239951665	−4.7461786284506475

Ar	4.3140367923270295	-11.637628034022729	2.8087446812628944
Ar	-2.1461542649640504	-3.5291643310028520	10.707550160317027
Ar	-6.1738550248766799	6.5557726788993200	-9.7650075276613819
Ar	-10.489975930523041	-7.9675590834254093	-2.2185596995225625
Ar	8.5569057328612956	8.0160116489891831	-6.3789774925033011
Ar	-2.2418275211999998	1.4974132268442661	9.0618493348909954
Ar	4.2742204104200834	-6.5324187053595972	1.2136609425717957
Ar	-10.618445169646904	-2.8656129553384679	-3.8919388066225045
Ar	-2.3459039871848586	6.5104189369029006	7.4315656797151135
Ar	4.4438150759134700	-1.3888117078063682	-0.33601089080249913
Ar	-6.6670068868738390	-7.8439550174572723	15.071799549780069
Ar	-10.664031419200768	2.2458820335139316	-5.5081447141966065
Ar	-14.932028679145132	-12.243989139991701	2.1855327861357869
Ar	-2.4577096029670167	11.576457906306281	5.8018996989549718
Ar	4.1969027612169327	3.8465916409851233	-2.0280856170070001
Ar	-0.23522786468981222	-10.911051678282201	5.4730090310201112
Ar	-6.7738322318798749	-2.7363757021759723	13.385272532753085
Ar	14.354774503058769	-9.4778201841904899	8.8870929113121946
Ar	-10.704905371602219	7.3335214131737851	-7.0929125142163434
Ar	-15.026638949665879	-7.1441587970522349	0.49768255636540454
Ar	3.9236346086069189	8.6683506300493089	-3.7400428137236226
Ar	6.1266947433900194	-13.790352664410221	-4.1624384923997484
Ar	-6.8757399858391945	2.2723493829879531	11.754962521153269
Ar	-0.34311236985287286	-5.7555185681253995	3.7957266858531873
Ar	14.285311010472777	-4.3536457049081623	7.2542421626868219
Ar	-15.127198818090699	-2.0774489938373879	-1.1732149809306283
Ar	-6.9782837612354545	7.2827467749679498	10.118035089539225
Ar	-0.40059908231660585	-0.77733921992845367	2.0191041455499419
Ar	8.3547546242384527	-11.531784011281422	-6.3205037107348261
Ar	14.211147047256333	0.72384340762692367	5.6026248292488683
Ar	-15.221273224662648	3.0184204157071521	-2.7893108372282445
Ar	-7.0753416148165060	12.328325236478706	8.4761163342020485
Ar	-0.51034086334290341	4.2527589670898269	0.45771886444678550
Ar	5.9503946302564001	-3.5368442182953728	-7.3630758098310096
Ar	-4.7964520032050268	-10.136333641763114	8.1301180641452380
Ar	14.101461315485102	5.8285510319455511	3.9835643491759050
Ar	9.8186616415371386	-8.7313138896740536	11.509534856444132
Ar	-15.280527479484375	8.0988643962617353	-4.3698069027460340
Ar	-0.64173825908897553	9.4106154984575756	-1.1323316632834506
Ar	1.5452359450495181	-13.048807036986178	-1.4911626627917909

Listing 2: Glycine(TS)-Krypton System

N. Kr Atoms 440

Kr (UFF)

Gly (MP2/aug-cc-pVDZ)

C	-1.6030482353048399	1.1769779215208207	-0.47448293648596906
O	-0.71383252974772338	1.4731505765229211	-1.5158442769228830
O	-2.7090812214302278	0.73295698059743419	-0.68916512172048516
H	-0.76947302161109499	2.4147884002010636	-1.7365059075315892
C	-0.98820216436799391	1.3669831679533591	0.90564942640776191
N	-1.8391757017248955	1.0578740173596373	2.0433216334909394
H	-0.63091279089302610	2.4073075885868684	0.98043365948143990
H	-8.1966184336219092E-002	0.74120029626554973	0.93261385968584065
H	-2.6940134496898391	1.6127414196605154	1.9913619528038959
H	-2.1466003550814823	8.7236093563986927E-002	1.9818073367766629
Kr	18.207926322396567	0.58573309912118166	-10.184964236745458
Kr	14.802261603358174	-1.6502467257688374	-10.156933676120611
Kr	-7.9030516376783240	12.004406518117205	4.1103711085179100
Kr	-1.1628241249112823	15.320950636664891	-2.0505722670856938
Kr	-8.1069283660925482	4.9331708292854444	-3.9949962748939689
Kr	-15.015639925620423	-5.3381771341317297	-6.0878872425752286
Kr	-14.856786954606880	1.6552369931315116	2.0179681793207283
Kr	11.528703503801017	0.79182832351419430	10.157570439192440
Kr	4.4097865196889741	-16.521066272982502	-3.6004854744397949E-002
Kr	18.108316827704321	-2.9288737553701711	-4.0406524087518987
Kr	18.317936064607700	4.0822908381690395	4.0955638805985268
Kr	11.368621283920195	-6.2155377447496400	2.0148030032829092
Kr	-14.935651657796640	-1.8566009655151765	8.0852249474394196
Kr	-1.2733177937654698	11.781923861651267	4.1146715630695887
Kr	5.4425354324323747	15.068497215513386	-2.0444077762133110
Kr	-1.4839470217817936	4.7657042537145120	-4.0025077296324039
Kr	-8.4215809363859062	-5.5539774761132730	-6.0573586704812765
Kr	-8.3291360261393326	1.4342153028426612	2.0452749477235246
Kr	-15.147659658532529	-8.8521485707131795	-2.3547314719228767E-002
Kr	18.147409520148869	0.56574068807790179	10.229793922856638
Kr	10.983712519116860	-16.729904394588353	-2.4355212251627234E-002
Kr	17.979100122090710	-6.4448632388631202	2.0390585079671144
Kr	-8.3374547570084019	-2.0660232850699258	8.0664635150101720
Kr	5.3083876804828343	11.528426701553094	4.0969781249050818
Kr	12.027931225982849	14.838379981378083	-2.0322251958777131

Kr	5.1425835740087740	4.5276796687257113	−4.0298022850863777
Kr	−1.8270322172823099	−5.7079048755863759	−5.9854380210777407
Kr	−8.5498766611378905	−9.0621239287383784	−8.9347465876951776E−003
Kr	−14.482379713445049	12.204185105754810	−4.0772945290485296
Kr	17.616230700971080	−17.022268086293327	−1.3707855215334800E−002
Kr	−1.7439630826793810	−2.2914745295076213	8.0247490765454561
Kr	11.904004579345065	11.308837366642495	4.1100266874116373
Kr	18.645948667860004	14.669212406641428	−2.0023856376115750
Kr	11.756573306523583	4.2999511908956940	−4.0452127890984544
Kr	4.7518910485298882	−5.9711019611105094	−6.0403814630939117
Kr	5.1016898597760099	0.92607039631374533	1.9930782526439186
Kr	−1.9513880863366992	−9.3137752869021266	3.8276630566586050E−004
Kr	−14.633264446232435	8.6773348007477740	2.0281794400602116
Kr	−7.8967646335784023	12.010905899869480	−4.0889699024635373
Kr	−14.803111536708469	1.6678347651078813	−6.0654379687232156
Kr	4.8565148875147592	−2.5110229413818197	8.0610066242476464
Kr	18.517587907065895	11.127763834333972	4.1405032440651750
Kr	18.353698302838584	4.0909548437156129	−4.0340772177089859
Kr	18.460133776679736	7.6025762098424003	−1.9957410703220895
Kr	11.353515793788288	−6.1959023117725893	−6.0609649255861253
Kr	11.501857031723874	−2.7048193394521682	−4.0342849324327528
Kr	11.615448526298637	0.78136684407393020	2.0183651607094242
Kr	4.6476310679850794	−9.5009526297299125	−6.4006403036254529E−003
Kr	−8.0384340560942338	8.5090674773430237	2.0382180703381345
Kr	−1.2805293688981172	11.849478447811091	−4.1418053288926746
Kr	−8.1781273620251955	1.4504150376909297	−5.9690644932063561
Kr	−14.954182328281332	−1.8496914756947698	−8.9489871702644625E−003
Kr	−14.719760087397701	5.1618228757369398	8.1274532268216344
Kr	11.443022994331839	−2.7123752000149013	8.0839082378210652
Kr	18.218231602491212	0.57315141160408600	2.0531447158011877
Kr	17.984982289936127	−6.4425719385026161	−6.0932785071364197
Kr	11.242529062379109	−9.7065179404491246	−6.8410577379321288E−003
Kr	−15.042211034278532	−5.3600233376867390	6.0525838108740926
Kr	5.3444210992703596	11.578314796741726	−4.1051199217254819
Kr	−1.5758158726742872	1.2608955136209343	−5.8587539128603625
Kr	−1.4111799200533379	8.3253238807502985	2.0144965818092664
Kr	−8.4139015216813604	−2.0854022980545466	2.5351723923396529E−002
Kr	−8.1095973061241651	4.9413124442400047	8.1049657436990650
Kr	−15.241571079560664	−12.358262058595640	−2.0621774933674222
Kr	18.070540929243542	−2.9463569195254755	8.1546736844993841
Kr	17.859111678911816	−9.9537454744725693	2.0154054901577534E−003

Kr	−8.4483651051962330	−5.5707106317441779	6.0471163901313778
Kr	11.944177816925571	11.333278393561859	−4.0701674042824223
Kr	5.0232102372481107	1.0281084206087794	−6.0617343775840391
Kr	5.2050652341690533	8.0351183680199298	2.0092169913286186
Kr	−1.6755213529042998	−2.4996890953879651	9.3543602129498304E−002
Kr	−1.5193787648772483	4.6429104074500307	7.9252752223213960
Kr	−8.6511779977459540	−12.559324343515863	−2.0483818912981469
Kr	−14.577347202883260	8.6861666082987892	−6.1003227196321630
Kr	−14.372354685963437	15.718098214658802	2.0612526103092312
Kr	−1.8509685571574721	−5.8323530087085613	6.0795558936370409
Kr	18.554978022582173	11.142482899752608	−4.0486098515056668
Kr	11.617924004092174	0.79831010803341906	−6.0593078253202819
Kr	11.828020002690854	7.7991617543223457	2.0318414494374419
Kr	4.9350060047859747	−2.5313844200609315	−1.5600641618481008E−002
Kr	5.0263699734774860	4.4803544407689220	8.0310270098797183
Kr	−2.0642132676229576	−12.791472574772254	−2.0504723183445113
Kr	−7.9883902798831201	8.4655853242436603	−6.0762111380344646
Kr	−7.7699446713188438	15.509434809655559	2.0773231659704874
Kr	−14.886501858249822	−1.8279968250475704	−8.1043231664306372
Kr	−14.744029870414892	5.1672244622913315	1.2703078313176909E−003
Kr	4.7619504263458552	−6.0383804925018172	6.0770264205375435
Kr	18.234060864593825	0.58269360515073965	−6.0714873204677522
Kr	18.439934151684547	7.5965802253664005	2.0724649837982287
Kr	11.509851230169216	−2.7191915593262403	2.8770248516099459E−003
Kr	11.650834424632205	4.2921067217571833	8.1247815241406549
Kr	4.5270857511243365	−12.994781851376056	−2.0501427219060124
Kr	11.711328827768057	4.2780303241768705	4.0480283213039421
Kr	4.7772151791795681	−6.0231174755170631	2.0210803933026593
Kr	−14.847646659857984	1.6480707512325081	6.0636481422804716
Kr	−1.3953401938451768	8.2846390934029692	−6.1252185184646448
Kr	−1.1614127195067263	15.297470357722650	2.0833676987170957
Kr	−8.2947186720887416	−2.0328231823051306	−8.0443755734038156
Kr	−8.2538879369004245	5.0525261510273021	1.8178326292211638E−002
Kr	−15.046060628398426	−5.3475370001910942	−2.0343981615013891
Kr	11.349789613192915	−6.2200787175942951	6.0634030550755336
Kr	18.104889181694777	−2.9338558905230276	1.7442595400437123E−002
Kr	18.270124674812845	4.0910790850188903	8.1935550379375961
Kr	11.115593696548345	−13.208028110588890	−2.0420981295937719
Kr	−15.147461400829869	−8.8639737289075242	4.0248766696356162
Kr	5.4325328450871488	15.048378058514245	2.0811802287543495
Kr	5.2384585586134387	8.0515623923564288	−6.1170390898296745

Kr	−1.7094010162883388	−2.2073175489616781	−7.9275439219833181
Kr	−1.6619322547489794	5.0584800252473494	−0.10493081274340449
Kr	−8.4428406235214624	−5.5598124237014614	−2.0099986129161564
Kr	−8.2642818181462232	1.4289125613683549	6.0566217427813189
Kr	17.970484453890421	−6.4573943448548414	6.1139795183604546
Kr	17.745074049723364	−13.477239749977604	−2.0492667337850174
Kr	−8.5585204537495443	−9.0775819945042393	4.0346182601634286
Kr	11.843229410163472	7.8238919550555126	−6.0936865655924732
Kr	12.012050723223920	14.826027878012841	2.0962568369470116
Kr	4.8730361058878726	−2.4633555797999702	−8.0523273656207532
Kr	5.3488880615471484	4.6607565770089669	−4.1324746084272210E−002
Kr	−1.8404351442265783	−5.8230688274224978	−1.9949021267748455
Kr	−1.6520951826455494	1.1535373646532969	5.8342981835923204
Kr	−14.503423409782794	12.186554111957248	4.6925128323175623E−003
Kr	−14.656441582884399	5.1799179582791135	−8.1250979437369093
Kr	−1.9552219571202569	−9.3444464288201896	4.0668987389800941
Kr	18.455210474740685	7.6244194732611321	−6.0906040274764841
Kr	18.629864149782254	14.660413326088685	2.1097474003619814
Kr	11.470268808990484	−2.6906378801510376	−8.0787848178510497
Kr	11.744210617922036	4.2939561565074547	2.1782410713781326E−003
Kr	4.7763370007462358	−6.0073453276864353	−2.0140005839469231
Kr	4.9529794935537463	0.97441777803587526	5.9725617687396513
Kr	−14.615282984448918	8.6771504313974113	6.1062353848920212
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Kr	7.8619843656393265	−11.980346174216779	4.0756223779296299
Kr	14.581495104217225	−8.6596299307944040	−2.0247479290442105
Kr	14.799884058887130	−1.6670793808036848	6.0785143097953824
Kr	−18.635085177658361	−14.670615155191916	2.0118849328695370
Kr	1.9404285652292399	9.3235258012006277	−3.0170390145849109E−002
Kr	1.7318924860909786	2.2845460183145110	−8.0260157182334417
Kr	−5.1768323450770488	−1.1225892758373455	−2.0073959430456920
Kr	−4.7876064288040974	5.9881196876626399	6.0334869241698490
Kr	−11.904229094944981	−11.307966995411210	−4.1096783553708667
Kr	−11.718304851936741	−4.2964241718137623	4.0273290068789649
Kr	−17.662836218724170	17.026497924365692	2.6333332865273217E−003
Kr	14.443579253349450	−12.196329353087123	4.0735159878838507
Kr	−12.019325747214310	−14.837910695536912	2.0320105004210194
Kr	8.5547440555725771	9.0568522628461796	−5.5594475666894598E−004
Kr	8.3440742347257757	2.0722336140469744	−8.0853401970850367
Kr	1.6414458992631611	−1.1377059285472337	−1.8793318006136996
Kr	1.7843490376347084	5.6724927901427113	5.8842794366698490
Kr	−5.3217662187151147	−11.527522192477985	−4.1041437526189828
Kr	−5.1103770306193725	−4.5184536043768624	4.0227905286523589
Kr	−11.023098854897045	16.752240160008157	1.5050691320343160E−002
Kr	−18.140432033210480	−0.56528638982668822	−10.227287613356864
Kr	−18.009687666650787	6.4427389060825027	−2.0386300869438330
Kr	−5.4392629418356844	−15.063759865250990	2.0344451024916030
Kr	15.166919156074545	8.8533037476239507	2.7286587574889554E−002
Kr	14.941965096196006	1.8523842714873775	−8.0836966418594915
Kr	8.2880853774350403	−1.4579035778240510	−2.0101175221877425
Kr	8.3960322196692836	5.5382041104709758	6.0450080587201596
Kr	1.2694806975411967	−11.740142463701169	−4.1076401678804597
Kr	1.5031001306764691	−4.8246791581663615	4.0709409262273191
Kr	−4.4270987339360497	16.558311833088169	1.8892285339442136E−002
Kr	−11.523272869795296	−0.77758401542536537	−10.150944107401079
Kr	−11.420363548470148	6.2435896242057627	−2.0190394791709667
Kr	−18.319420613092287	−4.0872444646143391	−4.0873925521246335
Kr	−18.135353408323628	2.9212523806494772	4.0468218119211521
Kr	1.1548558643755553	−15.287047161970023	2.0289776648665865
Kr	14.835138455003975	−1.6549754221216697	−2.0104427825784326

Kr	15.012221428340679	5.3390595289238227	6.0941915843929300
Kr	7.8623176386916551	−11.952802760966616	−4.1028635880523723
Kr	8.1155456432549435	−4.9680766033039090	4.0416885343451030
Kr	−18.210347983629216	−0.60045970915855440	10.187427555635749
Kr	2.1773139893696563	16.324966429660890	1.8390803442970109E−002
Kr	−4.9466357460646933	−0.99143023562276844	−10.082643479572550
Kr	−4.8618698039352362	6.1162776738925677	−2.0237196856756245
Kr	−11.710593456391639	−4.2911279719698889	−4.0400930099875101
Kr	−11.535149359797771	2.7221460218774540	4.0434843864968526
Kr	−18.440099344233658	−7.6097430471806637	2.0047343302098386
Kr	7.7364869614289660	−15.484885354694546	2.0374722978210364
Kr	14.448737467096656	−12.179982007673329	−4.0886510071044189
Kr	14.696508740200008	−5.1664047914604723	4.0517111687170368
Kr	−11.590194155381859	−0.81109821754174161	10.148811054551656
Kr	−18.648340352884205	−18.246125397327301	−5.2092580672871217E−002
Kr	8.7663106719821613	16.084543164759943	2.7158359646811597E−002
Kr	1.5985081490062263	−1.2062710574609157	−10.085985756760254
Kr	1.8416717457908300	5.8769943520012919	−2.0620714780970690
Kr	−5.0979556759980271	−4.5251484821390831	−4.0197615178815091
Kr	−4.9817135338853094	2.4957791011590764	4.0542900692865533
Kr	−11.817730162189747	−7.7972506306045402	2.0080748518166249
Kr	14.322607750914646	−15.711851581400429	2.0382708799541711
Kr	−17.783408996595355	13.486740708459322	−2.0454068067293472
Kr	−4.9940843920711746	−1.0325295082551311	10.123384613205632
Kr	−12.124058841662823	−18.402160033511262	−4.1465719199947570E−002
Kr	15.338814688016877	15.875347048645283	4.5384006029576034E−002
Kr	8.2045018190221093	−1.4278744063787767	−10.141389228533209
Kr	8.5407660157222125	5.5961060209996836	−2.0592213099176271
Kr	1.4901761088398879	−4.6657637923312203	−3.9688078319110862
Kr	1.6320093604677901	2.1612819580587641	3.7781064300998666
Kr	−5.2210194724558132	−8.0399689830245293	2.0264953815214413
Kr	−17.915414685760801	9.9606262041619544	4.0719921056176869
Kr	−11.150240325421645	13.238824987127000	−2.0164763950686879
Kr	−18.106337120167733	2.9310714358687342	−4.0701692642978706
Kr	1.5819834613924988	−1.2506176275103815	10.116789237370774
Kr	−5.5565979639907095	−18.619431075602268	−4.2747067689074505E−002

Listing 3: Glycine(TS)-Xenon System

N. Xe Atoms 440

Xe (UFF)

Gly (MP2/aug-cc-pVDZ)

C	1.7430815789163816	−1.1419342532833145	−0.28551610088893808
O	0.86215571934804647	−1.4283498403698611	−1.3366390680829094
O	2.8357790669192293	−0.65977435037606891	−0.48601323565085980
H	0.93728923075702597	−2.3619272885137601	−1.5843641756063145
C	1.1379385932328303	−1.3931287865975635	1.0894334427180385
N	1.9775818714852174	−1.0764315291876727	2.2336594174483961
H	0.82618817241595099	−2.4495597818345232	1.1380387090699922
H	0.20576407639167646	−0.80812264574431592	1.1341154536055484
H	2.8593263394571951	−1.5852781004226930	2.1614002029205799
H	2.2355091127810929	−8.9945080200699246E−002	2.1995941850762284
Xe	−19.314889723150952	−0.61854708815198989	−10.849053923199341
Xe	−15.695505368657997	1.7598789258597483	−10.812172055705270
Xe	8.3703946236314017	−12.753714830632020	4.3631403406639810
Xe	1.2218652243309231	−16.271605391989848	−2.1832352970642126
Xe	8.6049554719202259	−5.2594966968748160	−4.2646697813957664
Xe	15.961537429901970	5.6629862950049814	−6.4631445846036470
Xe	15.760689416964180	−1.7723062885937115	2.1476022279262716
Xe	−12.258804446616516	−0.84130175007148300	10.803455472108539
Xe	−4.6761792108728679	17.568784096108647	−2.8045167206699907E−002
Xe	−19.222420323634811	3.1156852818283891	−4.3113140942000383
Xe	−19.464241601767625	−4.3350822777262046	4.3387857966773522
Xe	−12.067131555091938	6.6068503058309389	2.1394886897541010
Xe	15.851996538524441	1.9545694293094513	8.6018116692922817
Xe	1.3457474802394698	−12.508219880007671	4.3606304668591003
Xe	−5.7905501674277469	−16.015416093868275	−2.1790490985434108
Xe	1.5893398583803053	−5.0171150622515901	−4.2411773320927146
Xe	8.9552752016215873	5.8921371931754996	−6.4345631581827814
Xe	8.7904678198661603	−1.5329013985752955	2.1511844150555097
Xe	16.103702010387291	9.3960561600851698	−1.4988564207226380E−002
Xe	−19.294551233270703	−0.59854530444256182	10.865832875876695
Xe	−11.665768863337277	17.792310211817835	−2.3618999176573209E−002
Xe	−19.098046866109755	6.8526825721212354	2.1555834095958244
Xe	8.8469617340299944	2.1849554654722789	8.5735768908857413
Xe	−5.6537636945489798	−12.258216196866980	4.3574008156852502
Xe	−12.785564451623854	−15.771537799194601	−2.1726797766404897
Xe	−5.4249140776257576	−4.7962026689984407	−4.2800795618439471
Xe	1.9546792305883365	6.0870228036337721	−6.3799929660966086
Xe	9.0916218162245297	9.6272737413326670	−6.5817059118708819E−003
Xe	15.371323457316789	−12.984211264857775	−4.3336665319157319
Xe	−18.719151012762978	18.101689714425348	−2.1676377709207040E−002

Xe	1.8469549637580751	2.4308843882024536	8.5443135644678225
Xe	−12.659572059765292	−12.022163817134057	4.3636397294998108
Xe	−19.821157984408217	−15.584615291593089	−2.1536236035520262
Xe	−12.454091829093812	−4.5645907041525078	−4.2977130491831934
Xe	−5.0359994994768735	6.3497678826476767	−6.4205063497474102
Xe	−5.3751290160545366	−1.0161037077411239	2.1281313545225449
Xe	2.0809800582957192	9.8996443638517135	2.6172213848963833E−003
Xe	15.519679520488172	−9.2317414799713049	2.1583575649333651
Xe	8.3703939489111701	−12.763311314063619	−4.3478810709020150
Xe	15.730353036457618	−1.7841977086434302	−6.4483590442022800
Xe	−5.1604550707360204	2.6636364083414565	8.5745468596679366
Xe	−19.689802463856420	−11.823216339651555	4.3829395600962622
Xe	−19.480423007367559	−4.3431143081429804	−4.3086201293527866
Xe	−19.604310496674966	−8.0731994155305404	−2.1426290879060237
Xe	−12.044194906722263	6.5894171645807020	−6.4455214452422851
Xe	−12.192187070279305	2.8753817059172402	−4.2878071214512063
Xe	−12.323852772564132	−0.83029910378507166	2.1450070610528886
Xe	−4.9300338193430662	10.101376952241385	−3.4850266411046477E−003
Xe	8.5110912514111554	−9.0253545211146271	2.1580317629307335
Xe	1.3489506283987822	−12.558573336899787	−4.3790914972502764
Xe	8.7030487163557471	−1.5510819570405543	−6.3803838170884664
Xe	15.872999220176666	1.9505238688271069	−4.3841831552308384E−003
Xe	15.608778948919115	−5.5035344712782734	8.6460781333899348
Xe	−12.158307387258793	2.8833575397199560	8.5928960982251361
Xe	−19.348639614797001	−0.60592243894980580	2.1677686326669843
Xe	−19.093282283050073	6.8518463083941956	−6.4925760639232211
Xe	−11.937970428402998	10.322259584086371	−8.5518753465396863E−003
Xe	15.975086652703398	5.6797330039167386	6.4426110399093952
Xe	−5.6760479503077015	−12.293251734235341	−4.3572756802715302
Xe	1.7122421465426012	−1.3145963367943185	−6.2949094072740746
Xe	1.4832658026375332	−8.8006040075513710	2.1339146076698476
Xe	8.8829991080724131	2.1958569190988424	1.3775547153812955E−002
Xe	8.5922584058552740	−5.2629652160269371	8.6196007941746320
Xe	16.213960548318457	13.126150419564988	−2.1804852660710203
Xe	−19.205998795902818	3.1349242970322293	8.6583380793804796
Xe	−18.972929180114559	10.584126796231079	−8.5278449362710326E−003
Xe	8.9697082590356185	5.9092290209511011	6.4288023557223912
Xe	−12.681476592829988	−12.040328271511985	−4.3350119472877662
Xe	−5.2922129681759147	−1.0899786889856278	−6.4173128523461225
Xe	−5.5409990308846302	−8.5312103007024778	2.1426090763750545
Xe	1.7831180588627711	2.6459032555793844	9.5808206559874681E−002

Xe	1.6053533679644534	−4.9554795439144765	8.4703010059248989
Xe	9.2067792889823110	13.348896964071587	−2.1719913153020647
Xe	15.480739271175956	−9.2476141575109150	−6.4867635916170849
Xe	15.247011892005483	−16.721537650204908	2.1948670731967472
Xe	1.9646866037722892	6.1850820231107280	6.4590754944651012
Xe	−19.708349226244234	−11.834840709920059	−4.3287928902893533
Xe	−12.310698131241626	−0.84714616826539235	−6.4401261517601212
Xe	−12.559529389560085	−8.2830051893026617	2.1580084174972267
Xe	−5.2040648910911358	2.6768140288859699	−7.7678064257241733E−003
Xe	−5.3588557764687534	−4.7753718343315228	8.5752616219991413
Xe	2.2044982795682744	13.601981766833779	−2.1738119029482812
Xe	8.4776904337949386	−9.0095624499350500	−6.4753340846473355
Xe	8.2343210885922300	−16.487023814060731	2.2069557681260834
Xe	15.828331713979049	1.9329668315272692	−8.6112906620704237
Xe	15.641580021808867	−5.5026116519346191	2.7427837041596229E−003
Xe	−5.0525800147531550	6.4049507357244231	6.4540026319524131
Xe	−19.349452408583797	−0.61610716847343772	−6.4732256586657977
Xe	−19.594291911115320	−8.0683071585083752	2.1848886261623548
Xe	−12.203466313805409	2.8882014612079532	7.0149286699564949E−005
Xe	−12.388895519081085	−4.5643262177500077	8.6408946141059122
Xe	−4.8006298245798504	13.819742741019684	−2.1734678161874723
Xe	−12.432949172629881	−4.5488920366940775	4.3007178689517325
Xe	−5.0666254067975371	6.3980190380691555	2.1489724522628522
Xe	15.750918492744448	−1.7687015816885605	6.4497119750868448
Xe	1.4746659751069859	−8.7808134937283935	−6.4897379496727794
Xe	1.2215643687828404	−16.253834601104376	2.2098425592611495
Xe	8.8269913244486471	2.1590349728798186	−8.5637375105376865
Xe	8.7012190600023782	−5.3333498523720673	8.8257891568268854E−003
Xe	15.983640132169159	5.6691401410444673	−2.1548911444782402
Xe	−12.053232341513162	6.6112628968497757	6.4429270545641959
Xe	−19.224812921361529	3.1206688306441235	4.1628340451250242E−003
Xe	−19.422646984377405	−4.3464481080322894	8.6985735080072981
Xe	−11.803030673886120	14.047547806874556	−2.1714216784365368
Xe	16.098516392293401	9.4061179993607098	4.2896622943801885
Xe	−5.7839804077514980	−16.000816608999386	2.2103962971024163
Xe	−5.5466123838725823	−8.5463516548402687	−6.4934634068762911
Xe	1.8329424168971373	2.3729425240015050	−8.4796982514461998
Xe	1.6740405479422369	−5.2321811612917477	−8.6347053242281452E−002
Xe	8.9710008937716026	5.9030083701020111	−2.1369994108157204
Xe	8.7482090895085900	−1.5298203401344483	6.4248053921893558
Xe	−19.095301604162142	6.8665383049320008	6.4891862313396569

Xe	-18.852144891668630	14.332088995562211	-2.1883137931262664
Xe	9.0959866513174799	9.6392761088952792	4.2923360819544545
Xe	-12.558646647617641	-8.3105411495164514	-6.4861708644364677
Xe	-12.777148536558849	-15.762077192445403	2.2188007858170677
Xe	-5.1581570528938387	2.6216531129394851	-8.5569996426591377
Xe	-5.5844294562202261	-4.8893298382150032	-2.4864532967901889E-002
Xe	1.9597916359886705	6.1916552446727486	-2.1241555309725610
Xe	1.7467189823105822	-1.2356722661844701	6.2353049419604876
Xe	15.389239494721833	-12.964516164578271	7.3044022448123212E-003
Xe	15.579595955368546	-5.5194949967715479	-8.6404280383158820
Xe	2.0833782177992570	9.9254322681296916	4.3239522683520883
Xe	-19.584969116522579	-8.0975359030990557	-6.4992833712619591
Xe	-19.813433862901608	-15.577747899636220	2.2198472025853206
Xe	-12.160962308288543	2.8622527575892986	-8.5907243326757516
Xe	-12.454725988840657	-4.5594232485105186	1.8626935668500885E-003
Xe	-5.0624070770516916	6.3841534099480315	-2.1379350532403811
Xe	-5.2642898619342011	-1.0463009298759731	6.3730085323717720
Xe	15.496812068777398	-9.2375092090933393	6.4966112355056644
Xe	8.3669773802570457	-12.740299087103795	6.9727362432912277E-003
Xe	8.5767652014313889	-5.2833488434571239	-8.6076424234711428
Xe	15.752701043792030	-1.7769593502919583	-2.1472687017635703
Xe	-4.9319002212811736	10.119093865699782	4.3026859866641392
Xe	-19.213980958364267	3.1185060946300283	-8.6501851462376482
Xe	-19.476823759168859	-4.3366632371555180	1.5329110270119429E-002
Xe	-12.063109019369190	6.5978517921992355	-2.1457551264009109
Xe	-12.294906488662654	-0.83086525473039741	6.4394312836321381
Xe	8.4827813185178300	-8.9990887267672601	6.4885557972429631
Xe	1.3506482272140778	-12.521737743270483	-3.4201298728961261E-003
Xe	1.5921570235643969	-5.0384011937972488	-8.5799481971843647
Xe	8.7613655873214018	-1.5457450623871334	-2.1110218829754506
Xe	16.088625684859490	9.3930504936993913	-4.3196899086435785
Xe	15.872673444896423	1.9529609138551625	4.2891737143076645
Xe	-11.932082580759598	10.333184953506040	4.2905888357605253
Xe	-19.096764214303846	6.8476300706593909	-2.1593374048251448
Xe	-19.335141422583181	-0.60466846153415676	6.4916082511633277
Xe	16.218969230031316	13.133384083086938	2.1376337818660023
Xe	-5.6620360612570284	-12.255994428932993	9.7044747295843754E-004
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Xe	11.689912903302211	−17.816177525241603	1.4142044244033144E−002
Xe	19.295439508013651	0.58969595451508727	−10.864081561870368
Xe	19.121339635313472	−6.8635994531449684	−2.1587911586182629
Xe	5.7932175881912240	16.011230111791093	2.1717029214268777
Xe	−16.109266738846575	−9.4043164595863367	1.6655472838802025E−002
Xe	−15.843954713360514	−1.9626231561897667	−8.6047031126930662
Xe	−8.7581980362512528	1.5383697297175132	−2.1353581573652796
Xe	−8.9300291848202544	−5.8905089957930690	6.4327623667309872
Xe	−1.3390706644181445	12.489112224892976	−4.3626380267359695
Xe	−1.5916250024663241	5.0933544554180123	4.3124901909182620
Xe	4.6866078561056970	−17.597995530190992	1.5027923199948390E−002
Xe	12.265019964406026	0.82590756058633663	−10.798653238292200
Xe	12.103393065785616	−6.6351973733557710	−2.1437825325585784
Xe	19.469021167303502	4.3285540804566089	−4.3342830226397595
Xe	19.246264364433468	−3.1231440011782388	4.3105620565747085
Xe	−1.2167546611773452	16.251887890651975	2.1685429324523509
Xe	−15.741235126296985	1.7627657921885111	−2.1456286927539794
Xe	−15.954941729923290	−5.6721783994219095	6.4692503606362619
Xe	−8.3426385650026571	12.713238287632230	−4.3607875248437473
Xe	−8.6078180471366768	5.2720624225551793	4.2965590128366582
Xe	19.328810498973475	0.61559624546941727	10.845208555787845
Xe	−2.3251089825686897	−17.353908473612524	1.5740873353491426E−002

Xe	5.2757885320070548	1.0627535023215169	-10.752491008073338
Xe	5.1128159736332570	-6.4729018740984001	-2.1485751169816187
Xe	12.434989020648594	4.5463030343629480	-4.2936910925046883
Xe	12.221140287249392	-2.8958282703678258	4.2899964618173305
Xe	19.598421937765181	8.0677442188945996	2.1457718382482232
Xe	-8.2149744640551390	16.465728035910125	2.1722976056843653
Xe	-15.343245775042726	12.954560697442057	-4.3534374797042759
Xe	-15.608915660881518	5.4939406750100286	4.3015254242036711
Xe	12.295853793976542	0.85083818543927170	10.797218193777013
Xe	19.845679999175069	19.380351268818703	-3.4997315624827038E-002
Xe	-9.3247312057607346	-17.100614153274947	2.1897010110897897E-002
Xe	-1.6886274539483568	1.2930858175287963	-10.741890776803659
Xe	-1.9680536983970935	-6.2281424834428680	-2.1665624124075125
Xe	5.4196006063123070	4.7866028168191308	-4.2679885244092555
Xe	5.2363873019913019	-2.6447359702478215	4.2682582854764570
Xe	12.558049196567174	8.2754451210728490	2.1405300726637733
Xe	-15.218487135689927	16.708308455924250	2.1646728511508027
Xe	18.879703535141982	-14.352365982178945	-2.1678487719522721
Xe	5.2997865853920940	1.0934694808590733	10.773958703535447
Xe	12.906186913684076	19.556848932150469	-3.0812886010624523E-002
Xe	-16.311368422369956	-16.873476784479276	3.0435643054720626E-002
Xe	-8.6905330709467066	1.5250435675909175	-10.788696969589106
Xe	-9.0228061303655096	-5.9323290822786010	-2.1662917366284411
Xe	-1.5754181452041220	4.9787061680660250	-4.2312786922898331
Xe	-1.7329988337365185	-2.3245166624920683	4.0863269111281735
Xe	5.5511236747805954	8.5368599397634579	2.1531003771877284
Xe	19.008856778689360	-10.603515194751813	4.3365004586030906
Xe	11.828300986006926	-14.079275175920761	-2.1464188851827908
Xe	19.233051791888361	-3.1314447922238111	-4.3181791430439080
Xe	-1.6863936028468043	1.3293671233300635	10.771840697646963
Xe	5.9218006385017929	19.795096484973602	-3.4023227599433360E-002

Listing 4: Formic Acid(TS)-Argon System

N. Ar Atoms 496

Ar (UFF)

AF (MP2/aug-cc-pVDZ)

C	0.32820751923190034	0.24878762656858178	-0.73056372892948862
O	-0.41426807581041425	0.86939200789680693	0.26786552883931863
O	0.52060179521256411	0.73126815470331019	-1.8207905679055385
H	-1.3336872421350090	0.56403879797382972	0.23470996152821824

H	0.78270495166240317	−0.70150403371954839	−0.39163721949431840
Ar	17.015156935037858	−2.4972294194540061	11.555660034065085
Ar	13.683757788299310	−0.67505706695729428	11.313822148779781
Ar	14.021881259893522	−4.2897519260257289	10.037920156171298
Ar	15.733668613203154	−1.4116980574631341	8.1416410167487605
Ar	11.229452712457766	8.8234845656181804	0.56371869498749339
Ar	2.1467431663864396	−5.5876496437813996	16.377954074298437
Ar	0.89438167562518123	−2.6780151807613337	−3.2494384234038045
Ar	−3.7099013468379209	5.7273091324452023	5.3479747536833049
Ar	12.860204184699871	4.2469397491308865	2.6762820769406823
Ar	2.5389814672500814	−7.3047492505006968	−1.1911249148999750
Ar	−2.0856715514860498	1.1627117437646677	7.4348459146086867
Ar	−3.3002383510840398	3.9834930604756962	−12.135246360643222
Ar	14.466232163438947	−0.34251538834349415	4.7787429747431300
Ar	8.6239884270158171	10.969838683555484	−6.1466232416599267
Ar	4.1999693298344578	−12.004515674684626	0.94728215993418219
Ar	−0.47216523304323765	−3.4195094406298860	9.5440970188228995
Ar	−6.3232197085935722	7.8961060559128464	−1.3638339437441660
Ar	−1.6763763868251174	−0.62663371128780099	−10.029969433491686
Ar	16.101322014968265	−4.9974986654228113	6.9357279704458596
Ar	5.5319836358031926	14.863601879128566	4.7334795651589356
Ar	10.280659998527430	6.3751436809218172	−4.0393766304099676
Ar	1.1765458896450087	−8.0949183317844948	11.712133576933827
Ar	−9.3100176160940009	11.782295217492559	9.4909590552991361
Ar	−5.7443005835792316E−002	−5.2056194846612307	−7.9388709506209763
Ar	−4.6544124339129409	3.2494477196334901	0.75586671094638402
Ar	0.50945110893786871	−0.92303604919245452	14.241890505477089
Ar	11.912434978886905	1.7901701787803859	−1.9302598124381052
Ar	7.1673490867901419	10.281503870030084	6.8598352561633718
Ar	1.5667287143258137	−9.7794278569361381	−5.8176442778016293
Ar	−3.0115438201810747	−1.2534362770361933	2.7472430295350572
Ar	−7.7069104207599191	7.2070711076740306	11.618780380269900
Ar	13.519852136716715	−2.8053761859011903	0.18671829024559286
Ar	8.7950513943727895	5.7057978280401827	8.9701119986123867
Ar	7.6544719551732232	8.5090710666610576	−10.737046229274972
Ar	3.2213211275065303	−14.442485508532473	−3.6748270208808083
Ar	−1.4318711971365206	−5.8772707876094517	4.9556318286692287
Ar	−6.0860129412714716	2.6264226173879273	13.725408560612037
Ar	−7.2771469909069957	5.4382082572289852	−5.9437211575735800
Ar	15.146837093331571	−7.4615638284926469	2.3333325922329213
Ar	10.399864662235624	1.1183116239441766	11.071054061717227

Ar	4.5475730534441174	12.372951457021202	6.0513256151253317E-002
Ar	9.3080782087534608	3.9159100883504547	-8.6247759859369868
Ar	0.21091157061424803	-10.570717986921240	7.1282625326814069
Ar	-4.4548758975085798	-1.9496907491925044	15.813815972297396
Ar	-10.310473415319784	9.3020938821847086	4.8284822098504989
Ar	-5.6277487437582518	0.82536359703856599	-3.8136159813361798
Ar	12.052756133983131	-3.5426152106142967	13.201996710308004
Ar	10.937213014155907	-0.66591366235854388	-6.5252070667973374
Ar	6.1796761072169382	7.7689710975208941	2.1779977153185079
Ar	-2.8070105999070836	-6.5951361155593533	17.929762238354854
Ar	-4.0129192486219418	-3.7349156628424440	-1.7081559622014306
Ar	-8.6942220823302510	4.7036305161927601	6.9478111846282555
Ar	12.543711429035705	-5.2544759460581556	-4.4089879873209048
Ar	7.8002050006114088	3.2004996300291260	4.2812486645229253
Ar	6.6723366087508618	6.0302089721708434	-15.309423806590566
Ar	-2.4029277978897610	-8.3327298677488866	0.38741939405179060
Ar	-7.0750551725280877	0.13029341473440384	9.0464937427813865
Ar	-8.2404229008865837	2.9634355891972426	-10.552680618620082
Ar	14.174717667940273	-9.9182209412453624	-2.2714269411838228
Ar	9.4206768114028385	-1.3836753316224115	6.3912616458738585
Ar	3.5849138916768122	9.9297424806495691	-4.5348493774554299
Ar	8.3109174437786688	1.4481902921262779	-13.229179189064967
Ar	-0.75414194897503462	-13.017656298542239	2.5354292946978272
Ar	-5.4447272664908866	-4.4458235798681862	11.143292430411339
Ar	-11.291615459597146	6.8576168928327457	0.23781840314007940
Ar	-6.6144386492478535	-1.6432721370626173	-8.4425361115645732
Ar	11.070466101452316	-6.0520280718849673	8.5403205241547919
Ar	-0.69294138368692626	1.8269406422836836	-5.3389169273130515
Ar	0.58428278723234872	13.857276608163914	6.3222871104765765
Ar	9.9368781560615034	-3.1344528712451836	-11.128151498607869
Ar	5.2153094329887342	5.3069442590804314	-2.4117675104636231
Ar	-3.7904234015316214	-9.1022193929941615	13.290662326799408
Ar	-5.0050366535813033	-6.2221069517524334	-6.3475183167255915
Ar	-9.6832126481576957	2.2506798194179725	2.3568418259740942
Ar	11.549646128710837	-7.7104565304539543	-9.0112397703946971
Ar	6.8585503518400550	0.74935828456598075	-0.31754416505468319
Ar	2.2166846230472550	9.2712448722903549	8.4603483147021876
Ar	-3.3765005869309976	-10.799904621281550	-4.2319626558216017
Ar	-8.0700854461266260	-2.3312999820570899	4.4643891514372589
Ar	13.173982180695761	-12.351938611981405	-6.8656889565616597
Ar	8.4607048294637721	-3.8405341989562212	1.7976398900030914

Ar	3.8406007265157966	4.6913872176837286	10.573077766894922
Ar	2.6177922164327505	7.4734896143705987	−9.1105024590744339
Ar	−1.7320952575115365	−15.462727200555413	−2.0848168309569513
Ar	−6.4212092272702499	−6.9077489052130998	6.5638753806943324
Ar	−12.251100268173879	4.4029039531296785	−4.3528257003469033
Ar	10.124560450103342	−8.5148240646623510	3.9490237025191295
Ar	5.4577550418467826	9.3193608140363204E−002	12.667440533002768
Ar	−0.40382825470451988	11.362027954468495	1.6477073110983871
Ar	4.2505261689800369	2.8648306254899705	−6.9814619978797481
Ar	−4.7671986854485420	−11.570133574788118	8.7149560939695192
Ar	−10.642016335906337	−0.20154777756226325	−2.2328995621825571
Ar	7.1006797186210830	−4.5683492854449916	14.796678348980807
Ar	5.8722729770234503	−1.6977113341006773	−4.8857082043332074
Ar	1.2273766061344071	6.7381410289428336	3.7632634856570517
Ar	−9.0291049617034584	−4.7847075588993286	−0.12694061320934874
Ar	7.4931304663181395	−6.2871315259645488	−2.7849593560292329
Ar	2.8448798035297664	2.1885012741255996	5.8748706500013945
Ar	1.6452869247231641	4.9987748912405330	−13.709161745885984
Ar	−7.3872750029090133	−9.3629123530815868	1.9817593531873892
Ar	−13.196506942043417	1.9359714557511407	−8.9558632712414337
Ar	9.1505830468198202	−10.964052624116006	−0.64507636247582956
Ar	4.4655010268760478	−2.4052104018913463	7.9728169421211810
Ar	−1.3750193630506422	8.9264093133854772	−2.9523965160059915
Ar	3.2755087428515735	0.40004808024489164	−11.604540642834431
Ar	10.544946126408151	15.882161153405367	3.1149624016853985
Ar	−5.7338796896308057	−14.026111658838300	4.1192469640672194
Ar	−11.591448011981676	−2.6631306338521616	−6.8486497206762387
Ar	6.1269571263504616	−7.0779375807312359	10.137233171409870
Ar	−4.3660775402858905	12.831082463616827	7.9110499870855371
Ar	4.8969732579359588	−4.1711156777218727	−9.5105520409054947
Ar	0.24671075523642003	4.2452872111804645	−0.82789293126005381
Ar	12.193609510137863	11.321877022537935	5.2345478703677841
Ar	−9.9781262894934457	−7.2457704753609091	−4.7446167137737163
Ar	6.5150495978468355	−8.7489452698817640	−7.3998038219909761
Ar	−2.7315666360007129	8.2416482529425341	10.042243172934786
Ar	13.820366175841023	6.7356119023090546	7.3471579094500843
Ar	−8.3447920130826283	−11.818442508389806	−2.6340907370110749
Ar	8.1661971199504819	−13.406931576298758	−5.2561114550547279
Ar	3.5074065537955867	−4.8789493605291687	3.3855631092284404
Ar	−1.1130167240660969	3.6672458203434837	12.152808537035677
Ar	−2.3381383464376073	6.4648167792872000	−7.5309150006466599

Ar	15.433480443974425	2.1420786258002389	9.4559598337968467
Ar	9.5834241763380135	13.409218773917731	−1.5483229673100858
Ar	−6.6832960620651800	−16.458359293648126	−0.48913201226117747
Ar	5.1692340292932810	−9.5546251306304946	5.5443750866114474
Ar	−5.3458014885815412	10.337458765953093	3.2333489437007814
Ar	7.8602611820414765	10.579156490475519	0.32307535301881951
Ar	−1.1540000769116152	−3.7381952551127289	16.074842118946272
Ar	−2.2980695496673769	−0.94653798854274984	−3.4702193257864256
Ar	−7.0050839831804010	7.5108467321528156	5.0892497697230752
Ar	9.4934380449842894	6.0040234802173913	2.4317024448251545
Ar	−0.74306207765535559	−5.4920836780888020	−1.4507692770998855
Ar	−5.3833130995768892	2.9284949951476120	7.1920760018980667
Ar	−6.6067685736200978	5.8277272642204538	−12.432114330196315
Ar	11.111642917199580	1.4277382637007769	4.5381912082205744
Ar	5.2500262240758184	12.797589197570712	−6.4140984727100596
Ar	0.89042404224038418	−10.148218494490852	0.65798882066159547
Ar	−3.7627646039489488	−1.6365349870664998	9.2834622552009396
Ar	−9.6415339535134184	9.7378657359476914	−1.6467008321651631
Ar	−4.9526421258530053	1.1628698207610373	−10.284856599935535
Ar	12.724786825491528	−3.1754246250634273	6.6536554512531909
Ar	2.2304337229780620	16.715946563657841	4.4442149891657738
Ar	6.9025442064023679	8.1317636331889247	−4.2714835631227768
Ar	−2.1335719562855542	−6.2399674240181415	11.405444917471531
Ar	−12.651854236068653	13.578246190449562	9.2032357281996759
Ar	−3.3402507953781950	−3.4288938619874720	−8.1975717568049902
Ar	−7.9760578762513203	5.0578755182667656	0.49733825246633340
Ar	−2.7808733729392916	0.85979669083719901	13.981731594034214
Ar	8.5500055905291905	3.5546939236739461	−2.1679940870603494
Ar	3.8747986232683007	12.064047382984405	6.5984559941903447
Ar	−1.7181383155819914	−8.0017196416348177	−6.0884410078794913
Ar	−6.3774185212500383	0.46821870135342158	2.6050045964230688
Ar	−11.054018436589384	8.9771049017169311	11.371334975012015
Ar	10.164355882890950	−1.0295347403490696	−5.9158036535974193E−002
Ar	5.5062637584435130	7.4896793526533001	8.7210979639041355
Ar	4.2798753357518828	10.336387334709700	−11.003278409172212
Ar	−8.6821436936687577E−002	−12.598277313458969	−3.9608464484985331
Ar	−4.7345159309427043	−4.0844454323566151	4.6908839330896637
Ar	−9.4378010970995518	4.3920787433670307	13.487733085032332
Ar	−10.596111349433022	7.2797833735292521	−6.2375638958717818
Ar	11.775366885968968	−5.6354221454737292	2.0632408966086810
Ar	7.1205687268560167	2.9050315712410080	10.822589869117200

Ar	1.2381778013651739	14.233252036154296	−0.22794360761249657
Ar	5.9346357255407334	5.6780731448941930	−8.8493693993154068
Ar	−3.1028969668116178	−8.7061918987682319	6.8267817851662844
Ar	−7.8115336836355107	−0.19206068062305373	15.590505100443847
Ar	−13.682032746777930	11.139128314501320	4.5753197006105255
Ar	−8.9382719595484232	2.6102314842641987	−4.0843972225236138
Ar	8.7443841490564314	−1.7053307899181396	12.921769721521494
Ar	7.5739468913897738	1.0987372283546331	−6.7511880057453864
Ar	2.8854080160174314	9.5522028884199628	1.9167453021992151
Ar	−6.1720750525000820	−4.7718893355377565	17.663604252489577
Ar	−7.3310021876597133	−1.9768043977934202	−1.9757748253093359
Ar	−12.049752326613858	6.4729110004401686	6.7098533685909407
Ar	9.1872643357048762	−3.4780861090634927	−4.6458007791926610
Ar	4.5022014045308225	4.9672330210097062	4.0241962358575405
Ar	3.2970403343922747	7.8580933210440147	−15.574934530913577
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Ar	−4.1352470366444507	−5.5102250074004129	14.504565942244868
Ar	−5.3079326056996043	−2.6889108927990719	−5.0651804274913328
Ar	−9.9931904845805555	5.7709682381823839	3.5927452047075477
Ar	11.244745175374701	−4.1862566057680102	−7.7656846320004593
Ar	6.5073595401381494	4.2485372547185190	0.92410023431551136
Ar	5.3267907530391634	7.1020995256672119	−18.703002154489923
Ar	−3.7016575132839646	−7.2648090018135152	−2.9718624455348999
Ar	−8.3845528429822203	1.1853203976431068	5.7048176647039854
Ar	−9.5757815457099884	4.0543760214195341	−13.995019186379947
Ar	12.852102382914710	−8.7819453293781944	−5.6448325626289604
Ar	8.1324309184228358	−0.31707215471927058	3.0330107249075153
Ar	2.2729433313301421	11.068386696764463	−7.9166747307507102
Ar	6.9932259353796491	2.4827877722043517	−16.633050268419211
Ar	−2.0709959053776541	−11.874060426566185	−0.85215750400580181
Ar	−6.7543716758340695	−3.3863478024156337	7.7976710983744262
Ar	−12.607993236325456	7.9839108400634267	−3.1419681548606433
Ar	−7.9254239291569668	−0.60783662120991633	−11.862210162838096
Ar	9.7598744108141471	−4.9265117466857040	5.1563836937854450
Ar	−1.9965992733768172	2.9078091276449678	−8.7456271533714833
Ar	−0.74514691425570967	14.950785499927683	2.8827554984538080
Ar	8.6246623337885975	−2.1012551965219677	−14.536742981696621
Ar	3.9181421110184469	6.3847752121829595	−5.7529031020323833
Ar	−5.1125110127324431	−7.9843320209836319	9.9151095129294067
Ar	−6.3158481136921365	−5.2015724253655229	−9.7681801096749261
Ar	−10.966376761922238	3.3230863484912234	−0.99399561587681207
Ar	10.246763139627619	−6.6873459816487015	−12.427606287140522
Ar	5.5637390606655108	1.8085121045771877	−3.6493906818913420
Ar	0.90319742810240222	10.285742065753487	5.0278671314443208
Ar	−4.6918867637886876	−9.7775758092347669	−7.6589992036412662
Ar	−9.3660785475237862	−1.2682278669665612	1.1167815301574111
Ar	11.846836443820575	−11.260039567357250	−10.296228961006568
Ar	7.1686555267739536	−2.7622781344471696	−1.5487962873763910

Ar	2.5316467005097105	5.7158283020014942	7.1520328294827724
Ar	1.2980637433524247	8.5986235400477344	-12.491588315713603
Ar	-3.0605203478034966	-14.369712771916699	-5.5256159746608366
Ar	-7.7311361767452986	-5.8464387020831108	3.2238358453670659
Ar	-13.552824335622722	5.5253204323542651	-7.7349907398410629
Ar	8.7986776937000606	-7.3792648165646586	0.56954292257848393
Ar	4.1465384882844534	1.1325083365305051	9.2484040400298664
Ar	-1.7248929576152547	12.511077202479594	-1.7378159703010332
Ar	2.9500088703323151	3.9299169372430929	-10.338093307764730
Ar	-6.0835130755295275	-10.444821070637396	5.3360061401845060
Ar	-11.915082632616816	0.86575566886154876	-5.5876093977654682
Ar	5.7722442196041257	-3.4774384658686288	11.354894406530351
Ar	4.5723016801076692	-0.64736704186713689	-8.2320053208489412
Ar	-7.2964215627628212E-002	7.8132630742959339	0.40385894209654116
Ar	-10.310748997888162	-3.7223132721841412	-3.4822953925631079
Ar	6.1934826239192979	-5.2179053803734066	-6.1403003839198922
Ar	1.5225393888542642	3.1662787741362024	2.4654004897793054
Ar	0.32699949780084525	6.0928814465015728	-17.157180934939078
Ar	-8.6849846777201236	-8.2978250494618671	-1.3759929149520751
Ar	-14.508013625774865	3.0246258833749731	-12.385516851809999
Ar	7.8212586912676754	-9.8236306991716162	-4.0245711132129873
Ar	3.1594397139601296	-1.3322310157527939	4.5890565312090725
Ar	-2.6927172781370299	10.062527002987592	-6.3326238772907528
Ar	1.9641641976770570	1.4294426905629545	-15.020039874496204
Ar	9.2205363641695453	16.971747513988284	-0.31719741889518654
Ar	-7.0424706181924952	-12.889124915453392	0.73985782528369537
Ar	-12.883929269810725	-1.6273455062551656	-10.261572954777836
Ar	4.8089986000238492	-5.9585989333969493	6.7478484995288746
Ar	-5.6965022959957707	13.924558268422272	4.4715527021486254
Ar	3.5949272835891315	-3.1489323117779198	-12.933326197799827
Ar	-1.0411327455562220	5.3802920752423029	-4.1686299036318868
Ar	10.883418590936920	12.340160232168058	1.8194320078038566
Ar	-11.282609251338952	-6.2133539434501754	-8.1580091352620805
Ar	5.2119806039485672	-7.7247258530808107	-10.825379853597905
Ar	-4.0383862577665406	9.2632526595240794	6.6121104239620880
Ar	12.517377109840460	7.7704863966714077	3.9341609153139547
Ar	-9.6582320858319353	-10.798708054993202	-6.0490789369359623
Ar	6.8341855313496724	-12.311256486264575	-8.6987853600285536
Ar	2.1764001847406487	-3.7237440324505822	4.5161575196335624E-002
Ar	-2.4165075857337057	4.6876614948983928	8.7286811991544333
Ar	-3.6529420072487349	7.5858036910852231	-10.921267121149954

Ar	14.137985280004145	3.1833630919209401	6.0443667258447329
Ar	8.2721047253679334	14.546513813679674	-4.9251220567097516
Ar	-8.0112743759938407	-15.365655036015093	-3.9317554270053505
Ar	3.8509051809994088	-8.4208437683294139	2.1629500496485008
Ar	-6.6746689096913228	11.481669371349835	-0.15023751882306918

Listing 5: Formic Acid(TS)-Krypton System

N. Kr Atoms 498

Kr (UFF)

AF (MP2/aug-cc-pVDZ)

C	1.4103237521702003	-0.96079922015686348	1.3280321292241393
O	0.13581686862545475	-1.3485818906956206	1.7178780436017194
O	2.4197825363933503	-1.4832890361999507	1.7342594904739468
H	-0.22093389787100973	-1.9928824172965971	1.0887648603199744
H	1.4012530615038765	-7.6704195466691757E-002	0.66266009373803481
Kr	10.947663228718055	-13.194289377181441	14.096930064412991
Kr	9.2178088996484906	-13.006869808036576	10.413799250883574
Kr	7.5923918957429946	-10.942085810252237	13.586497740231659
Kr	11.183130283845847	-9.7314407316694211	11.964917064447461
Kr	14.960517277153022	-3.5112271259303096	-0.58216202541847528
Kr	-4.7173641081536735	-16.188559303796740	8.0347281958705956
Kr	-0.15570031448602265	3.9091964704584021	2.4993560262463492
Kr	-0.84979667927089342	-6.4419631940296078	-6.6516285939661737
Kr	13.190985357904676	-4.9286625236372066	4.6432638699517543
Kr	-1.9390819256467491	2.5331612398712191	7.7621085370188876
Kr	-2.6378957691647118	-7.9091785383381161	-1.4826633720294295
Kr	1.9335791531933395	12.210748611287539	-6.8847405639163277
Kr	11.411681062129622	-6.3158863884475611	9.8626847504126403
Kr	15.295038277721567	3.3431741097236971	-4.8273198196006337
Kr	-3.7236289603702257	1.0959569241442439	13.074764796148443
Kr	-4.3742620210571017	-9.2834476640953749	3.7574697462534985
Kr	-0.48030265229011276	0.39467052740112668	-10.887639175026585
Kr	0.16922044583590293	10.809914667441451	-1.6524834542002331
Kr	9.5871768414468370	-7.7515384617700933	15.140480865054094
Kr	12.757460415197846	-8.5785927727404978	-8.8703349563814431
Kr	13.559870102458053	1.9287657927557471	0.41951532123842317
Kr	-6.1467207589690505	-10.708961432071353	9.0617755556659354
Kr	-2.8918052437158219	-11.471130061979236	-14.896268416544682
Kr	-1.5852640895567420	9.3955152666645052	3.5516675411763323
Kr	-2.2573338967659518	-1.0206011415059568	-5.6560973701726267

Kr	−2.9362842410403007	−14.776217742956380	2.7444747825694460
Kr	11.795128789810576	0.51032167188197919	5.6364472477502048
Kr	11.037941232155797	−10.015189703411178	−3.6448406458309082
Kr	−3.3339974672257138	7.9699846389628943	8.7576639346099778
Kr	−4.0035068309045307	−2.4357023084146627	−0.43926173144712610
Kr	−4.6704470293871116	−12.916725819196540	−9.7150605840673538
Kr	10.016723112526037	−0.90132149582959264	10.855075730818946
Kr	9.2943898985181352	−11.417541263300256	1.5819475193406074
Kr	13.872662939281957	8.7732881227471680	−3.8251187571850105
Kr	−5.1097078641241875	6.5360636011628728	14.061724948309406
Kr	−5.8745039870862916	−3.8819864205281585	4.7993901291481036
Kr	−6.4329479860744323	−14.349126940256042	−4.5061406773375747
Kr	−1.8758854705529591	5.7993014253302331	−9.9032542434385356
Kr	8.2039542203940208	−2.3401209252707544	16.140083620364550
Kr	7.5068804665905651	−12.819577651851143	6.7851796096319088
Kr	11.353827058251214	−3.0767513427951458	−7.8543581886324567
Kr	12.151254889010659	7.3586589515265688	1.4244854117502912
Kr	−7.5655876579735359	−5.2901031520029447	10.060424862265849
Kr	−8.1758128849020384	−15.746791453500716	0.71552829795616590
Kr	−4.3195528920360591	−5.9875126840362185	−13.901622366626212
Kr	−3.6592611242579403	4.3941437779001520	−4.6806901377940591
Kr	5.7079901340599930	−14.219585629779186	12.077005658672155
Kr	10.388781231282294	5.9364899371138646	6.6378473760365821
Kr	9.6406872975688742	−4.5054350755366350	−2.6319891297341775
Kr	−9.9413197715699066	−17.148269997939469	5.9954221229593907
Kr	−5.4839560115289121	3.0233019203790676	0.52093686161673447
Kr	−6.1016274609388566	−7.4191838956949736	−8.6925291448513793
Kr	8.6134762584228444	4.5081468013830923	11.844868988285596
Kr	7.9580501783461299	−5.9622100020868567	2.5967205092154182
Kr	12.429810958247883	14.170578634768008	−2.8197951711123768
Kr	−7.1954726146403036	1.5751048660791793	5.7647059709415513
Kr	−7.8588035945401229	−8.8413923596548738	−3.4912618284250336
Kr	−3.2786867791609349	11.232943697469874	−8.9035892278993636
Kr	6.8037015346547713	3.0736924875620408	17.128011833312634
Kr	6.0947472822659474	−7.3064679998946716	7.7925229712597499
Kr	9.9723046612250457	2.3462245542662745	−6.8535300593480155
Kr	10.704830523663201	12.783076035606536	2.4107921364194667
Kr	−8.9599093827696343	0.13147446835264490	11.071435909741648
Kr	−9.6152463431526414	−10.254330692985240	1.7244599797104536
Kr	−5.7245920838423450	−0.58704332508229506	−12.926059815599269
Kr	−5.0528496170787989	9.8351732175911160	−3.6773505157669217

Kr	4.2852989310653218	−8.7231234497592602	13.077153546035937
Kr	1.5780423320487791	5.3383773028149202	−2.6325460134210337
Kr	7.5444626912995414	−9.5479797475501815	−10.880197307160827
Kr	8.9522545034943644	11.364811369910154	7.6354732888763612
Kr	8.3110054859647224	0.95844911101073638	−1.6540566064787467
Kr	−11.383158201642839	−11.687652657069309	7.0219186070702708
Kr	−6.8127422286261794	8.4214869886908801	1.5309126595885421
Kr	−7.5098324678212851	−2.0052029880368765	−7.7007022185361444
Kr	7.1846812632337889	9.9272625802830330	12.831133556030705
Kr	6.4791538305509233	−0.48891854656261774	3.5633948039830092
Kr	5.7999920030419609	−10.994941338890966	−5.6541722926693474
Kr	−8.5618889495865371	7.0058047051509522	6.7515676460855270
Kr	−9.2703156459887275	−3.4178713544836525	−2.4888024886172100
Kr	5.3834360848253793	8.4775164403190733	18.088465992630667
Kr	4.7056979512948658	−1.8888647550166129	8.7904954172799670
Kr	4.0498216248685255	−12.399826325154477	−0.44934810790300306
Kr	8.5683033071861239	7.7624080027910614	−5.8683180442568110
Kr	−10.340844199260777	5.5691283204410205	12.047533267276272
Kr	−11.024263597083525	−4.8316805939798941	2.7326896712229676
Kr	−7.1178256953609189	4.8206450628275368	−11.933812669012223
Kr	2.9068837904726803	−3.3283881753500890	14.083152498433723
Kr	2.2886983463715005	−13.801602728037762	4.7603528964078503
Kr	6.1283606222039815	−4.0438080722263985	−9.8605080713886206
Kr	6.8326019267257854	6.3603004229157918	−0.63156646767821667
Kr	−12.813432620863843	−6.2753998304931198	8.0365093833851056
Kr	−8.9075219557290435	3.4104927136593273	−6.7142092702017582
Kr	0.50489323126242314	−15.202595230863828	10.055557365207601
Kr	5.0849648500551234	4.9520287012622228	4.5786392478084510
Kr	4.3692233144514008	−5.4617620312115456	−4.6093925811003551
Kr	−10.671090236663508	2.0053741141270520	−1.4985939254678009
Kr	3.2997313784020905	3.5101772330589505	9.7763023395270494
Kr	2.6363383661658597	−6.8943883746857804	0.56403814917786765
Kr	7.1428084080135150	13.181748523762334	−4.8659348449853086
Kr	−12.429913184217105	0.59275922662655156	3.7258137574535697
Kr	−8.5020351832465391	10.243176519051520	−10.925322284703634
Kr	1.5064063315080107	2.0687806535708000	15.079523702107647
Kr	0.86409497823303649	−8.2470785231904333	5.7417425578852512
Kr	4.7430992191729144	1.3707130960114706	−8.8754429796482412
Kr	5.3976304322875208	11.778062578707416	0.36841405922056386
Kr	18.042227856042569	−7.5793494807958099	−6.8429320581315372
Kr	−14.204295176299278	−0.83343047859658159	9.0265727462848915

Kr	−10.291624051840815	8.8495982095991597	−5.7120268002477248
Kr	−0.92417410406624823	−9.7145758614936106	11.072198622323883
Kr	2.3305079104162703	−10.515585393915725	−12.891200907212557
Kr	3.6493671142585704	10.362774146688080	5.5712367477938223
Kr	2.9638420407917918	−2.1536921429755732E−002	−3.5672495656328711
Kr	16.344070386136174	−9.0104977037879106	−1.6157366072154642
Kr	−12.064203182890520	7.4498761866393632	−0.49869313198032450
Kr	1.8871296664671693	8.9380154195168071	10.770180133450660
Kr	0.57514174005963281	−11.960776114184492	−7.6752673302537273
Kr	14.590571658944279	−10.434115631613910	3.6377940077549900
Kr	−13.800485907682365	6.0301731784782975	4.7191270991308283
Kr	0.10310664788958818	7.4934073298696022	16.060193840232543
Kr	−0.55165572205502322	−2.8685965681677064	6.7530455811867913
Kr	−1.1883764933693355	−13.374651923262238	−2.4758330444846179
Kr	3.3427858465309006	6.7796219498328751	−7.8902427593694338
Kr	12.795120461135891	−11.826812698488499	8.8702120792927879
Kr	16.666643559104735	−2.0926125395048691	−5.8245308621795457
Kr	−15.557221654134315	4.5909501571895364	10.006675757289102
Kr	−2.3324932563438217	−4.3078924262829696	12.070597448037878
Kr	0.91725413256593469	−5.0136050539764305	−11.871198406033606
Kr	13.129122476841259	−3.2998291305418657	−4.2252411227450466
Kr	−6.4294195401741741	−15.958418436473055	4.3494119087646155
Kr	−1.9196276933523093	4.1884020463064395	−1.0772818678422160
Kr	−2.5846534245241282	−6.2147755283726358	−10.267632869329754
Kr	11.417043008456703	−4.7247988168796624	0.99115997121076937
Kr	−3.6978979396284104	2.7705300301386018	4.1609955100135334
Kr	−4.3559186904372034	−7.6456232913920736	−5.0805356540837208
Kr	0.22773478125956603	12.443889520297745	−10.568429127618852
Kr	9.6330117245036977	−6.1267480905272667	6.2214901111488752
Kr	13.490072238808219	3.5574929308609344	−8.5196345572692440
Kr	−5.4467668610595998	1.3459327723756418	9.3993369803901423
Kr	−6.1206356164389266	−9.0721758303748494	0.12840088662992571
Kr	−2.1926538849526556	0.62857194070607947	−14.583530377446786
Kr	−1.5576294256774321	11.022693470647040	−5.2730192242146350
Kr	7.8242368915171365	−7.5152893649916157	11.425873304212139
Kr	11.046261536470382	−8.3366887295088201	−12.549920804323305
Kr	11.765101574606323	2.1412300287144439	−3.2340091761632883
Kr	−7.8677056370488616	−10.474064390639715	5.3696169447640028
Kr	−4.6469921116134154	−11.211929509454496	−18.563159076301897
Kr	−3.3229485334771236	9.6169768717204942	−5.9946750105082214E−002
Kr	−3.9886919638328053	−0.80493500300572984	−9.2843408826417022

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Kr	10.002651302991845	0.71725216704414874	1.9911505367933371
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Kr	13.378630268270344	−1.5008785330802024	2.5319029974368310
Kr	−1.7501921746526039	5.9477870103158432	5.6364343732932127
Kr	−2.4452528446016268	−4.4383455215002563	−3.5704093023391996
Kr	2.1162790039028216	15.708294749079222	−9.0485376064878409
Kr	11.606101060783470	−2.9040773875801555	7.7463158246727017
Kr	15.460278356556900	6.7790271970482037	−6.9989233197014613
Kr	−3.5172153401151505	4.5338786554951112	10.888591664005274
Kr	−4.2324587081101770	−5.8950210699595011	1.6451109824380186
Kr	−0.27516453573066796	3.8197604999804757	−13.082407823858818
Kr	0.33123833515068368	14.293613373552697	−3.7531848528751683
Kr	9.8139869214860322	−4.3192600605750213	12.976175050396789
Kr	12.933384942547391	−5.0708724820627626	−11.031966064184889
Kr	13.732633971613144	5.3570451951639466	−1.6976498470638193
Kr	−5.9660450403962422	−7.2852233626018519	6.8885604928862607
Kr	−2.7020021549754381	−7.9671169267207915	−17.053281273443524

Kr	-1.4279583317537234	12.886838825068805	1.4644226125483650
Kr	-2.0661669009858028	2.3862505544342478	-7.7683401527785385
Kr	-2.7843038091012238	-11.301051280850423	0.64466462104873978
Kr	11.975880038030098	3.9330581150535830	3.5317684419520128
Kr	11.183870338531783	-6.5183769410416517	-5.7377889219089173
Kr	-3.1786217157035845	11.468949927418612	6.6676741368454131
Kr	-3.8769384730017600	0.98709587212776106	-2.5921495167866886
Kr	-4.5041261249434790	-9.4220042753173665	-11.787556828490933
Kr	10.208273010954697	2.5135377444764115	8.7422427746864262
Kr	9.4700443874920399	-7.9444875581727468	-0.52828759318534191
Kr	14.039661912440922	12.201945848659792	-5.9997124226509424
Kr	-4.9261763023767964	10.034558419225572	11.894635471912771
Kr	-5.6613299530643344	-0.41582504026252509	2.6582464361405869
Kr	-6.2724168966975480	-10.857950882028030	-6.5988843077156476
Kr	-1.6700238701471641	9.2322031815743255	-12.083739418390117
Kr	8.4156450783164480	1.0911008387012116	13.966942535402234
Kr	7.6914319787935215	-9.3470471180014041	4.6983661636452094
Kr	11.556937811517612	0.36267478150722710	-10.032672442706678
Kr	12.295459162667832	10.765624312249578	-0.69451786537283844
Kr	-7.3843524987416362	-1.8501832966464600	7.8980130097801950
Kr	-8.0287434079198334	-12.275641585175068	-1.3872026969756719
Kr	-4.1145441171536365	-2.5667240072749991	-16.087789261217853
Kr	-3.4644908855980154	7.8060893206830331	-6.7844750963835532
Kr	5.8954396441697217	-10.726347287161097	9.9041813816224682
Kr	10.558216756220595	9.3645582688906757	4.5322125940228890
Kr	9.8047259115333834	-1.0777057942138759	-4.7365435753509182
Kr	-9.7734004993874439	-13.671312852771450	3.8417870940736187
Kr	-5.2401156506703268	6.4108698819997327	-1.5811635753528197
Kr	-5.9192615943229017	-3.9987565596028696	-10.799152217331200
Kr	8.7924214056817895	7.9315968792200193	9.7379365900476191
Kr	8.1216646318884393	-2.4993743288670252	0.46240278429505471
Kr	12.562806114523863	17.624228317090452	-4.9766461901804968
Kr	-7.0019242267727737	4.9952225165793331	3.6424934612912567
Kr	-7.6889137831234571	-5.4200021870220896	-5.5919326299550187
Kr	-3.0972431607606015	14.727498672763518	-11.070326929460922
Kr	7.0061708954536757	6.4974036326871918	14.944140373271194
Kr	6.3153979096137016	-3.9029904754229383	5.7091975309502372
Kr	10.171656382064246	5.7778316248249268	-9.0404526497751068
Kr	10.844477730745979	16.252802271759045	0.29890141583804342
Kr	-8.7503726923662946	3.5694443554300892	8.8820016163214177
Kr	-9.4418867055713651	-6.8327242696763086	-0.38370112134841938

Kr	−5.5153180050240245	2.8406356204160605	−15.101877151115060
Kr	−4.8841857901452874	13.316401055712099	−5.7742747032295219
Kr	4.5014647892632667	−5.2993784763146010	10.897338555474585
Kr	1.7546806813186488	8.7756474780713063	−4.7597482175622323
Kr	7.7266258879207914	−6.0436181789198535	−13.038604639083960
Kr	9.1018722130723049	14.841626165791673	5.5306332663428108
Kr	8.4076461322125766	4.3585886795096060	−3.7411944420361238
Kr	−11.203714509826773	−8.2582116968545165	4.8550601041477810
Kr	−6.6523363757166658	11.912321416555402	−0.56022834496857876
Kr	−7.3196216215765189	1.4062987236572091	−9.8171701359984436
Kr	7.3417482384355983	13.418028737687646	10.750933637196551
Kr	6.7059926454757548	2.9708188301893093	1.4795839175676380
Kr	5.9500214818926338	−7.4878989658086965	−7.7395919624862630
Kr	−8.3987706158654909	10.496729188666164	4.6501451225828969
Kr	−9.0918180793317838	−3.3986013636842661E−003	−4.5999387771405056
Kr	5.5658282082261659	11.971655702753587	15.934878763877446
Kr	4.9006100475600407	1.5274257632036246	6.6789326246173761
Kr	4.2124164646724838	−8.9198314396559226	−2.5380495291612069
Kr	8.7513499710987475	11.186581623630746	−8.0521765475610305
Kr	−10.151980782093787	9.0676121868245154	9.8822691379275174
Kr	−10.848857138694784	−1.4139566622352311	0.61571178135889437
Kr	−6.8983057798849492	8.2485754495973964	−14.101072119598214
Kr	3.1114701875890525	9.7059897849467502E−002	11.904351808757312
Kr	2.4524500668787956	−10.322844036746382	2.6592597006229526
Kr	6.3374145507012569	−0.60912281004668256	−12.052358939496973
Kr	6.9825548828412227	9.7613456706371515	−2.7437950166118363
Kr	−12.614333232041792	−2.8294480487774840	5.8595932607851697
Kr	−8.7060209560418755	6.8220537997754747	−8.8164302457141108
Kr	0.68535901326327653	−11.702878372996755	7.8830574627406627
Kr	5.2388459295425864	8.3509879404661120	2.4687124254526815
Kr	4.5480303646810922	−2.0371017700164598	−6.7260445677787013
Kr	−10.488886925239850	5.4263144192127450	−3.6101681618129216
Kr	3.4783270265651614	6.9292508169087466	7.6685276908734643
Kr	2.7806524381631248	−3.4166879100995917	−1.4090306890119184
Kr	7.3256438544806608	16.682834368344359	−7.0283690542475314
Kr	−12.246968072598499	4.0163449867775949	1.6078765468850227
Kr	−8.3025012855818563	13.725650730463858	−13.077032927797815
Kr	1.7074162876663836	5.5007303011608109	12.891002438604588
Kr	1.0359347502055074	−4.6831713780705035	3.5185656160278134
Kr	4.9461038466329397	4.7977037476060591	−11.065722842058324
Kr	5.5422661607102812	15.258644876766853	−1.7290837701046342

Kr	18.213692806455569	-4.0865283765100981	-8.9993113967661458
Kr	-13.987074994948516	2.5958796480672732	6.8427899980020648
Kr	-10.108168950373413	12.324014435612007	-7.8057078093076644
Kr	-0.72914617630796330	-6.2808869063677175	8.8920530881930109
Kr	2.5151848682530837	-7.0118709653339257	-15.048338344530327
Kr	3.8065336923301811	13.856225222993409	3.4866353784300252
Kr	3.1636343863999259	3.3652396140118399	-5.7615540230955640
Kr	16.496911945956661	-5.5237237432724475	-3.7077050028352350
Kr	-11.887944077023226	10.927788614223200	-2.5981278006494386
Kr	2.0489809585156764	12.434378964033336	8.6844587101268065
Kr	0.73574966792877783	-8.4559892332613664	-9.7558857789256006
Kr	14.774552524660464	-6.9516036979400218	1.5246166900849134
Kr	-13.642785382467986	9.5166822937318507	2.6269242716697745
Kr	0.28642500189139941	10.999735636715288	13.895702183102916
Kr	-0.37376953726192669	0.52197641018377128	4.6320788694665049
Kr	-1.0254573053463538	-9.8913202404647471	-4.5694081133520177
Kr	3.5416424717163006	10.214897573426931	-10.069746159414816
Kr	12.996203106375365	-8.3561523810323095	6.7635027152531251
Kr	16.859137921978206	1.3375658961109671	-8.0028537754656011
Kr	-15.365089502308946	8.0921986319123640	7.8432980020981482
Kr	-2.1284338783905028	-0.88201495082454628	9.8923025513051250
Kr	1.1220142130473203	-1.5802290144248785	-14.063143265239143

Listing 6: Formic Acid(TS)-Xenon System

N. Xe Atoms 499

Xe (UFF)

AF (MP2/ aug-cc-pVDZ)

C	0.29287783591214034	-1.2949017696527163	1.8977901795508136
O	1.6184663144511808	-1.7060008212309024	1.9184868412639839
O	-0.63412096239693183	-2.0362902490117669	1.6794003475045143
H	1.8801920376224732	-1.9308206665090386	2.8238100339949437
H	0.18720130157223133	-0.20229582004762009	2.0327689443860719
Xe	3.9396156997587988	-15.649713613446279	17.208655337254118
Xe	5.5673400045393038	-12.196765007844396	15.161151711831970
Xe	3.2570341613611715	-15.197378778366971	12.954654246790989
Xe	1.2481760278239080	-12.555193836209158	15.813619596745179
Xe	-2.1755846195892601	2.4132232420932542	15.949544416317048
Xe	14.616639290458748	-13.226324970942274	2.7019327664072716
Xe	-4.4896890523563027	-1.6126101490134055	-1.6270039071324505
Xe	8.5089143995448495	4.9623852938733144	1.3776983418343902

Xe	-1.7873790371609959	-3.5511827709527797	15.204150036068683
Xe	-4.0893746480600530	-7.6115107227265346	-2.4008134136404937
Xe	9.0032693711434373	-1.0192405827353821	0.61443673632156770
Xe	-10.140878737582824	10.505391658589911	-3.6953551421701851
Xe	-1.4029923169289562	-9.5068139557405686	14.433456450031112
Xe	-7.4465618739872399	8.5532256418571286	13.159031507211985
Xe	-3.6728050553130496	-13.680205615131984	-3.1530695634562385
Xe	9.2811829497486844	-7.0279111774028342	-0.12480891571806924
Xe	3.1848189765570258	11.076391057297599	-1.4138706192050354
Xe	-9.7710022715526410	4.5018137427910787	-4.4546855761207613
Xe	-0.99372182814929988	-15.574632580092491	13.671464795268410
Xe	5.9887160725295256	9.1241687571093273	15.376937212883998
Xe	-7.0836132899019608	2.5505515819028513	12.419767954194175
Xe	9.6432256437516610	-13.101430292891049	-0.88535425988588645
Xe	16.555600237001602	11.655791197481610	0.86855072190528726
Xe	-9.3903349945512993	-1.4787999257255318	-5.2011484419504477
Xe	3.5849498041948369	5.0663836168717511	-2.1694813410988134
Xe	14.260156875373399	-7.1608060855148059	3.4832099362142688
Xe	-6.7020414896669145	-3.4232055121202882	11.664069565047686
Xe	6.3945188045389454	3.1334542048466183	14.641858380701688
Xe	-8.9889730616757628	-7.4655990704971336	-5.9531927575691661
Xe	3.9906686447263366	-0.90413667501932293	-2.9062546594163874
Xe	17.001436571309100	5.6853523439329949	0.11455141386492106
Xe	-6.2970255636087638	-9.4014308572411185	10.906373409518830
Xe	6.7849436366895022	-2.8303936715258673	13.899516193128067
Xe	-12.345837300437649	8.6932263813574018	9.6113063226058664
Xe	-8.5824253473507426	-13.543530508148503	-6.7140187033460208
Xe	4.3434697718774515	-6.8664156481323024	-3.6433751742046705
Xe	17.415194012559194	-0.32099805963989092	-0.63624232931625646
Xe	-1.7011737681517762	11.203552393552648	-4.9541036752045651
Xe	-5.8797622396758689	-15.462692168965525	10.134457428516114
Xe	7.1692795660747191	-8.7934347782501092	13.139555425508110
Xe	1.0248970865066247	9.2603900709137310	11.776010727258809
Xe	-11.987104837601729	2.6907560116397460	8.8799037942603363
Xe	4.7435885466600682	-12.976694464065147	-4.4283751042140684
Xe	17.764448894647668	-6.3230465112361935	-1.3890481648892814
Xe	11.604103282561749	11.785438171969213	-2.7267703572035069
Xe	-1.3139870545455503	5.1911274854361924	-5.7083373513829905
Xe	7.5342471690924970	-14.868362768574569	12.382617216068986
Xe	-11.604942209202550	-3.2970263491681133	8.1200471428929308
Xe	1.4168192671504833	3.2590505677753683	11.027822489228866

Xe	18.107109591594142	-12.376436930594405	-2.1557051772588101
Xe	-0.92812563166687123	-0.77618754344131835	-6.4345769995815898
Xe	12.029629877108611	5.7960894117218462	-3.4847080972288205
Xe	-11.192086620670366	-9.2859150460611488	7.3639601943971975
Xe	1.8042887404777124	-2.6961627300182940	10.272871350707938
Xe	-17.219705268560404	8.8167728022970131	6.0416205891898302
Xe	-0.54034075870360765	-6.7479526565822825	-7.1964278458338971
Xe	12.427106197385445	-0.19110618477825547	-4.2255864965501742
Xe	-6.6063888683376266	11.326606131452232	-8.5164444871206104
Xe	-10.775146506907227	-15.346313961698371	6.5839677003984569
Xe	2.1914955593236560	-8.6615605659167851	9.5248763382795101
Xe	-3.8686540306269621	9.3999679401930951	8.2440717284054763
Xe	-16.885037624390012	2.8347440974687426	5.2995509345609362
Xe	-0.14473823765752775	-12.841508573182002	-7.9670935803625085
Xe	12.792158929723046	-6.1814713801578991	-4.9815079734186796
Xe	6.7247054047278736	11.913384903799733	-6.2692264938790423
Xe	-6.2333659690158436	5.3261247316321896	-9.2786380746358077
Xe	2.5820434278887556	-14.746736046025623	8.7629347588113493
Xe	-4.8699526131996835	4.3823492556067940	-0.89352713412970630
Xe	9.5215143257465886	9.9811239446142501	10.566816475550281
Xe	-16.508665809447294	-3.1704760156959568	4.5505223880255850
Xe	-3.4939210432053391	3.3959698359486614	7.4956922901468301
Xe	13.156346245753328	-12.255588876514688	-5.7374111023075480
Xe	-5.8527354591153875	-0.64359288006340887	-10.029386944307486
Xe	7.1285615892155318	5.9114610605463138	-7.0314015389744338
Xe	-16.085458643788950	-9.1574607097939520	3.7919775015002228
Xe	-3.1214809844960323	-2.5732252519477141	6.7399843717594550
Xe	9.9431423498871929	3.9822095344735722	9.8206844870430210
Xe	-5.4570780085580353	-6.6204841842179638	-10.770320861202997
Xe	7.5229298387083654	-6.3384981372422322E-002	-7.7750282468016660
Xe	-15.652315221939698	-15.201340874100111	3.0178029393959966
Xe	-2.6989691737236745	-8.5244674380844021	5.9724413280772906
Xe	10.339845850027235	-1.9943251059945915	9.0648839620513346
Xe	-8.7580208501604151	9.5374098402129164	4.7040735356770851
Xe	-5.0496995481821090	-12.696039616010818	-11.535018461297994
Xe	7.8956862170771940	-6.0447508283323632	-8.5222077613706428
Xe	1.8403729363589547	12.030679047968336	-9.8021620272986567
Xe	-2.3055714531994118	-14.634376041771109	5.2269459931619968
Xe	10.714562108535464	-7.9845254660451861	8.3188384621605209
Xe	4.5567277431978797	10.106158253452385	6.9569542496732746
Xe	-8.4073243242486271	3.5441177919013187	3.9583231064426312

Xe	8.2743203824785230	-12.119616410439006	-9.2769276996742267
Xe	2.2358088543594987	6.0304783474116537	-10.564163220351626
Xe	11.079137189348749	-14.057133815271975	7.5553783495868014
Xe	-8.0795480656379759	-2.4479919019430376	3.2138435044025928
Xe	4.9646600323862833	4.1069100300086028	6.2071559937456300
Xe	2.6228931446110977	6.3900879780267955E-002	-11.313746264806909
Xe	-7.6116058236136812	-8.4352117283063439	2.4475026828242266
Xe	5.3592847038581661	-1.8655930566511045	5.4360279360347485
Xe	-13.657033614940653	9.6680310040212003	1.1378293256731427
Xe	3.0048119046781956	-5.9086191313585630	-12.047381911086463
Xe	-3.0578943076118219	12.143948523442694	-13.341450241556108
Xe	-7.1952336903909986	-14.510695172680547	1.6833559389146699
Xe	5.7595327148071132	-7.8682312254274720	4.7172487635168494
Xe	-0.33962807074622658	10.241632045123701	3.4124673614042624
Xe	-13.304916845280520	3.6713951287851372	0.38621182577314156
Xe	2.4030667169235880	8.2661338836055673	20.246613084844586
Xe	3.3882327634777001	-11.985522776902343	-12.809178043899674
Xe	-2.6773008907311904	6.1599042447854941	-14.114770330487707
Xe	6.1243906950699758	-13.929170929204682	3.9505800407652765
Xe	13.054077039158180	10.828389642345313	5.7262027436125198
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Xe	4.2798477850214711	4.5887418005069902	2.0153298254005576
Xe	1.9805084449585442	0.55488650930681127	−15.573345230268647
Xe	−8.2982847021941950	−7.9548281433520245	−1.7549925975989213
Xe	4.9409797592557032	−1.3520542693965700	1.2283355673328418
Xe	−14.411226790471048	10.158855134627673	−3.0956324014116512
Xe	2.3708871553128219	−5.4141805486342802	−16.299813852315467
Xe	−3.7483624492051617	12.630201758086780	−17.617483567175867
Xe	−7.8823310847616703	−14.033061222870742	−2.5143865343268827
Xe	5.0567241722294334	−7.3717474745468383	0.51417789862231011
Xe	−1.0213635353233641	10.724572928436414	−0.76916971554645275
Xe	−14.046778599826421	4.1524498850044758	−3.8596672476298939
Xe	1.7082052340787812	8.7642993654860639	15.972429919063027
Xe	2.7464755382647437	−11.488170216127543	−17.052705113539584
Xe	−3.3718947950033975	6.6641931169453574	−18.407853258997779
Xe	5.4342601148987555	−13.456325869802560	−0.23990851260061138
Xe	12.296006897694470	11.302143078363164	1.4890149595751569
Xe	−13.666768570374394	−1.8302557400005131	−4.6058091622021360
Xe	−0.63038115889360302	4.7020229279689163	−1.5213961135645484
Xe	2.1008873514239803	2.7776974642661552	15.241331364789758
Xe	−2.9859702323987785	0.68118825769632751	−19.162546688900889
Xe	−13.262152442729963	−7.8191321919166370	−5.3596914442061365
Xe	−0.25744278455752923	−1.2535028117511073	−2.1710323480302960
Xe	12.731823748733545	5.3171247183634369	0.73994308217113813
Xe	2.4890807395803516	−3.1841313307674834	14.496642214019165
Xe	−2.5949090425579153	−5.2998246568290091	−19.895617955964600
Xe	−12.849966189788809	−13.894468100007380	−6.1103586025763024
Xe	0.14850090623304735	−7.2311514515467161	−3.0137749952714445
Xe	13.164605915160998	−0.67103051753273379	−1.4951984472315848E−002
Xe	−5.9152617950310846	10.853559880933309	−4.3208245545477473
Xe	2.8732405118062729	−9.1406717820054979	13.732722348534216
Xe	−3.1949441670542997	8.9069679929658268	12.440202798687221
Xe	−2.1932933971904172	−11.318960570333948	−20.576435609532805
Xe	0.53637580758657433	−13.330200703866979	−3.7860950663887487
Xe	7.3920961746498177	11.430228746973658	−2.0656298744566888
Xe	−4.8178884827718349	5.4722622474621243	14.554008443972990
Xe	11.920958097355999	−10.096357573881937	1.2813641204613979

Xe	-7.1221841837353494	1.4462801276349477	-3.0403112698040595
Xe	5.8333909427578989	8.0022207045177147	-2.3727229088373283E-002
Xe	-4.4394698443908895	-0.50629220936576869	13.811544743128138
Xe	-6.7307654323750485	-4.5356940254205425	-3.7900014303101113
Xe	6.2788043919941412	2.0553888497241304	-0.78743097008468732
Xe	-12.835736745415399	13.637489136936484	-5.1251572871670685
Xe	-4.0525044146711489	-6.4666811474440600	13.054312022330393
Xe	-10.086012811169162	11.685284537376099	11.766767821790303
Xe	-6.3282454032627484	-10.546530261799091	-4.5480370601574167
Xe	6.6502516937756608	-3.9761388644615030	-1.5341917294499974
Xe	0.54313722730643976	14.217855340385055	-2.7979112030706847
Xe	-12.467974797391049	7.5680033604907129	-5.8981377268153281
Xe	-3.6406476916910990	-12.454922479375076	12.284951819704087
Xe	3.2786937596945993	12.259261006387961	13.940781050664903
Xe	-9.7188822547390465	5.6199778474244590	11.024592042661668
Xe	6.9955546610002308	-9.9632119076042382	-2.2744741976021854
Xe	13.833613712814719	14.778033247455850	-0.55878955773955885
Xe	-12.094904915144559	1.5770585151925816	-6.6517006968870600
Xe	0.93871410583126491	8.1250998268897607	-3.5609904211832104
Xe	11.579229584854202	-4.0971493689617011	2.0375262117850812
Xe	-9.3467610607962399	-0.37098470831057928	10.272051846192882
Xe	3.6834544549988339	6.1855651540286862	13.183135825443637
Xe	-11.703621524782243	-4.4050993020519025	-7.4009840578529129
Xe	1.3292422329488800	2.1306259445869298	-4.2994705626793985
Xe	14.273203283846746	8.7236483418277242	-1.3244414519239447
Xe	-8.9517236223131587	-6.3515959299844260	9.5163202648641789
Xe	4.0782132629975854	0.21459830723010767	12.443061822258391
Xe	-14.977857536798769	11.822255350367389	8.2067008830275885
Xe	-11.291507391685672	-10.410391567467267	-8.1460095490499818
Xe	1.7105197268196024	-3.8095875486961406	-5.0176912825659823
Xe	14.701142327797815	2.7467115389936385	-2.0723093067938563
Xe	-4.3460368798066398	14.339790355401721	-6.3445023032322068
Xe	-8.5335080122650666	-12.346232030365259	8.7483962790491905
Xe	4.4662918992202272	-5.7403124431085750	11.694114124717794
Xe	-1.6206194027174439	12.406065740284255	10.397723202050132
Xe	-14.608683810093231	5.7513135568071441	7.4676039393193534
Xe	2.1017852091484599	-9.8298040444624331	-5.8059848925758493
Xe	15.080620089517904	-3.2555482958329174	-2.8235698514871044
Xe	8.9624609723179649	14.917467179465316	-4.1094608725227708
Xe	-3.9577145410140036	8.2530950785736508	-7.1097902462735743
Xe	4.8432087149871332	-11.730733243060731	10.932008554341422

Xe	-14.255507024124581	-0.23436132257590311	6.7211102782474033
Xe	-1.2298605630804953	6.3184286410244894	9.6309812458923112
Xe	15.424077573436810	-9.2521159877339123	-3.5777223929024644
Xe	-3.5781100243463033	2.2717453940499142	-7.8646914404276682
Xe	9.3711132933267063	8.8466195773101095	-4.8839956033066976
Xe	-13.851407682646892	-6.2307004353620981	5.9658678761030552
Xe	-0.84821301536073557	0.33994005234997660	8.8811757668658391
Xe	-19.863477629287008	11.928328405995375	4.5925672730415235
Xe	-3.1918279413600059	-3.6914540047354172	-8.6084365414629769
Xe	9.7774373173150604	2.8616894245039317	-5.6302658674170480
Xe	-9.3000016273457540	14.462153791127722	-9.9576045188999345
Xe	-13.424212193870224	-12.219027933905533	5.1968041092225805
Xe	-0.45666705580595424	-5.6016388138778579	8.1100455615327220
Xe	-6.5103903243465835	12.542002115378155	6.8642868071084511
Xe	-19.559411377553836	5.9059420594833476	3.8496404086198344
Xe	-2.7941866258744588	-9.6962582157923727	-9.3563924291078369
Xe	10.159295809395726	-3.1173690385589667	-6.3774000771463371
Xe	4.0795088500130792	15.041126067090470	-7.6517310244924834
Xe	-8.9315590001564260	8.3890042263937197	-10.723794051889037
Xe	-6.3661724790883431E-002	-11.612785751886422	7.3739061123024934
Xe	-7.4960640364582183	7.4343446306808580	-2.2919489204969539
Xe	6.8120093052852209	13.107122505017525	9.1294741104655710
Xe	-19.191667786645720	-9.7029403990594065E-002	3.1026186721345175
Xe	-6.1296669954850040	6.4611295549373748	6.1033443702448418
Xe	10.525153521550147	-9.1222306495432193	-7.1275181982517601
Xe	-8.5567151464004390	2.4081793177269835	-11.483332039756565
Xe	4.4835546548925649	8.9638138403384655	-8.4182568687761918
Xe	-18.796008548794106	-6.1076857197440901	2.3459049155209102
Xe	-5.7908600469043208	0.49631605789558442	5.3691162032214557
Xe	7.2238881695334349	7.0367752823881284	8.3695535110295545
Xe	-8.1701110880903283	-3.5641716841678432	-12.226323344123580
Xe	4.8794263355560084	2.9837721896485774	-9.1739287016427244
Xe	-18.359672877496184	-12.083098826769575	1.5861845944822646
Xe	-5.3697871459438256	-5.5067757210394372	4.5989785630002569
Xe	7.6308049145457657	1.0561355365845111	7.6178626518835895
Xe	-11.388944917384583	12.675745395269946	3.3106592644190580
Xe	-7.7579537330654178	-9.5635846107557221	-12.971823765648702
Xe	5.2638253841819358	-2.9847667235575170	-9.9170804121252445
Xe	-0.80470060835581736	15.154523002300484	-11.180053669134663
Xe	-4.9522755527942168	-11.497803715158195	3.8412945555254914
Xe	8.0178368698791598	-4.9178534523750619	6.8677841049982726

Xe	1.9077651782624911	13.251783404215939	5.5712123509790397
Xe	−11.025106386514807	6.5982198769837002	2.5488838956304458
Xe	5.6371153079632990	−8.9842330875477145	−10.657473907571777
Xe	−0.40802534347203667	9.0819261557890396	−11.951294821505721
Xe	8.3931133418589763	−10.928315875148296	6.1213922078066707
Xe	−10.676071738713190	0.61740118109781827	1.8031995300836736
Xe	2.3026608250685423	7.1552963874768896	4.8011865475264202
Xe	−2.3538463589523231E−002	3.1094323261781773	−12.712194451722723
Xe	−10.275339478992102	−5.3781363153745190	1.0471694295644813
Xe	2.7275037690007329	1.1816225855621747	4.0408387159869266
Xe	−16.358169064059087	12.804290838772463	−0.28520148400026463
Xe	0.36287247950116980	−2.8546358586370228	−13.450352366622973
Xe	−5.7507849603067900	15.263436494730117	−14.763103160854323
Xe	−9.8483279324839508	−11.374969607211911	0.28975644715039650
Xe	3.1595494090424516	−4.8520791959018510	3.3251090616063173
Xe	−2.9817630955224681	13.385566411069718	2.0291743790164798
Xe	−15.990248251884955	6.7310030905128970	−1.0653248915547255
Xe	−0.29570644286541331	11.391028203360348	18.817698846069984
Xe	0.74918196171768847	−8.8469330384592251	−14.184737441268757
Xe	−5.3749220579190373	9.2148588373972888	−15.547550921705074
Xe	3.4762235159855952	−10.792396643973161	2.5546572903050104
Xe	10.336102213965455	13.949852807284865	4.2942205838224137
Xe	−15.625465506412731	0.74403778943596532	−1.8051831886688088
Xe	−2.5908416590814141	7.2886238105065466	1.2636415488949566
Xe	9.3207695093675311E−002	5.3373362232084656	18.083304719274754
Xe	−4.9918933806905894	3.2448999614633647	−16.316799702350441
Xe	−15.228974911039645	−5.2426020695995561	−2.5611206306650662
Xe	−2.2922053202771635	1.3379161870284173	0.50166059730505053
Xe	10.756207203590485	7.8837090239957179	3.5402561066985849
Xe	0.48500375113508820	−0.63063771784386502	17.352612620855247
Xe	−4.6050320237505460	−2.7319610043521760	−17.060586203453422
Xe	−14.810948594212727	−11.240255243510836	−3.3142853256641551
Xe	−1.8787228726807772	−4.7116769678341788	−0.27530987472804314
Xe	11.191250327511984	1.9127724837531663	2.7907149429491107
Xe	−7.8759682186898310	13.512065689336369	−1.5230322649696730
Xe	0.87100580031063368	−6.5963101976369103	16.595030915995512
Xe	−5.1901649245711763	11.546994557405389	15.309048654241021
Xe	−4.2111648829329758	−8.7059392749186308	−17.771781773465651
Xe	−1.4265253428999860	−10.668032702200533	−0.99201228360442195
Xe	5.4252828320419884	14.086888765729793	0.74421538817904465

Listing 7: Acetic Acid(TS)-Xenon System

N. Xe Atoms 429

Xe (UFF)

AA (MP2/aug-cc-pVDZ)

C	-1.6847698545182528	1.1908943798627896	-1.8687476448983491
H	-0.87560398132844797	1.9160022023768990	-1.7646630377471142
H	-2.6105891270946930	1.7620158983637269	-1.9552685047774265
H	-1.5327862038127291	0.58936421284886120	-2.7604689171978363
C	-1.7615291329262805	0.31361460886361936	-0.64946602996235625
O	-1.7394134597125948	-0.87906245878128886	-0.65639000477808351
O	-1.9596949112073316	1.0224171429648619	0.52821408402782344
H	-1.1225607015580088	1.3041941225098028	0.91515710178926790
Xe	19.278241873956102	0.57767124814980919	-10.856932779190842
Xe	15.661389166131167	-1.7987975993355911	-10.817901212314407
Xe	-8.3242368792509964	12.724059126377087	4.3453498304327516
Xe	-1.2027113790217923	16.192322752447705	-2.2037524024933473
Xe	-8.5767569270369091	5.2384736605510787	-4.2770713205546338
Xe	-15.956157165962892	-5.6581904992716838	-6.4500612941935378
Xe	-15.711963196779895	1.7852219679404782	2.1460198794207632
Xe	12.250989213552243	0.84569493468391466	10.811160486811048
Xe	4.6288129033949019	-17.543762716406263	1.7940382755257459E-002
Xe	19.180261671612890	-3.1433470328191904	-4.3112168304814666
Xe	19.439974636729815	4.3163174185205246	4.3179843528266799
Xe	12.015538343649643	-6.6003506163008669	2.1437793284644928
Xe	-15.817471230869351	-1.9210633626098599	8.6068088046148787
Xe	-1.3319455922093635	12.465121555338104	4.3376475046106764
Xe	5.7830859899184910	15.965158203473607	-2.2067727644585085
Xe	-1.5976300892507371	4.8844892282898238	-4.1622195870045502
Xe	-8.9624788343532416	-5.8917510594890450	-6.4400886390502619
Xe	-8.7001968805724488	1.5380263444611539	2.1407835729613458
Xe	-16.095386214775175	-9.3721817392728344	6.1555869720511611E-003
Xe	19.276672441320738	0.59323031324873021	10.855194205550964
Xe	11.608659207487223	-17.792993247001501	1.6997030243882810E-002
Xe	19.049846572481552	-6.8661732832461793	2.1621140712169229
Xe	-8.8241128276417857	-2.1512429564993942	8.5752254564671695
Xe	5.6608657670984615	12.241356997386047	4.3474271503085609
Xe	12.768129352986218	15.736247657158229	-2.2091331260991076
Xe	5.3934577161558170	4.7544535729217747	-4.2753490218513788
Xe	-1.9702995196651902	-6.1305756142926775	-6.4286499817704028

Xe	−9.0899268319101889	−9.5948203439630024	2.2922506517158198E−003
Xe	−15.315660183192925	12.970217454916979	−4.3507778318294683
Xe	18.660061294372472	−18.118468975659280	1.8641848185794032E−002
Xe	−1.8427874418815309	−2.3849945125644272	8.5486380932922330
Xe	12.655124124766754	12.007783421033723	4.3399538063302181
Xe	19.802303814532340	15.547870981679456	−2.2015074479686754
Xe	12.400751133591010	4.5335299465432746	−4.2991163568550395
Xe	5.0228058233986230	−6.3723671920845746	−6.4417323206374073
Xe	5.2700697668536964	1.0560062574441409	2.1434168700787271
Xe	−2.0974544696215043	−9.8232299098521167	1.3898997063844284E−003
Xe	−15.465273372640587	9.2283562788143545	2.1473270569870540
Xe	−8.3174929121124190	12.708704872306329	−4.3526261467205059
Xe	−15.708296342423088	1.7822598044826605	−6.4533741126430835
Xe	5.1387898371308243	−2.6292360262923076	8.5737947392200038
Xe	19.680104543032552	11.802402768890236	4.3447064848529866
Xe	19.437384552114363	4.3104912341743660	−4.3275676462137307
Xe	19.569581762210873	8.0397676575255446	−2.1717955505993203
Xe	12.011194150010303	−6.6112737430395061	−6.4384186689597600
Xe	12.146729334537163	−2.8920333304247419	−4.2843255600042918
Xe	12.276772116307360	0.82312765192295168	2.1427355441355149
Xe	4.8927418321174798	−10.072218467721648	2.4725624748395520E−003
Xe	−8.4601630937247592	8.9729786819659285	2.1517167473778311
Xe	−1.3330757110145626	12.434154346799939	−4.3320764713329547
Xe	−8.6987070879166790	1.5348682211031799	−6.4177264221957948
Xe	−15.836956389752297	−1.9327484674981543	−5.1214822815954993E−005
Xe	−15.562021446719708	5.5268199533822289	8.6437349913336519
Xe	12.126522124251375	−2.8746665636013820	8.5913063953432420
Xe	19.308960434922035	0.58652698644989221	2.1557092594093241
Xe	19.054130453388979	−6.8839824862985450	−6.4828039075738531
Xe	11.891541125396945	−10.322408046826899	6.9642391103512044E−003
Xe	−15.947486430838602	−5.6454437900799448	6.4534247081915987
Xe	5.6525447362055301	12.224827782544521	−4.3540628484009467
Xe	−1.7223841100829911	1.2407118118990139	−6.2845877426063286
Xe	−1.4619128734994191	8.6906910950779448	2.1450054498921300
Xe	−8.8023690170778490	−2.1584881528474371	−2.9025049951113655E−003
Xe	−8.5706701174886462	5.2866593907287411	8.6429516484863544
Xe	−16.214889447280378	−13.108613196813709	−2.1480194837034472
Xe	19.172502284187580	−3.1417752268917258	8.6532961566238686
Xe	18.924950340625998	−10.601269723981231	1.0001991364290259E−002
Xe	−8.9533450092656643	−5.8652253801828484	6.4290273525657353
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