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**Probing the Interaction of Ionic Liquids with CO₂:
A Raman Spectroscopy and *Ab Initio* Study**

by

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Abstract

This research project involves an investigation of the interaction of carbon dioxide (CO₂) with selected ionic liquids (ILs). Raman spectroscopy and first principle quantum mechanical calculations were performed on selected IL solvents in contact with CO₂ in the effort to discover how the solvents interact with the gas.

ILs are salts (mixtures of cations and anions) that are liquid at room-temperature. Recent work has shown that gas solubilities in ILs vary dramatically depending on the cation and anion that comprise the IL. Tailoring the ion structures may therefore optimize the IL's ability to dissolve CO₂. Further, the CO₂ solubility, negligible vapor pressure, and high thermal stability of ILs point to their potential application as CO₂ scrubbing chemicals in harsh operating environments.

A combined experimental and computational effort was aimed at investigating the factors which govern the CO₂ solubility mechanism. Studies focused on six ILs formed by the permutations of three anions: hexafluorophosphate, tetrafluoroborate, bis(trifluoromethylsulfonyl)imide; and two cations: 1-ethyl-3-methylimidazolium, 1-butyl-3-methylimidazolium.

In situ variable-temperature Raman spectroscopy was performed on the selected ILs in equilibrium with atmospheres of different CO₂ and nitrogen (N₂) partial pressures. Raman spectroscopy is an optical technique capable of resolving molecular vibrations characteristic to inter-molecular interactions. The vibrational frequency bands attributed to the IL molecules shifted in response to the externally varied temperature and partial pressure of CO₂. The

observed IL band shifts were reversible with respect to changes in atmosphere. The solvation mechanism was explored by systematically varying the temperature and gas composition. Experimental considerations included enabling requisite convective mass transport of gas to establish equilibrium and limiting the sample water content.

Computational modeling was used to investigate the molecular pair interactions of CO₂ and N₂ with select IL cations and anions. Gaussian03®, a first principles computational software suite, was used to compute optimized geometries, binding energies of interaction, electrostatic potentials, and vibrational frequencies. The results indicate that interaction energies between CO₂ and the IL cations and anions are greater than those of N₂. CO₂ is found to engage in an interaction where its oxygen is aligned with the most positively charged hydrogens on the imidazole cation ring. For interactions with the anions, CO₂ orients the carbon toward the geometric center of the anion and the O-C-O angle is reduced. The computed Raman vibrational modes were attributed, scaled, and compared to the experiment.

Knowledge gained from this effort will help guide the further improvement of ILs for carbon dioxide removal in applications ranging from sequestration of greenhouse gas emissions to purification of submarine air.

Keywords: Ionic Liquids, Carbon Dioxide, Raman Spectroscopy, *Ab Initio*, Solubility

Preface

The first time I was on a submarine, I was struck by a strong, sickly-sweet odor. I learned that this characteristic "submarine smell" was caused by the chemical monoethanolamine, the carbon dioxide capture agent. Ever since, the chemical physics of carbon dioxide and liquid sorbents has captured my attention.

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Thanks go to my patient advisers, Dr. John Bendler (modeling molecules and genuine “good form”), Assistant Research Professor W. Matthew Reichert, Dr. Wesley Henderson (the nocturnal researcher who introduced me to the world of green science), Dr. Patrik Johansson and coworkers at the Chalmers University of Technology Applied Physics Department, Ms. Jackie Brown, Ms. Kristen Selde, Mr. Jeff Walbert, Professor Mary Wintersgill, Captain Kathy Shanebrook, USN, Dr. Fred Saalfeld, Dr. Hugh De Long (perpetually embodying “COOLBIZ”), the Trident Scholar Committee, and, if appropriate, the gracious spouses of all those mentioned above. The Office of Naval Research and the Air Force Office of Scientific Research funded portions of this Project. Presented opinions do not necessarily reflect those of the U.S. Navy or U.S. Air Force

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I. Introduction

Stringently designed and constructed atmosphere purification systems are vital to maintain U.S. Navy submarines as operational national assets. As such, new carbon dioxide (CO₂) capture methods, implementing less volatile and less toxic chemicals, should be researched as replacements for monoethanolamine (MEA) in submarine atmosphere purification systems. The premise of the research project is: ionic liquids (ILs) offer a potential long-term replacement of corrosive and volatile MEA in submarine CO₂ scrubbers.

Before this premise may be evaluated in terms of fleet efficiency and viability, a scientific task-specific optimization of ILs should take place. Currently, the gas solvent properties of ILs are not well understood. While the marginal performance of commercially available ILs over MEA could be studied without understanding how ILs selectively capture CO₂, this “black box” approach limits the applied functionality and benefit of ILs from the start. Instead, the fundamental gas solvent properties of ILs were investigated to enable more enlightened, and thus more resource-effective, fleet efficiency and viability studies in the future.

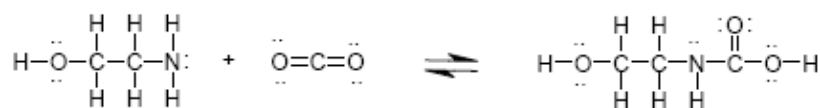
This research project involves a basic science investigation of the interaction of CO₂ with selected ILs. A combined experimental and computational approach was undertaken to explore the underlying physics that explain why one IL dissolves more CO₂ than another, and why ILs dissolve more CO₂ than N₂. Knowledge gained from this effort will help guide the further improvement of ILs for carbon dioxide removal in applications ranging from sequestration of greenhouse gas emissions to purification of submarine air.

II. Background Information

A. Current Submarine Atmosphere Control System

On submarines, the gases contained by the pressure hull comprise a closed atmospheric system. As sailors live and work onboard, each crew member produces approximately 1.5 grams per hour of CO₂.¹ As an asphyxiant, CO₂ interferes with oxidative metabolism by displacing the oxygen in breathable air. Exposures to atmospheres with high CO₂ partial pressures have the same effect as hypoxia, the insufficient delivery of oxygen (O₂) to the body as the result of low O₂ partial pressures. Symptoms vary with relative percentage of CO₂ and can include: impaired night vision, heavy breathing, impaired judgment, dizziness, slow thinking, impaired muscular coordination, unconsciousness, and death. To both ensure the health of the crew and prevent contaminant damage to the ship's machinery, an efficient and reliable system needs to maintain a troposphere-like gas composition of the closed submarine atmosphere.

On U.S. submarines, CO₂ is currently removed from the closed atmosphere by bubbling ambient air through a scrubber consisting of cold MEA in the liquid state (Figure 1).¹ The MEA chemically bonds with the CO₂ and forms a carbamate molecule in a reversible reaction (Eq. 1).² Upon heating, the MEA desorbs CO₂ and the gas is then discharged from the pressurized hull.³



(Eq. 1)

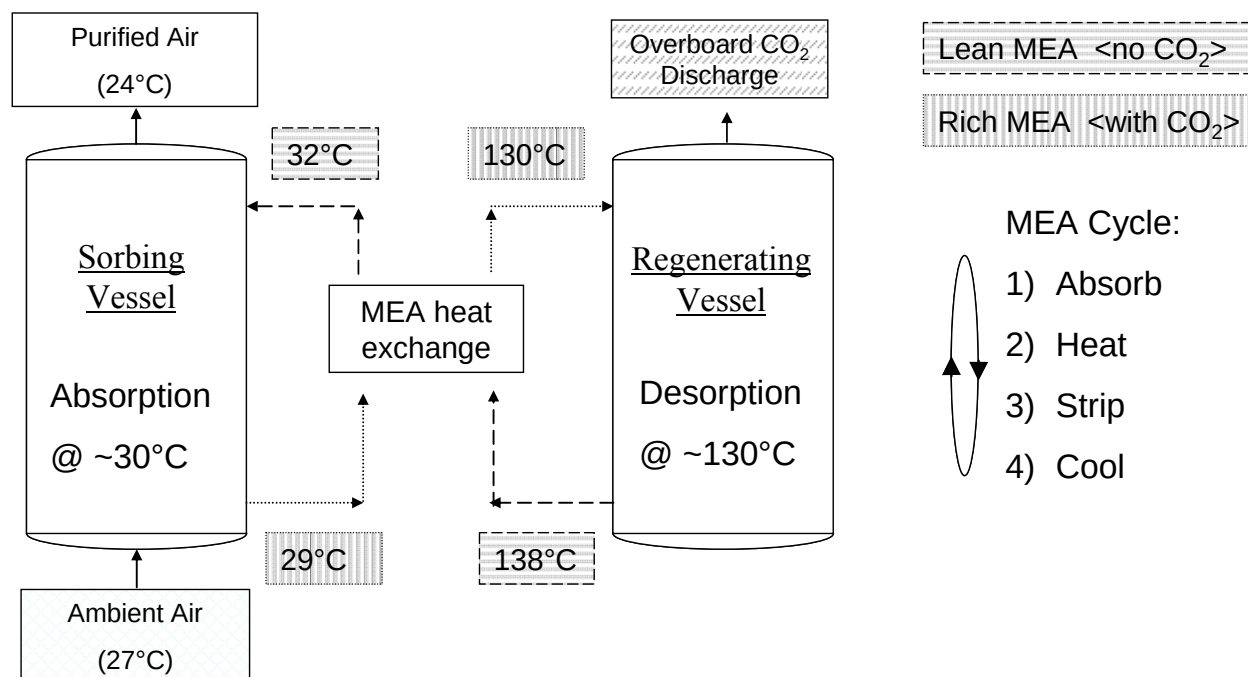


Figure 1: Schematic of a Current Submarine CO₂ Scrubber

In addition to MEA's high vapor pressure, which leads to fugitive emissions during regeneration, high concentrations of MEA in the submarine atmosphere cause a breakdown of the protective film on the commutators in motor generators.⁴ Further, U.S. Submarine Force leadership has expressed overall dissatisfaction with the current bulky and heavy atmosphere purification systems because they limit onboard placement of other war fighting technologies.⁵

B. Solvation Theory

The composition of the gas solute and liquid solvent determines if the solvation occurs via a chemical reaction or a physical interaction. Monoethanolamine solvent dissolves carbon dioxide by breaking and forming bonds in a chemical reaction. This process is called chemisorption.² When water is exposed to nitrogen, the water solvent dissolves nitrogen without

breaking or forming any bonds. This process is called physisorption. Regardless of the sorption mechanism, a few quantitative parameters can be used to describe a gas-liquid interaction at a certain temperature and pressure. The bulk solubility is the amount of gas solute that can dissolve in a given amount of liquid solvent at equilibrium. Diffusion describes how fast a given gas molecule will transport through a liquid. Solubility selectivity is the ratio of bulk equilibrium solubility of one gas solute to the bulk equilibrium solubility of another gas solute. These quantitative parameters help describe gas-liquid interactions and help compare different gas sorbents.

C. Ionic Liquids



Figure 2: An IL Sample in Vial

Ionic liquids (ILs), a class of chemicals, may offer a less problematic solution to the challenge of capturing CO_2 from submarine atmospheres. ILs, typically composed of nitrogen-containing organic cations and inorganic anions,⁶ are molten salts which are in the liquid phase at ambient temperatures (Figure 2).⁷ While alkylpyridinium chloroaluminate-based ILs have been known since the 1950s,⁸ the 1982 discovery of imidazolium-based ILs⁹ stimulated academic interest into their ability to replace volatile organic solvents in chemical processes.^{10,11} ILs have

been shown to possess widely different chemical and physical properties depending on their constituent ions. Many of these ions are chemically benign, i.e. “green.” ILs have been called “tunable” solvents¹² due to the ability to vary the constituent ions, thereby modifying and optimizing the IL physical properties for a specific application. As such, the variety of cations and anions that could be combined to make an IL is virtually limitless. Figure 3 showcases a selection of commonly synthesized IL ions.

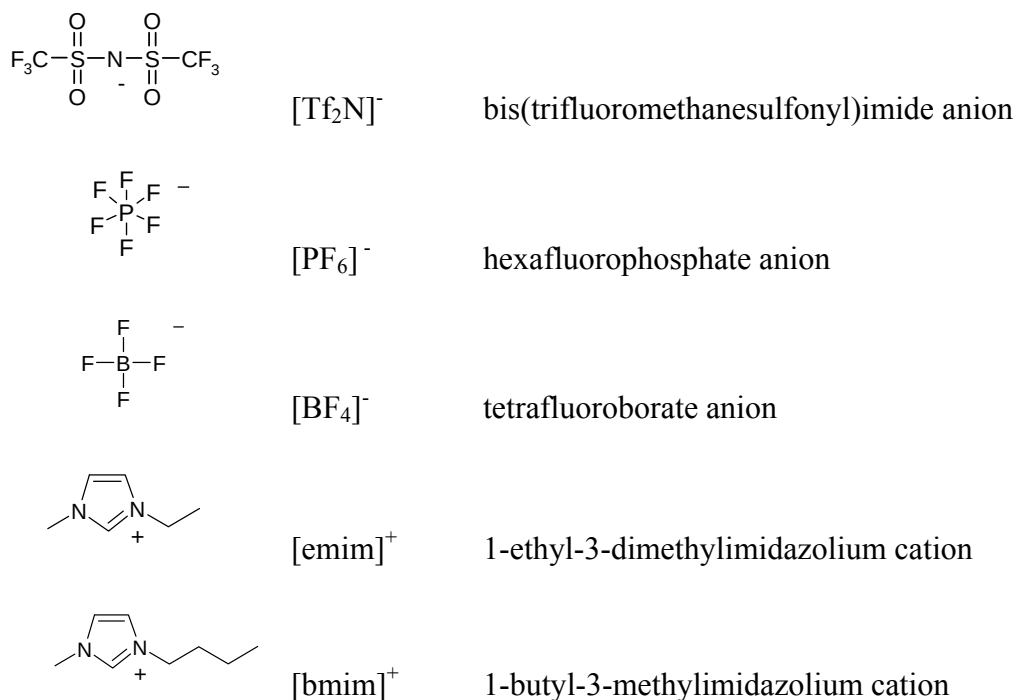


Figure 3: Common IL Ions

Experimental data from Noble et al. and Brennecke et al. have shown that gas solubilities in ILs vary dramatically depending on the constituent cation and anion (Table 1).^{13,14,15,16,17,18,19,20} Furthermore, Brennecke’s research group has been able to enhance CO₂ solubility as much as 25-fold over the first ILs investigated by simply changing the cation and anion that comprise the

IL. It follows that judicious tailoring of cations, and anions may further optimize the IL's ability to dissolve carbon dioxide to a level which surpasses MEA.

Table 1: CO₂ Solubility and Selectivity for Select Solvents

Solvent	CO ₂ Solubility (g/L)	CO ₂ /N ₂ Selectivity Ratio
MEA	6.63 ⁽²⁰⁾	<i>No Data</i>
[bmim][Tf ₂ N]	3.61 ⁽¹⁸⁾	22.3 ⁽¹⁸⁾
[bmim][PF ₆]	3.43 ⁽¹⁸⁾	23.5 ⁽¹⁸⁾
[emim][BF ₄]	2.85 ⁽¹⁸⁾	38.0 ⁽¹⁸⁾

Further, CO₂ has been shown to have a much higher solubility in IL systems than other gases, such as O₂ and N₂.¹⁷ Anthony et al. reported CO₂ solubility to be two to three orders of magnitude greater than N₂ or O₂ solubility in imidazolium-based ILs at room-temperature, indicating that ILs have the potential to selectively capture CO₂ from troposphere-like gas mixtures in industrial settings. Yet despite the wide applicability of ILs, relatively little is understood on the molecular scale regarding their physical properties.²¹ Because of their negligible vapor pressures, high thermal and electrochemical stabilities, low flammabilities, and excellent solvation capabilities,²² ILs offer a potential long-term replacement for corrosive and effervescent monoethanolamine (MEA) in submarine CO₂ scrubbers.

D. Raman Spectroscopy

The effects of intermolecular interactions can be probed through observing optically excited molecular vibrations because vibrations are influenced by interactions. Raman

spectroscopy is an optical technique capable of resolving characteristic molecular vibrations through analyzing the scattering of light.²³ As opposed to Rayleigh scattering, Raman scattering occurs as an inelastic process, in which the scattered photons are of a different energy than the incident photons. The energy difference, or Raman shift, between the scattered and incident photons correspond to the characteristic vibrational energies of a molecule.²⁴ Observation of the Raman effect is experimentally demanding because the lines are weak; only one thousandth of the total scattered radiation is Raman scattered. The rest of the incident radiation is Rayleigh scattered without change in frequency. For a vibration to be Raman active, it must change the molecular polarizability. “Stokes” and “Anti-Stokes” label Raman processes that scatter photons with lower and higher energy, respectively, than the incident photons. The energy diagram for these three mechanisms is shown in Figure 4.

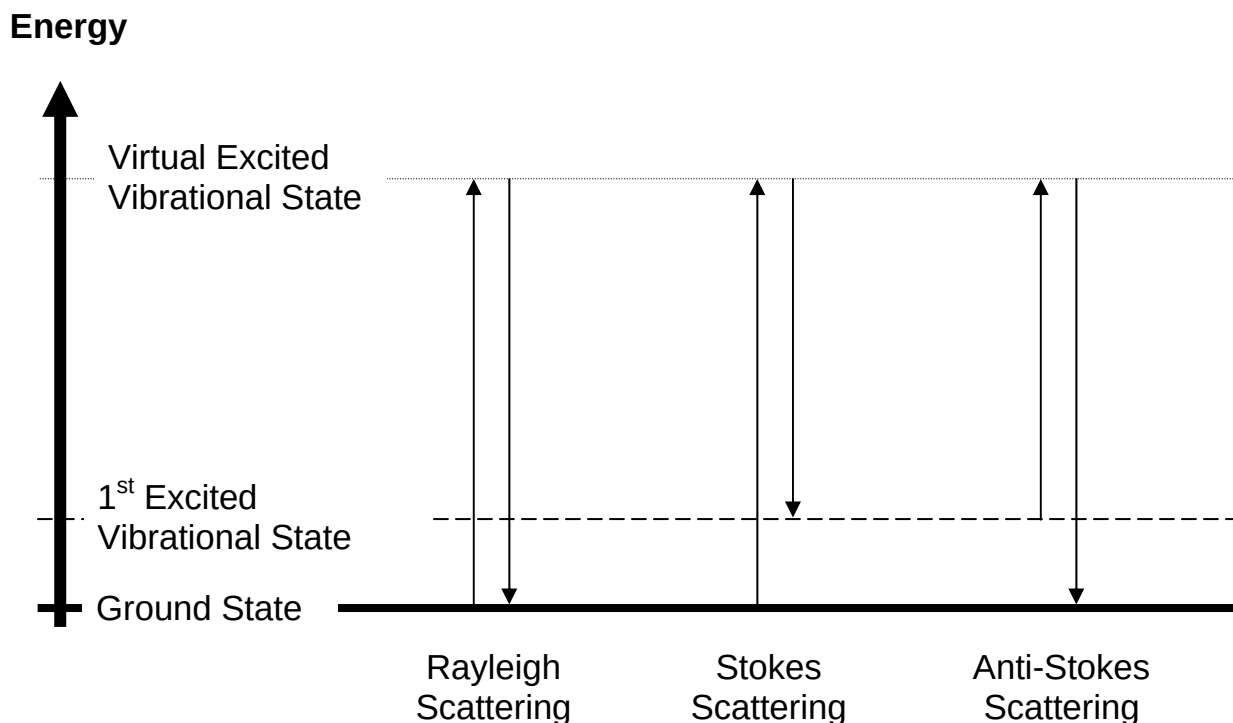


Figure 4: Optical Scattering Mechanisms

The wavelength shift of the Raman scattering depends on the type of vibration (activated normal mode) and, more subtly, on the local chemical environment. As the temperature and sample atmosphere vary, the chemical environment changes around the anions, cations, and solute gas molecules. As the chemical environment changes, the molecules and their vibrational energies themselves change. Changes in internal geometry and energy of molecules result in altered Raman shifts. As such, Raman spectroscopy has proven to be a powerful tool in probing intermolecular interactions and has been used to study ILs.^{25,26,27}

E. *Ab Initio* Molecular Orbital Theory

To more fully explain the nature of intermolecular interactions for a particular system, a self-consistent theoretical model can be used to predict specific effects. The model may then be tested by systematic comparison of its findings with observed experimental results. A number of successful molecular modeling methods, including molecular mechanics, semi-empirical, and *ab initio*, have served to expand the understanding of molecular interactions by successfully guiding experiments. Of these methods, *ab initio* is the only one that predicts molecular behavior without any experimental parameters and, as such, is applied often to novel systems. While *ab initio* calculations are also the most computationally demanding molecular modeling method listed, it was selected for this study because it offered an experimentally independent guide to the exploration and explanation of CO₂ selective solubility in ILs.

Ab initio is Latin for “from the beginning,” and signifies that the method deduces results from a first principles approach to determining an approximate solution to the Schrödinger equation.²⁸ The time independent Schrödinger equation (Eq. 2) describes electrons as waves and

permits a mathematical treatment of electron distribution that in turn affects molecular structures, energies, and properties.²⁹

$$\hat{H}\Psi = E\Psi \quad (\text{Eq. 2})$$

In the equation, the Hamiltonian, $\hat{H}$, operates on the many-electron wavefunction Ψ to produce the eigenvalue total energy E .³⁰ The “total energy” is the energy of the system, which is a sum of kinetic and potential energies of the constituent particles (i.e. nuclei and electrons).

A system in equilibrium is at an energy minimum. *Ab initio* calculations allow the determination of total energy, E , versus nuclear coordinates to find minima and thus elucidate equilibrium structure. In this manner, the total energy of one calculated minima can be compared to that of another minima to indicate the relative energetic stability of the system. The lower energy minima will, in theory, correspond to the true, experimentally observable, physical behavior. The Schrödinger equation can only be solved in exact analytic terms for one-electron systems; hence approximations are required to apply the Schrödinger wave function approach to many-electron molecular systems. The accuracy of the *ab initio* model depends on the nature of the approximations (level of theory) and the size of the mathematical orbital representation (basis set).

Hartree-Fock (HF) theory is a standard level of theory comprised of a set of approximations often used in *ab initio* calculations. These approximations include, among others; the Born-Oppenheimer approximation for which the motion of nuclei are treated as stationary as compared to the rapid electron motion; and the self-consistent field (SCF) approximation for which each electron is treated in the presence of the average field of all other electrons. In addition, molecular orbitals are treated as a linear combination of atomic orbitals

(LCAO). The HF approach neglects the correlation between and amongst electrons. As a result, the energy corresponding to the ground state of any anti-symmetric normalized trial function will be greater than the energy of the exact wavefunction. Implementing the variational principle, coefficients are computed that minimize the energy of the resultant wavefunction for a given set of nuclear coordinates (the Born-Oppenheimer approximation). The larger the basis set from which the wavefunction is constructed, the more accurate the result. However, there is a difference between the exact energy and the result obtained with HF theory employing an infinitely large basis set (i.e., at the HF limit) which is the energy due to electron correlation. Post HF methods, using Many-Body Perturbation theory, attempt to account for electron correlation. Results obtained with one such post-HF approach, the Møller-Plesser-2nd order (MP2), are presented in this work.

For a given level of theory and basis set, the *ab initio* method provides a calculation process to minimize the total energy of the molecular system. Since the total energy of a molecular system varies with small changes in relative positions of all constituent particles, the nuclear coordinates may be systematically perturbed to minimize the total energy. The potential energy surface (PES) is the mathematical relationship linking molecular structure, i.e. coordinates of nuclei, and the resultant total energy. The goal of geometry optimization calculations is to locate the molecular geometry corresponding to the lowest-energy point on the PES which, in turn, better approximates the true physical geometry. The PES may contain many local minima and maxima, thus many input geometries may need to be optimized to ensure that the structure that corresponds to the global minimum is found.

The distribution of charge in molecular systems has great significance for molecular interactions and structures. The electrostatic potential (ESP), which can be calculated using the *ab initio* approach, is useful in describing such interactions and in explaining complex structures. ESP is the interaction energy experienced by a positive elementary point charge (i.e. a test point of +1 charge) along a molecule's surface at a given set of coordinates. Several ESP surfaces are displayed in this work.

Beyond characterizing structures and comparing relative total energies, *ab initio* calculations offer a theoretical method capable of calculating vibrational frequencies. These calculated vibrational frequencies are sufficiently accurate to characterize molecular potential surfaces, generate zero-point vibration and thermal energy corrections to the total energy, and assign and explain spectral lines. Frequency calculations allow the characterization of the stationary points that have been found along the PES as minima or transition states. Minima will possess zero imaginary frequencies while transition states will possess one or more imaginary frequencies. Zero point energy (ZPE) is the lowest possible energy that a quantum mechanical physical system may possess due to finite particle vibration as a result of the Heisenberg uncertainty principle.²⁹ Without the ZPE correction, calculated total energies assume isolated molecules at a temperature of zero Kelvin contain stationary, not vibrating, nuclei. Finally, for each calculated vibrational frequency, the *ab initio* method calculates displacements of nuclei corresponding to the normal modes associated with the spectral line.

III. Materials

High purity (99.999+ %) nitrogen and carbon dioxide were purchased from Airgas and used as received. Commercially available ILs, of purity greater than 97%, were purchased from Sigma-Aldrich (Table 2). Additionally, one salt was synthesized: 1-ethyl-3-methylimidazolium- d_3 -tetrafluoroborate ([emim- d_3][BF₄]). The identity of the deuterated ([emim- d_3][BF₄]) IL was confirmed using NMR spectroscopy.

Table 2: Commercially Purchased ILs

Abbreviation	Chemical Name
[emim][BF₄]	1-ethyl-3-methylimidazolium tetrafluoroborate
[emim][PF₆]	1-ethyl-3-methylimidazolium hexafluorophosphate
[emim][Tf₂N]	1-ethyl-3-methylimidazolium bis(trifluoro-methylsulfonyl)imide
[bmim][BF₄]	1-butyl-3-methylimidazolium tetrafluoroborate
[bmim][PF₆]	1-butyl-3-methyl-imidazolium hexafluorophosphate
[bmim][Tf₂N]	1-butyl-3-methylimidazolium bis(trifluoro-methylsulfonyl)imide

Trace water was removed from the ILs using evacuation. The procedure was as follows. The IL was loaded into a Schlenk flask in the inert atmosphere drybox. The flask was then sealed, removed from the drybox, and attached to a vacuum gas manifold. Water was removed from the IL sample via evacuation at less than 10^{-3} torr for at least 48 hours while stirring. Following evacuation the Schlenk tube, containing the dry IL, was sealed and removed from the vacuum gas manifold and transferred into the drybox.

IV. Methods

A. Raman Experiment

The standard Raman spectroscopy instrumental setup consisted of a Horiba Jobin-Yvon LabRam High Resolution Confocal Raman Microscope (operating with a 633 nm He-Ne laser) controlled by LabSpec spectroscopy data acquisition and processing software (loaded on a Windows-based computer processor). The sample temperature and gas environment were controlled using a Linkam LTS350 temperature stage with a TMS94 temperature programmer.

Microscope glass slides with a concave depression in the center (18 mm wide by 1.75 mm deep, concavity slide, Carolina Biological Supply) were used to contain the ILs for the Raman spectroscopy measurements. The glass microscope slides were deep-welled and able to contain a stir bar and approximately 0.2 mL of IL. To fit the Linkam sample stage, the outside corners of the glass slides were machined in-house.

The internal cavity of the Linkam LTS350 stage was prepared by cleaning with ethanol and cotton swabs. The hermetic seal was ensured through coating the rubber o-ring with vacuum grease. Ethanol was used to wash the surface of a Teflon stir bar and the concave microscope slide. The residual ethanol in the Linkam stage and on the microscope slide was removed by placing them under vacuum in the drybox antechamber for > 30 min. Using a sterile syringe and under drybox atmosphere, approximately 0.2 mL of the dry IL was transferred into the recess of a cleaned concave microscope slide, already supporting a cleaned stir bar. The concave microscope slide was placed in the Linkam LTS350 stage and sealed.

The Linkam stage, containing dried IL sample under drybox the atmosphere (N_2), was removed from the drybox, clamped with standard binder clips (for increased seal integrity),

connected to the TMS94 temperature programmer, and connected to the nitrogen-flushed gas handling system using stainless steel quick connects (Figure 5). Positive pressure in the Linkam cavity (and throughout the gas handling system) was visually verified through the observation of gas bubbling through a bubbler containing de-ionized water in the last stage of the gas handling system. Setting the Tylan Mass Flow Controller to 25 standard cubic centimeters per minute (SCCM), N_2 was streamed at a constant rate at a fixed-temperature and continuously stirred IL sample for two hours to achieve equilibrium saturation at room-temperature.

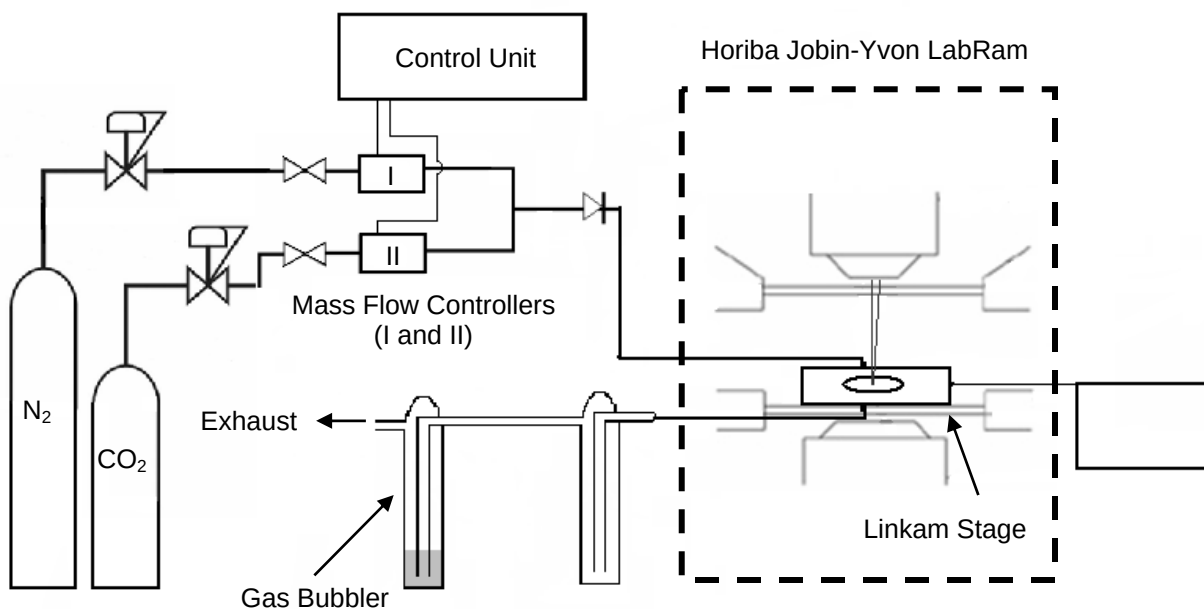


Figure 5: Gas Handling System Attached to the Raman Microscope

The constructed gas handling system (Figure 5) includes: Union Carbide Corporation gas cylinders, Victor SR253C-320 Single Stage Medium Duty Carbon Dioxide Regulator, Airgas Y12-N145A580 High Pressure Two Stage Regulator, Swagelock stainless steel quick connects

and tube fittings, 0.062 inch perfluoroalkoxy (PFA) tubing, Tylan General Model FC-128 Flow Controllers, Tylan General RO-28 control unit, stainless steel union elbows, stainless steel union tee, Linkam LTS350 temperature stage, ring stand, clamps, glassware, plastic connecting tubing, and de-ionized water.

The Horiba Jobin-Yvon LabRam High Resolution Raman microscope was calibrated before every spectra acquisition with a single-crystal silicon sample with 520.7 cm^{-1} Raman peak. The Linkam stage, containing the equilibrated sample under constant gas flow, was placed on the manual microscope stage and under the confocal Raman microscope objective (Figure 6). A “confocal microscope” uses point source illumination and a pinhole in an optically conjugate plane in front of the detector to eliminate out-of-focus information.³¹ The confocal optics were manually focused on the surface of the sample. The confocal optics of the Raman microscope allow for the precise sampling of the spectra of a defined volume of sample without interference from other molecules in the path of the Raman laser excitation source.³² Thus, if the Raman is properly focused on the IL, the observed spectra will be from a thickness of IL of less than 0.1 mm.

Temperatures and gas environments were cycled while acquiring *in situ* Raman spectra of equilibrated ILs. Raman spectra of the IL sample were acquired under constant gas flow at varying temperatures. Fifteen minutes were allotted between variable temperature spectroscopic acquisitions to allow for sample equilibrium. Spectra were acquired during temperature increase and decrease so that at least two data sets existed for each temperature. Once the temperature was stable at 22.5°C , the Linkam stage was removed from under the Raman microscope objective and placed on top of the magnetic stir plate.

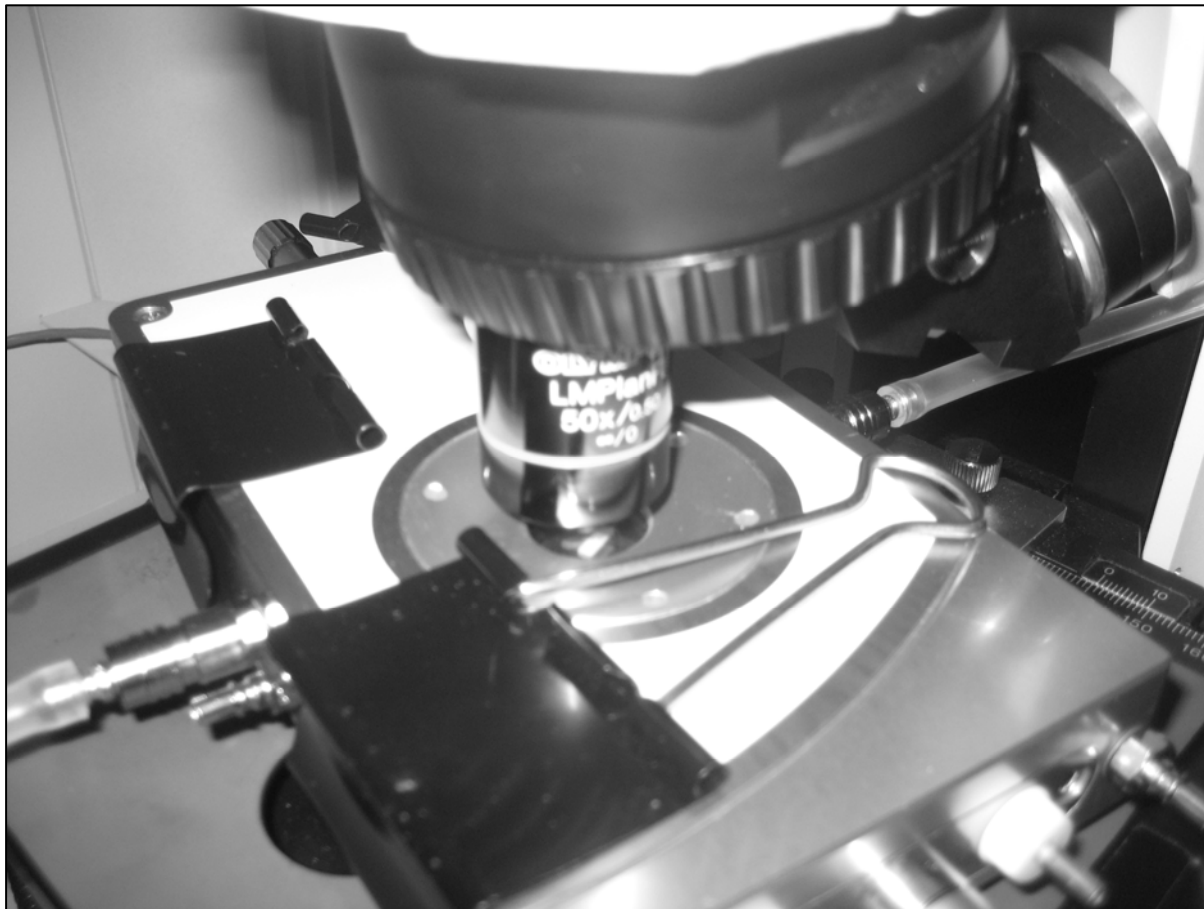


Figure 6: *In situ* IL Sample in Linkam Stage Connected to Gas Handling System

The composition of gas atmosphere in the Linkam stage was varied by manually setting the N_2 and CO_2 stream rates using the Tylan General Model FC-128 Flow Controller. Setting the Tylan Mass Flow Controller to 25 standard cubic centimeters per minute (SCCM), CO_2 was streamed at a constant rate over a fixed-temperature and continuously stirred IL sample for two hours to achieve equilibrium gas saturation at room-temperature. The Linkam stage, containing the equilibrated sample under constant CO_2 flow, was placed on the manual microscope stage and under the confocal Raman microscope objective. The confocal optics were manually focused on the surface of the sample, and *in situ* variable-temperature spectra were acquired.

In the effort to improve signal to noise ratio, an optical grade, gas tight, 1cm^2 quartz cuvette cell was also used to acquire Raman spectra of ILs and gases. Samples were pre-saturated with the appropriate gas prior to obtaining spectra. Figure 7 shows the cuvette cell attached to the vacuum line system. The cuvette cell was mounted on a JY Double Pass 1cm^2 Cell holder that provides for an overall sample path length of 2 cm (compared to less than 0.1 mm for the confocal optics). The cuvette cell has a square base with internal cavity 1 cm in internal width.

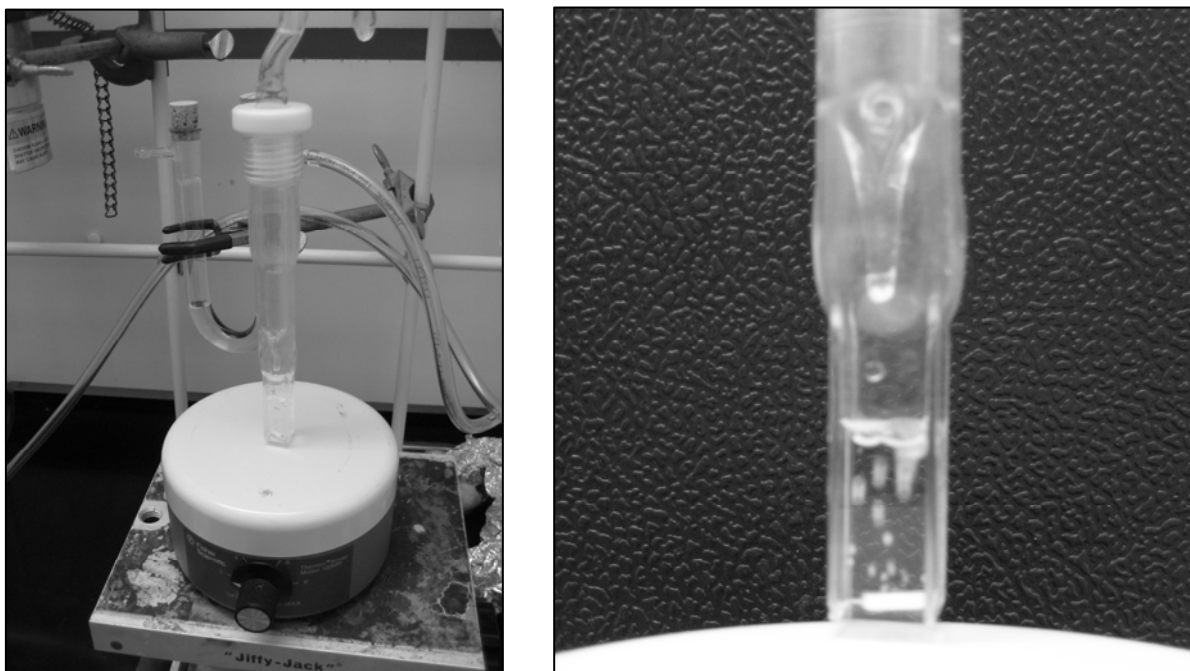


Figure 7: Quartz Cuvette Cell Attached to the Evacuation and Gas Loading System

All acquired spectra were processed using a Savitzky-Golay smoothing filter,³³ a baseline correction, and a normalizing intensity coefficient. The peaks were calculated using a Gaussian-Lorenz algorithm that analyzes the area under the curve.

B. *Ab Initio* Computation

The resources used in the computational components of the study included Gaussian03®³⁴ and GaussView®³⁵ software suites operating on a variety of computational platforms. Gaussian03® was used to calculate total energies, optimize geometries, and generate normal mode vibrational frequencies. GaussView®, a graphical user interface, was used in tandem with Gaussian03® output to gain a greater understanding of a molecular system. One of the computational platforms is the Air Force Research Laboratory Major Shared Resource Center. This supercomputing facility is part of the Department of Defense High Performance Computing Modernization Office. Another platform is the U.S. Naval Academy's Computer Aided Design & Interactive Graphics (CADIG) primary compute server Orthrus, a 40-processor Linux cluster. In addition, Linux and Windows workstations in the Naval Academy Chemistry Department were used.

Isolated IL molecular ions were individually constructed using the graphical user interface GaussView® and subsequently submitted to Gaussian03® for full geometry optimization (i.e. no geometric constraints) followed by a frequency calculation. The first goal was to develop a suitable computational protocol that provides reasonable agreement with the highest levels of theory attainable at sufficient computational efficiency to allow us to explore the IL-gas system. Implementing a variety of levels of theory and basis sets, the BF_4^- anion, CO_2 molecule, and $[\text{BF}_4(\text{CO}_2)]^-$ complex were explored. The geometry-optimized potential energy profiles were computed for these three systems because the $[\text{BF}_4(\text{CO}_2)]^-$ complex represents the simplest IL ion interacting with CO_2 . The input geometry of the $[\text{BF}_4(\text{CO}_2)]^-$ complex was the global minimum configuration calculated previously.³⁶ A Hartree-Fock approach with a

moderately sized basis set (HF/6-31+G(d) is the denotation for such calculations) was selected and used for the prototype study to allow for greater computational efficiency. The moderate size of the basis set is especially important for probing the potential energy surfaces in this study since the surfaces have many local minima and maxima (transition states) to evaluate.

The interaction, or binding energy, ΔE , of $[\text{BF}_4(\text{CO}_2)]^-$ was calculated by evaluating the energetic difference between isolated constituent molecules and the complex (Eq. 3).

$$\Delta E = E([\text{BF}_4(\text{CO}_2)]^-) - (E([\text{BF}_4]^-) + E([\text{CO}_2])) \quad (\text{Eq. 3})$$

Specifically, the sum of the total energies of the BF_4^- anion and CO_2 molecule was subtracted from the total energy of the $[\text{BF}_4(\text{CO}_2)]^-$ complex. Subsequently, corrections to this ΔE were applied including corrections for differences in zero-point energies coming from the components in Eq. 3 and a correction for basis set superposition error (BSSE). BSSE is a false stabilization of the complex relative to the isolated molecules that arises from the fact that there are additional basis functions available to the molecules in the complex that are not present in calculations of the isolated molecules (i.e., a molecule in a complex is better described simply due to proximity of the basis sets describing other molecules of the complex). The result is an overestimation of the magnitude of the binding energy. A commonly employed method for accounting for the BSSE is the “counterpoise correction” for which calculations on the isolated molecules incorporating the additional basis functions of the complex are used to estimate the false stabilization arising from BSSE. Using standard literature procedures, counterpoise corrections at Hartree-Fock and MP2 were performed to correct for BSSE.³⁷ The $[\text{BF}_4(\text{CO}_2)]^-$ binding energies for various levels of theory and basis sets were computed. Subsequently, further calculations

corrected for the electron correlation effect by means of Møller-Plesset second-order perturbation theory (MP2).

Substituting a methyl for an alkyl group is a common practice to reduce the expense of *ab initio* calculations. As such, 1,3-dimethylimidazolium, [mmim]⁺, replaced 1-ethyl-3-methylimidazolium, [emim]⁺, and 1-butyl-3-methylimidazolium, [bmim]⁺, for the majority of calculations. The [mmim]⁺ cation, was selected as a preliminary approximation to the [emim]⁺ and [bmim]⁺ cations primarily to eliminate the numerous degrees of freedom in the alkyl chain. After the optimized geometry was computed for [mmim]⁺, a HF/6-31+G(d) geometry optimized CO₂ molecule was systematically placed in ten relative positions around the hemisphere of the [mmim]⁺ cation at a nearest neighbor atomic distance of approximately 5 Å. Many input geometries were used to allow for adequate sampling of the phase space. Similar protocols were used to scan the PES for the following complexes: anion-CO₂, anion-N₂, cation-CO₂, cation-N₂, anion-cation, anion-cation-CO₂, and anion-cation-CO₂. Further, to better understand the electrostatic interactions between molecular species, GaussView® was used to calculate and visualize molecular electrostatic potentials (ESPs), which is the distribution of charge along the surface of a molecule.

The calculated normal modes were animated and tabulated using GaussView®. While normal mode intensities are also reported in the output of any Gaussian03® frequency calculation, intensities are less reliable than the calculated frequency.³⁸ However, normal mode intensities may be used as a way to assess the relative Raman activity of a normal mode. The output frequencies were scaled as per Pople and coworkers.³⁹ Raw frequencies computed at the Hartree Fock level contain known systematic errors due to a neglect of electron correlation and

use of the harmonic oscillator approximation, resulting in overestimates.³⁸ It is standard practice to scale frequencies predicted by the Hartree Fock level by an empirical factor of 0.8929.³⁸

V. Results

A. Raman Spectra

The gas phase CO₂ Raman spectra were acquired using both the Linkam stage and glass cuvette cell. Three Raman lines were detected at the following frequencies: 1285.3 cm⁻¹, 1388.0 cm⁻¹, and 1409.6 cm⁻¹. These spectroscopic features correspond well to reported CO₂ Raman lines: Hanson reported Raman lines for gaseous CO₂ at 1285 cm⁻¹, 1388 cm⁻¹ and 1409 cm⁻¹.⁴⁰

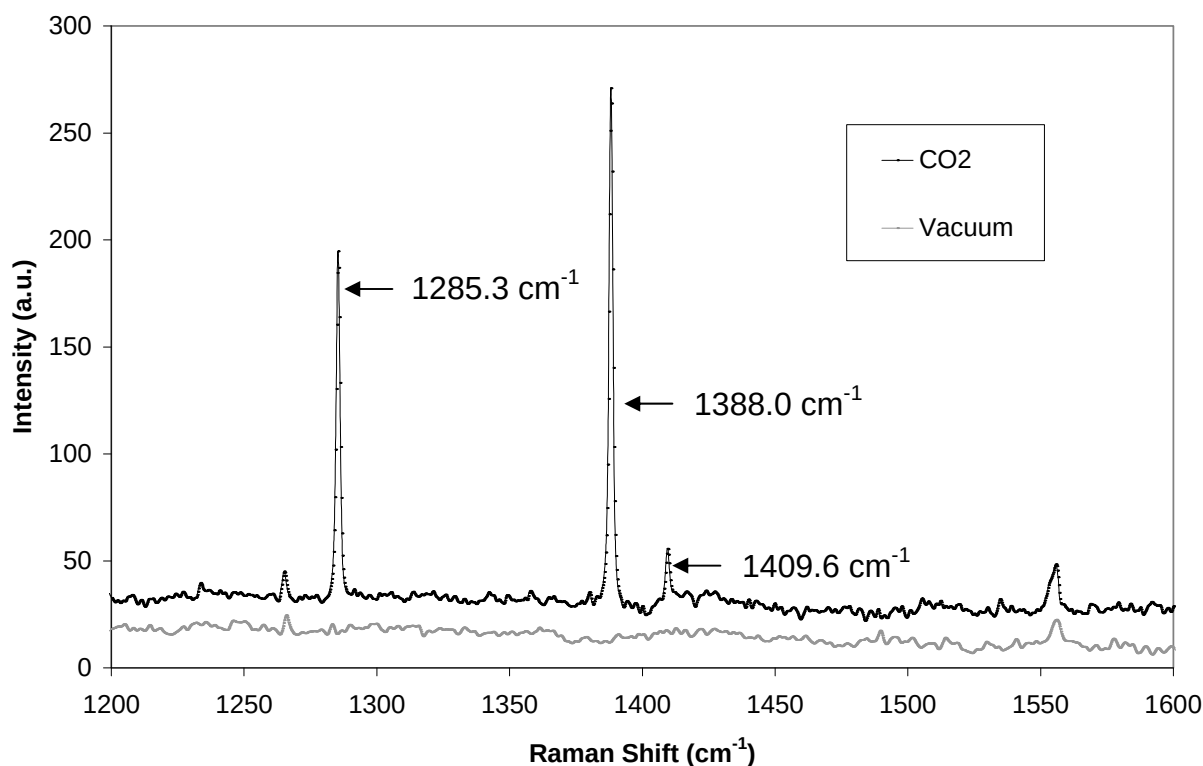


Figure 8: Raman Spectra of Evacuated and CO₂-Filled Cuvette Cell

The Raman spectra for a [emim- d_3][BF₄] sample at 23°C under sequentially alternating N₂ and CO₂ atmospheres are presented in Figure 9 for the frequency range from 1360 cm⁻¹ to 1420 cm⁻¹. The intensity of all spectra have been normalized to the 1425 cm⁻¹ peak (not shown) and the baselines have been shifted for clarity of presentation. Due to the need to remove the Linkam stage and place it on magnetic stir plate to establish equilibrium, the spectra were acquired with approximately the same focus point (i.e. static vertical but not lateral position).

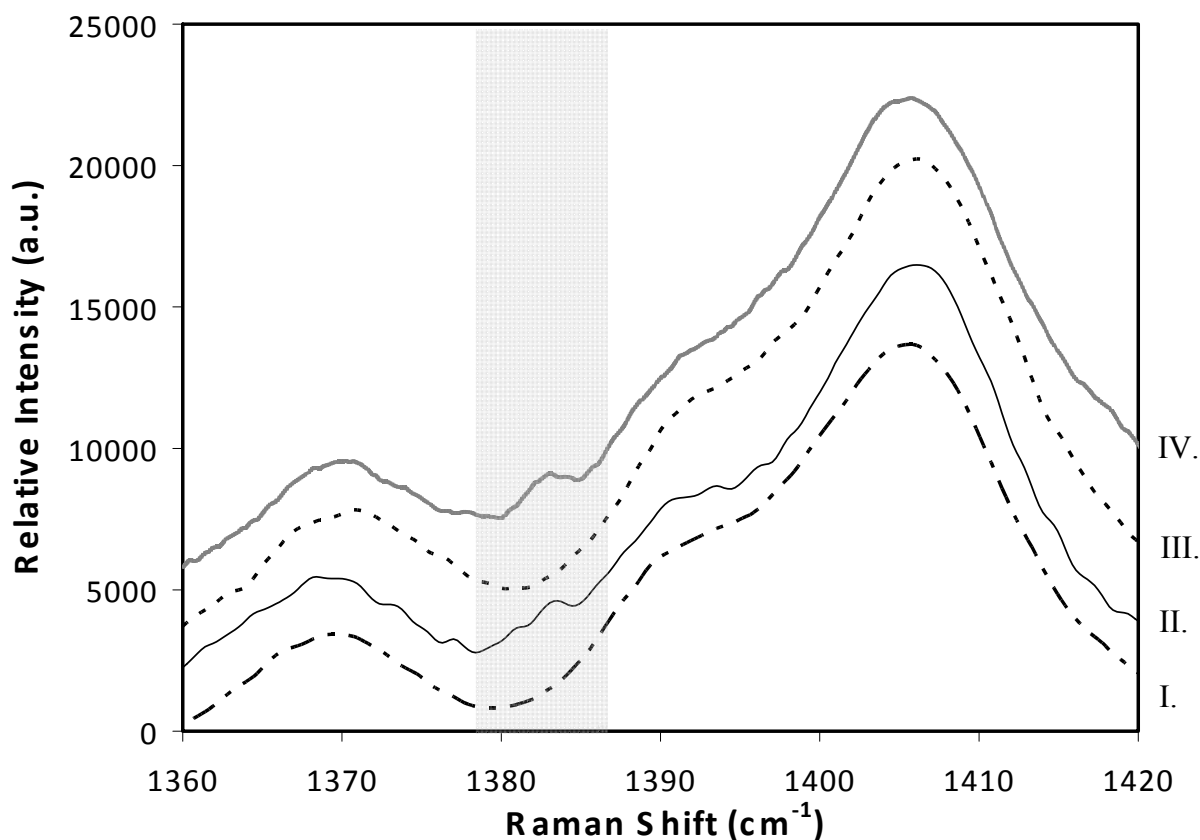


Figure 9: Raman Spectra of [emim- d_3][BF₄] under Cycled N₂ and CO₂ Flow at 23°C

- - - I. N₂ Atmosphere (1st exposure) — II. CO₂ Atmosphere (1st exposure)
 III. N₂ Atmosphere (2nd exposure) ——— IV. CO₂ Atmosphere (2nd exposure)

The experimental data show the effect of gas atmosphere composition on the Raman spectra of an imidazolium-based IL. A small peak at 1383 cm^{-1} is present under CO_2 atmosphere but not under N_2 atmosphere (Figure 9, I and II). The appearance and disappearance of this feature when the gases are switched is caused by the presence of CO_2 in the IL. Furthermore, the new observed Raman band is most likely the 1388 cm^{-1} CO_2 band shifted to lower energy due to interaction of the IL with CO_2 . This phenomenon occurs for all other tested ILs.

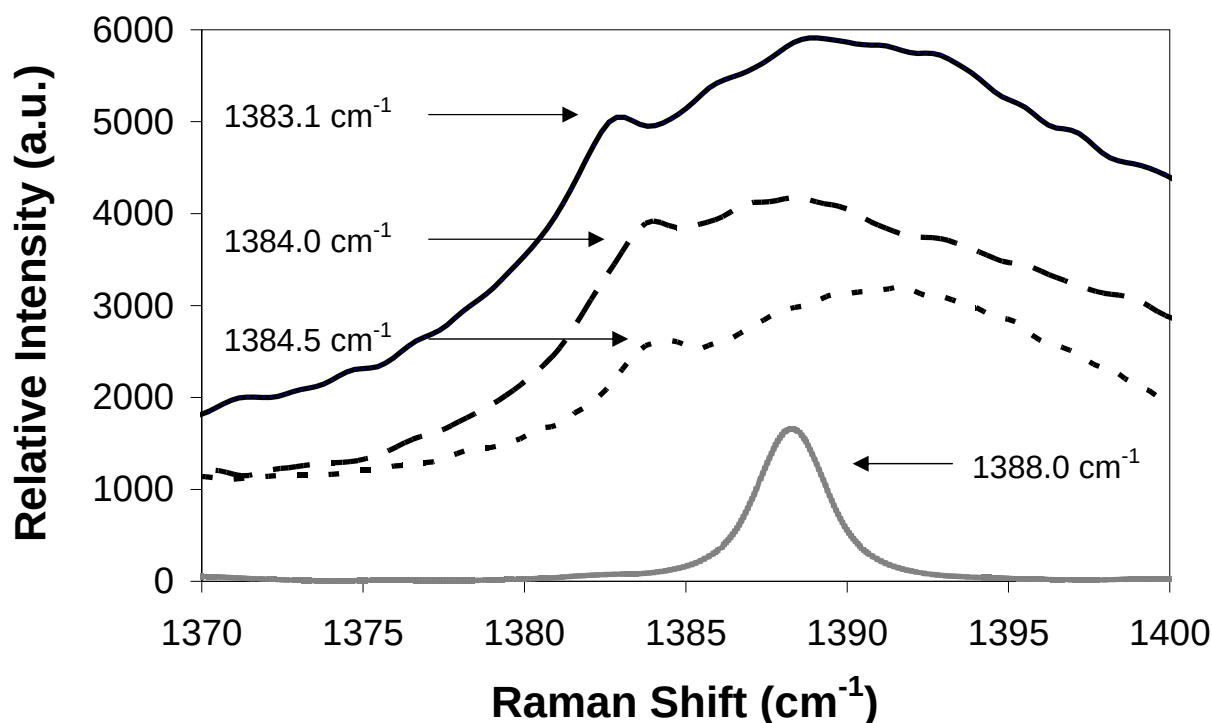


Figure 10: Raman Spectra of ILs under CO_2 Flow at 23°C

— I. $[\text{emim}][\text{BF}_4]$ — · II. $[\text{bmim}][\text{Tf}_2\text{N}]$ ····· III. $[\text{bmim}][\text{PF}_6]$ — IV. Gas Phase CO_2

Figure 10 plots the spectra of three different ILs saturated with CO_2 . For comparison, the experimental gas phase 1388 cm^{-1} CO_2 Raman line is provided. The shifted 1388 cm^{-1} “ CO_2

interaction peak” is distinct and repeatable for each reported IL system. The magnitude of the shift is greatest for [emim][BF₄], and less for [bmim][Tf₂N] and [bmim][PF₆].

The presence of the second main CO₂ Raman band (1285 cm⁻¹) in any of the studied ILs has yet to be identified. This may be due to a variety of factors. The 1285 cm⁻¹ band is less intense than the 1388 cm⁻¹ band, so it may be lost in the spectra baseline noise. A sinusoidal perturbation of the baseline is consistently observed (Figure 11).

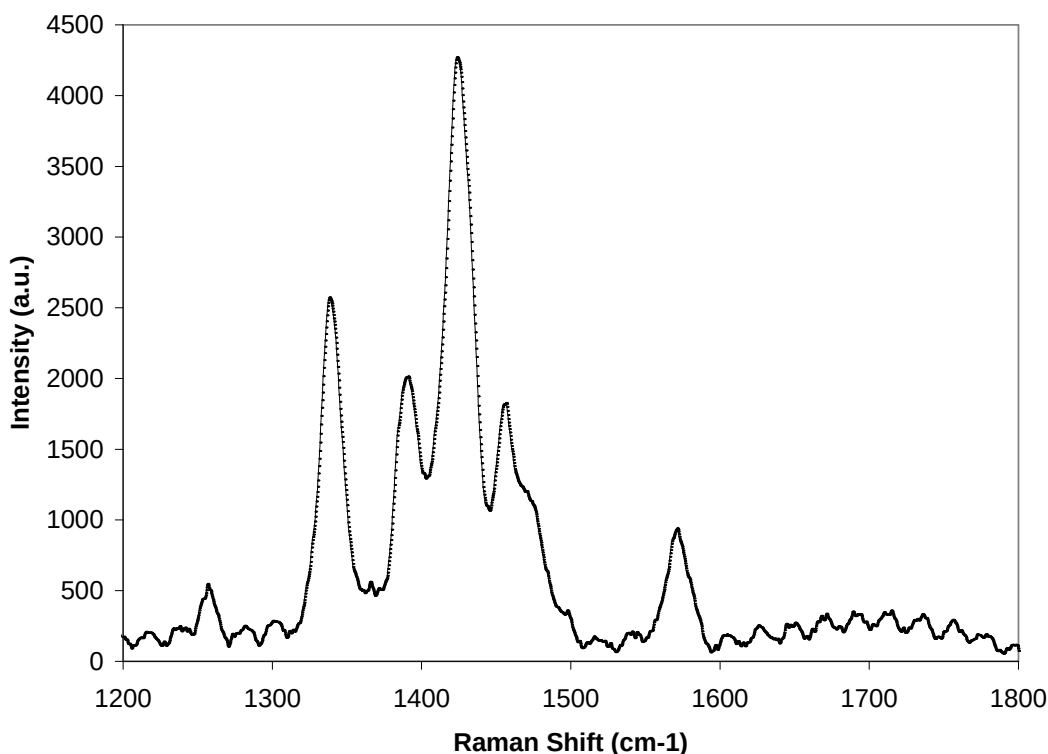


Figure 11: Raman Spectra of [emim][BF₄] under N₂ Flow at 23°C

This oscillating baseline is evident when there is no IL sample present (glass slide only) and when the confocal spectroscopy is focused in the gas phase above the sample. This instrument-specific perturbation is not prohibitive of taking data. The low-energy CO₂ line could

possibly be masked by the oscillating baseline. Alternatively, the 1285 cm^{-1} line may simply not be present.

B. *Ab Initio* Computations

One $[\text{BF}_4(\text{CO}_2)]^-$ configuration was found to optimize to a stable minimum at HF/6-31+G(d). The optimization for the $[\text{BF}_4(\text{CO}_2)]^-$ complex is visually dramatic (Figure 12). A molecular pair of BF_4^- and CO_2 exists in the most stable state when the CO_2 molecule, linear when isolated, bends to approach the BF_4^- anion. The $\angle\text{OCO}$ is 180° in the HF/6-31+G(d) optimized geometry for CO_2 in isolation and 174.5° in the corresponding complex with BF_4^- anion. The carbon in the CO_2 orients toward the geometric center of the anion.

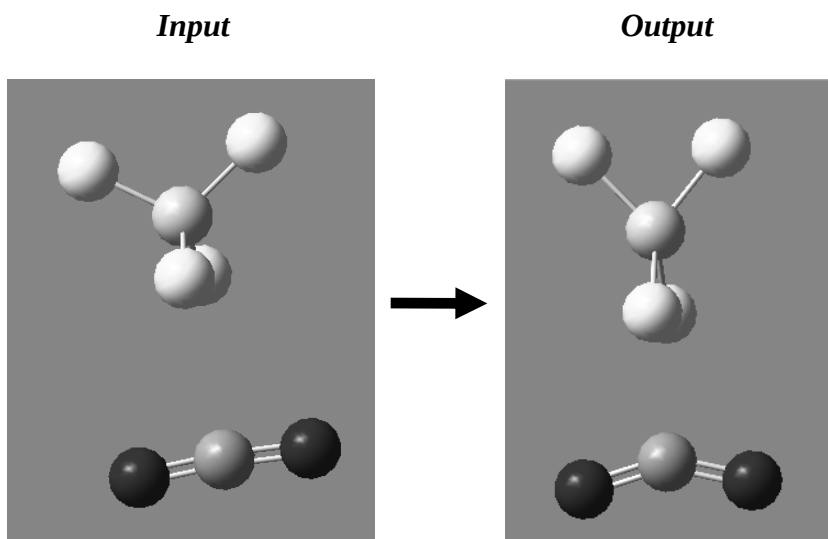


Figure 12: Geometry Optimization of $[\text{BF}_4(\text{CO}_2)]^-$

Upon optimization, many intra-molecular geometric parameters are altered from initial input geometry, including $d(\text{C}=\text{O})$, the internal CO_2 carbon-oxygen bond length, and $d(\text{BC})$, the

distance between the CO₂ carbon and the [BF₄]⁻ boron. These geometric parameters are tabulated for a series of *ab initio* methods (Table 3).

Table 3: Optimized Geometry Parameters Computed for [BF₄(CO₂)]⁻ Complex

Level of Theory/Basis Set	<OCO (°)	d(C=O) (Å)	d(BC) (Å)
HF/6-31+G(d)	174.5	1.14	3.45
MP2/cc-PVDZ	173.5	1.18	3.25
MP2/cc-PVTZ	174.7	1.17	3.32
MP2/cc-PVQZ	175.0	1.17	3.31
MP2/aug-cc-PVDZ	175.2	1.18	3.31
MP2/aug-cc-PVTZ	175.1	1.17	3.31

Figure 13 plots the binding energies computed from the tabulated total energies as a function of the time expended during the Gaussian03® geometry optimization calculation. Like the geometric parameters of the optimized [BF₄(CO₂)]⁻ complex, the binding energies converge as the level of theory becomes more robust and as the basis set size increases. HF/6-31+G(d) yielded calculated binding energies that are in reasonable agreement with MP2/aug-cc-pVTZ, the most computationally demanding methods attempted in this work. Thus, HF/6-31+G(d) was selected as the protocol with sufficient computational efficiency to allow efficient probing of novel potential energy surfaces while providing reasonable computational accuracy.

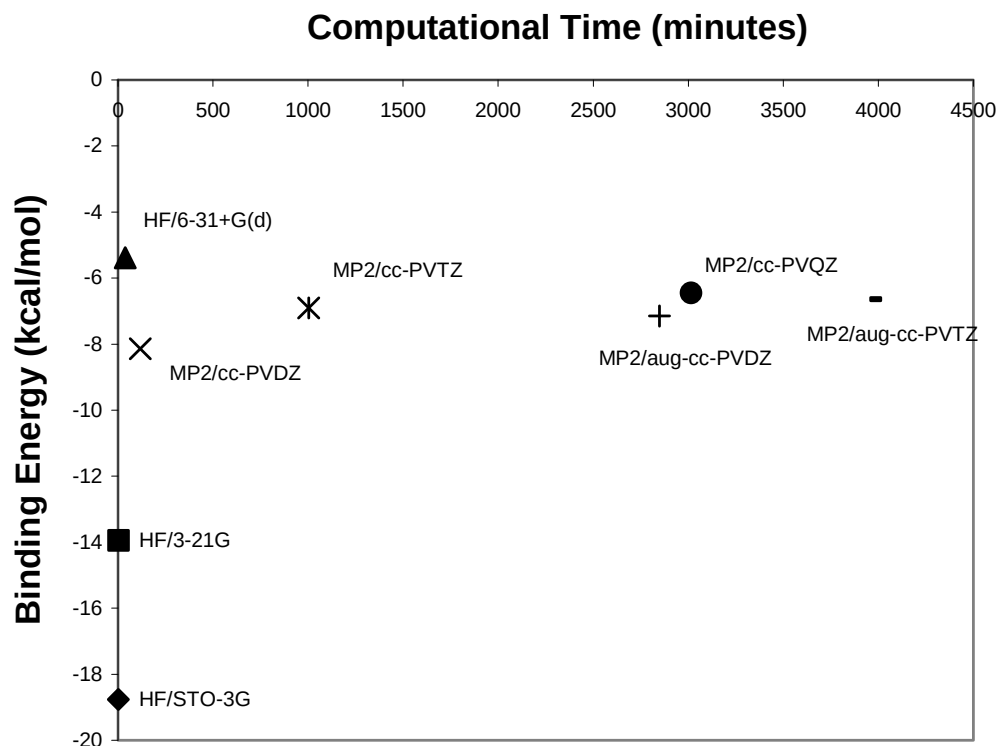


Figure 13: Binding Energy vs. Computational Expense

For interactions with the other anions, CO_2 orients the carbon toward the geometric center of the anion and the O-C-O angle is reduced. The O-C-O angle reduction is greatest in the $[\text{BF}_4(\text{CO}_2)]^-$ complex. In the one stable configuration of $[\text{PF}_6(\text{CO}_2)]^-$, the CO_2 carbon situates itself in the middle of two adjacent P-F bonds and along one of the equators of the octahedrally symmetric PF_6^- anion. In the stable configurations of $[\text{Tf}_2\text{N}(\text{CO}_2)]^-$, fluorine atoms were never nearest-neighbors to CO_2 oxygen atoms. Instead, a variety of optimized $[\text{Tf}_2\text{N}(\text{CO}_2)]^-$ structures yielding energy minima were calculated, each with the carbon of the CO_2 drawn into the anion center at different orientations.

Table 4: Lowest Energy Configurations of Anion-CO₂ Complexes at HF/6-31+G(d)

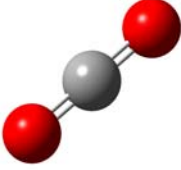
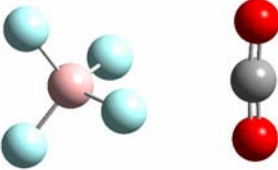
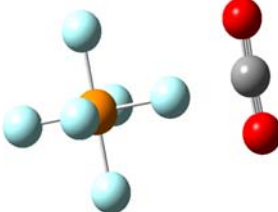
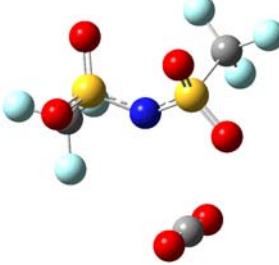
Complex	Structure	d(C=O) (Å)	<OCO (°)
[CO ₂]		1.1434	180.0
[BF ₄ (CO ₂)] ⁻		1.1444	174.5
[PF ₆ (CO ₂)] ⁻		1.1439	175.6
[Tf ₂ N(CO ₂)] ⁻		1.1439	176.2

Table 5 displays the computed interaction energies, in kcal/mol, for the anion-CO₂ complexes. As the series of corrections are made to the computed interaction energy across a given level of theory, the magnitude of the interaction decreases. The BF₄⁻ interacts with CO₂ more strongly than PF₆⁻ and Tf₂N⁻.

Table 5: Interaction Energies (in kcal/mol) of Anion-CO₂ Complexes

CO ₂ Complex	HF/6-31+G(d)// HF/6-31+G(d)		MP2/6-31+G(d)// HF/6-31+G(d)		
	$\Delta E^{(a)}$	$\Delta(E+ZPE)^{(b)}$	$\Delta E^{(a)}$	$\Delta E + CP^{(c)}$	$\Delta(E + ZPE) + CP^{(d)}$
[BF ₄ (CO ₂)] ⁻	-5.39	-4.91	-6.71	-5.06	-4.58
[PF ₆ (CO ₂)] ⁻	-4.02	-3.64	-5.68	-3.86	-3.48
[Tf ₂ N(CO ₂)] ⁻	-4.14	-3.76	-7.23	-4.18	-3.80

(a) $\Delta E = E([Complex]) - (E([ion]) + E([CO_2]))$

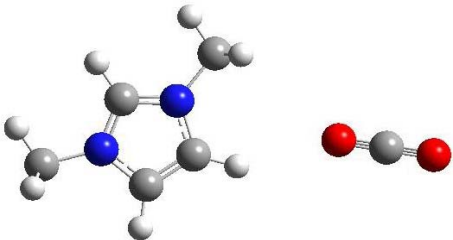
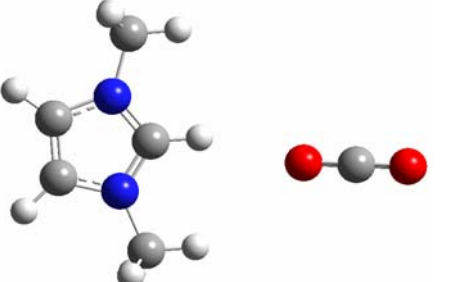
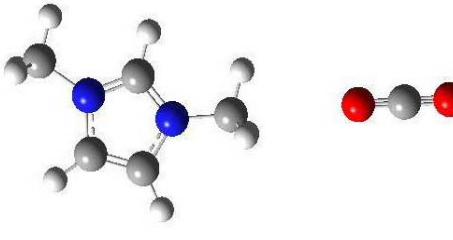
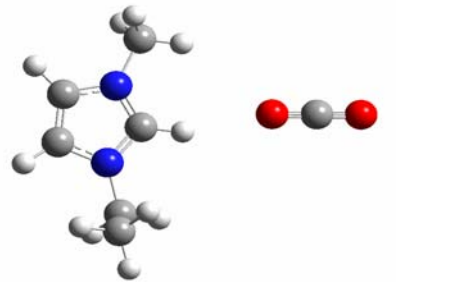
(b) $\Delta(E+ZPE) = (E([Complex]) + ZPE([Complex]) - (E([ion] + ZPE([ion]) + E([CO_2]) + ZPE([CO_2])))$

(c) $\Delta E + CP = E([Complex]) - (E([ion]) + E([CO_2])) + E(CP)$

(d) $\Delta(E+ZPE) + CP = \Delta(E+ZPE) + E(CP)$

Cation-CO₂ complexes were also explored. For several input configurations, the geometry optimization did not converge because the molecules collided or drifted away. The remainder of the calculations successfully converged to one of three different optimized configurations of the [mmim(CO₂)]⁺ complex. These results, along with an optimized [emim(CO₂)]⁺ complex are reported in Table 6.

Table 6: Lowest Energy Configurations of Cation-CO₂ Complexes at HF/6-31+G(d)

Complex	Structure	d(C=O) (Å)	<OCO (°)
[mmim(CO ₂)] ⁺ A		1.1436	179.9
[mmim(CO ₂)] ⁺ B		1.1436	180.0
[mmim(CO ₂)] ⁺ C		1.1435	180.0
[emim(CO ₂)] ⁺ B1		1.1436	180.0

The total energies of the these local minima were compared, and configuration B was determined to be the $[\text{mmim}(\text{CO}_2)]^+$ global minimum. Computed binding energies were extracted for configurations A, B, and C of the $[\text{mmim}(\text{CO}_2)]^+$ complex (Table 7).

Table 7: Interaction Energies (in kcal/mol) of Cation-CO₂ Complexes

CO ₂ Complex	HF/6-31+G(d)// HF/6-31+G(d)		MP2/6-31+G(d)// HF/6-31+G(d)		
	$\Delta E^{(a)}$	$\Delta(E+ZPE)^{(b)}$	$\Delta E^{(a)}$	$\Delta E + CP^{(c)}$	$\Delta(E + ZPE) + CP^{(d)}$
$[\text{mmim}(\text{CO}_2)]^+ \text{ A}$	-3.01	-2.66	-4.14	-3.32	-2.97
$[\text{mmim}(\text{CO}_2)]^+ \text{ B}$	-3.87	-3.47	-4.69	-3.88	-3.48
$[\text{mmim}(\text{CO}_2)]^+ \text{ C}$	-2.32	-2.07	-3.07	-2.46	-2.21
$[\text{emim}(\text{CO}_2)]^+ \text{ B1}$	-3.77	-3.37	-4.65	-3.80	-3.41

(a) $\Delta E = E([\text{Complex}]) - (E([\text{ion}]) + E([\text{CO}_2]))$

(b) $\Delta(E+ZPE) = (E([\text{Complex}]) + ZPE([\text{Complex}])) - (E([\text{ion}]) + ZPE([\text{ion}]) + E([\text{CO}_2]) + ZPE([\text{CO}_2]))$

(c) $\Delta E + CP = E([\text{Complex}]) - (E([\text{ion}]) + E([\text{CO}_2])) + E(CP)$

(d) $\Delta(E+ZPE) + CP = \Delta(E+ZPE) + E(CP)$

The magnitude of the binding energy for configuration B is larger than the other two configurations, indicating the CO₂ molecule most strongly interacts with the $[\text{mmim}]^+$ cation when it is positioned in penetrating alignment, within the imidazolium plane, closest to the proton attached to the position 2 carbon. For comparison, the ambient energy available at 298 K is approximately 0.6 kcal/mol.

To better understand why the B geometry of $[\text{mmim}(\text{CO}_2)]^+$ is energetically favored, GaussView® was used to calculate and visualize molecular electrostatic potentials. The distribution of charge along the surface of $[\text{mmim}]^+$ and CO₂ were computed. The acidic proton on the 2nd position carbon of the imidazolium ring gave rise to the most positive (blue) surface

relative to the more neutral surfaces of the $[\text{mmim}]^+$ cation. The electronegative oxygen atoms gave rise to the most negative surfaces of the CO_2 molecule. When the $[\text{mmim}]^+$ and CO_2 were paired together, the most negative part of the CO_2 molecule (the poles of the oxygens) would naturally seek the most positive part of the $[\text{mmim}]^+$ cation (the most acidic hydrogen). Thus, the global minimum, configuration B of the $[\text{mmim}(\text{CO}_2)]^+$ complex, may be visually explained with help of the electrostatic potential surfaces.

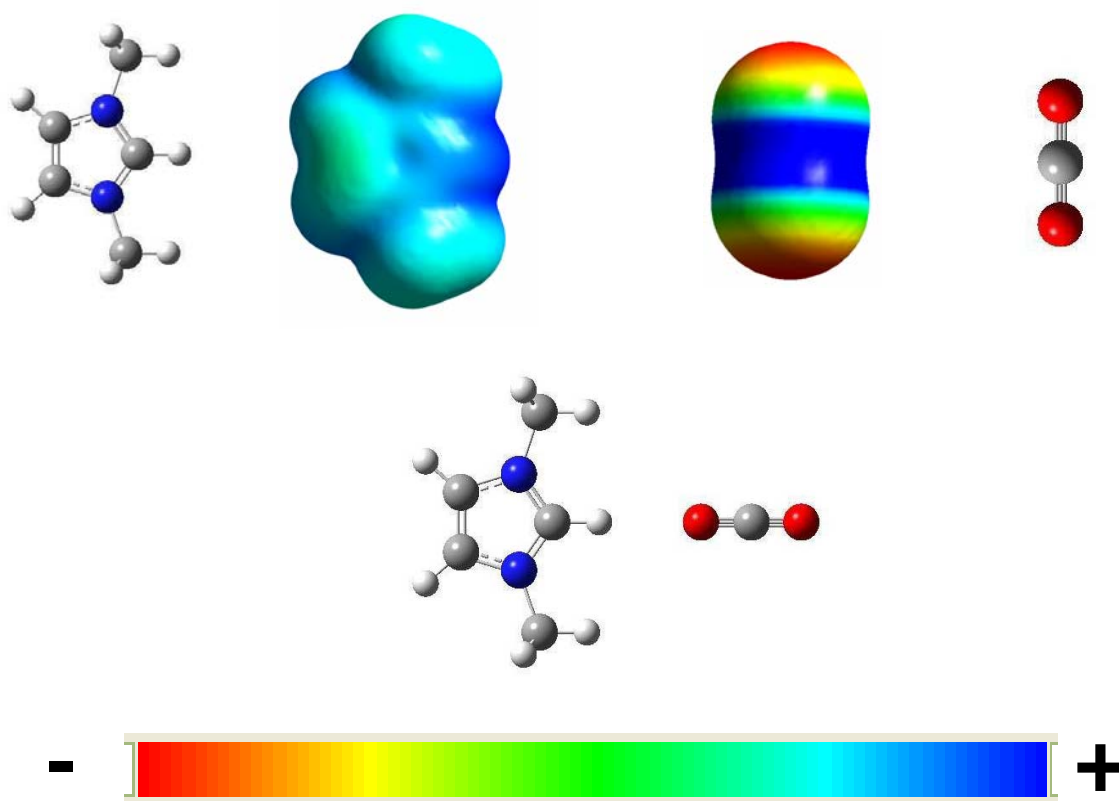


Figure 14: Electrostatic Potential Explaining the Formation of $[\text{mmim}(\text{CO}_2)]^+$

Structures are calculated at HF/6-31+G(d), and both ESPs are on the same scale.

Implementing the HF/6-31+G(d) protocol, the interaction energetics of N_2 with $[\text{mmim}]^+$ and $[\text{BF}_4]^-$ were explored. The same method that was used to find the global minimum of

$[\text{mmim}(\text{CO}_2)]^+$ and $[\text{BF}_4(\text{CO}_2)]^-$, was used to find the global minimum of $[\text{mmim}(\text{N}_2)]^+$ and $[\text{BF}_4(\text{N}_2)]^-$. The binding energies of the global minimum configurations of $[\text{mmim}(\text{N}_2)]^+$ and $[\text{BF}_4(\text{N}_2)]^-$ were computed.

For the two simplest IL ions, the magnitude of the N_2 binding energies was calculated to be less than the magnitude of the CO_2 binding energies. Since CO_2 has a greater ability to dissolve in imidazolium-based ionic liquids than N_2 , and CO_2 has a greater interaction energy with $[\text{mmim}]^+$ and $[\text{BF}_4]^-$ than N_2 , stronger (solute gas)-(solvent ion) pair interaction may give rise to greater gas solvation. Table 8 displays the computed interaction energies, in kcal/mol, for the anion- N_2 and cation- N_2 complexes. The results indicate interaction energies between CO_2 and the IL cations and anions that are greater than those of N_2 .

Table 8: Interaction Energies (in kcal/mol) for N_2 Complexes

N_2 Complex	HF/6-31+G(d)// HF/6-31+G(d)		MP2/6-31+G(d)// HF/6-31+G(d)		
	$\Delta E^{(a)}$	$\Delta(E+\text{ZPE})^{(b)}$	$\Delta E^{(a)}$	$\Delta E + \text{CP}^{(c)}$	$\Delta(E + \text{ZPE}) + \text{CP}^{(d)}$
$[\text{BF}_4(\text{N}_2)]^-$	-1.21	-0.97	-2.44	-1.60	-1.35
$[\text{PF}_6(\text{N}_2)]^-$	-1.00	-0.81	-2.29	-1.31	-1.12
$[\text{PF}_6(\text{N}_2)]^-$	-0.86	-0.69	-1.92	-1.05	-0.89
$[\text{TF}_2\text{N}(\text{N}_2)]^-$	-1.18	-0.94	-3.35	-1.56	-1.32
$[\text{mmim}(\text{N}_2)]^+ \text{ A}$	-1.17	-0.84	-2.35	-1.68	-1.35
$[\text{mmim}(\text{N}_2)]^+ \text{ B}$	-1.57	-1.20	-2.69	-2.05	-1.68
$[\text{mmim}(\text{N}_2)]^+ \text{ C}$	-0.93	-0.67	-1.83	-1.24	-0.98

(a) $\Delta E = E([\text{Complex}]) - (E([\text{ion}]) + E([\text{N}_2]))$

(b) $\Delta(E+\text{ZPE}) = (E([\text{Complex}]) + \text{ZPE}([\text{Complex}])) - (E([\text{ion}]) + \text{ZPE}([\text{ion}]) + E([\text{N}_2]) + \text{ZPE}([\text{N}_2]))$

(c) $\Delta E + \text{CP} = E([\text{Complex}]) - (E([\text{ion}]) + E([\text{N}_2])) + E(\text{CP})$

(d) $\Delta(E+\text{ZPE}) + \text{CP} = \Delta(E+\text{ZPE}) + E(\text{CP})$

Complexes between IL cations and anions were also explored (Table 9). The lowest energy complexes for all systems placed the anion above the plane of the imidazole ring, closest to the C2 position.

Table 9: Lowest Energy Configurations of Cation-Anion Complexes at HF/6-31+G(d)

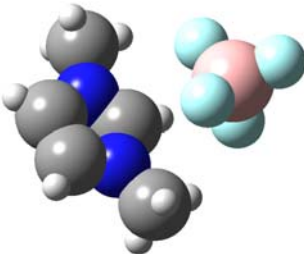
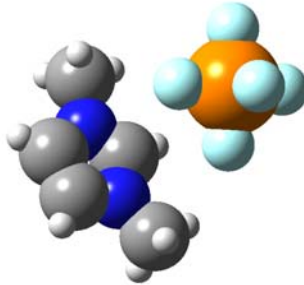
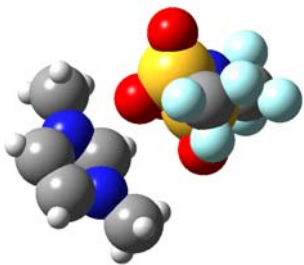
Complex	Structure
[mmim(BF ₄)]	
[mmim(PF ₆)]	
[mmim(Tf ₂ N)]	

Table 10 displays the computed interaction energies, in kcal/mol, for several IL anion-cation pairs. The interaction energies between mmim⁺ and a given anion does not differ greatly

from that between emim^+ and the same anion. This result further substantiates the validity of our methyl for alkyl simplification of IL cations modeled in this study.

Table 10: Binding Energies (in kcal/mol) of IL Ion Pairs:

Ion Pair Complex	HF/6-31+G(d)// HF/6-31+G(d)		MP2/6-31+G(d)// HF/6-31+G(d)		
	$\Delta E^{(a)}$	$\Delta(E+ZPE)^{(b)}$	$\Delta E^{(a)}$	$\Delta E + CP^{(c)}$	$\Delta(E + ZPE) + CP^{(d)}$
[mmim(BF ₄)]	-82.94	-81.98	-87.13	-83.70	-82.74
[emim(BF ₄)]	-82.61	-81.57	-87.24	-83.62	-82.58
[mmim(PF ₆)]	-77.33	-76.46	-81.84	-77.93	-77.06
[emim(PF ₆)]	-77.12	-76.20	-82.15	-78.02	-77.11
[mmim(Tf ₂ N)]	-77.46	-76.56	-83.78	-78.17	-77.27

(a) $\Delta E = E([Complex]) - (E([cation]) + E([anion]))$

(b) $\Delta(E+ZPE) = (E([Complex]) + ZPE([Complex])) - (E([cation]) + ZPE([cation]) + E([anion]) + ZPE([anion]))$

(c) $\Delta E + CP = E([Complex]) - (E([cation]) + E([anion])) + E(CP)$

(d) $\Delta(E+ZPE) + CP = \Delta(E+ZPE) + E(CP)$

To incorporate anion-cation interaction in the CO₂ interaction model, ion pair-CO₂ complexes were explored. The lowest energy structures for the [mmim(BF₄)(CO₂)], [mmim(PF₆)(CO₂)], and [mmim(Tf₂N)(CO₂)] complexes are reported in Table 11. As with all previously reported structures, the d(C=O) bond is slightly lengthened and the $\angle\text{OCO}$ of the CO₂ is decreased upon complexation. In the [mmim(BF₄)(CO₂)] optimized structure, the CO₂ exists slightly tilted away from the imidazole plane. This geometry is similar, but distorted from the lowest energy structure reported for the [mmim(CO₂)]⁺ complex. However, like the [BF₄(CO₂)]⁻ complex, the CO₂ carbon in [mmim(BF₄)(CO₂)] aligns to the boron center of the anion. Similarly in the other ion pair-CO₂ structures, the anion-CO₂ interaction seems to dominate.

Table 11: Lowest Energy Configurations of Ion Pair-CO₂ Complexes at HF/6-31+G(d)

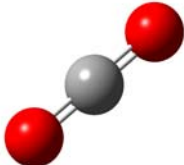
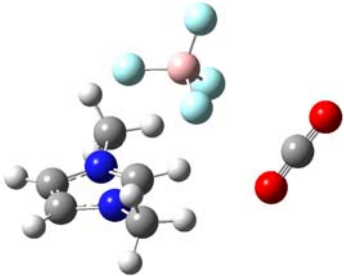
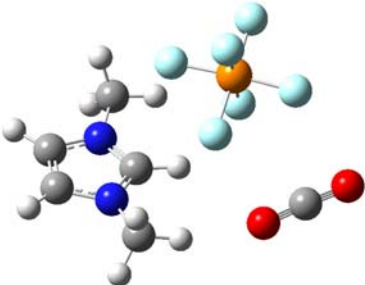
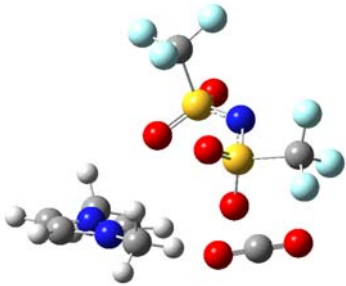
Complex	Structure	d(C=O) (Å)	<OCO (°)
[CO ₂]		1.1434	180.0
[mmim(BF ₄)(CO ₂)]		1.1439	177.0
[mmim(PF ₆)(CO ₂)]		1.1437	177.6
[mmim(Tf ₂ N)(CO ₂)]		1.1437	177.8

Table 12 reports the energies that result when a CO₂ molecule interacts with a stable anion-cation pair. The most stable complex was found to be [mmim(BF₄)(CO₂)]. Similarly, the interaction energy of CO₂ with the [mmim(BF₄)] complex is greatest in magnitude compared to its interaction with other cation-anion complexes.

Table 12: CO₂ Interaction Energies (in kcal/mol) in Ion Pair-CO₂ Complexes

Ion Pair –CO ₂ Complex	HF/6-31+G(d)// HF/6-31+G(d)		MP2/6-31+G(d)// HF/6-31+G(d)		
	$\Delta E^{(a)}$	$\Delta(E+ZPE)^{(b)}$	$\Delta E^{(a)}$	$\Delta E + CP^{(c)}$	$\Delta(E + ZPE) + CP^{(d)}$
[mmim(BF ₄)(CO ₂)]	-4.61	-4.18	-7.70	-5.17	-4.74
[mmim(PF ₆)(CO ₂)]	-4.02	-3.60	-6.93	-4.49	-4.07
[mmim(Tf ₂ N)(CO ₂)]	-3.77	-3.27	-6.61	-3.31	-2.82

(a) $\Delta E = E([Complex]) - (E([ion\ pair]) + E([CO_2]))$

(b) $\Delta(E+ZPE) = (E([Complex]) + ZPE([Complex])) - (E([ion\ pair]) + ZPE([ion\ pair]) + E([CO_2]) + ZPE([CO_2]))$

(c) $\Delta E + CP = E([Complex]) - (E([ion\ pair]) + E([CO_2])) + E(CP)$

(d) $\Delta(E+ZPE) + CP = \Delta(E+ZPE) + E(CP)$

As with [mmim(CO₂)]⁺ complexes, ion pair-CO₂ complexes can be explained using electrostatic potentials. Figure 15 shows the ESP of the lowest energy optimized configurations of the anion-cation complexes. Presumably, the areas of most negative (most red), will attract the carbon center of the CO₂. Similarly, the areas of most positive (most blue), will attract the electron-dense oxygen in CO₂. The relative magnitude of negative surface charge density in the anion region is greatest for [mmim(BF₄)], and weakest for [mmim(TF₂N)]. This result makes sense because of the anion and cation in each case have the same charge, yet BF₄⁻ is a much

smaller anion than Tf_2N^- . Since the mmim^+ cation is constant throughout the presented series, the relative magnitude of positive surface charge density in the cation region is mostly constant.

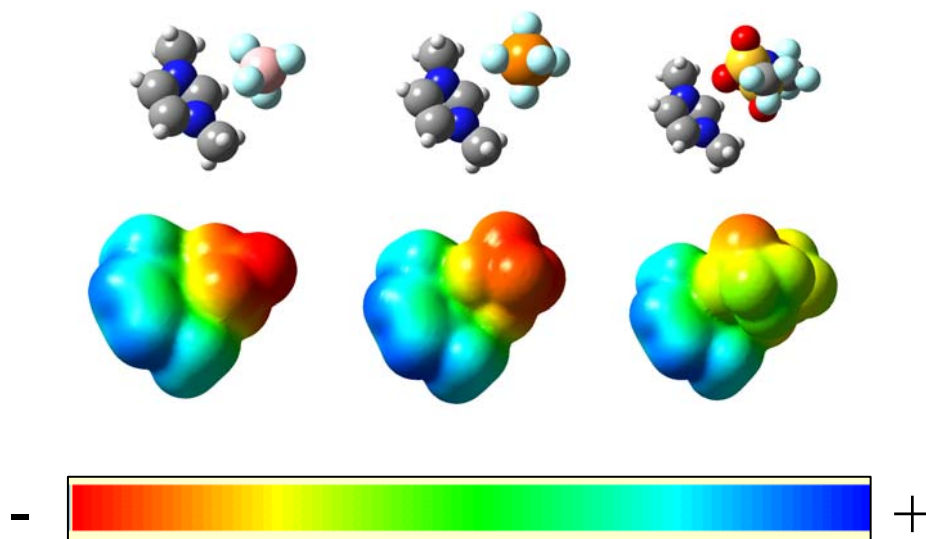


Figure 15: Electrostatic Potentials of Anion-Cation Pairs

Structures are calculated at HF/6-31+G(d), and ESPs are on the same scale.

Frequency Calculations:

CO_2 has four normal modes, a doubly-degenerate IR-active mode (1 and 2), a symmetric breathing Raman-active mode (3), and a non-degenerate asymmetric IR-active mode (4). These modes are tabulated in Table 13. The doubly degenerate CO_2 bending mode (modes 1 and 2) split when complexed with $[\text{BF}_4(\text{CO}_2)]^-$ compared to the $[\text{mmim}(\text{CO}_2)]^+$. Similarly, the anion- CO_2 interaction shifted the most Raman active frequency (mode 3) more than the cation- CO_2 interaction. The symmetric CO_2 stretching mode shifted from 1349.0 cm^{-1} in CO_2 to 1346.7 cm^{-1} in $[\text{BF}_4(\text{CO}_2)]^-$. Again, the shifts upon complexation as predicted at HF/6-31+G(d) are rather small in magnitude, but in principle resolvable in experiment.

Table 13: CO₂ Frequency Shifts Due to Interaction with [BF₄]⁻ and [mmim]⁺

CO ₂ Mode	Frequency (cm ⁻¹)	
	CO ₂	[BF ₄ (CO ₂)] ⁻
1	669.2	662.6
2	669.2	674.9
3	1349.0	1346.7
4	2289.4	2280.4

A Raman line in region of 1388 cm⁻¹ was detected in the IL phase upon loading the IL with CO₂. The presence of this line is reversible and repeatable. Experimental frequency shift from gas phase CO₂, $\Delta_{\text{obs.}}$, indicated the strength of the IL-CO₂ interaction: BF₄⁻ > Tf₂N⁻ > PF₆⁻. The experimental frequency shift is proportional to the computed anion-CO₂ ΔE .

Table 14 summarizes the experimental and calculated CO₂ Raman line shifts. The trends and relative magnitudes of differences between the CO₂ gas phase and CO₂-IL Raman Line for the experimental (Δ_{obs}) and *ab initio* calculations (Δ_{calc}) are in good agreement. Furthermore, the agreement is best for the calculations involving both cation and anion interactions with CO₂.

Table 14: Observed and Calculated CO₂ Raman Line Shifts (in cm⁻¹)

Sample	Experimental		Calculated at HF/6-31+G(d)			
	Freq.	$\Delta_{\text{obs.}}$ ^(a)	X ^(b)	$\Delta_{\text{calc.}}$ ^(c)	Y ^(d)	$\Delta_{\text{calc.}}$ ^(c)
Gas Phase CO₂	1388.0					
[emim][BF₄]	1383.1	4.9	BF₄	2.3	BF₄	3.7
[bmim][Tf₂N]	1384.0	4.0	Tf₂N	1.4	Tf₂N	2.5
[bmim][PF₆]	1384.5	3.5	PF₆	1.0	PF₆	2.5

(a) $\Delta_{\text{obs.}}$ is the magnitude of the shift in frequency from gas phase to liquid phase CO₂ peak

(b) X represents anion component of anion-CO₂ complex $[X(\text{CO}_2)]^-$, e.g. $[\text{BF}_4(\text{CO}_2)]^-$

(c) $\Delta_{\text{calc.}}$ is the magnitude of the shift in frequency from isolated CO₂ vibration to vibration in the complex

(d) Y represents anion component of ion pair-CO₂ complex $[\text{mmim}(Y)(\text{CO}_2)]$, e.g. $[\text{mmim}(\text{BF}_4)(\text{CO}_2)]$

C. A Selective Solvation Model

Figure 16 displays the relationship between CO₂ solubility and CO₂/N₂ selectivity ratio using reported data.¹⁸ The inverse dependence of solubility and selectivity ratio (also see Table 1) points to factors, other than electrostatic binding, that govern the selective gas solubility mechanism in ILs. There are two competing models to explain the selective IL solvation of CO₂ compared to other small molecular gases like N₂.

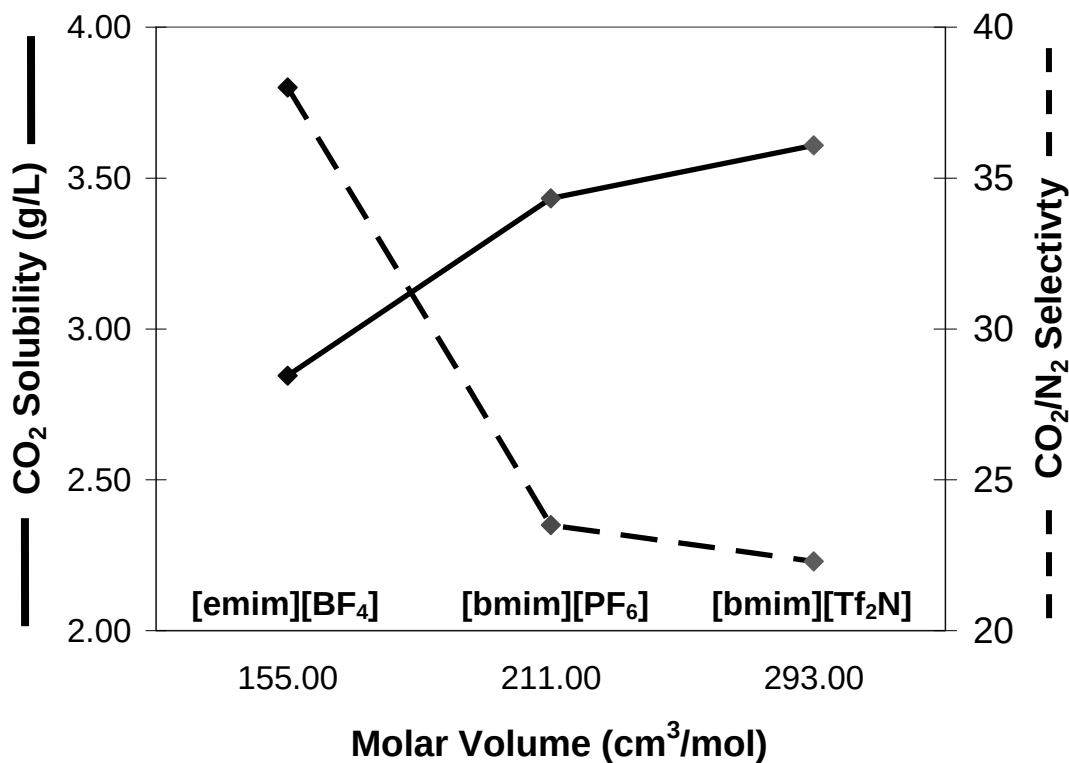


Figure 16: Experimental CO₂ Solubility and Selectivity Trends in Several ILs

One model holds that specific fluorine-CO₂ electrostatic interactions give rise to the selective solvation. Brennecke and co-workers have proposed that anions containing fluorine have specific fluorine-CO₂ interactions which give rise to increased CO₂ solubility in ILs.¹⁹ By

this model, an increase in fluorine content in the anion would result in higher CO₂ solubility which is in agreement with the observed trend of Tf₂N⁺ > PF₆⁻ > BF₄⁻. The Raman results reported in this work confirm a specific interaction of CO₂ and ionic liquid ions, but do not provide much insight into the nature of this interaction. The *ab initio* computations, however, do provide a glimpse of the potential interactions between CO₂ and the ionic liquid ions. These computational results show stable configurations of [Tf₂N(CO₂)]⁻, where fluorine atoms were never nearest-neighbors to CO₂ oxygen atoms. The CO₂ preferentially interacts with the N, at the center of the anion. These results do not support the model proposed by Brennecke.

Alternatively, Noble has proposed that as IL molecular volume increases, the importance of Van der Waals forces to the CO₂ solubility mechanism correspondingly increases. Camper and coworkers discovered that increased IL molar volume correlates with increased CO₂ solubility.¹⁵ Similarly, it has been proposed by Welton and co-workers that strength of anion-cation interaction in the IL affects the available free volume, and one would anticipate that a weaker interacting anion leads to more free volume being available.⁴¹ For an IL with a large cation and anion, like [bmim][Tf₂N], the electrostatic binding between cation and anion is not extremely strong (relative to [emim][BF₄], as validated in the *ab initio* calculations in this study). This weakened anion-cation interaction enlarges the IL free volume, which can be filled with N₂ and CO₂ gas solute molecules alike. However, unlike N₂, CO₂ will preferentially interact with anion centers or cation rings due to the localized charge distribution in CO₂. When an IL with a smaller cation and anion, like [emim][BF₄], is considered, the electrostatic binding between cation and anion is stronger (relative to [bmim][Tf₂N], as validated in the *ab initio* calculations in this study). With smaller IL free volume, the CO₂-anion electrostatic interaction is not only

stronger, but the electrostatic interactions dominate the mechanism because there is less space for any gas solute. In other words, molecules that have weaker electrostatic interactions with IL anions and cations, e.g. N_2 , will be preferentially “pushed” out of the smaller void space. This proposed model is represented schematically by Figure 17.

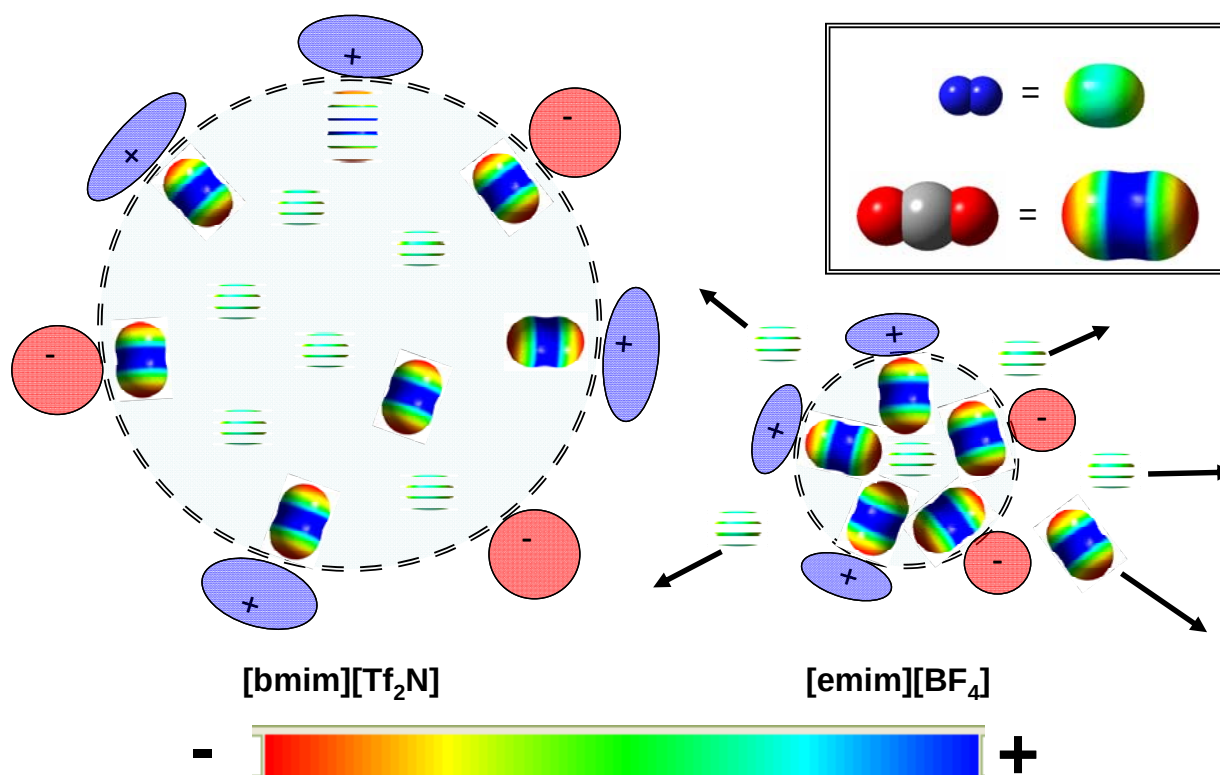


Figure 17: IL Selective Solubility Model

In this model, more charge localization gives rise to increased electrostatic attraction between the IL anion and cation. The greater the charge density of the IL ions (because the ILs ions will be involved in tight binding with each other), the less likely any gas solute can enter in the liquid phase (decreased bulk CO_2 solubility). However, the greater charge density of the IL ions also gives rise to stronger IL ion- CO_2 interactions (increased CO_2 selectivity). Thus, to increase

equilibrium CO₂ concentration in solvents, the inter-ion electrostatic attraction should be relaxed. However, to increase ratio of CO₂ concentration to N₂ concentration, the inter-ion electrostatic attraction should be magnified. Thus, there is some optimal situation that appropriately balances these two competing factors.

VI. Summary

A new *in situ* variable temperature and atmosphere Raman spectroscopy apparatus has been assembled and refined for use at the Naval Academy. The apparatus was validated and calibrated and the experimental procedures were established for acquiring IL Raman spectra at varying temperatures and gas atmospheres. Experimental results confirm that the presence of CO₂ affects the Raman spectra of the studied ILs. Observed, repeatable, and reversible frequency shifts of the main CO₂ Raman line confirmed an electrostatic interaction between the CO₂ and IL molecules. The lower vibration energy of the main CO₂ Raman line in liquid phase indicates a weakening of the C=O bonds when CO₂ enters the IL phase and suggests that CO₂ is sharing electron density with IL ions.

Computationally, the Hartree Fock level of theory with the 6-31+G(d) basis set was selected for its reasonable accuracy and limited expense as the method to calculate binding energies, Raman-active normal mode frequencies, and electrostatic potentials. Stable complexes between gas molecules (CO₂ and N₂) and selected ionic liquid ions ([BF₄]⁻, [PF₆]⁻, [Tf₂N]⁻, [mmim]⁺, [emim]⁺) were found. The sophistication of the computation was increased by investigating ion pair interactions with CO₂ and with N₂. In all cases, the binding energy of a complex with N₂ was smaller than the corresponding complex with CO₂. The calculated CO₂ binding energies for [BF₄]⁻ complexes were larger in magnitude than for the [PF₆]⁻ or [Tf₂N]⁻

complexes. Similarly, the shift of CO₂ vibrational frequencies in complexes with [BF₄]⁻ were larger in magnitude than the shifts in complexes with [PF₆]⁻ or [Tf₂N]⁻. Similarly, a greater experimental frequency shift of the main CO₂ Raman line was observed in the [BF₄]⁻ IL as compared with [PF₆]⁻ or [Tf₂N]⁻ ILs. Increased quantitative agreement between calculated and observed frequency shifts were reported with ion pair-CO₂ complexes, as a more sophisticated *ab initio* treatment.

Using the combined experimental and computational approach, a model explaining the inverse experimental correlation of CO₂ solubility and selectivity points was formulated. The fluorine interaction model proposed by Brennecke and co-workers was not supported by the calculated geometries in this study. Rather, it was found that the greater the charge density of the IL ions (because the ILs ions will be involved in tight binding with each other), the less likely any gas solute can enter in the liquid phase (decreased bulk CO₂ solubility). However, the greater charge density of the IL ions also gives rise to stronger IL ion-CO₂ interactions (increased CO₂ selectivity). The predictions of this model fit the available experimental spectroscopic and solubility data.

Future work should be aimed at both further investigating the basic science of CO₂ solvation in ionic liquids, and also designing CO₂ scrubbing systems that can incorporate the unique properties of ILs. Specifically, future basic scientific work could involve an investigation of a larger ensemble of anions and cations, targeting interactions with fluorinated anions, and target specific binding sites (e.g. C-H-O hydrogen bonds). A possible goal of a continued experimental work could be to provide quantitative measurements of the bulk CO₂ solubility, diffusion, and solubility selectivity of a wide array of ILs. Using the results of this work,

engineers can incorporate the understanding of the solubility/selectivity trade-off to design a pressure-swing or temperature-swing CO₂ scrubber that meets the application requirements. Knowledge gained from this effort will help guide the further improvement of ILs for carbon dioxide removal in applications ranging from sequestration of greenhouse gas emissions to purification of submarine air.

VII. References

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Appendix 1

Output Gaussian03® file for a sequential geometry optimization and frequency job for the [CO₂] complex at HF/6-31+G(d):

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smdir=/nishome/scratch/
Entering Link 1 = /usr/software/g03/l1.exe PID=      28922.
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 Gaussian, Inc., Wallingford CT, 2004.

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 1-Nov-2007

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 Initialization pass.

 ! Initial Parameters !
 ! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.
! R1	R(1,2)	1.1434	estimate D2E/DX2
! R2	R(1,3)	1.1434	estimate D2E/DX2
! A1	L(2,1,3, -1, -1)	180.0	estimate D2E/DX2
! A2	L(2,1,3, -2, -2)	180.0	estimate D2E/DX2

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07

Number of steps in this run= 20 maximum allowed number of steps= 100.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	8	0	0.000000	0.000000	1.143360
3	8	0	0.000000	0.000000	-1.143360

```

                        Distance matrix (angstroms):
                        1           2           3
1  C      0.000000
2  O      1.143360    0.000000
3  O      1.143360    2.286720    0.000000
Stoichiometry      C02
Framework group    D*H[0(C),C*(0.0)]
Deg. of freedom    1
Full point group           D*H      NOp    8
Largest Abelian subgroup   D2H      NOp    8
Largest concise Abelian subgroup C2      NOp    2
                        Standard orientation:
-----
Center      Atomic      Atomic      Coordinates (Angstroms)
Number      Number      Type          X          Y          Z
-----
1           6           0           0.000000    0.000000    0.000000
2           8           0           0.000000    0.000000    1.143360
3           8           0           0.000000    0.000000   -1.143360
-----
Rotational constants (GHZ):      0.00000000    12.0847949    12.0847949
Standard basis: 6-31+G(d) (6D, 7F)
There are 17 symmetry adapted basis functions of AG symmetry.
There are 2 symmetry adapted basis functions of B1G symmetry.
There are 5 symmetry adapted basis functions of B2G symmetry.
There are 5 symmetry adapted basis functions of B3G symmetry.
There are 1 symmetry adapted basis functions of AU symmetry.
There are 13 symmetry adapted basis functions of B1U symmetry.
There are 7 symmetry adapted basis functions of B2U symmetry.
There are 7 symmetry adapted basis functions of B3U symmetry.
Integral buffers will be 262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
57 basis functions, 96 primitive gaussians, 57 cartesian basis
functions
11 alpha electrons 11 beta electrons
nuclear repulsion energy 59.2417809460 Hartrees.
NAtoms= 3 NActive= 3 NUniq= 2 SFac= 2.76D+00 NATFMM= 60 Big=F
One-electron integrals computed using PRISM.
NBasis= 57 RedAO= T NBF= 17 2 5 5 1 13 7 7
NBsUse= 57 1.00D-06 NBFU= 17 2 5 5 1 13 7 7
Harris functional with IExCor= 205 diagonalized for initial guess.
ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn= 4
AccDes= 0.00D+00
HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 4 IDoV=1
ScaDFX= 1.000000 1.000000 1.000000 1.000000
Initial guess orbital symmetries:
Occupied (SGU) (SGG) (SGG) (SGG) (SGU) (SGG) (SGU) (PIU)
(PIU) (PIG) (PIG)
Virtual (PIU) (PIU) (SGG) (SGU) (PIU) (PIU) (SGG) (SGG)
(PIG) (PIG) (SGU) (PIU) (PIU) (SGU) (SGG) (PIU)
(PIU) (SGU) (SGU) (SGG) (PIG) (PIG) (SGG) (PIU)
(PIU) (SGU) (DLTG) (DLTG) (PIG) (PIG) (SGG) (DLTU)
(DLTU) (DLTG) (DLTG) (PIU) (PIU) (SGU) (SGG) (PIG)
(PIG) (SGU) (SGG) (SGG) (SGG) (SGU)

```

The electronic state of the initial guess is 1-SGG.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 Keep R1 integrals in memory in canonical form, NReq= 1921281.
 SCF Done: E(RHF) = -187.638786758 A.U. after 10 cycles
 Convrg = 0.1904D-08 -V/T = 2.0029
 S**2 = 0.0000

Population analysis using the SCF density.

Orbital symmetries:

Occupied	(SGU)	(SGG)	(SGG)	(SGG)	(SGU)	(SGG)	(SGU)	(PIU)
	(PIU)	(PIG)	(PIG)					
Virtual	(SGG)	(PIU)	(PIU)	(SGU)	(PIU)	(PIU)	(SGG)	(PIG)
	(PIG)	(SGG)	(SGU)	(PIU)	(PIU)	(SGU)	(SGG)	(PIU)
	(PIU)	(SGU)	(SGU)	(SGG)	(SGG)	(PIG)	(PIG)	(PIU)
	(PIU)	(SGU)	(DLTG)	(DLTG)	(SGG)	(PIG)	(PIG)	(DLTU)
	(DLTU)	(DLTG)	(DLTG)	(SGU)	(PIU)	(PIU)	(SGG)	(PIG)
	(PIG)	(SGU)	(SGG)	(SGG)	(SGG)	(SGU)		

The electronic state is 1-SGG.

Alpha occ. eigenvalues --	-20.66724	-20.66721	-11.46905	-1.55030	-
1.49539					
Alpha occ. eigenvalues --	-0.79977	-0.74667	-0.72620	-0.72620	-
0.54743					
Alpha occ. eigenvalues --	-0.54743				
Alpha virt. eigenvalues --	0.05692	0.09536	0.09536	0.10145	
0.22124					
Alpha virt. eigenvalues --	0.22124	0.24447	0.28061	0.28061	
0.28432					
Alpha virt. eigenvalues --	0.32554	0.35114	0.35114	0.39090	
0.53438					
Alpha virt. eigenvalues --	0.86423	0.86423	0.88353	1.21852	
1.22981					
Alpha virt. eigenvalues --	1.35582	1.38398	1.38398	1.50525	
1.50525					
Alpha virt. eigenvalues --	1.60387	1.62739	1.62739	1.68831	
1.70084					
Alpha virt. eigenvalues --	1.70084	2.00525	2.00525	2.34970	
2.34970					
Alpha virt. eigenvalues --	2.40463	2.48506	2.48506	3.24404	
3.37165					
Alpha virt. eigenvalues --	3.37165	3.66658	3.73260	4.44107	
5.04220					
Alpha virt. eigenvalues --	5.24768				

Condensed to atoms (all electrons):

		1	2	3
1	C	4.182061	0.481489	0.481489
2	O	0.481489	8.039985	-0.093992
3	O	0.481489	-0.093992	8.039985

Mulliken atomic charges:

```

      1
  1  C    0.854962
  2  O   -0.427481
  3  O   -0.427481

```

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

```

      1
  1  C    0.854962
  2  O   -0.427481
  3  O   -0.427481

```

Sum of Mulliken charges= 0.00000

Electronic spatial extent (au): $\langle R^2 \rangle = 111.7043$

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

```

  X= 0.0000  Y= 0.0000  Z= 0.0000  Tot= 0.0000

```

Quadrupole moment (field-independent basis, Debye-Ang):

```

  XX= -14.7229  YY= -14.7229  ZZ= -20.3347
  XY= 0.0000   XZ= 0.0000   YZ= 0.0000

```

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

```

  XX= 1.8706   YY= 1.8706   ZZ= -3.7412
  XY= 0.0000   XZ= 0.0000   YZ= 0.0000

```

Octapole moment (field-independent basis, Debye-Ang**2):

```

  XXX= 0.0000  YYY= 0.0000  ZZZ= 0.0000  XYY= 0.0000
  XXY= 0.0000  XXZ= 0.0000  XZZ= 0.0000  YZZ= 0.0000
  YYZ= 0.0000  XYZ= 0.0000

```

Hexadecapole moment (field-independent basis, Debye-Ang**3):

```

  XXXX= -11.3271  YYYY= -11.3271  ZZZZ= -102.5896  XXXY= 0.0000
  XXXZ= 0.0000   YYYY= 0.0000   YYYZ= 0.0000   ZZZX= 0.0000
  ZZZY= 0.0000   XXYY= -3.7757  XXZZ= -18.7983  YYZZ= -18.7983
  XXYZ= 0.0000   YYXZ= 0.0000  ZZXY= 0.0000

```

N-N= 5.924178094598D+01 E-N= -5.6097778837645D+02 KE= 1.871025207670D+02

Symmetry AG KE= 1.012475638439D+02

Symmetry B1G KE= 1.347431541639D-33

Symmetry B2G KE= 4.685219822022D+00

Symmetry B3G KE= 4.685219822022D+00

Symmetry AU KE= 2.025683826077D-34

Symmetry B1U KE= 6.915203788184D+01

Symmetry B2U KE= 3.666239698597D+00

Symmetry B3U KE= 3.666239698597D+00

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	0.0000000000	0.0000000000	0.0000000000
2	8	0.0000000000	0.0000000000	-0.000004204
3	8	0.0000000000	0.0000000000	0.000004204

Cartesian Forces: Max 0.000004204 RMS 0.000001982

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Berny optimization.

Internal Forces: Max 0.000004204 RMS 0.000002972

Search for a local minimum.


```

B2=1.14336
A1=179.99999915
1\1\GINC-HERCULES\FOpt\RHF\6-31+G(d)\C102\EUCKER\01-Nov-2007\0\#\# OPT
FREQ=RAMAN HF/6-31+G(D) GEOM=CONNECTIVITY\CO2_hf_of\0,1\C,0.,0.,0.\0
,0.,0.,1.14336\0,0.,0.,-1.14336\Version=IA32L-G03RevC.02\State=1-SGG\
HF=-187.6387868\RMSD=1.904e-09\RMSF=1.982e-06\Dipole=0.,0.,0.\PG=D*H [
O(C1),C*(01.01)]\ \@

```

```

ERWIN WITH HIS PSI CAN DO
CALCULATIONS QUITE A FEW.
BUT ONE THING HAS NOT BEEN SEEN
JUST WHAT DOES PSI REALLY MEAN.

```

```
-- WALTER HUCKEL, TRANS. BY FELIX BLOCH
```

```
Job cpu time: 0 days 0 hours 0 minutes 14.3 seconds.
```

```
File lengths (MBytes): RWF= 12 Int= 0 D2E= 0 Chk= 7 Scr=
1
```

```
Normal termination of Gaussian 03 at Thu Nov 1 23:17:16 2007.
```

```
Link1: Proceeding to internal job step number 2.
```

```
-----
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31+G(d) Freq
-----
```

```
1/10=4, 29=7, 30=1, 38=1, 40=1, 46=1/1, 3;
```

```
2/40=1/2;
```

```
3/5=1, 6=6, 7=11, 11=1, 16=1, 25=1, 30=1, 70=2, 71=2/1, 2, 3;
```

```
4/5=1, 7=1/1;
```

```
5/5=2, 38=6/2;
```

```
8/6=4, 10=90, 11=11/1;
```

```
10/13=10/2;
```

```
11/6=2, 8=1, 9=11, 15=111, 16=1/1, 2, 10;
```

```
10/6=1/2;
```

```
6/7=2, 8=2, 9=2, 10=2, 18=1, 28=1/1;
```

```
7/8=1, 10=1, 25=1/1, 2, 3, 16;
```

```
1/10=4, 30=1, 46=1/3;
```

```
99//99;
```

```
-----
CO2_hf_of
-----
```

```
Redundant internal coordinates taken from checkpoint file:
```

```
CO2_hf_of_.chk
```

```
Charge = 0 Multiplicity = 1
```

```
C,0,0.,0.,0.
```

```
O,0,0.,0.,1.14336
```

```
O,0,0.,0.,-1.14336
```

```
Recover connectivity data from disk.
```

```
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```

```
Berny optimization.
```

```
Initialization pass.
```

```

-----
! Initial Parameters !
! (Angstroms and Degrees) !
-----
-----

```

```

! Name      Definition      Value      Derivative Info.
! -----
! R1      R(1,2)      1.1434      calculate D2E/DX2
analytically !
! R2      R(1,3)      1.1434      calculate D2E/DX2
analytically !
! A1      L(2,1,3,-1,-1)      180.0      calculate D2E/DX2
analytically !
! A2      L(2,1,3,-2,-2)      180.0      calculate D2E/DX2
analytically !
! -----
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run= 2 maximum allowed number of steps= 2.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Input orientation:
! -----
Center      Atomic      Atomic      Coordinates (Angstroms)
Number      Number      Type      X      Y      Z
! -----
1      6      0      0.000000      0.000000      0.000000
2      8      0      0.000000      0.000000      1.143360
3      8      0      0.000000      0.000000      -1.143360
! -----
Distance matrix (angstroms):
      1      2      3
1 C      0.000000
2 O      1.143360      0.000000
3 O      1.143360      2.286720      0.000000
Stoichiometry      C02
Framework group      D*H[0(C),C*(0.0)]
Deg. of freedom      1
Full point group      D*H      NOp      8
Largest Abelian subgroup      D2H      NOp      8
Largest concise Abelian subgroup      C2      NOp      2
Standard orientation:
! -----
Center      Atomic      Atomic      Coordinates (Angstroms)
Number      Number      Type      X      Y      Z
! -----
1      6      0      0.000000      0.000000      0.000000
2      8      0      0.000000      0.000000      1.143360
3      8      0      0.000000      0.000000      -1.143360
! -----
Rotational constants (GHZ):      0.0000000      12.0847949      12.0847949
Standard basis: 6-31+G(d) (6D, 7F)
There are 17 symmetry adapted basis functions of AG symmetry.
There are 2 symmetry adapted basis functions of B1G symmetry.
There are 5 symmetry adapted basis functions of B2G symmetry.
There are 5 symmetry adapted basis functions of B3G symmetry.
There are 1 symmetry adapted basis functions of AU symmetry.
There are 13 symmetry adapted basis functions of B1U symmetry.

```

There are 7 symmetry adapted basis functions of B2U symmetry.
 There are 7 symmetry adapted basis functions of B3U symmetry.
 Integral buffers will be 262144 words long.
 Raffenetti 1 integral format.
 Two-electron integral symmetry is turned on.
 57 basis functions, 96 primitive gaussians, 57 cartesian basis functions
 11 alpha electrons 11 beta electrons
 nuclear repulsion energy 59.2417809460 Hartrees.
 NAtoms= 3 NActive= 3 NUniq= 2 SFac= 2.76D+00 NATFMM= 60 Big=F
 One-electron integrals computed using PRISM.
 NBasis= 57 RedAO= T NBF= 17 2 5 5 1 13 7 7
 NBsUse= 57 1.00D-06 NBFU= 17 2 5 5 1 13 7 7
 Initial guess read from the checkpoint file:
 C02_hf_of_.chk
 Initial guess orbital symmetries:
 Occupied (SGU) (SGG) (SGG) (SGG) (SGU) (SGG) (SGU) (PIU)
 (PIU) (PIG) (PIG)
 Virtual (SGG) (PIU) (PIU) (SGU) (PIU) (PIU) (SGG) (PIG)
 (PIG) (SGG) (SGU) (PIU) (PIU) (SGU) (SGG) (PIU)
 (PIU) (SGU) (SGU) (SGG) (SGG) (PIG) (PIG) (PIU)
 (PIU) (SGU) (DLTG) (DLTG) (SGG) (PIG) (PIG) (DLTU)
 (DLTU) (DLTG) (DLTG) (SGU) (PIU) (PIU) (SGG) (PIG)
 (PIG) (SGU) (SGG) (SGG) (SGG) (SGU)
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 Keep R1 integrals in memory in canonical form, NReq= 1921281.
 SCF Done: E(RHF) = -187.638786758 A.U. after 1 cycles
 Conv = 0.1440D-09 -V/T = 2.0029
 S**2 = 0.0000
 Range of M.O.s used for correlation: 1 57
 NBasis= 57 NAE= 11 NBE= 11 NFC= 0 NFV= 0
 NR0rb= 57 NOA= 11 NOB= 11 NVA= 46 NVB= 46
 **** Warning!!!: The largest alpha MO coefficient is 0.11461806D+02
 Differentiating once with respect to electric field.
 with respect to dipole field.
 Electric field/nuclear overlap derivatives assumed to be zero.
 Store integrals in memory, NReq= 1797610.
 There are 3 degrees of freedom in the 1st order CPHF.
 3 vectors were produced by pass 0.
 AX will form 3 AO Fock derivatives at one time.
 3 vectors were produced by pass 1.
 3 vectors were produced by pass 2.
 3 vectors were produced by pass 3.
 3 vectors were produced by pass 4.
 3 vectors were produced by pass 5.
 3 vectors were produced by pass 6.
 3 vectors were produced by pass 7.
 1 vectors were produced by pass 8.
 Inv2: IOpt= 1 Iter= 1 AM= 3.05D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension 25 with in-core refinement.

End of Minotr Frequency-dependent properties file 721 does not exist.
 Symmetrizing basis deriv contribution to polar:
 IMax=3 JMax=2 DiffMx= 0.00D+00
 G2DrvN: will do 4 centers at a time, making 1 passes doing MaxLOS=2.
 FoFDir/FoFCou used for L=0 through L=2.
 DoAtom=TTT
 Differentiating once with respect to electric field.
 with respect to dipole field.
 Differentiating once with respect to nuclear coordinates.
 Store integrals in memory, NReq= 1797645.
 There are 9 degrees of freedom in the 1st order CPHF.
 9 vectors were produced by pass 0.
 AX will form 9 AO Fock derivatives at one time.
 9 vectors were produced by pass 1.
 9 vectors were produced by pass 2.
 9 vectors were produced by pass 3.
 9 vectors were produced by pass 4.
 9 vectors were produced by pass 5.
 9 vectors were produced by pass 6.
 6 vectors were produced by pass 7.
 Inv2: IOpt= 1 Iter= 1 AM= 4.63D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension 69 with in-core refinement.
 Isotropic polarizability for W= 0.000000 13.24 Bohr**3.
 End of Minotr Frequency-dependent properties file 721 does not exist.

Population analysis using the SCF density.

Orbital symmetries:

Occupied	(SGU)	(SGG)	(SGG)	(SGG)	(SGU)	(SGG)	(SGU)	(PIU)
	(PIU)	(PIG)	(PIG)					
Virtual	(SGG)	(PIU)	(PIU)	(SGU)	(PIU)	(PIU)	(SGG)	(PIG)
	(PIG)	(SGG)	(SGU)	(PIU)	(PIU)	(SGU)	(SGG)	(PIU)
	(PIU)	(SGU)	(SGU)	(SGG)	(SGG)	(PIG)	(PIG)	(PIU)
	(PIU)	(SGU)	(DLTG)	(DLTG)	(SGG)	(PIG)	(PIG)	(DLTU)
	(DLTU)	(DLTG)	(DLTG)	(SGU)	(PIU)	(PIU)	(SGG)	(PIG)
	(PIG)	(SGU)	(SGG)	(SGG)	(SGG)			

The electronic state is 1-SGG.

Alpha occ. eigenvalues --	-20.66724	-20.66721	-11.46905	-1.55030	-
1.49539					
Alpha occ. eigenvalues --	-0.79977	-0.74667	-0.72620	-0.72620	-
0.54743					
Alpha occ. eigenvalues --	-0.54743				
Alpha virt. eigenvalues --	0.05692	0.09536	0.09536	0.10145	
0.22124					
Alpha virt. eigenvalues --	0.22124	0.24447	0.28061	0.28061	
0.28432					
Alpha virt. eigenvalues --	0.32554	0.35114	0.35114	0.39090	
0.53438					
Alpha virt. eigenvalues --	0.86423	0.86423	0.88353	1.21852	
1.22981					

```

Alpha virt. eigenvalues --      1.35582   1.38398   1.38398   1.50525
1.50525
Alpha virt. eigenvalues --      1.60387   1.62739   1.62739   1.68831
1.70084
Alpha virt. eigenvalues --      1.70084   2.00525   2.00525   2.34970
2.34970
Alpha virt. eigenvalues --      2.40463   2.48506   2.48506   3.24404
3.37165
Alpha virt. eigenvalues --      3.37165   3.66658   3.73260   4.44107
5.04220
Alpha virt. eigenvalues --      5.24768
Condensed to atoms (all electrons):
      1      2      3
1  C      4.182061   0.481489   0.481489
2  O      0.481489   8.039985  -0.093992
3  O      0.481489  -0.093992   8.039985
Mulliken atomic charges:
      1
1  C      0.854962
2  O     -0.427481
3  O     -0.427481
Sum of Mulliken charges=    0.00000
Atomic charges with hydrogens summed into heavy atoms:
      1
1  C      0.854962
2  O     -0.427481
3  O     -0.427481
Sum of Mulliken charges=    0.00000
APT atomic charges:
      1
1  C      1.571860
2  O     -0.785930
3  O     -0.785930
Sum of APT charges=    0.00000
APT Atomic charges with hydrogens summed into heavy atoms:
      1
1  C      1.571860
2  O     -0.785930
3  O     -0.785930
Sum of APT charges=    0.00000
Electronic spatial extent (au):  <R**2>=   111.7043
Charge=    0.0000 electrons
Dipole moment (field-independent basis, Debye):
X=    0.0000   Y=    0.0000   Z=    0.0000   Tot=    0.0000
Quadrupole moment (field-independent basis, Debye-Ang):
XX=   -14.7229   YY=   -14.7229   ZZ=   -20.3347
XY=    0.0000   XZ=    0.0000   YZ=    0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
XX=    1.8706   YY=    1.8706   ZZ=   -3.7412
XY=    0.0000   XZ=    0.0000   YZ=    0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
XXX=    0.0000   YYY=    0.0000   ZZZ=    0.0000   XYY=    0.0000
XXY=    0.0000   XXZ=    0.0000   XZZ=    0.0000   YZZ=    0.0000
YYZ=    0.0000   XYZ=    0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):

```

```

XXXX=  -11.3271  YYYY=  -11.3271  ZZZZ=  -102.5896  XXXY=    0.0000
XXXZ=   0.0000  YYYY=   0.0000  YYYZ=   0.0000  ZZZX=   0.0000
ZZZY=   0.0000  XXYY=  -3.7757  XXZZ=  -18.7983  YYZZ=  -18.7983
XXYZ=   0.0000  YYXZ=   0.0000  ZZXY=   0.0000
N-N= 5.924178094598D+01 E-N=-5.609778837220D+02 KE= 1.871025207387D+02
Symmetry AG KE= 1.012475638274D+02
Symmetry B1G KE= 1.347431545227D-33
Symmetry B2G KE= 4.685219823576D+00
Symmetry B3G KE= 4.685219823576D+00
Symmetry AU KE= 2.025683833114D-34
Symmetry B1U KE= 6.915203786671D+01
Symmetry B2U KE= 3.666239698699D+00
Symmetry B3U KE= 3.666239698699D+00
Exact polarizability: 8.352 0.000 8.352 0.000 0.000 23.016
Approx polarizability: 7.572 0.000 7.572 0.000 0.000 22.804
Full mass-weighted force constant matrix:
Low frequencies --- 0.0011 0.0011 0.0016 1.7897 1.7897
749.5133
Low frequencies --- 749.5133 1510.8188 2563.9836
Diagonal vibrational polarizability:
3.3155225 3.3155225 4.5128396
Diagonal vibrational hyperpolarizability:
0.0000000 0.0000000 0.0000000
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering
activities (A**4/AMU), depolarization ratios for plane and unpolarized
incident light, reduced masses (AMU), force constants (mDyne/A),
and normal coordinates:

```

			1 PIU			2 PIU			3 SGG		
Frequencies --			749.5133			749.5133			1510.8188		
Red. masses --			12.8774			12.8774			15.9949		
Frc consts --			4.2622			4.2622			21.5108		
IR Inten --			69.2114			69.2114			0.0000		
Raman Activ --			0.0000			0.0000			15.0076		
Depolar (P) --			0.0000			0.0000			0.1539		
Depolar (U) --			0.0000			0.0000			0.2667		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z		
1 6	0.88	0.00	0.00	0.00	0.88	0.00	0.00	0.00	0.00		
2 8	-0.33	0.00	0.00	0.00	-0.33	0.00	0.00	0.00	0.00		
3 8	-0.33	0.00	0.00	0.00	-0.33	0.00	0.00	0.00	-0.71		

			4 SGU		
Frequencies --			2563.9836		
Red. masses --			12.8774		
Frc consts --			49.8779		
IR Inten --			1102.4205		
Raman Activ --			0.0000		
Depolar (P) --			0.0000		
Depolar (U) --			0.0000		
Atom AN	X	Y	Z		
1 6	0.00	0.00	0.88		
2 8	0.00	0.00	-0.33		
3 8	0.00	0.00	-0.33		

- Thermochemistry -

 Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Atom 1 has atomic number 6 and mass 12.00000

Atom 2 has atomic number 8 and mass 15.99491

Atom 3 has atomic number 8 and mass 15.99491

Molecular mass: 43.98983 amu.

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	0.00000	149.33983	149.33983
X	0.00000	1.00000	0.00000
Y	0.00000	0.00000	1.00000
Z	1.00000	0.00000	0.00000

This molecule is a prolate symmetric top.

Rotational symmetry number 2.

Rotational temperature (Kelvin) 0.57998

Rotational constant (GHZ): 12.084795

Zero-point vibrational energy 33338.9 (Joules/Mol)

7.96819 (Kcal/Mol)

Vibrational temperatures: 1078.38 1078.38 2173.73 3689.00
 (Kelvin)

Zero-point correction= 0.012698 (Hartree/Particle)

Thermal correction to Energy= 0.015252

Thermal correction to Enthalpy= 0.016196

Thermal correction to Gibbs Free Energy= -0.007941

Sum of electronic and zero-point Energies= -187.626089

Sum of electronic and thermal Energies= -187.623535

Sum of electronic and thermal Enthalpies= -187.622591

Sum of electronic and thermal Free Energies= -187.646728

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	9.571	6.516	50.801
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	37.270
Rotational	0.592	1.987	13.015
Vibrational	8.089	1.548	0.516

	Q	Log10(Q)	Ln(Q)
Total Bot	0.449483D+04	3.652713	8.410683
Total V=0	0.311479D+10	9.493429	21.859429
Vib (Bot)	0.152488D-05	-5.816764	-13.393593
Vib (V=0)	0.105670D+01	0.023952	0.055152
Electronic	0.100000D+01	0.000000	0.000000
Translational	0.114679D+08	7.059484	16.255062
Rotational	0.257036D+03	2.409993	5.549215

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	0.0000000000	0.0000000000	0.0000000000
2	8	0.0000000000	0.0000000000	-0.000004204
3	8	0.0000000000	0.0000000000	0.000004204

```

1\1\GINC-HERCULES\Freq\RHF\6-31+G(d)\C102\EUCKER\01-Nov-2007\0\#\#N GEO
M=ALLCHECK GUESS=READ SCRF=CHECK GENCHK RHF/6-31+G(D) FREQ\CO2_hf_of\
\0,1\C,0.,0.,0.\0,0.,0.,1.14336\0,0.,0.,-1.14336\Version=IA32L-G03Rev
C.02\State=1-SGG\HF=-187.6387868\RMSD=1.440e-10\RMSF=1.982e-06\Dipole=
0.,0.,0.\DipoleDeriv=0.7871067,0.,0.,0.,0.7871067,0.,0.,0.,3.1413653,-
0.3935533,0.,0.,0.,-0.3935533,0.,0.,0.,-1.5706827,-0.3935533,0.,0.,0.,
-0.3935533,0.,0.,0.,-1.5706827\Polar=8.3521462,0.,8.3521462,0.,0.,23.0
160136\PolarDeriv=0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,
0.,0.,0.,3.3934126,0.,0.,0.,0.,0.,3.3934126,0.,2.0910169,0.,2.091
0169,0.,0.,10.3393307,0.,0.,0.,-3.3934126,0.,0.,0.,0.,0.,-3.3934126
,0.,-2.0910169,0.,-2.0910169,0.,0.,-10.3393307\HyperPolar=0.,0.,0.,0.,
0.,0.,0.,0.,0.,0.\PG=D*H [O(C1),C*(01.01)]\NImag=0\0.18552012,0.,0.18
552012,0.,0.,2.17101500,-0.09276006,0.,0.,0.04638100,0.,-0.09276006,0.
,0.,0.04638100,0.,0.,-1.08550750,0.,0.,1.23357892,-0.09276006,0.,0.,0.
04637906,0.,0.,0.04638100,0.,-0.09276006,0.,0.,0.04637906,0.,0.,0.0463
8100,0.,0.,-1.08550750,0.,0.,-0.14807142,0.,0.,1.23357892\0.,0.,0.,0.
,0.,0.00000420,0.,0.,-0.00000420\ \@

```

WE SHOULD BE CAREFUL TO GET OUT OF AN EXPERIENCE ONLY THE WISDOM
 THAT IS IN IT -- AND STOP THERE;
 LEST WE BE LIKE THE CAT THAT SITS DOWN ON A HOT STOVE-LID.
 SHE WILL NEVER SIT DOWN ON A HOT STOVE LID AGAIN;
 BUT ALSO SHE WILL NEVER SIT DOWN ON A COLD ONE ANY MORE.

-- MARK TWAIN

Job cpu time: 0 days 0 hours 0 minutes 25.1 seconds.

File lengths (MBytes): RWF= 12 Int= 0 D2E= 0 Chk= 7 Scr=

1

Normal termination of Gaussian 03 at Thu Nov 1 23:17:43 2007.

Appendix 2

Output Gaussian03 file for a sequential geometry optimization and frequency job for the
 $[\text{BF}_4(\text{CO}_2)]^-$ complex at HF/6-31+G(d):

Entering Link 1 = C:\G03W\l1.exe PID= 2332.

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Cite this work as:

Gaussian 03, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,

P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Gaussian 03: IA32W-G03RevD.01 13-Oct-2005

11-Apr-2008

%chk=BC_HF631+G(d).chk

%mem=50MW

%nproc=1

Will use up to 1 processors via shared memory.

opt freq=raman hf/6-31+g(d) geom=connectivity

1/18=20, 38=1, 57=2/1, 3;

2/9=110, 17=6, 18=5, 40=1/2;

3/5=1, 6=6, 7=11, 11=9, 16=1, 25=1, 30=1/1, 2, 3;

4//1;

5/5=2, 38=5/2;

6/7=2, 8=2, 9=2, 10=2, 28=1/1;

7//1, 2, 3, 16;

1/18=20/3(3);

2/9=110/2;

6/7=2, 8=2, 9=2, 10=2, 19=2, 28=1/1;

99//99;

2/9=110/2;

3/5=1, 6=6, 7=11, 11=9, 16=1, 25=1, 30=1/1, 2, 3;

4/5=5, 16=3/1;

5/5=2, 38=5/2;

7//1, 2, 3, 16;

1/18=20/3(-5);

2/9=110/2;

6/7=2, 8=2, 9=2, 10=2, 19=2, 28=1/1;

99/9=1/99;

BC_HF631+G(d)

Symbolic Z-matrix:

Charge = -1 Multiplicity = 1

B	0.	0.	0.
F	1.39647	0.	0.
F	-0.46546	1.31661	0.
F	-0.46546	-0.65831	1.14022
F	-0.46546	-0.65831	-1.14022
O	2.64568	3.00134	-1.14002
C	2.6383	3.00656	0.00331
O	2.63092	3.01178	1.14663

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Initialization pass.

! Initial Parameters !			
! (Angstroms and Degrees) !			

! Name	Definition	Value	Derivative Info.
! -----			
! R1	R(1,2)	1.3965	estimate D2E/DX2
! R2	R(1,3)	1.3965	estimate D2E/DX2
! R3	R(1,4)	1.3965	estimate D2E/DX2
! R4	R(1,5)	1.3965	estimate D2E/DX2
! R5	R(1,6)	4.1602	estimate D2E/DX2
! R6	R(1,7)	4.0	estimate D2E/DX2
! R7	R(1,8)	4.1602	estimate D2E/DX2
! R8	R(2,6)	3.445	estimate D2E/DX2
! R9	R(2,7)	3.2529	estimate D2E/DX2
! R10	R(2,8)	3.451	estimate D2E/DX2
! R11	R(3,6)	3.7171	estimate D2E/DX2
! R12	R(3,7)	3.534	estimate D2E/DX2
! R13	R(3,8)	3.7116	estimate D2E/DX2
! R14	R(6,7)	1.1434	estimate D2E/DX2
! R15	R(7,8)	1.1434	estimate D2E/DX2
! A1	A(2,1,3)	109.47	estimate D2E/DX2
! A2	A(2,1,4)	109.47	estimate D2E/DX2
! A3	A(2,1,5)	109.47	estimate D2E/DX2
! A4	A(3,1,4)	109.4724	estimate D2E/DX2
! A5	A(3,1,5)	109.4725	estimate D2E/DX2
! A6	A(4,1,5)	109.4724	estimate D2E/DX2
!			

```

! A7      A(4,1,6)           140.8784      estimate D2E/DX2
!
! A8      A(4,1,7)           124.9945      estimate D2E/DX2
!
! A9      A(4,1,8)           109.088       estimate D2E/DX2
!
! A10     A(5,1,6)           109.1667      estimate D2E/DX2
!
! A11     A(5,1,7)           125.089       estimate D2E/DX2
!
! A12     A(5,1,8)           140.9965      estimate D2E/DX2
!
! A13     A(6,1,8)           31.9041       estimate D2E/DX2
!
! A14     A(6,2,8)           38.7317       estimate D2E/DX2
!
! A15     A(6,3,8)           35.8559       estimate D2E/DX2
!
! A16     A(2,6,3)           36.8847       estimate D2E/DX2
!
! A17     A(2,7,3)           38.9899       estimate D2E/DX2
!
! A18     A(2,8,3)           36.903        estimate D2E/DX2
!
! A19     L(6,7,8,-2,-1)     180.0        estimate D2E/DX2
!
! A20     L(6,7,8,-1,-2)     180.0        estimate D2E/DX2
!
! D1      D(8,2,6,3)         -85.2783      estimate D2E/DX2
!
! D2      D(6,2,8,3)         86.0896       estimate D2E/DX2
!
! D3      D(8,3,6,2)         81.8085       estimate D2E/DX2
!
! D4      D(6,3,8,2)         -80.9904      estimate D2E/DX2
!

```

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07

Number of steps in this run= 49 maximum allowed number of steps= 100.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

```

-----
Center   Atomic   Atomic   Coordinates (Angstroms)
Number   Number   Type      X           Y           Z
-----
  1         5         0      0.000000    0.000000    0.000000
  2         9         0      1.396470    0.000000    0.000000
  3         9         0     -0.465462    1.316615    0.000000
  4         9         0     -0.465462   -0.658307    1.140222
  5         9         0     -0.465462   -0.658308   -1.140221
  6         8         0      2.645678    3.001337   -1.140017
  7         6         0      2.638297    3.006556    0.003307
  8         8         0      2.630916    3.011775    1.146631

```

```

-----
                        Distance matrix (angstroms):
                        1           2           3           4           5
1  B      0.000000
2  F      1.396470      0.000000
3  F      1.396470      2.280409      0.000000
4  F      1.396470      2.280409      2.280443      0.000000
5  F      1.396470      2.280409      2.280444      2.280443      0.000000
6  O      4.160201      3.445023      3.717138      5.317111      4.803352
7  C      4.000000      3.252925      3.534010      4.935293      4.936821
8  O      4.160201      3.451001      3.711588      4.801781      5.318530
                        6           7           8
6  O      0.000000
7  C      1.143360      0.000000
8  O      2.286720      1.143360      0.000000
Stoichiometry      CBF402(1-)
Framework group    C1[X(CBF402)]
Deg. of freedom    18
Full point group    C1
Largest Abelian subgroup    C1      NOp      1
Largest concise Abelian subgroup    C1      NOp      1
                        Standard orientation:
-----
Center      Atomic      Atomic      Coordinates (Angstroms)
Number      Number      Type          X          Y          Z
-----
1           5           0          -1.396833      0.000000      0.000017
2           9           0          -0.475764      0.009015     -1.049591
3           9           0          -0.714214     -0.009015      1.218245
4           9           0          -2.197707     -1.140186     -0.093289
5           9           0          -2.199593      1.140186     -0.075359
6           8           0           2.603167      1.143360     -0.000006
7           6           0           2.603167      0.000000     -0.000006
8           8           0           2.603167     -1.143360     -0.000006
-----
Rotational constants (GHZ):      3.5939893      0.8924699      0.8310914
Standard basis: 6-31+G(d) (6D, 7F)
There are 152 symmetry adapted basis functions of A symmetry.
Integral buffers will be 262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
152 basis functions, 256 primitive gaussians, 152 cartesian basis
functions
32 alpha electrons      32 beta electrons
nuclear repulsion energy      355.6334611828 Hartrees.
NAtoms= 8 NActive= 8 NUniq= 8 SFac= 7.50D-01 NAtFMM= 80 NAOKFM=F
Big=F
One-electron integrals computed using PRISM.
NBasis= 152 RedAO= T NBF= 152
NBsUse= 152 1.00D-06 NBFU= 152
Harris functional with IExCor= 205 diagonalized for initial guess.
ExpMin= 3.15D-02 ExpMax= 7.00D+03 ExpMxC= 1.05D+03 IAcc=3 IRadAn= 5
AccDes= 0.00D+00
HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 5 IDoV=1
ScaDFX= 1.000000 1.000000 1.000000 1.000000

```

Initial guess orbital symmetries:

```

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

```

The electronic state of the initial guess is 1-A.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

```

SCF Done: E(RHF) = -610.406768171      A.U. after   11 cycles
           Convrg =  0.3971D-08          -V/T =  2.0028
           S**2   =  0.0000

```

Population analysis using the SCF density.

Orbital symmetries:

```

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

```

The electronic state is 1-A.

```

Alpha occ. eigenvalues -- -26.07615 -26.07456 -26.07059 -26.07058 -
20.54020
Alpha occ. eigenvalues -- -20.54018 -11.34318 -7.51902 -1.42297 -
1.41554
Alpha occ. eigenvalues -- -1.36842 -1.35574 -1.35307 -1.35075 -
0.67470
Alpha occ. eigenvalues -- -0.62201 -0.60580 -0.59939 -0.59764 -
0.53583
Alpha occ. eigenvalues -- -0.53471 -0.53387 -0.45273 -0.45230 -
0.42170

```

```

Alpha occ. eigenvalues -- -0.42143 -0.41476 -0.41453 -0.41345 -
0.38882
Alpha occ. eigenvalues -- -0.38719 -0.38583
Alpha virt. eigenvalues -- 0.15848 0.20249 0.20453 0.21393
0.22503
Alpha virt. eigenvalues -- 0.22794 0.23530 0.27352 0.34525
0.34629
Alpha virt. eigenvalues -- 0.36923 0.39561 0.39808 0.40939
0.45175
Alpha virt. eigenvalues -- 0.46101 0.46640 0.49656 0.50040
0.50328
Alpha virt. eigenvalues -- 0.52869 0.53795 0.54686 0.55124
0.56832
Alpha virt. eigenvalues -- 0.58028 0.58947 0.62031 0.62282
0.63412
Alpha virt. eigenvalues -- 0.64501 0.68714 0.73658 0.75228
0.75302
Alpha virt. eigenvalues -- 0.75807 0.78180 0.78588 0.86779
0.99285
Alpha virt. eigenvalues -- 1.01507 1.03983 1.09813 1.10514
1.12848
Alpha virt. eigenvalues -- 1.34478 1.36673 1.48574 1.51129
1.54087
Alpha virt. eigenvalues -- 1.60233 1.60365 1.60975 1.63630
1.65629
Alpha virt. eigenvalues -- 1.73384 1.76230 1.77554 1.82703
1.83045
Alpha virt. eigenvalues -- 1.88075 2.02385 2.04628 2.04641
2.06562
Alpha virt. eigenvalues -- 2.08602 2.08713 2.09156 2.12242
2.12832
Alpha virt. eigenvalues -- 2.14295 2.15666 2.16142 2.17080
2.20141
Alpha virt. eigenvalues -- 2.27927 2.28010 2.28384 2.34914
2.34994
Alpha virt. eigenvalues -- 2.35380 2.37360 2.37847 2.47619
2.47729
Alpha virt. eigenvalues -- 2.48098 2.48215 2.48862 2.51287
2.51952
Alpha virt. eigenvalues -- 2.52354 2.52471 2.52656 2.53419
2.54371
Alpha virt. eigenvalues -- 2.61139 2.62168 2.82275 3.07506
3.07649
Alpha virt. eigenvalues -- 3.07730 3.32602 3.33517 3.38880
3.49725
Alpha virt. eigenvalues -- 3.50142 3.63271 3.63656 3.64127
3.79576
Alpha virt. eigenvalues -- 3.86276 3.92258 4.36596 4.65237
5.18387
Alpha virt. eigenvalues -- 5.38358 5.88155 5.94053 5.94806
6.46715

```

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	B	2.562937	0.138985	0.138382	0.156980	0.156951	-0.000354
2	F	0.138985	9.587451	0.004776	-0.004485	-0.004441	0.001246

```

      3 F      0.138382    0.004776    9.587926   -0.005895   -0.005910
0.000303
      4 F      0.156980   -0.004485   -0.005895    9.558202   -0.006770    0.000021
      5 F      0.156951   -0.004441   -0.005910   -0.006770    9.558226   -0.000533
      6 O     -0.000354    0.001246    0.000303    0.000021   -0.000533    8.012739
      7 C     -0.011304    0.000846    0.004571    0.000880    0.000893    0.508783
      8 O     -0.000358    0.001256    0.000317   -0.000533    0.000019   -0.099358

```

```

      7      8
      1 B     -0.011304   -0.000358
      2 F      0.000846    0.001256
      3 F      0.004571    0.000317
      4 F      0.000880   -0.000533
      5 F      0.000893    0.000019
      6 O      0.508783   -0.099358
      7 C      4.151736    0.508693
      8 O      0.508693    8.012867

```

Mulliken atomic charges:

```

      1
      1 B      1.857783
      2 F     -0.725634
      3 F     -0.724470
      4 F     -0.698398
      5 F     -0.698435
      6 O     -0.422845
      7 C      0.834902
      8 O     -0.422903

```

Sum of Mulliken charges= -1.00000

Atomic charges with hydrogens summed into heavy atoms:

```

      1
      1 B      1.857783
      2 F     -0.725634
      3 F     -0.724470
      4 F     -0.698398
      5 F     -0.698435
      6 O     -0.422845
      7 C      0.834902
      8 O     -0.422903

```

Sum of Mulliken charges= -1.00000

Electronic spatial extent (au): $\langle R^2 \rangle = 1258.9217$

Charge= -1.0000 electrons

Dipole moment (field-independent basis, Debye):

```

X=      6.2703    Y=      0.0003    Z=     -0.0119    Tot=      6.2703

```

Quadrupole moment (field-independent basis, Debye-Ang):

```

XX=    -57.1353    YY=    -51.9968    ZZ=    -46.1798
XY=      0.0004    XZ=    -0.0213    YZ=    -0.0007

```

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

```

XX=    -5.3646    YY=    -0.2262    ZZ=      5.5908
XY=      0.0004    XZ=    -0.0213    YZ=    -0.0007

```

Octapole moment (field-independent basis, Debye-Ang**2):

```

XXX=     22.2257    YYY=      0.0008    ZZZ=    -1.6491    XYY=    -4.9458
XXY=    -0.0165    XXZ=     1.0204    XZZ=      0.2275    YZZ=      0.0174
YYZ=      0.5308    XYZ=      0.0807

```

Hexadecapole moment (field-independent basis, Debye-Ang**3):

```

XXXX=  -1129.7217    YYYY=   -214.4009    ZZZZ=   -122.2372    XXXY=      0.0733
XXXZ=    -3.9942    YYYY=      0.0071    YYYZ=    -0.0557    ZZZX=      1.8971

```

ZZZY= 0.0517 XXYY= -274.3485 XXZZ= -189.6045 YYZZ= -53.5896
 XXYZ= -0.2278 YYXZ= -1.1494 ZZXY= -0.0295
 N-N= 3.556334611828D+02 E-N=-2.178080609963D+03 KE= 6.087153757993D+02
 ***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	5	-0.003513808	-0.003250886	0.000000288
2	9	0.001849663	0.001832448	0.000014604
3	9	0.001504337	0.001355083	-0.000007660
4	9	0.000690720	0.000755488	-0.000872440
5	9	0.000689895	0.000756924	0.000872415
6	8	0.004176201	0.005184192	-0.000922973
7	6	-0.009568171	-0.011803844	-0.000032404
8	8	0.004171162	0.005170596	0.000948169

Cartesian Forces: Max 0.011803844 RMS 0.003864882

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 Berny optimization.

Internal Forces: Max 0.004240792 RMS 0.001503044

Search for a local minimum.

Step number 1 out of a maximum of 49

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Second derivative matrix not updated -- first step.

Eigenvalues --- 0.00508 0.00889 0.00971 0.01158 0.07745
 Eigenvalues --- 0.08733 0.17976 0.21555 0.25000 0.25000
 Eigenvalues --- 0.25000 0.25000 0.42892 0.46144 0.46211
 Eigenvalues --- 0.46211 1.19584 1.379841000.000001000.00000
 Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
 Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
 Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
 Eigenvalues --- 1000.000001000.000001000.000001000.00000

RFO step: Lambda=-9.79317886D-04.

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.00910566 RMS(Int)= 0.00019880

Iteration 2 RMS(Cart)= 0.00016964 RMS(Int)= 0.00008263

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00008263

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.63895	0.00111	0.00000	0.00304	0.00304	2.64199
R2	2.63895	0.00047	0.00000	0.00122	0.00122	2.64016
R3	2.63895	-0.00130	0.00000	-0.00280	-0.00280	2.63614
R4	2.63895	-0.00130	0.00000	-0.00281	-0.00281	2.63614
R5	7.86164	0.00228	0.00000	0.00984	0.00982	7.87146
R6	7.55890	-0.00307	0.00000	-0.05162	-0.05160	7.50731
R7	7.86164	0.00227	0.00000	0.00943	0.00941	7.87105
R8	6.51015	0.00120	0.00000	-0.00030	-0.00035	6.50980
R9	6.14714	-0.00407	0.00000	-0.06076	-0.06070	6.08644
R10	6.52145	0.00118	0.00000	-0.00258	-0.00263	6.51882
R11	7.02437	0.00110	0.00000	-0.00538	-0.00543	7.01894
R12	6.67831	-0.00370	0.00000	-0.06180	-0.06173	6.61658
R13	7.01389	0.00111	0.00000	-0.00372	-0.00376	7.01012
R14	2.16064	-0.00031	0.00000	0.00065	0.00081	2.16144

R15	2.16064	-0.00029	0.00000	0.00067	0.00082	2.16146
A1	1.91061	-0.00059	0.00000	-0.00944	-0.00943	1.90118
A2	1.91061	-0.00009	0.00000	0.00131	0.00130	1.91192
A3	1.91061	-0.00008	0.00000	0.00133	0.00132	1.91193
A4	1.91065	0.00021	0.00000	0.00236	0.00235	1.91300
A5	1.91066	0.00021	0.00000	0.00236	0.00235	1.91300
A6	1.91065	0.00035	0.00000	0.00209	0.00208	1.91274
A7	2.45879	-0.00031	0.00000	-0.00129	-0.00138	2.45741
A8	2.18157	-0.00020	0.00000	-0.00109	-0.00108	2.18048
A9	1.90394	-0.00007	0.00000	-0.00083	-0.00073	1.90321
A10	1.90532	-0.00007	0.00000	-0.00077	-0.00067	1.90464
A11	2.18322	-0.00020	0.00000	-0.00109	-0.00109	2.18213
A12	2.46085	-0.00031	0.00000	-0.00136	-0.00145	2.45940
A13	0.55683	-0.00025	0.00000	-0.00053	-0.00072	0.55612
A14	0.67600	-0.00023	0.00000	0.00037	0.00014	0.67614
A15	0.62580	-0.00019	0.00000	0.00062	0.00040	0.62621
A16	0.64376	-0.00005	0.00000	-0.00135	-0.00135	0.64241
A17	0.68050	0.00049	0.00000	0.00498	0.00501	0.68551
A18	0.64408	-0.00005	0.00000	-0.00138	-0.00139	0.64269
A19	3.14159	-0.00292	0.00000	-0.03572	-0.03582	3.10577
A20	3.14159	0.00424	0.00000	0.04434	0.04444	3.18603
D1	-1.48839	-0.00003	0.00000	-0.00132	-0.00135	-1.48974
D2	1.50255	0.00002	0.00000	-0.00119	-0.00116	1.50139
D3	1.42783	0.00006	0.00000	-0.00104	-0.00098	1.42685
D4	-1.41355	-0.00008	0.00000	-0.00156	-0.00162	-1.41517

Item	Value	Threshold	Converged?
Maximum Force	0.004241	0.000450	NO
RMS Force	0.001503	0.000300	NO
Maximum Displacement	0.039696	0.001800	NO
RMS Displacement	0.009110	0.001200	NO

Predicted change in Energy=-4.941394D-04

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Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.000027	0.000090	0.000012
2	9	0	1.398039	0.005926	0.000517
3	9	0	-0.458771	1.319743	-0.000571
4	9	0	-0.464386	-0.656418	1.139904
5	9	0	-0.463578	-0.657141	-1.139792
6	8	0	2.648026	3.006535	-1.140005
7	6	0	2.620915	2.985550	0.003268
8	8	0	2.634760	3.015384	1.146590

Distance matrix (angstroms):

		1	2	3	4	5
1	B	0.000000				
2	F	1.398078	0.000000			
3	F	1.397114	2.274612	0.000000		
4	F	1.394986	2.281562	2.281649	0.000000	
5	F	1.394985	2.281574	2.281648	2.279695	0.000000
6	O	4.165396	3.444838	3.714265	5.319991	4.806724

7	C	3.972696	3.220806	3.501342	4.906623	4.908144
8	O	4.165182	3.449609	3.709598	4.804881	5.321155
		6	7	8		
6	O	0.000000				
7	C	1.143787	0.000000			
8	O	2.286651	1.143795	0.000000		

Stoichiometry CBF402(1-)

Framework group C1[X(CBF402)]

Deg. of freedom	18
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Full point group

Largest Abelian subgroup	C1
--------------------------	----

Largest concise Abelian subgroup C1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.397908	-0.000011	0.000339
2	9	0	0.471591	-0.007455	-1.046802
3	9	0	0.708353	0.007202	1.215407
4	9	0	2.196737	1.139925	-0.091334
5	9	0	2.198594	-1.139723	-0.076746
6	8	0	-2.607516	-1.143299	0.000036
7	6	0	-2.574788	0.000018	-0.001282
8	8	0	-2.607272	1.143351	0.000123

Rotational constants (GHZ):	3.6011617	0.8951058	0.8330880
-----------------------------	-----------	-----------	-----------

Standard basis: $6-31+G(d)$ (6D, 7F)

There are 152 symmetry adapted basis functions of A symmetry.

Integral buffers will be 262144 words long.

Raffenetti 1 integral format.

Two-electron integral symmetry is turned on.

152 basis functions, 256 primitive gaussians, 152 cartesian basis functions

32 alpha electrons 32 beta electrons

nuclear repulsion energy 355.8870128948 Hartrees.

NAtoms= 8 NActive= 8 NUniq= 8 SFac= 7.50D-01 NAtFMM= 80 NAOKFM=F
Big=F

One-electron integrals computed using PRISM.

NBasis= 152 RedAO= T NBF= 152

NBsUse= 152 1.00D-06 NBFU= 152

Initial guess read from the read-write file:

Initial guess orbital symmetries:

[illegible]

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor= 205 diagonalized for initial guess.
 ExpMin= 3.15D-02 ExpMax= 7.00D+03 ExpMxC= 1.05D+03 IAcc=3 IRadAn=
 AccDes= 0.00D+00
 HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 5 IDoV=1
 ScaDFX= 1.000000 1.000000 1.000000 1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 SCF Done: E(RHF) = -610.407395389 A.U. after 12 cycles
 Conv = 0.7372D-08 -V/T = 2.0028
 S**2 = 0.0000
 ***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	5	-0.001927327	-0.001652846	0.000001449
2	9	0.001729514	0.001020963	0.000011556
3	9	0.000591375	0.001138125	-0.000006432
4	9	0.000490580	0.000572694	-0.000670448
5	9	0.000491093	0.000574436	0.000670301
6	8	0.000629108	0.000796500	-0.000207443
7	6	-0.002637395	-0.003229854	-0.000001224
8	8	0.000633052	0.000779982	0.000202242

Cartesian Forces: Max 0.003229854 RMS 0.001184535

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 Berny optimization.

Internal Forces: Max 0.001233359 RMS 0.000486184

Search for a local minimum.

Step number 2 out of a maximum of 49

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Update second derivatives using D2CorX and points 1 2

Trust test= 1.27D+00 RLast= 1.18D-01 DXMaxT set to 3.53D-01

Eigenvalues ---	0.00508	0.00890	0.00893	0.01135	0.07034
Eigenvalues ---	0.07902	0.17962	0.21520	0.24976	0.25000
Eigenvalues ---	0.25000	0.25000	0.42764	0.45938	0.46147
Eigenvalues ---	0.46211	1.18952	1.379631000	0.000001000	0.00000
Eigenvalues ---	1000.000001000	0.000001000	0.000001000	0.000001000	0.00000
Eigenvalues ---	1000.000001000	0.000001000	0.000001000	0.000001000	0.00000
Eigenvalues ---	1000.000001000	0.000001000	0.000001000	0.000001000	0.00000
Eigenvalues ---	1000.000001000	0.000001000	0.000001000	0.000001000	0.00000

RFO step: Lambda=-6.98050200D-05.

Quartic linear search produced a step of 0.38090.

Iteration 1 RMS(Cart)= 0.00836429 RMS(Int)= 0.00005248

Iteration 2 RMS(Cart)= 0.00002691 RMS(Int)= 0.00004355

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00004355

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.64199	0.00116	0.00116	0.00238	0.00353	2.64552
R2	2.64016	0.00062	0.00046	0.00118	0.00163	2.64180
R3	2.63614	-0.00098	-0.00107	-0.00205	-0.00312	2.63302

R4	2.63614	-0.00098	-0.00107	-0.00205	-0.00312	2.63302
R5	7.87146	0.00041	0.00374	-0.02582	-0.02209	7.84936
R6	7.50731	-0.00086	-0.01965	-0.02744	-0.04708	7.46023
R7	7.87105	0.00040	0.00359	-0.02618	-0.02260	7.84845
R8	6.50980	0.00003	-0.00013	-0.02568	-0.02584	6.48396
R9	6.08644	-0.00123	-0.02312	-0.02862	-0.05170	6.03474
R10	6.51882	0.00002	-0.00100	-0.02768	-0.02872	6.49010
R11	7.01894	0.00007	-0.00207	-0.02457	-0.02667	6.99227
R12	6.61658	-0.00107	-0.02351	-0.02539	-0.04886	6.56771
R13	7.01012	0.00008	-0.00143	-0.02308	-0.02454	6.98559
R14	2.16144	0.00008	0.00031	-0.00004	0.00035	2.16179
R15	2.16146	0.00008	0.00031	-0.00004	0.00035	2.16181
A1	1.90118	-0.00005	-0.00359	-0.00051	-0.00411	1.89707
A2	1.91192	-0.00012	0.00050	-0.00034	0.00015	1.91207
A3	1.91193	-0.00012	0.00050	-0.00034	0.00016	1.91209
A4	1.91300	0.00004	0.00089	0.00021	0.00109	1.91410
A5	1.91300	0.00004	0.00089	0.00020	0.00109	1.91409
A6	1.91274	0.00022	0.00079	0.00078	0.00157	1.91431
A7	2.45741	-0.00012	-0.00053	0.00049	-0.00009	2.45732
A8	2.18048	-0.00012	-0.00041	-0.00046	-0.00087	2.17961
A9	1.90321	-0.00010	-0.00028	-0.00141	-0.00164	1.90157
A10	1.90464	-0.00011	-0.00026	-0.00136	-0.00157	1.90308
A11	2.18213	-0.00012	-0.00041	-0.00047	-0.00088	2.18125
A12	2.45940	-0.00013	-0.00055	0.00043	-0.00017	2.45923
A13	0.55612	-0.00002	-0.00027	0.00187	0.00150	0.55762
A14	0.67614	0.00001	0.00005	0.00286	0.00281	0.67894
A15	0.62621	0.00001	0.00015	0.00218	0.00223	0.62844
A16	0.64241	0.00021	-0.00051	0.00279	0.00228	0.64469
A17	0.68551	0.00036	0.00191	0.00334	0.00529	0.69081
A18	0.64269	0.00021	-0.00053	0.00276	0.00223	0.64493
A19	3.10577	-0.00068	-0.01364	-0.00028	-0.01398	3.09179
A20	3.18603	0.00097	0.01693	0.00027	0.01726	3.20329
D1	-1.48974	0.00004	-0.00051	-0.00049	-0.00102	-1.49075
D2	1.50139	-0.00006	-0.00044	-0.00182	-0.00224	1.49914
D3	1.42685	-0.00004	-0.00037	-0.00252	-0.00286	1.42398
D4	-1.41517	0.00002	-0.00062	0.00013	-0.00050	-1.41567
Item	Value	Threshold	Converged?			
Maximum Force	0.001233	0.000450	NO			
RMS Force	0.000486	0.000300	NO			
Maximum Displacement	0.029036	0.001800	NO			
RMS Displacement	0.008362	0.001200	NO			

Predicted change in Energy=-8.931049D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.002945	0.004006	0.000030
2	9	0	1.402863	0.012899	0.001184
3	9	0	-0.453534	1.325357	-0.001312
4	9	0	-0.460174	-0.651019	1.139261
5	9	0	-0.458316	-0.652678	-1.138997
6	8	0	2.642214	3.002060	-1.139793

7	6	0	2.608085	2.970184	0.003226
8	8	0	2.630894	3.008859	1.146324

Distance matrix (angstroms):

		1	2	3	4	5
1	B	0.000000				
2	F	1.399946	0.000000			
3	F	1.397979	2.273491	0.000000		
4	F	1.393335	2.281866	2.281888	0.000000	
5	F	1.393334	2.281883	2.281880	2.278259	0.000000
6	O	4.153705	3.431166	3.700152	5.306966	4.792744
7	C	3.947782	3.193447	3.475484	4.880359	4.881867
8	O	4.153222	3.434413	3.696613	4.790560	5.307803

		6	7	8
6	O	0.000000		
7	C	1.143972	0.000000	
8	O	2.286156	1.143980	0.000000

Stoichiometry CBF402(1-)

Framework group C1[X(CBF402)]

Deg. of freedom 18

Full point group

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.393879	-0.000027	0.000653
2	9	0	0.464017	-0.005518	-1.045854
3	9	0	0.701582	0.004947	1.215167
4	9	0	2.190799	1.139341	-0.089593
5	9	0	2.192616	-1.138894	-0.079213
6	8	0	-2.599470	-1.143017	0.000112
7	6	0	-2.553902	0.000046	-0.001710
8	8	0	-2.598918	1.143139	0.000190

Rotational constants (GHZ): 3.6044416 0.9016998 0.8388428

Standard basis: 6-31+G(d) (6D, 7F)

There are 152 symmetry adapted basis functions of A symmetry.

Integral buffers will be 262144 words long.

Raffenetti 1 integral format.

Two-electron integral symmetry is turned on.

152 basis functions, 256 primitive gaussians, 152 cartesian basis functions

32 alpha electrons 32 beta electrons

nuclear repulsion energy 356.4065555517 Hartrees.

NAtoms= 8 NActive= 8 NUniq= 8 SFac= 7.50D-01 NAtFMM= 80 NAOKFM=F
Big=F

One-electron integrals computed using PRISM.

NBasis= 152 RedA0= T NBF= 152

NBsUse= 152 1.00D-06 NBFU= 152

Initial guess read from the read-write file:

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

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Virtual      (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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Harris functional with IExCor= 205 diagonalized for initial guess.
 ExpMin= 3.15D-02 ExpMax= 7.00D+03 ExpMxC= 1.05D+03 IAcc=3 IRadAn=
 AccDes= 0.00D+00

HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 5 IDoV=1

ScaDFX= 1.000000 1.000000 1.000000 1.000000

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RHF) = -610.407516396 A.U. after 8 cycles

Conv = 0.9867D-08 -V/T = 2.0028

S**2 = 0.0000

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	5	-0.000506256	-0.000364558	0.000002068
2	9	0.001151877	0.000776431	0.000008085
3	9	0.000374337	0.000791669	-0.000004112
4	9	0.000206158	0.000262613	-0.000138942
5	9	0.000207818	0.000262837	0.000137947
6	8	-0.000726135	-0.000863758	-0.000132150
7	6	0.000014314	0.000010461	0.000010573
8	8	-0.000722113	-0.000875693	0.000116531

Cartesian Forces: Max 0.001151877 RMS 0.000497535

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 Berny optimization.

Internal Forces: Max 0.000706519 RMS 0.000242994

Search for a local minimum.

Step number 3 out of a maximum of 49

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Update second derivatives using D2CorX and points 1 2 3

Trust test= 1.35D+00 RLast= 1.08D-01 DXMaxT set to 3.53D-01

Eigenvalues --- 0.00421 0.00510 0.00892 0.01104 0.07707

Eigenvalues --- 0.11952 0.17911 0.21507 0.24927 0.25000

Eigenvalues --- 0.25000 0.25023 0.41964 0.45791 0.46150

Eigenvalues --- 0.46211 1.18861 1.379451000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.00000

RFO step: Lambda=-8.77673444D-05.

Quartic linear search produced a step of 0.61226.

Iteration 1 RMS(Cart)= 0.01321016 RMS(Int)= 0.00003129

Iteration 2 RMS(Cart)= 0.00001755 RMS(Int)= 0.00001996

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001996

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.64552	0.00071	0.00216	0.00151	0.00365	2.64917
R2	2.64180	0.00043	0.00100	0.00068	0.00166	2.64346
R3	2.63302	-0.00031	-0.00191	-0.00093	-0.00284	2.63018
R4	2.63302	-0.00031	-0.00191	-0.00093	-0.00284	2.63018
R5	7.84936	-0.00031	-0.01353	-0.03491	-0.04844	7.80093
R6	7.46023	-0.00004	-0.02883	-0.03636	-0.06519	7.39504
R7	7.84845	-0.00031	-0.01384	-0.03523	-0.04906	7.79939
R8	6.48396	-0.00039	-0.01582	-0.03461	-0.05042	6.43354
R9	6.03474	-0.00017	-0.03165	-0.03771	-0.06935	5.96539
R10	6.49010	-0.00040	-0.01758	-0.03671	-0.05431	6.43579
R11	6.99227	-0.00031	-0.01633	-0.03342	-0.04977	6.94250
R12	6.56771	-0.00009	-0.02992	-0.03407	-0.06397	6.50375
R13	6.98559	-0.00031	-0.01502	-0.03176	-0.04678	6.93880
R14	2.16179	0.00036	0.00021	0.00013	0.00035	2.16215
R15	2.16181	0.00035	0.00021	0.00013	0.00034	2.16215
A1	1.89707	0.00007	-0.00252	-0.00109	-0.00364	1.89343
A2	1.91207	-0.00007	0.00009	-0.00009	0.00001	1.91208
A3	1.91209	-0.00007	0.00010	-0.00009	0.00001	1.91210
A4	1.91410	-0.00006	0.00067	0.00006	0.00073	1.91483
A5	1.91409	-0.00005	0.00067	0.00006	0.00073	1.91482
A6	1.91431	0.00018	0.00096	0.00113	0.00209	1.91640
A7	2.45732	-0.00003	-0.00005	0.00070	0.00064	2.45796
A8	2.17961	-0.00009	-0.00053	-0.00061	-0.00114	2.17847
A9	1.90157	-0.00015	-0.00100	-0.00193	-0.00293	1.89864
A10	1.90308	-0.00015	-0.00096	-0.00188	-0.00283	1.90025
A11	2.18125	-0.00009	-0.00054	-0.00062	-0.00116	2.18008
A12	2.45923	-0.00003	-0.00011	0.00063	0.00052	2.45975
A13	0.55762	0.00012	0.00092	0.00259	0.00350	0.56112
A14	0.67894	0.00016	0.00172	0.00393	0.00566	0.68460
A15	0.62844	0.00014	0.00137	0.00307	0.00444	0.63288
A16	0.64469	0.00019	0.00139	0.00337	0.00480	0.64948
A17	0.69081	0.00019	0.00324	0.00406	0.00739	0.69820
A18	0.64493	0.00019	0.00137	0.00334	0.00473	0.64965
A19	3.09179	0.00023	-0.00856	0.00015	-0.00843	3.08337
A20	3.20329	-0.00030	0.01057	-0.00006	0.01053	3.21382
D1	-1.49075	0.00005	-0.00062	-0.00037	-0.00097	-1.49172
D2	1.49914	-0.00007	-0.00137	-0.00210	-0.00348	1.49566
D3	1.42398	-0.00008	-0.00175	-0.00298	-0.00474	1.41924
D4	-1.41567	0.00007	-0.00031	0.00044	0.00016	-1.41551

Item	Value	Threshold	Converged?
Maximum Force	0.000707	0.000450	NO
RMS Force	0.000243	0.000300	YES
Maximum Displacement	0.035836	0.001800	NO
RMS Displacement	0.013212	0.001200	NO

Predicted change in Energy=-6.533129D-05

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Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.009091	0.011591	0.000055
2	9	0	1.410915	0.023821	0.002091
3	9	0	-0.445998	1.334351	-0.002320
4	9	0	-0.452724	-0.641703	1.138972
5	9	0	-0.449423	-0.644644	-1.138503
6	8	0	2.629788	2.990501	-1.139694
7	6	0	2.592184	2.951221	0.003172
8	8	0	2.621145	2.994528	1.146148

Distance matrix (angstroms):

		1	2	3	4	5
1	B	0.000000				
2	F	1.401879	0.000000			
3	F	1.398859	2.272803	0.000000		
4	F	1.391833	2.282229	2.281969	0.000000	
5	F	1.391831	2.282248	2.281961	2.277480	0.000000
6	O	4.128073	3.404484	3.673814	5.280824	4.764013
7	C	3.913285	3.156749	3.441634	4.844647	4.846136
8	O	4.127259	3.405675	3.671857	4.761397	5.281248
		6	7	8		
6	O	0.000000				
7	C	1.144159	0.000000			
8	O	2.285861	1.144162	0.000000		

Stoichiometry CBF402(1-)

Framework group C1[X(CBF402)]

Deg. of freedom 18

Full point group C1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.385224	-0.000049	0.000866
2	9	0	0.451474	-0.002885	-1.044776
3	9	0	0.691093	0.001883	1.215355
4	9	0	2.180005	1.139131	-0.087409
5	9	0	2.181769	-1.138343	-0.082764
6	8	0	-2.581519	-1.142826	0.000215
7	6	0	-2.528060	0.000082	-0.001975
8	8	0	-2.580583	1.143036	0.000268

Rotational constants (GHZ): 3.6063712 0.9133773 0.8489598

Standard basis: 6-31+G(d) (6D, 7F)

There are 152 symmetry adapted basis functions of A symmetry.

Integral buffers will be 262144 words long.

Raffenetti 1 integral format.

Two-electron integral symmetry is turned on.

152 basis functions, 256 primitive gaussians, 152 cartesian basis functions
 32 alpha electrons 32 beta electrons
 nuclear repulsion energy 357.2714790096 Hartrees.
 NAToms= 8 NActive= 8 NUniq= 8 SFac= 7.50D-01 NATFMM= 80 NAOKFM=F
 Big=F
 One-electron integrals computed using PRISM.
 NBasis= 152 RedAO= T NBF= 152
 NBsUse= 152 1.00D-06 NBFU= 152
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
 Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor= 205 diagonalized for initial guess.
 ExpMin= 3.15D-02 ExpMax= 7.00D+03 ExpMxC= 1.05D+03 IAcc=3 IRadAn= 5
 AccDes= 0.00D+00
 HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 5 IDoV=1
 ScaDFX= 1.000000 1.000000 1.000000 1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 SCF Done: E(RHF) = -610.407624093 A.U. after 8 cycles
 Convg = 0.7895D-08 -V/T = 2.0028
 S**2 = 0.0000
 ***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	5	0.000858160	0.000911144	0.000002875
2	9	0.000493190	0.000540522	0.000002977
3	9	0.000223317	0.000438060	-0.000001482
4	9	-0.000057753	-0.000064617	0.000265325
5	9	-0.000054622	-0.000065634	-0.000266768
6	8	-0.001495634	-0.001806105	0.000018996
7	6	0.001524999	0.001857294	0.000016187
8	8	-0.001491657	-0.001810664	-0.000038111

Cartesian Forces: Max 0.001857294 RMS 0.000896286

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 Berny optimization.

Internal Forces: Max 0.001007251 RMS 0.000374635

Search for a local minimum.

Step number 4 out of a maximum of 49

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Update second derivatives using D2CorX and points 1 2 3 4

Trust test= 1.65D+00 RLast= 1.69D-01 DXMaxT set to 4.99D-01

Eigenvalues ---	0.00103	0.00513	0.00894	0.01103	0.07782
Eigenvalues ---	0.17820	0.19446	0.21756	0.24915	0.25000
Eigenvalues ---	0.25000	0.25036	0.42130	0.46147	0.46211
Eigenvalues ---	0.48137	1.18343	1.379191000	0.000001000	0.00000
Eigenvalues ---	1000.000001000	0.000001000	0.000001000	0.000001000	0.00000
Eigenvalues ---	1000.000001000	0.000001000	0.000001000	0.000001000	0.00000
Eigenvalues ---	1000.000001000	0.000001000	0.000001000	0.000001000	0.00000
Eigenvalues ---	1000.000001000	0.000001000	0.000001000	0.000001000	0.00000

RFO step: Lambda=-1.78226433D-04.

Quartic linear search produced a step of 2.000000.

Iteration 1 RMS(Cart)= 0.04181905 RMS(Int)= 0.00099554

Iteration 2 RMS(Cart)= 0.00055907 RMS(Int)= 0.00022110

Iteration 3 RMS(Cart)= 0.00000032 RMS(Int)= 0.00022110

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.64917	0.00018	0.00730	0.00132	0.00839	2.65756
R2	2.64346	0.00021	0.00333	0.00065	0.00375	2.64721
R3	2.63018	0.00027	-0.00568	-0.00087	-0.00655	2.62364
R4	2.63018	0.00027	-0.00568	-0.00087	-0.00655	2.62363
R5	7.80093	-0.00079	-0.09688	-0.06822	-0.16507	7.63586
R6	7.39504	0.00037	-0.13038	-0.06886	-0.19925	7.19578
R7	7.79939	-0.00078	-0.09813	-0.06853	-0.16664	7.63275
R8	6.43354	-0.00060	-0.10084	-0.06558	-0.16625	6.26730
R9	5.96539	0.00048	-0.13870	-0.06881	-0.20750	5.75789
R10	6.43579	-0.00060	-0.10861	-0.06827	-0.17692	6.25887
R11	6.94250	-0.00050	-0.09954	-0.06190	-0.16154	6.78097
R12	6.50375	0.00051	-0.12793	-0.06159	-0.18941	6.31433
R13	6.93880	-0.00050	-0.09356	-0.05958	-0.15302	6.78578
R14	2.16215	0.00042	0.00071	0.00007	0.00057	2.16271
R15	2.16215	0.00041	0.00069	0.00005	0.00053	2.16268
A1	1.89343	0.00016	-0.00728	-0.00023	-0.00787	1.88556
A2	1.91208	-0.00004	0.00002	-0.00052	-0.00043	1.91165
A3	1.91210	-0.00004	0.00002	-0.00053	-0.00043	1.91167
A4	1.91483	-0.00008	0.00146	0.00005	0.00158	1.91641
A5	1.91482	-0.00007	0.00147	0.00006	0.00159	1.91642
A6	1.91640	0.00007	0.00419	0.00115	0.00535	1.92176
A7	2.45796	0.00006	0.00128	0.00185	0.00320	2.46116
A8	2.17847	-0.00003	-0.00229	-0.00070	-0.00301	2.17546
A9	1.89864	-0.00012	-0.00586	-0.00326	-0.00924	1.88940
A10	1.90025	-0.00013	-0.00566	-0.00320	-0.00895	1.89130
A11	2.18008	-0.00003	-0.00232	-0.00072	-0.00306	2.17702
A12	2.45975	0.00006	0.00104	0.00175	0.00284	2.46259
A13	0.56112	0.00019	0.00701	0.00510	0.01230	0.57342
A14	0.68460	0.00022	0.01132	0.00747	0.01926	0.70386
A15	0.63288	0.00019	0.00888	0.00578	0.01494	0.64781
A16	0.64948	0.00014	0.00959	0.00656	0.01649	0.66597
A17	0.69820	0.00004	0.01478	0.00770	0.02325	0.72145
A18	0.64965	0.00014	0.00946	0.00650	0.01628	0.66593
A19	3.08337	0.00073	-0.01685	0.00149	-0.01540	3.06797
A20	3.21382	-0.00101	0.02105	-0.00159	0.01946	3.23328

D1	-1.49172	0.00005	-0.00193	0.00005	-0.00159	-1.49330
D2	1.49566	-0.00005	-0.00696	-0.00331	-0.01038	1.48528
D3	1.41924	-0.00008	-0.00948	-0.00498	-0.01469	1.40455
D4	-1.41551	0.00008	0.00033	0.00167	0.00239	-1.41312

Item	Value	Threshold	Converged?
Maximum Force	0.001007	0.000450	NO
RMS Force	0.000375	0.000300	NO
Maximum Displacement	0.104788	0.001800	NO
RMS Displacement	0.042021	0.001200	NO

Predicted change in Energy=-1.845406D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.029998	0.037279	0.000122
2	9	0	1.436159	0.058023	0.004543
3	9	0	-0.423276	1.362751	-0.005053
4	9	0	-0.428174	-0.612052	1.138549
5	9	0	-0.420951	-0.618469	-1.137508
6	8	0	2.588440	2.949907	-1.139352
7	6	0	2.545689	2.895769	0.003026
8	8	0	2.587091	2.946458	1.145595

Distance matrix (angstroms):

		1	2	3	4	5
1	B	0.000000				
2	F	1.406321	0.000000			
3	F	1.400842	2.271543	0.000000		
4	F	1.388369	2.282697	2.282037	0.000000	
5	F	1.388366	2.282713	2.282037	2.276077	0.000000
6	O	4.040721	3.316511	3.588333	5.193876	4.667949
7	C	3.807844	3.046943	3.341402	4.736885	4.738316
8	O	4.039079	3.312054	3.590882	4.664211	5.193225
		6	7	8		
6	O	0.000000				
7	C	1.144459	0.000000			
8	O	2.284951	1.144443	0.000000		

Stoichiometry CBF402(1-)

Framework group C1[X(CBF402)]

Deg. of freedom 18

Full point group C1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.355317	-0.000114	0.001477
2	9	0	0.411853	0.004223	-1.041402
3	9	0	0.658480	-0.006424	1.216688
4	9	0	2.144763	1.138902	-0.082114

4	9	-0.000717464	-0.000839900	0.001162278
5	9	-0.000707438	-0.000847060	-0.001164699
6	8	-0.002771353	-0.003354965	-0.000001180
7	6	0.004085213	0.004963165	0.000026551
8	8	-0.002772609	-0.003330492	-0.000020574

 Cartesian Forces: Max 0.004963165 RMS 0.002180698

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 Berny optimization.

Internal Forces: Max 0.002245765 RMS 0.000872201

Search for a local minimum.

Step number 5 out of a maximum of 49

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Update second derivatives using D2CorX and points 4 5

Trust test= 1.44D+00 RLast= 5.34D-01 DXMaxT set to 7.06D-01

Eigenvalues ---	0.00045	0.00526	0.00903	0.01113	0.07802
Eigenvalues ---	0.17522	0.20301	0.21900	0.24996	0.25000
Eigenvalues ---	0.25000	0.25353	0.42652	0.46143	0.46211
Eigenvalues ---	0.51875	1.17252	1.378371000	0.000001000	0.00000
Eigenvalues ---	1000.000001000	0.000001000	0.000001000	0.000001000	0.00000
Eigenvalues ---	1000.000001000	0.000001000	0.000001000	0.000001000	0.00000
Eigenvalues ---	1000.000001000	0.000001000	0.000001000	0.000001000	0.00000
Eigenvalues ---	1000.000001000	0.000001000	0.000001000	0.000001000	0.00000

RFO step: Lambda=-2.79784370D-04.

Quartic linear search produced a step of 1.00491.

Iteration 1 RMS(Cart)= 0.04763918 RMS(Int)= 0.02712824

Iteration 2 RMS(Cart)= 0.01349035 RMS(Int)= 0.00064220

Iteration 3 RMS(Cart)= 0.00002760 RMS(Int)= 0.00064131

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00064131

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.65756	-0.00096	0.00844	-0.00022	0.00757	2.66513
R2	2.64721	-0.00029	0.00377	-0.00023	0.00289	2.65010
R3	2.62364	0.00158	-0.00658	0.00083	-0.00574	2.61789
R4	2.62363	0.00158	-0.00658	0.00084	-0.00574	2.61789
R5	7.63586	-0.00162	-0.16588	-0.08387	-0.24967	7.38619
R6	7.19578	0.00100	-0.20023	-0.07920	-0.27947	6.91631
R7	7.63275	-0.00161	-0.16745	-0.08347	-0.25086	7.38189
R8	6.26730	-0.00089	-0.16706	-0.07824	-0.24480	6.02250
R9	5.75789	0.00159	-0.20852	-0.07580	-0.28438	5.47351
R10	6.25887	-0.00088	-0.17779	-0.07846	-0.25621	6.00267
R11	6.78097	-0.00079	-0.16233	-0.07273	-0.23517	6.54580
R12	6.31433	0.00152	-0.19034	-0.06845	-0.25858	6.05575
R13	6.78578	-0.00079	-0.15377	-0.07168	-0.22509	6.56069
R14	2.16271	0.00073	0.00057	0.00020	0.00003	2.16274
R15	2.16268	0.00071	0.00053	0.00018	-0.00003	2.16266
A1	1.88556	0.00032	-0.00791	0.00143	-0.00753	1.87803
A2	1.91165	0.00010	-0.00043	-0.00032	-0.00054	1.91111
A3	1.91167	0.00010	-0.00044	-0.00035	-0.00056	1.91111
A4	1.91641	-0.00014	0.00159	-0.00051	0.00130	1.91771
A5	1.91642	-0.00013	0.00160	-0.00049	0.00133	1.91775
A6	1.92176	-0.00024	0.00538	0.00026	0.00570	1.92745
A7	2.46116	0.00032	0.00322	0.00309	0.00659	2.46775
A8	2.17546	0.00013	-0.00302	-0.00022	-0.00329	2.17218

A9	1.88940	-0.00005	-0.00928	-0.00352	-0.01319	1.87621
A10	1.89130	-0.00006	-0.00899	-0.00352	-0.01286	1.87844
A11	2.17702	0.00014	-0.00308	-0.00022	-0.00335	2.17368
A12	2.46259	0.00032	0.00286	0.00304	0.00613	2.46872
A13	0.57342	0.00037	0.01236	0.00665	0.01968	0.59310
A14	0.70386	0.00041	0.01936	0.00942	0.03026	0.73413
A15	0.64781	0.00036	0.01501	0.00736	0.02325	0.67106
A16	0.66597	0.00000	0.01657	0.00822	0.02578	0.69175
A17	0.72145	-0.00028	0.02336	0.00922	0.03455	0.75600
A18	0.66593	0.00000	0.01636	0.00816	0.02544	0.69138
A19	3.06797	0.00165	-0.01548	0.00506	-0.01043	3.05754
A20	3.23328	-0.00225	0.01956	-0.00574	0.01374	3.24702
D1	-1.49330	0.00005	-0.00160	0.00196	0.00120	-1.49210
D2	1.48528	-0.00003	-0.01043	-0.00269	-0.01357	1.47172
D3	1.40455	-0.00010	-0.01476	-0.00449	-0.02002	1.38453
D4	-1.41312	0.00012	0.00240	0.00388	0.00743	-1.40568

Item	Value	Threshold	Converged?
Maximum Force	0.002246	0.000450	NO
RMS Force	0.000872	0.000300	NO
Maximum Displacement	0.141375	0.001800	NO
RMS Displacement	0.060614	0.001200	NO

Predicted change in Energy=-2.540265D-04

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Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.062022	0.076007	0.000186
2	9	0	1.471997	0.106629	0.007094
3	9	0	-0.390978	1.403175	-0.007922
4	9	0	-0.392043	-0.569719	1.138606
5	9	0	-0.380679	-0.579792	-1.136949
6	8	0	2.527670	2.886774	-1.138823
7	6	0	2.482874	2.820956	0.002879
8	8	0	2.534113	2.875637	1.144851

Distance matrix (angstroms):

		1	2	3	4	5
1	B	0.000000				
2	F	1.410324	0.000000			
3	F	1.402372	2.269787	0.000000		
4	F	1.385330	2.283071	2.281850	0.000000	
5	F	1.385327	2.283071	2.281877	2.275605	0.000000
6	O	3.908602	3.186970	3.463887	5.065447	4.524995
7	C	3.659956	2.896457	3.204567	4.588214	4.589579
8	O	3.906331	3.176474	3.471770	4.520278	5.063853
		6	7	8		
6	O	0.000000				
7	C	1.144475	0.000000			
8	O	2.283711	1.144429	0.000000		

Stoichiometry CBF402(1-)
Framework group C1[X(CBF402)]
Deg. of freedom 18

Full point group C1
 Largest Abelian subgroup C1 NOp 1
 Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.309338	-0.000182	0.002003
2	9	0	0.355211	0.011594	-1.036515
3	9	0	0.611893	-0.015123	1.218554
4	9	0	2.093380	1.139161	-0.077466
5	9	0	2.094857	-1.136282	-0.104619
6	8	0	-2.428910	-1.141529	0.000672
7	6	0	-2.350614	0.000258	-0.003150
8	8	0	-2.426225	1.142180	0.000490

Rotational constants (GHZ): 3.6138949 1.0138848 0.9351696

Standard basis: 6-31+G(d) (6D, 7F)

There are 152 symmetry adapted basis functions of A symmetry.

Integral buffers will be 262144 words long.

Raffenetti 1 integral format.

Two-electron integral symmetry is turned on.

152 basis functions, 256 primitive gaussians, 152 cartesian basis functions

32 alpha electrons 32 beta electrons

nuclear repulsion energy 364.5280793942 Hartrees.

NAtoms= 8 NActive= 8 NUniq= 8 SFac= 7.50D-01 NATFMM= 80 NAOKFM=F
 Big=F

One-electron integrals computed using PRISM.

NBasis= 152 RedAO= T NBF= 152

NBsUse= 152 1.00D-06 NBFU= 152

Initial guess read from the read-write file:

Initial guess orbital symmetries:

Occupied	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
Virtual	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)

Harris functional with IExCor= 205 diagonalized for initial guess.

ExpMin= 3.15D-02 ExpMax= 7.00D+03 ExpMxC= 1.05D+03 IAcc=3 IRadAn=
 AccDes= 0.00D+00

HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 5 IDoV=1

ScaDFX= 1.000000 1.000000 1.000000 1.000000

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RHF) = -610.408237731 A.U. after 9 cycles

Convg = 0.8050D-08 -V/T = 2.0028

S**2 = 0.0000

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	5	0.006281045	0.006010076	0.000008249
2	9	-0.002119975	-0.000657481	-0.000046748
3	9	-0.000382653	-0.000915328	0.000021725
4	9	-0.001281894	-0.001548820	0.001790290
5	9	-0.001263344	-0.001563421	-0.001792542
6	8	-0.003340157	-0.003989434	-0.000723437
7	6	0.005452466	0.006585561	0.000023872
8	8	-0.003345489	-0.003921153	0.000718591

Cartesian Forces: Max 0.006585561 RMS 0.003053455

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Berny optimization.

Internal Forces: Max 0.002980005 RMS 0.001248042

Search for a local minimum.

Step number 6 out of a maximum of 49

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Update second derivatives using D2CorX and points 5 6

Trust test= 1.37D+00 RLast= 7.67D-01 DXMaxT set to 9.98D-01

Eigenvalues --- 0.00031 0.00546 0.00917 0.01134 0.07849
 Eigenvalues --- 0.16988 0.17071 0.21078 0.25000 0.25000
 Eigenvalues --- 0.25011 0.25280 0.42395 0.46137 0.46211
 Eigenvalues --- 0.50369 1.16189 1.377091000.000001000.00000
 Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
 Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
 Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
 Eigenvalues --- 1000.000001000.000001000.000001000.00000

RFO step: Lambda=-3.22232538D-04.

Quartic linear search produced a step of 0.73092.

Iteration 1 RMS(Cart)= 0.04745868 RMS(Int)= 0.01750937

Iteration 2 RMS(Cart)= 0.00925539 RMS(Int)= 0.00078175

Iteration 3 RMS(Cart)= 0.00001184 RMS(Int)= 0.00078161

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00078161

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.66513	-0.00182	0.00553	-0.00311	0.00161	2.66674
R2	2.65010	-0.00060	0.00211	-0.00138	-0.00007	2.65003
R3	2.61789	0.00261	-0.00420	0.00337	-0.00083	2.61707
R4	2.61789	0.00262	-0.00420	0.00338	-0.00082	2.61707
R5	7.38619	-0.00208	-0.18249	-0.06303	-0.24541	7.14078
R6	6.91631	0.00123	-0.20427	-0.04712	-0.25140	6.66491
R7	7.38189	-0.00207	-0.18336	-0.06090	-0.24416	7.13773
R8	6.02250	-0.00085	-0.17893	-0.05167	-0.23007	5.79243
R9	5.47351	0.00223	-0.20786	-0.03511	-0.24309	5.23042
R10	6.00267	-0.00080	-0.18727	-0.04484	-0.23188	5.77078
R11	6.54580	-0.00082	-0.17189	-0.04940	-0.22121	6.32458

R12	6.05575	0.00206	-0.18900	-0.03764	-0.22649	5.82926
R13	6.56069	-0.00083	-0.16452	-0.05266	-0.21681	6.34388
R14	2.16274	0.00140	0.00002	0.00040	-0.00061	2.16214
R15	2.16266	0.00139	-0.00002	0.00039	-0.00065	2.16200
A1	1.87803	0.00048	-0.00550	0.00532	-0.00144	1.87659
A2	1.91111	0.00020	-0.00039	-0.00058	-0.00070	1.91041
A3	1.91111	0.00020	-0.00041	-0.00061	-0.00075	1.91036
A4	1.91771	-0.00011	0.00095	-0.00097	0.00024	1.91795
A5	1.91775	-0.00011	0.00097	-0.00097	0.00029	1.91803
A6	1.92745	-0.00062	0.00416	-0.00200	0.00225	1.92970
A7	2.46775	0.00065	0.00482	0.00379	0.00900	2.47676
A8	2.17218	0.00033	-0.00240	0.00104	-0.00143	2.17075
A9	1.87621	0.00000	-0.00964	-0.00164	-0.01180	1.86441
A10	1.87844	0.00000	-0.00940	-0.00186	-0.01175	1.86669
A11	2.17368	0.00033	-0.00245	0.00108	-0.00143	2.17225
A12	2.46872	0.00065	0.00448	0.00394	0.00878	2.47750
A13	0.59310	0.00064	0.01439	0.00559	0.02090	0.61400
A14	0.73413	0.00070	0.02212	0.00675	0.03070	0.76482
A15	0.67106	0.00063	0.01699	0.00596	0.02406	0.69512
A16	0.69175	-0.00011	0.01884	0.00657	0.02661	0.71836
A17	0.75600	-0.00052	0.02525	0.00597	0.03334	0.78934
A18	0.69138	-0.00011	0.01860	0.00656	0.02631	0.71768
A19	3.05754	0.00225	-0.00762	0.01106	0.00349	3.06103
A20	3.24702	-0.00298	0.01004	-0.01278	-0.00290	3.24413
D1	-1.49210	0.00008	0.00088	0.00561	0.00748	-1.48462
D2	1.47172	-0.00003	-0.00992	0.00042	-0.01025	1.46147
D3	1.38453	-0.00015	-0.01463	0.00052	-0.01521	1.36932
D4	-1.40568	0.00020	0.00543	0.00605	0.01282	-1.39286

Item	Value	Threshold	Converged?
Maximum Force	0.002980	0.000450	NO
RMS Force	0.001248	0.000300	NO
Maximum Displacement	0.123997	0.001800	NO
RMS Displacement	0.056322	0.001200	NO

Predicted change in Energy=-3.018379D-04

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Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.094226	0.114078	0.000184
2	9	0	1.504963	0.148571	0.007660
3	9	0	-0.360471	1.440620	-0.008573
4	9	0	-0.357506	-0.531340	1.139176
5	9	0	-0.345120	-0.542230	-1.137428
6	8	0	2.470601	2.822346	-1.138664
7	6	0	2.428952	2.757602	0.002898
8	8	0	2.479331	2.810021	1.144669

Distance matrix (angstroms):

		1	2	3	4	5
1	B	0.000000				
2	F	1.411178	0.000000			
3	F	1.402334	2.269250	0.000000		


```

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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Harris functional with IExCor= 205 diagonalized for initial guess.
 ExpMin= 3.15D-02 ExpMax= 7.00D+03 ExpMxC= 1.05D+03 IAcc=3 IRadAn= 5
 AccDes= 0.00D+00

HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 5 IDoV=1
 ScaDFX= 1.000000 1.000000 1.000000 1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RHF) = -610.408593637 A.U. after 9 cycles
 Conv = 0.5874D-08 -V/T = 2.0028
 S**2 = 0.0000

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	5	0.006236845	0.005733572	0.000005092
2	9	-0.002424327	-0.001231669	-0.000061626
3	9	-0.000439401	-0.000922915	0.000030176
4	9	-0.001356097	-0.001604382	0.001572427
5	9	-0.001343982	-0.001615179	-0.001573877
6	8	-0.002442339	-0.002790029	-0.001596393
7	6	0.004216252	0.005128102	-0.000033890
8	8	-0.002446951	-0.002697501	0.001658091

Cartesian Forces: Max 0.006236845 RMS 0.002664428

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.

Internal Forces: Max 0.002484659 RMS 0.001130572

Search for a local minimum.

Step number 7 out of a maximum of 49

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Update second derivatives using D2CorX and points 6 7

Trust test= 1.18D+00 RLast= 7.08D-01 DXMaxT set to 1.00D+00

```

Eigenvalues --- 0.00054 0.00566 0.00932 0.01166 0.07498
Eigenvalues --- 0.09364 0.16627 0.20717 0.24972 0.25000
Eigenvalues --- 0.25000 0.25024 0.41114 0.45736 0.46139
Eigenvalues --- 0.46211 1.14395 1.375851000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.00000

```

RFO step: Lambda=-2.87708846D-04.

Quartic linear search produced a step of 0.42333.

Iteration 1 RMS(Cart)= 0.01895700 RMS(Int)= 0.00025099

Iteration 2 RMS(Cart)= 0.00007496 RMS(Int)= 0.00022934

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00022934

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
----------	-------	--------	---------------------	-------------------	--------------------	-------

R1	2.66674	-0.00189	0.00068	-0.00732	-0.00688	2.65986
R2	2.65003	-0.00056	-0.00003	-0.00302	-0.00329	2.64674
R3	2.61707	0.00248	-0.00035	0.00644	0.00609	2.62316
R4	2.61707	0.00248	-0.00035	0.00644	0.00609	2.62316
R5	7.14078	-0.00164	-0.10389	0.00677	-0.09709	7.04368
R6	6.66491	0.00081	-0.10642	0.03650	-0.06990	6.59501
R7	7.13773	-0.00162	-0.10336	0.01053	-0.09281	7.04492
R8	5.79243	-0.00031	-0.09740	0.02723	-0.07010	5.72233
R9	5.23042	0.00188	-0.10291	0.06309	-0.03986	5.19056
R10	5.77078	-0.00025	-0.09816	0.04256	-0.05545	5.71533
R11	6.32458	-0.00050	-0.09365	0.01173	-0.08178	6.24280
R12	5.82926	0.00156	-0.09588	0.03209	-0.06377	5.76549
R13	6.34388	-0.00052	-0.09178	0.00228	-0.08947	6.25441
R14	2.16214	0.00182	-0.00026	0.00037	-0.00019	2.16195
R15	2.16200	0.00187	-0.00028	0.00043	-0.00015	2.16185
A1	1.87659	0.00047	-0.00061	0.01001	0.00903	1.88562
A2	1.91041	0.00028	-0.00030	-0.00031	-0.00053	1.90988
A3	1.91036	0.00028	-0.00032	-0.00029	-0.00052	1.90984
A4	1.91795	-0.00009	0.00010	-0.00206	-0.00188	1.91607
A5	1.91803	-0.00009	0.00012	-0.00207	-0.00187	1.91616
A6	1.92970	-0.00080	0.00095	-0.00487	-0.00391	1.92579
A7	2.47676	0.00080	0.00381	0.00295	0.00688	2.48364
A8	2.17075	0.00043	-0.00060	0.00301	0.00239	2.17313
A9	1.86441	0.00005	-0.00500	0.00323	-0.00193	1.86247
A10	1.86669	0.00005	-0.00498	0.00269	-0.00243	1.86425
A11	2.17225	0.00042	-0.00060	0.00309	0.00247	2.17472
A12	2.47750	0.00080	0.00372	0.00341	0.00723	2.48474
A13	0.61400	0.00075	0.00885	-0.00011	0.00903	0.62303
A14	0.76482	0.00081	0.01299	-0.00401	0.00945	0.77427
A15	0.69512	0.00075	0.01018	-0.00004	0.01048	0.70560
A16	0.71836	-0.00017	0.01126	-0.00081	0.01085	0.72921
A17	0.78934	-0.00050	0.01411	-0.00500	0.00965	0.79899
A18	0.71768	-0.00017	0.01114	-0.00063	0.01087	0.72856
A19	3.06103	0.00189	0.00148	0.01688	0.01838	3.07941
A20	3.24413	-0.00241	-0.00123	-0.02000	-0.02127	3.22285
D1	-1.48462	0.00011	0.00317	0.00882	0.01226	-1.47236
D2	1.46147	-0.00005	-0.00434	0.00483	0.00012	1.46159
D3	1.36932	-0.00014	-0.00644	0.01043	0.00359	1.37292
D4	-1.39286	0.00022	0.00543	0.00416	0.00992	-1.38294
Item	Value		Threshold	Converged?		
Maximum Force	0.002485		0.000450	NO		
RMS Force	0.001131		0.000300	NO		
Maximum Displacement	0.052288		0.001800	NO		
RMS Displacement	0.018953		0.001200	NO		
Predicted change in Energy=-1.939133D-04						
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad						

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.108857	0.128660	0.000086
2	9	0	1.516196	0.151699	0.005057
3	9	0	-0.346559	1.453133	-0.005559

4	9	0	-0.346334	-0.519818	1.139885
5	9	0	-0.338121	-0.526824	-1.138956
6	8	0	2.451319	2.794676	-1.139390
7	6	0	2.416622	2.746641	0.003127
8	8	0	2.452997	2.791499	1.145672

Distance matrix (angstroms):

		1	2	3	4	5
1	B	0.000000				
2	F	1.407536	0.000000			
3	F	1.400595	2.272378	0.000000		
4	F	1.388115	2.282058	2.281354	0.000000	
5	F	1.388116	2.282028	2.281422	2.278866	0.000000
6	O	3.727355	3.028125	3.303548	4.899778	4.337434
7	C	3.489931	2.746725	3.050969	4.426726	4.428153
8	O	3.728012	3.024425	3.309693	4.336025	4.901136
		6	7	8		
6	O	0.000000				
7	C	1.144053	0.000000			
8	O	2.285065	1.144003	0.000000		

Stoichiometry CBF402(1-)

Framework group C1[X(CBF402)]

Deg. of freedom 18

Full point group

C1

Largest Abelian subgroup

C1

NOp

1

Largest concise Abelian subgroup

C1

NOp

1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.242888	0.000041	0.002076
2	9	0	0.296560	0.005598	-1.039841
3	9	0	0.548637	-0.007912	1.218471
4	9	0	2.029451	1.140667	-0.082503
5	9	0	2.031347	-1.138155	-0.096447
6	8	0	-2.304994	-1.142635	0.000840
7	6	0	-2.247039	-0.000058	-0.003226
8	8	0	-2.305776	1.142430	0.000642

Rotational constants (GHZ): 3.6061037 1.0976657 1.0058337

Standard basis: 6-31+G(d) (6D, 7F)

There are 152 symmetry adapted basis functions of A symmetry.

Integral buffers will be 262144 words long.

Raffenetti 1 integral format.

Two-electron integral symmetry is turned on.

152 basis functions, 256 primitive gaussians, 152 cartesian basis functions

32 alpha electrons 32 beta electrons

nuclear repulsion energy 370.2005272212 Hartrees.

NAtoms= 8 NActive= 8 NUniq= 8 SFac= 7.50D-01 NATFMM= 80 NAOKFM=F

Big=F

One-electron integrals computed using PRISM.

NBasis= 152 RedAO= T NBF= 152

NBsUse= 152 1.00D-06 NBFU= 152

Initial guess read from the read-write file:

Initial guess orbital symmetries:

```

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

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Harris functional with IExCor= 205 diagonalized for initial guess.

ExpMin= 3.15D-02 ExpMax= 7.00D+03 ExpMxC= 1.05D+03 IAcc=3 IRadAn=

5

AccDes= 0.00D+00

HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 5 IDoV=1

ScaDFX= 1.000000 1.000000 1.000000 1.000000

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RHF) = -610.40882507 A.U. after 9 cycles

Convrg = 0.9983D-08 -V/T = 2.0028

S**2 = 0.0000

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	5	0.003123919	0.002349002	0.000000502
2	9	-0.001537540	-0.000700273	-0.000020448
3	9	0.000209985	-0.000253184	0.000016369
4	9	-0.000730863	-0.000799531	0.000465164
5	9	-0.000731863	-0.000795020	-0.000463726
6	8	-0.000448499	-0.000409508	-0.000998897
7	6	0.000581585	0.000984654	-0.000109798
8	8	-0.000466724	-0.000376139	0.001110834

Cartesian Forces: Max 0.003123919 RMS 0.001026569

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Internal Forces: Max 0.001164983 RMS 0.000446911

Search for a local minimum.

Step number 8 out of a maximum of 49

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Update second derivatives using D2CorX and points 7 8

Trust test= 1.20D+00 RLast= 2.31D-01 DXMaxT set to 1.00D+00

Eigenvalues --- 0.00062 0.00569 0.00937 0.01075 0.06471

Eigenvalues --- 0.08906 0.16491 0.20615 0.24653 0.25000

Eigenvalues --- 0.25000 0.25013 0.39774 0.44736 0.46170

Eigenvalues --- 0.46211 1.13100 1.375521000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
 Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
 Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
 Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

RFO step: Lambda=-3.22361470D-05.

Quartic linear search produced a step of 0.33604.

Iteration 1 RMS(Cart)= 0.00585010 RMS(Int)= 0.00002847

Iteration 2 RMS(Cart)= 0.00001858 RMS(Int)= 0.00001693

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001693

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.65986	-0.00116	-0.00231	-0.00333	-0.00564	2.65422
R2	2.64674	-0.00023	-0.00110	-0.00089	-0.00200	2.64474
R3	2.62316	0.00100	0.00205	0.00194	0.00399	2.62715
R4	2.62316	0.00099	0.00205	0.00193	0.00398	2.62714
R5	7.04368	-0.00038	-0.03263	0.02760	-0.00504	7.03864
R6	6.59501	-0.00001	-0.02349	0.03033	0.00684	6.60185
R7	7.04492	-0.00037	-0.03119	0.02732	-0.00388	7.04104
R8	5.72233	0.00019	-0.02356	0.04082	0.01725	5.73957
R9	5.19056	0.00050	-0.01339	0.04729	0.03390	5.22445
R10	5.71533	0.00022	-0.01863	0.04396	0.02536	5.74069
R11	6.24280	-0.00011	-0.02748	0.01330	-0.01416	6.22864
R12	5.76549	0.00012	-0.02143	0.01295	-0.00847	5.75702
R13	6.25441	-0.00013	-0.03007	0.00930	-0.02078	6.23363
R14	2.16195	0.00086	-0.00006	0.00048	0.00041	2.16236
R15	2.16185	0.00097	-0.00005	0.00058	0.00052	2.16237
A1	1.88562	0.00008	0.00303	0.00156	0.00457	1.89019
A2	1.90988	0.00026	-0.00018	0.00074	0.00057	1.91045
A3	1.90984	0.00027	-0.00018	0.00081	0.00065	1.91049
A4	1.91607	-0.00001	-0.00063	-0.00039	-0.00103	1.91505
A5	1.91616	-0.00002	-0.00063	-0.00043	-0.00105	1.91511
A6	1.92579	-0.00057	-0.00131	-0.00220	-0.00355	1.92224
A7	2.48364	0.00047	0.00231	0.00063	0.00293	2.48657
A8	2.17313	0.00031	0.00080	0.00173	0.00252	2.17566
A9	1.86247	0.00014	-0.00065	0.00282	0.00215	1.86462
A10	1.86425	0.00015	-0.00082	0.00268	0.00186	1.86612
A11	2.17472	0.00030	0.00083	0.00169	0.00250	2.17722
A12	2.48474	0.00047	0.00243	0.00079	0.00319	2.48793
A13	0.62303	0.00032	0.00303	-0.00233	0.00072	0.62375
A14	0.77427	0.00033	0.00317	-0.00581	-0.00263	0.77164
A15	0.70560	0.00034	0.00352	-0.00112	0.00242	0.70803
A16	0.72921	-0.00018	0.00365	-0.00311	0.00055	0.72976
A17	0.79899	-0.00024	0.00324	-0.00407	-0.00085	0.79814
A18	0.72856	-0.00018	0.00365	-0.00289	0.00075	0.72930
A19	3.07941	0.00039	0.00618	0.00066	0.00683	3.08624
A20	3.22285	-0.00056	-0.00715	-0.00154	-0.00868	3.21417
D1	-1.47236	0.00004	0.00412	0.00341	0.00752	-1.46484
D2	1.46159	-0.00001	0.00004	0.00059	0.00059	1.46218
D3	1.37292	-0.00003	0.00121	0.00618	0.00736	1.38027
D4	-1.38294	0.00005	0.00333	-0.00232	0.00101	-1.38194

Item	Value	Threshold	Converged?
Maximum Force	0.001165	0.000450	NO
RMS Force	0.000447	0.000300	NO
Maximum Displacement	0.022976	0.001800	NO
RMS Displacement	0.005850	0.001200	NO

Predicted change in Energy=-3.188545D-05

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Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.112027	0.128561	0.000062
2	9	0	1.516530	0.139540	0.003437
3	9	0	-0.337783	1.453841	-0.003577
4	9	0	-0.348826	-0.520205	1.139994
5	9	0	-0.343364	-0.524689	-1.139500
6	8	0	2.451060	2.793652	-1.139909
7	6	0	2.417699	2.753207	0.003160
8	8	0	2.447633	2.795760	1.146256

Distance matrix (angstroms):

		1	2	3	4	5
1	B	0.000000				
2	F	1.404550	0.000000			
3	F	1.399539	2.272864	0.000000		
4	F	1.390226	2.281793	2.281389	0.000000	
5	F	1.390222	2.281822	2.281432	2.279504	0.000000
6	O	3.724690	3.037251	3.296056	4.900915	4.338224
7	C	3.493551	2.764662	3.046486	4.434104	4.435509
8	O	3.725958	3.037843	3.298697	4.337724	4.903032
		6	7	8		
6	O	0.000000				
7	C	1.144271	0.000000			
8	O	2.286169	1.144280	0.000000		

Stoichiometry CBF402(1-)

Framework group C1[X(CBF402)]

Deg. of freedom 18

Full point group

C1

Largest Abelian subgroup

C1

NOp 1

Largest concise Abelian subgroup

C1

NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.240492	0.000088	0.001566
2	9	0	0.306637	0.000733	-1.047565
3	9	0	0.540151	-0.002097	1.213270
4	9	0	2.031067	1.140632	-0.081363
5	9	0	2.033019	-1.138869	-0.084432
6	8	0	-2.304368	-1.143275	0.000667
7	6	0	-2.253056	-0.000161	-0.002898
8	8	0	-2.305881	1.142893	0.000628

Rotational constants (GHZ): 3.6038124 1.0966281 1.0048687

Standard basis: 6-31+G(d) (6D, 7F)

There are 152 symmetry adapted basis functions of A symmetry.

Integral buffers will be 262144 words long.

```

Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
152 basis functions, 256 primitive gaussians, 152 cartesian basis
functions
32 alpha electrons 32 beta electrons
nuclear repulsion energy 370.0633799160 Hartrees.
NAtoms= 8 NActive= 8 NUniq= 8 SFac= 7.50D-01 NATFMM= 80 NAOKFM=F
Big=F
One-electron integrals computed using PRISM.
NBasis= 152 RedAO= T NBF= 152
NBsUse= 152 1.00D-06 NBFU= 152
Initial guess read from the read-write file:
Initial guess orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
Harris functional with IExCor= 205 diagonalized for initial guess.
ExpMin= 3.15D-02 ExpMax= 7.00D+03 ExpMxC= 1.05D+03 IAcc=3 IRadAn=
AccDes= 0.00D+00
HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 5 IDoV=1
ScaDFX= 1.000000 1.000000 1.000000 1.000000
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RHF) = -610.408865279 A.U. after 9 cycles
Convrg = 0.4100D-08 -V/T = 2.0028
S**2 = 0.0000
***** Axes restored to original set *****
-----
Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
-----
1 5 0.000955465 0.000400240 0.000006431
2 9 -0.000538928 -0.000312779 -0.000001516
3 9 0.000442905 0.000266333 0.000004167
4 9 -0.000268974 -0.000265100 -0.000117462
5 9 -0.000265853 -0.000258023 0.000118215
6 8 0.000188567 0.000339878 -0.000097654
7 6 -0.000685976 -0.000501157 -0.000030554
8 8 0.000172795 0.000330608 0.000118372
-----
Cartesian Forces: Max 0.000955465 RMS 0.000357807

```

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.000375759 RMS 0.000154930

Search for a local minimum.

Step number 9 out of a maximum of 49

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Update second derivatives using D2CorX and points 7 8 9

Trust test= 1.25D+00 RLast= 5.72D-02 DXMaxT set to 1.00D+00

Eigenvalues --- 0.00061 0.00552 0.00674 0.00939 0.07364

Eigenvalues --- 0.11294 0.16512 0.20585 0.23501 0.25000

Eigenvalues --- 0.25000 0.25020 0.39241 0.44737 0.46211

Eigenvalues --- 0.46354 1.14354 1.375541000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.00000

RFO step: Lambda=-2.16471129D-05.

Quartic linear search produced a step of 0.33477.

Iteration 1 RMS(Cart)= 0.00856505 RMS(Int)= 0.00003241

Iteration 2 RMS(Cart)= 0.00001974 RMS(Int)= 0.00001884

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001884

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.65422	-0.00038	-0.00189	-0.00138	-0.00324	2.65097
R2	2.64474	0.00008	-0.00067	-0.00013	-0.00078	2.64396
R3	2.62715	0.00012	0.00134	0.00050	0.00184	2.62899
R4	2.62714	0.00011	0.00133	0.00049	0.00182	2.62896
R5	7.03864	0.00009	-0.00169	-0.02784	-0.02954	7.00911
R6	6.60185	-0.00022	0.00229	-0.03131	-0.02903	6.57282
R7	7.04104	0.00008	-0.00130	-0.02844	-0.02976	7.01128
R8	5.73957	0.00023	0.00577	-0.01052	-0.00475	5.73482
R9	5.22445	-0.00002	0.01135	-0.01254	-0.00118	5.22327
R10	5.74069	0.00023	0.00849	-0.01017	-0.00167	5.73902
R11	6.22864	-0.00005	-0.00474	-0.04146	-0.04618	6.18246
R12	5.75702	-0.00036	-0.00284	-0.04669	-0.04953	5.70749
R13	6.23363	-0.00006	-0.00696	-0.04297	-0.04992	6.18371
R14	2.16236	0.00001	0.00014	0.00008	0.00021	2.16257
R15	2.16237	0.00004	0.00017	0.00010	0.00027	2.16264
A1	1.89019	-0.00004	0.00153	-0.00046	0.00106	1.89125
A2	1.91045	0.00016	0.00019	0.00063	0.00084	1.91129
A3	1.91049	0.00016	0.00022	0.00061	0.00085	1.91134
A4	1.91505	0.00004	-0.00034	0.00015	-0.00019	1.91486
A5	1.91511	0.00003	-0.00035	0.00012	-0.00022	1.91489
A6	1.92224	-0.00034	-0.00119	-0.00104	-0.00228	1.91996
A7	2.48657	0.00018	0.00098	0.00246	0.00342	2.48999
A8	2.17566	0.00018	0.00084	0.00107	0.00190	2.17756
A9	1.86462	0.00018	0.00072	-0.00032	0.00038	1.86500
A10	1.86612	0.00018	0.00062	-0.00037	0.00025	1.86637
A11	2.17722	0.00018	0.00084	0.00102	0.00184	2.17906
A12	2.48793	0.00018	0.00107	0.00248	0.00351	2.49144
A13	0.62375	0.00000	0.00024	0.00258	0.00283	0.62658
A14	0.77164	-0.00003	-0.00088	0.00147	0.00058	0.77222
A15	0.70803	0.00001	0.00081	0.00501	0.00587	0.71389
A16	0.72976	-0.00006	0.00018	0.00353	0.00369	0.73345
A17	0.79814	-0.00002	-0.00028	0.00489	0.00457	0.80271
A18	0.72930	-0.00006	0.00025	0.00364	0.00385	0.73315

A19	3.08624	-0.00022	0.00229	-0.00125	0.00104	3.08727
A20	3.21417	0.00018	-0.00291	0.00103	-0.00187	3.21230
D1	-1.46484	0.00001	0.00252	0.00464	0.00716	-1.45768
D2	1.46218	0.00000	0.00020	-0.00350	-0.00331	1.45887
D3	1.38027	0.00004	0.00246	0.00147	0.00393	1.38420
D4	-1.38194	-0.00004	0.00034	-0.00051	-0.00018	-1.38212

Item	Value	Threshold	Converged?
Maximum Force	0.000376	0.000450	YES
RMS Force	0.000155	0.000300	YES
Maximum Displacement	0.029744	0.001800	NO
RMS Displacement	0.008565	0.001200	NO

Predicted change in Energy=-1.359786D-05

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Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.118522	0.131996	0.000088
2	9	0	1.521354	0.131833	0.002707
3	9	0	-0.322043	1.459945	-0.002631
4	9	0	-0.348271	-0.514963	1.139817
5	9	0	-0.344083	-0.518271	-1.139451
6	8	0	2.443205	2.787726	-1.140119
7	6	0	2.409126	2.749420	0.003113
8	8	0	2.437166	2.791981	1.146398

Distance matrix (angstroms):

		1	2	3	4	5
1	B	0.000000				
2	F	1.402834	0.000000			
3	F	1.399126	2.272007	0.000000		
4	F	1.391199	2.281855	2.281695	0.000000	
5	F	1.391186	2.281888	2.281706	2.279274	0.000000
6	O	3.709059	3.034737	3.271617	4.888579	4.324187
7	C	3.478186	2.764037	3.020275	4.421711	4.423055
8	O	3.710210	3.036960	3.272281	4.323723	4.890626
		6	7	8		
6	O	0.000000				
7	C	1.144381	0.000000			
8	O	2.286530	1.144421	0.000000		

Stoichiometry CBF402(1-)

Framework group C1[X(CBF402)]

Deg. of freedom 18

Full point group C1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.233904	0.000081	0.001221
2	9	0	0.311361	-0.001541	-1.055593

```

3          9          0          0.523373      0.000551      1.206500
4          9          0          2.027188      1.140310      -0.076319
5          9          0          2.029056     -1.138962      -0.074363
6          8          0         -2.294480     -1.143433       0.000483
7          6          0         -2.244280     -0.000158      -0.002696
8          8          0         -2.295851      1.143096       0.000522
-----
Rotational constants (GHZ):      3.6046538      1.1039113      1.0109014
Standard basis: 6-31+G(d) (6D, 7F)
There are 152 symmetry adapted basis functions of A symmetry.
Integral buffers will be 262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
152 basis functions, 256 primitive gaussians, 152 cartesian basis
functions
32 alpha electrons      32 beta electrons
nuclear repulsion energy      370.5392246276 Hartrees.
NAtoms= 8 NActive= 8 NUniq= 8 SFac= 7.50D-01 NATFMM= 80 NAOKFM=F
Big=F
One-electron integrals computed using PRISM.
NBasis= 152 RedAO= T NBF= 152
NBsUse= 152 1.00D-06 NBFU= 152
Initial guess read from the read-write file:
Initial guess orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A)
Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
Harris functional with IExCor= 205 diagonalized for initial guess.
ExpMin= 3.15D-02 ExpMax= 7.00D+03 ExpMxC= 1.05D+03 IAcc=3 IRadAn=
AccDes= 0.00D+00
HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 5 IDoV=1
ScaDFX= 1.000000 1.000000 1.000000 1.000000
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RHF) = -610.408886942 A.U. after 8 cycles
Convrg = 0.4805D-08 -V/T = 2.0028
S**2 = 0.0000
***** Axes restored to original set *****
-----
Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
-----
1 5 -0.000277740 -0.000577711 0.000008116

```

2	9	0.000091375	-0.000307522	0.000007905
3	9	0.000412156	0.000513569	0.000000002
4	9	0.000003558	0.000048551	-0.000359347
5	9	0.000005777	0.000050832	0.000355886
6	8	0.000349189	0.000557022	0.000241312
7	6	-0.000924629	-0.000814988	0.000027534
8	8	0.000340315	0.000530247	-0.000281408

Cartesian Forces: Max 0.000924629 RMS 0.000392367

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Berny optimization.

Internal Forces: Max 0.000452512 RMS 0.000191858

Search for a local minimum.

Step number 10 out of a maximum of 49

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Update second derivatives using D2CorX and points 7 8 9 10

Trust test= 1.59D+00 RLast= 9.97D-02 DXMaxT set to 1.00D+00

Eigenvalues ---	0.00060	0.00229	0.00572	0.00941	0.07709
Eigenvalues ---	0.12653	0.16473	0.20563	0.23111	0.25000
Eigenvalues ---	0.25000	0.25016	0.42928	0.45824	0.46211
Eigenvalues ---	0.49344	1.20418	1.37561	1000.00000	1000.00000
Eigenvalues ---	1000.00000	1000.00000	1000.00000	1000.00000	1000.00000
Eigenvalues ---	1000.00000	1000.00000	1000.00000	1000.00000	1000.00000
Eigenvalues ---	1000.00000	1000.00000	1000.00000	1000.00000	1000.00000
Eigenvalues ---	1000.00000	1000.00000	1000.00000	1000.00000	1000.00000

RFO step: Lambda=-3.12343113D-05.

Quartic linear search produced a step of 1.42152.

Iteration 1 RMS(Cart)= 0.01728142 RMS(Int)= 0.00019788

Iteration 2 RMS(Cart)= 0.00011797 RMS(Int)= 0.00013293

Iteration 3 RMS(Cart)= 0.00000002 RMS(Int)= 0.00013293

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.65097	0.00017	-0.00461	-0.00118	-0.00561	2.64536
R2	2.64396	0.00026	-0.00111	0.00037	-0.00059	2.64337
R3	2.62899	-0.00032	0.00261	0.00040	0.00301	2.63200
R4	2.62896	-0.00032	0.00259	0.00040	0.00299	2.63195
R5	7.00911	0.00023	-0.04199	0.01028	-0.03180	6.97731
R6	6.57282	-0.00021	-0.04127	0.00862	-0.03275	6.54007
R7	7.01128	0.00023	-0.04230	0.00898	-0.03344	6.97784
R8	5.73482	0.00024	-0.00675	0.03745	0.03070	5.76552
R9	5.22327	-0.00012	-0.00168	0.03908	0.03745	5.26072
R10	5.73902	0.00023	-0.00237	0.03690	0.03459	5.77362
R11	6.18246	-0.00005	-0.06565	-0.01980	-0.08537	6.09709
R12	5.70749	-0.00045	-0.07041	-0.02391	-0.09434	5.61316
R13	6.18371	-0.00005	-0.07096	-0.02171	-0.09262	6.09109
R14	2.16257	-0.00030	0.00030	0.00003	0.00028	2.16285
R15	2.16264	-0.00033	0.00038	0.00001	0.00035	2.16300
A1	1.89125	-0.00003	0.00151	0.00014	0.00159	1.89284
A2	1.91129	0.00007	0.00119	0.00075	0.00205	1.91334
A3	1.91134	0.00007	0.00121	0.00075	0.00209	1.91343
A4	1.91486	0.00002	-0.00026	-0.00006	-0.00026	1.91460
A5	1.91489	0.00002	-0.00031	-0.00006	-0.00029	1.91460
A6	1.91996	-0.00015	-0.00324	-0.00149	-0.00507	1.91489
A7	2.48999	0.00003	0.00486	0.00140	0.00610	2.49609

A8	2.17756	0.00008	0.00270	0.00166	0.00422	2.18178
A9	1.86500	0.00015	0.00054	0.00191	0.00232	1.86732
A10	1.86637	0.00014	0.00036	0.00189	0.00218	1.86855
A11	2.17906	0.00008	0.00262	0.00159	0.00406	2.18313
A12	2.49144	0.00002	0.00499	0.00141	0.00617	2.49761
A13	0.62658	-0.00012	0.00402	-0.00090	0.00315	0.62973
A14	0.77222	-0.00016	0.00083	-0.00529	-0.00445	0.76777
A15	0.71389	-0.00011	0.00834	0.00249	0.01104	0.72493
A16	0.73345	0.00005	0.00525	-0.00028	0.00474	0.73820
A17	0.80271	0.00011	0.00650	-0.00006	0.00612	0.80883
A18	0.73315	0.00005	0.00547	-0.00010	0.00508	0.73823
A19	3.08727	-0.00037	0.00147	-0.00132	0.00018	3.08745
A20	3.21230	0.00039	-0.00266	0.00070	-0.00196	3.21034
D1	-1.45768	0.00001	0.01018	0.00515	0.01529	-1.44239
D2	1.45887	-0.00002	-0.00470	-0.00419	-0.00889	1.44998
D3	1.38420	0.00005	0.00559	0.00560	0.01121	1.39541
D4	-1.38212	-0.00006	-0.00026	-0.00504	-0.00536	-1.38748

Item	Value	Threshold	Converged?
Maximum Force	0.000453	0.000450	NO
RMS Force	0.000192	0.000300	YES
Maximum Displacement	0.069330	0.001800	NO
RMS Displacement	0.017278	0.001200	NO

Predicted change in Energy=-2.806312D-05

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Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.129218	0.133561	0.000166
2	9	0	1.528768	0.103957	0.001550
3	9	0	-0.285355	1.469527	-0.001053
4	9	0	-0.353369	-0.506707	1.139041
5	9	0	-0.351258	-0.508125	-1.138776
6	8	0	2.431334	2.785324	-1.140439
7	6	0	2.395016	2.749605	0.002958
8	8	0	2.420622	2.792524	1.146475

Distance matrix (angstroms):

		1	2	3	4	5
1	B	0.000000				
2	F	1.399864	0.000000			
3	F	1.398813	2.270645	0.000000		
4	F	1.392792	2.282374	2.282530	0.000000	
5	F	1.392769	2.282429	2.282512	2.277818	0.000000
6	O	3.692231	3.050983	3.226441	4.877302	4.311569
7	C	3.460857	2.783853	2.970354	4.409974	4.411165
8	O	3.692512	3.055266	3.223267	4.310453	4.878521
		6	7	8		
6	O	0.000000				
7	C	1.144532	0.000000			
8	O	2.286951	1.144609	0.000000		

Stoichiometry CBF402(1-)
Framework group C1[X(CBF402)]

Deg. of freedom 18

Full point group

C1

Largest Abelian subgroup

C1

NOp

1

Largest concise Abelian subgroup

C1

NOp

1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.225935	0.000008	0.000343
2	9	0	0.332787	-0.005312	-1.077560
3	9	0	0.486677	0.004754	1.187842
4	9	0	2.024956	1.139226	-0.059802
5	9	0	2.026524	-1.138569	-0.049715
6	8	0	-2.284754	-1.143509	0.000162
7	6	0	-2.234921	-0.000065	-0.002066
8	8	0	-2.285076	1.143442	0.000313

Rotational constants (GHZ): 3.6074063 1.1114041 1.0171572

Standard basis: 6-31+G(d) (6D, 7F)

There are 152 symmetry adapted basis functions of A symmetry.

Integral buffers will be 262144 words long.

Raffenetti 1 integral format.

Two-electron integral symmetry is turned on.

152 basis functions, 256 primitive gaussians, 152 cartesian basis functions

32 alpha electrons 32 beta electrons

nuclear repulsion energy 371.0164317327 Hartrees.

NAtoms= 8 NActive= 8 NUniq= 8 SFac= 7.50D-01 NATFMM= 80 NAOKFM=F

Big=F

One-electron integrals computed using PRISM.

NBasis= 152 RedAO= T NBF= 152

NBsUse= 152 1.00D-06 NBFU= 152

Initial guess read from the read-write file:

Initial guess orbital symmetries:

Occupied	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)				
Virtual	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)

Harris functional with IExCor= 205 diagonalized for initial guess.

ExpMin= 3.15D-02 ExpMax= 7.00D+03 ExpMxC= 1.05D+03 IAcc=3 IRadAn=

5

AccDes= 0.00D+00

HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 5 IDoV=1

ScaDFX= 1.000000 1.000000 1.000000 1.000000

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 SCF Done: E(RHF) = -610.408925406 A.U. after 9 cycles
 Conv = 0.3396D-08 -V/T = 2.0028
 S**2 = 0.0000

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	5	-0.002462963	-0.002105973	0.000015023
2	9	0.001104561	-0.000205798	0.000016017
3	9	0.000387841	0.000786683	-0.000012393
4	9	0.000553960	0.000627816	-0.000613296
5	9	0.000558294	0.000625886	0.000605105
6	8	0.000443875	0.000670541	0.000681107
7	6	-0.001044521	-0.001023898	0.000123142
8	8	0.000458953	0.000624742	-0.000814705

Cartesian Forces: Max 0.002462963 RMS 0.000894664

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 Berny optimization.

Internal Forces: Max 0.001029419 RMS 0.000398144

Search for a local minimum.

Step number 11 out of a maximum of 49

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Update second derivatives using D2CorX and points 7 8 9 10 11

Trust test= 1.37D+00 RLast= 1.80D-01 DXMaxT set to 1.00D+00

Eigenvalues --- 0.00052 0.00152 0.00565 0.00945 0.07846
 Eigenvalues --- 0.09878 0.16442 0.20532 0.24982 0.25000
 Eigenvalues --- 0.25003 0.25137 0.43478 0.46018 0.46211
 Eigenvalues --- 0.54060 1.21242 1.375821000.000001000.00000
 Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
 Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
 Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
 Eigenvalues --- 1000.000001000.000001000.000001000.00000

RFO step: Lambda=-3.19275870D-05.

Quartic linear search produced a step of 0.60189.

Iteration 1 RMS(Cart)= 0.01673417 RMS(Int)= 0.00022803

Iteration 2 RMS(Cart)= 0.00011156 RMS(Int)= 0.00018098

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00018098

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.64536	0.00103	-0.00338	0.00100	-0.00212	2.64324
R2	2.64337	0.00044	-0.00036	0.00098	0.00085	2.64422
R3	2.63200	-0.00098	0.00181	-0.00121	0.00060	2.63259
R4	2.63195	-0.00098	0.00180	-0.00121	0.00059	2.63254
R5	6.97731	0.00039	-0.01914	-0.00157	-0.02085	6.95645
R6	6.54007	-0.00012	-0.01971	-0.00732	-0.02716	6.51292
R7	6.97784	0.00038	-0.02013	-0.00269	-0.02298	6.95486
R8	5.76552	0.00017	0.01848	0.02107	0.03958	5.80510
R9	5.26072	-0.00023	0.02254	0.01666	0.03927	5.29999
R10	5.77362	0.00014	0.02082	0.01790	0.03878	5.81240

R11	6.09709	-0.00008	-0.05138	-0.02968	-0.08097	6.01612
R12	5.61316	-0.00050	-0.05678	-0.03594	-0.09274	5.52041
R13	6.09109	-0.00006	-0.05575	-0.02836	-0.08403	6.00707
R14	2.16285	-0.00065	0.00017	-0.00003	0.00011	2.16296
R15	2.16300	-0.00078	0.00021	-0.00009	0.00009	2.16309
A1	1.89284	-0.00005	0.00096	-0.00176	-0.00087	1.89197
A2	1.91334	-0.00014	0.00123	0.00035	0.00173	1.91506
A3	1.91343	-0.00015	0.00126	0.00029	0.00170	1.91513
A4	1.91460	0.00001	-0.00016	0.00035	0.00029	1.91489
A5	1.91460	0.00001	-0.00017	0.00032	0.00027	1.91487
A6	1.91489	0.00032	-0.00305	0.00042	-0.00308	1.91181
A7	2.49609	-0.00029	0.00367	0.00053	0.00394	2.50003
A8	2.18178	-0.00017	0.00254	0.00032	0.00267	2.18445
A9	1.86732	-0.00003	0.00140	0.00010	0.00137	1.86869
A10	1.86855	-0.00004	0.00131	0.00016	0.00137	1.86992
A11	2.18313	-0.00016	0.00245	0.00027	0.00253	2.18565
A12	2.49761	-0.00030	0.00371	0.00044	0.00386	2.50146
A13	0.62973	-0.00026	0.00190	0.00011	0.00203	0.63175
A14	0.76777	-0.00030	-0.00268	-0.00283	-0.00548	0.76229
A15	0.72493	-0.00025	0.00665	0.00351	0.01039	0.73532
A16	0.73820	0.00020	0.00286	0.00098	0.00348	0.74168
A17	0.80883	0.00028	0.00368	0.00203	0.00526	0.81408
A18	0.73823	0.00020	0.00306	0.00102	0.00369	0.74192
A19	3.08745	-0.00049	0.00011	-0.00346	-0.00332	3.08413
A20	3.21034	0.00056	-0.00118	0.00333	0.00216	3.21250
D1	-1.44239	0.00001	0.00920	0.00326	0.01240	-1.42999
D2	1.44998	-0.00003	-0.00535	-0.00558	-0.01089	1.43909
D3	1.39541	0.00004	0.00675	0.00246	0.00926	1.40467
D4	-1.38748	-0.00007	-0.00323	-0.00509	-0.00839	-1.39587

Item	Value	Threshold	Converged?
Maximum Force	0.001029	0.000450	NO
RMS Force	0.000398	0.000300	NO
Maximum Displacement	0.068784	0.001800	NO
RMS Displacement	0.016730	0.001200	NO

Predicted change in Energy=-2.357837D-05

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Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.137789	0.133142	0.000258
2	9	0	1.535346	0.075619	0.001371
3	9	0	-0.248956	1.477894	-0.000660
4	9	0	-0.359683	-0.498162	1.138119
5	9	0	-0.357992	-0.499186	-1.137741
6	8	0	2.419903	2.786775	-1.140524
7	6	0	2.380916	2.749751	0.002802
8	8	0	2.407653	2.793836	1.146298

Distance matrix (angstroms):

		1	2	3	4	5
1	B	0.000000				
2	F	1.398741	0.000000			

```

3 F 1.399261 2.269387 0.000000
4 F 1.393109 2.283102 2.283392 0.000000
5 F 1.393082 2.283135 2.283350 2.275861 0.000000
6 O 3.681195 3.071927 3.183593 4.869202 4.302819
7 C 3.446487 2.804634 2.921277 4.398724 4.399778
8 O 3.680351 3.075789 3.178802 4.300635 4.869252
      6      7      8
6 O 0.000000
7 C 1.144589 0.000000
8 O 2.286866 1.144658 0.000000
Stoichiometry CBF402(1-)
Framework group C1[X(CBF402)]
Deg. of freedom 18
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:
-----
Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z
-----
1 5 0 1.220979 -0.000078 -0.000266
2 9 0 0.355409 -0.006162 -1.099005
3 9 0 0.451366 0.005493 1.168322
4 9 0 2.023274 1.138119 -0.040042
5 9 0 2.024521 -1.137712 -0.028321
6 8 0 -2.278201 -1.143292 -0.000020
7 6 0 -2.225508 0.000082 -0.001369
8 8 0 -2.277170 1.143573 0.000140
-----
Rotational constants (GHZ): 3.6111180 1.1172118 1.0220847
Standard basis: 6-31+G(d) (6D, 7F)
There are 152 symmetry adapted basis functions of A symmetry.
Integral buffers will be 262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
152 basis functions, 256 primitive gaussians, 152 cartesian basis
functions
32 alpha electrons 32 beta electrons
nuclear repulsion energy 371.4123454627 Hartrees.
NAtoms= 8 NActive= 8 NUniq= 8 SFac= 7.50D-01 NATFMM= 80 NAOKFM=F
Big=F
One-electron integrals computed using PRISM.
NBasis= 152 RedAO= T NBF= 152
NBsUse= 152 1.00D-06 NBFU= 152
Initial guess read from the read-write file:
Initial guess orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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Harris functional with IExCor= 205 diagonalized for initial guess.
 ExpMin= 3.15D-02 ExpMax= 7.00D+03 ExpMxC= 1.05D+03 IAcc=3 IRadAn= 5
 AccDes= 0.00D+00

HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 5 IDoV=1
 ScaDFX= 1.000000 1.000000 1.000000 1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 SCF Done: E(RHF) = -610.408959355 A.U. after 9 cycles
 Convrg = 0.4155D-08 -V/T = 2.0028
 S**2 = 0.0000

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	5	-0.003234790	-0.002478398	0.000013908
2	9	0.001391487	-0.000237641	0.000016390
3	9	0.000229986	0.000700322	-0.000016575
4	9	0.000833133	0.000895641	-0.000500010
5	9	0.000834038	0.000888553	0.000488238
6	8	0.000222245	0.000381505	0.000724466
7	6	-0.000530192	-0.000495820	0.000147762
8	8	0.000254093	0.000345836	-0.000874177

Cartesian Forces: Max 0.003234790 RMS 0.001017141

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 Berny optimization.

Internal Forces: Max 0.001276921 RMS 0.000438943

Search for a local minimum.

Step number 12 out of a maximum of 49

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Update second derivatives using D2CorX and points 8 9 10 11 12

Trust test= 1.44D+00 RLast= 1.71D-01 DXMaxT set to 1.00D+00

```

Eigenvalues --- 0.00055 0.00113 0.00559 0.00949 0.07515
Eigenvalues --- 0.08929 0.16411 0.20498 0.25000 0.25000
Eigenvalues --- 0.25015 0.27602 0.43468 0.46056 0.46211
Eigenvalues --- 0.55696 1.18757 1.375571000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.00000

```

RFO step: Lambda=-1.97017721D-05.

Quartic linear search produced a step of 0.79325.

Iteration 1 RMS(Cart)= 0.01484321 RMS(Int)= 0.00021947

Iteration 2 RMS(Cart)= 0.00009204 RMS(Int)= 0.00018749

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00018749

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.64324	0.00128	-0.00168	0.00204	0.00062	2.64386
R2	2.64422	0.00040	0.00067	0.00083	0.00175	2.64597
R3	2.63259	-0.00111	0.00048	-0.00162	-0.00115	2.63145
R4	2.63254	-0.00110	0.00047	-0.00160	-0.00113	2.63141
R5	6.95645	0.00028	-0.01654	0.01199	-0.00471	6.95174
R6	6.51292	0.00005	-0.02154	0.01118	-0.01050	6.50242
R7	6.95486	0.00028	-0.01823	0.01223	-0.00616	6.94869
R8	5.80510	0.00006	0.03140	0.01853	0.04998	5.85508
R9	5.29999	-0.00010	0.03115	0.01717	0.04839	5.34838
R10	5.81240	0.00004	0.03077	0.01581	0.04663	5.85903
R11	6.01612	-0.00012	-0.06423	-0.00053	-0.06467	5.95145
R12	5.52041	-0.00028	-0.07357	-0.00037	-0.07394	5.44647
R13	6.00707	-0.00009	-0.06665	0.00273	-0.06384	5.94323
R14	2.16296	-0.00062	0.00009	-0.00017	-0.00011	2.16285
R15	2.16309	-0.00077	0.00007	-0.00024	-0.00019	2.16290
A1	1.89197	-0.00002	-0.00069	-0.00111	-0.00188	1.89009
A2	1.91506	-0.00028	0.00137	-0.00063	0.00088	1.91595
A3	1.91513	-0.00030	0.00135	-0.00065	0.00083	1.91597
A4	1.91489	-0.00004	0.00023	0.00002	0.00038	1.91527
A5	1.91487	-0.00004	0.00021	0.00003	0.00037	1.91524
A6	1.91181	0.00067	-0.00244	0.00230	-0.00059	1.91122
A7	2.50003	-0.00046	0.00312	-0.00161	0.00122	2.50124
A8	2.18445	-0.00035	0.00212	-0.00107	0.00086	2.18531
A9	1.86869	-0.00021	0.00109	-0.00049	0.00050	1.86919
A10	1.86992	-0.00022	0.00109	-0.00046	0.00052	1.87044
A11	2.18565	-0.00033	0.00200	-0.00105	0.00077	2.18642
A12	2.50146	-0.00047	0.00306	-0.00168	0.00110	2.50256
A13	0.63175	-0.00024	0.00161	-0.00122	0.00040	0.63215
A14	0.76229	-0.00027	-0.00434	-0.00247	-0.00674	0.75555
A15	0.73532	-0.00024	0.00824	-0.00024	0.00819	0.74352
A16	0.74168	0.00025	0.00276	-0.00092	0.00144	0.74312
A17	0.81408	0.00030	0.00417	-0.00106	0.00262	0.81670
A18	0.74192	0.00025	0.00293	-0.00102	0.00152	0.74344
A19	3.08413	-0.00031	-0.00264	-0.00113	-0.00374	3.08039
A20	3.21250	0.00036	0.00171	0.00106	0.00278	3.21528
D1	-1.42999	0.00001	0.00984	-0.00078	0.00898	-1.42101
D2	1.43909	-0.00004	-0.00864	-0.00252	-0.01108	1.42801
D3	1.40467	0.00001	0.00735	0.00031	0.00773	1.41240
D4	-1.39587	-0.00004	-0.00665	-0.00352	-0.01024	-1.40611

Item	Value	Threshold	Converged?
Maximum Force	0.001277	0.000450	NO
RMS Force	0.000439	0.000300	NO
Maximum Displacement	0.060311	0.001800	NO
RMS Displacement	0.014839	0.001200	NO

Predicted change in Energy=-1.942390D-05

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Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.142979	0.130125	0.000326

2	9	0	1.539593	0.047274	0.001918
3	9	0	-0.217041	1.483238	-0.001094
4	9	0	-0.367129	-0.491018	1.137441
5	9	0	-0.364655	-0.492694	-1.136958
6	8	0	2.410999	2.792383	-1.140424
7	6	0	2.370414	2.752822	0.002703
8	8	0	2.399815	2.797537	1.146009

Distance matrix (angstroms):

		1	2	3	4	5
1	B	0.000000				
2	F	1.399070	0.000000			
3	F	1.400189	2.268868	0.000000		
4	F	1.392501	2.283584	2.283960	0.000000	
5	F	1.392484	2.283586	2.283918	2.274401	0.000000
6	O	3.678701	3.098373	3.149369	4.866968	4.300697
7	C	3.440931	2.830239	2.882149	4.393662	4.394633
8	O	3.677089	3.100463	3.145022	4.297748	4.866194
		6	7	8		
6	O	0.000000				
7	C	1.144531	0.000000			
8	O	2.286466	1.144557	0.000000		

Stoichiometry CBF4O2(1-)

Framework group C1[X(CBF4O2)]

Deg. of freedom 18

Full point group

C1

Largest Abelian subgroup

C1

NOp

1

Largest concise Abelian subgroup C1

NOp

1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.220112	-0.000127	-0.000472
2	9	0	0.379239	-0.004790	-1.118644
3	9	0	0.421760	0.003894	1.149809
4	9	0	2.023083	1.137384	-0.019565
5	9	0	2.024117	-1.137000	-0.010835
6	8	0	-2.276562	-1.142978	-0.000091
7	6	0	-2.220819	0.000195	-0.000644
8	8	0	-2.274617	1.143487	0.000007

Rotational constants (GHZ): 3.6137481 1.1192071 1.0238656

Standard basis: 6-31+G(d) (6D, 7F)

There are 152 symmetry adapted basis functions of A symmetry.

Integral buffers will be 262144 words long.

Raffenetti 1 integral format.

Two-electron integral symmetry is turned on.

152 basis functions, 256 primitive gaussians, 152 cartesian basis functions

32 alpha electrons

32 beta electrons

nuclear repulsion energy

371.5622783950 Hartrees.

NAtoms= 8 NActive= 8 NUniq= 8 SFac= 7.50D-01 NATFMM= 80 NAOKFM=F

Big=F

One-electron integrals computed using PRISM.

NBasis= 152 RedAO= T NBF= 152

NBsUse= 152 1.00D-06 NBFU= 152

Initial guess read from the read-write file:

Initial guess orbital symmetries:

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Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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```

Harris functional with IExCor= 205 diagonalized for initial guess.

ExpMin= 3.15D-02 ExpMax= 7.00D+03 ExpMxC= 1.05D+03 IAcc=3 IRadAn=

AccDes= 0.00D+00

HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 5 IDoV=1

ScaDFX= 1.000000 1.000000 1.000000 1.000000

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RHF) = -610.408985178 A.U. after 9 cycles

Convrg = 0.3639D-08 -V/T = 2.0028

S**2 = 0.0000

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	5	-0.002752208	-0.002026288	0.000006239
2	9	0.001097313	-0.000238814	0.000012191
3	9	0.000036147	0.000392085	-0.000014191
4	9	0.000809513	0.000870226	-0.000200092
5	9	0.000807148	0.000862909	0.000190571
6	8	-0.000039316	0.000021811	0.000439161
7	6	0.000048076	0.000108956	0.000093159
8	8	-0.000006673	0.000009114	-0.000527038

Cartesian Forces: Max 0.002752208 RMS 0.000828597

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Berny optimization.

Internal Forces: Max 0.001012127 RMS 0.000354994

Search for a local minimum.

Step number 13 out of a maximum of 49

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Update second derivatives using D2CorX and points 9 10 11 12 13

Trust test= 1.33D+00 RLast= 1.46D-01 DXMaxT set to 1.00D+00

Eigenvalues --- 0.00062 0.00099 0.00552 0.00953 0.06884

```

Eigenvalues --- 0.09037 0.16398 0.20481 0.25000 0.25000
Eigenvalues --- 0.25025 0.29037 0.42556 0.45934 0.46210
Eigenvalues --- 0.47380 1.14633 1.375061000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.00000

```

RFO step: Lambda=-1.18672849D-05.

Quartic linear search produced a step of 0.60635.

Iteration 1 RMS(Cart)= 0.00860884 RMS(Int)= 0.00010032

Iteration 2 RMS(Cart)= 0.00003182 RMS(Int)= 0.00009232

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00009232

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.64386	0.00101	0.00038	0.00170	0.00221	2.64607
R2	2.64597	0.00023	0.00106	0.00038	0.00157	2.64754
R3	2.63145	-0.00085	-0.00070	-0.00128	-0.00198	2.62947
R4	2.63141	-0.00084	-0.00069	-0.00126	-0.00195	2.62946
R5	6.95174	0.00009	-0.00286	0.00956	0.00661	6.95835
R6	6.50242	0.00015	-0.00637	0.01096	0.00453	6.50695
R7	6.94869	0.00010	-0.00374	0.01036	0.00654	6.95524
R8	5.85508	-0.00002	0.03030	0.00740	0.03774	5.89282
R9	5.34838	0.00006	0.02934	0.00759	0.03695	5.38533
R10	5.85903	-0.00004	0.02827	0.00596	0.03426	5.89328
R11	5.95145	-0.00012	-0.03922	0.00827	-0.03091	5.92054
R12	5.44647	-0.00003	-0.04483	0.01090	-0.03393	5.41255
R13	5.94323	-0.00009	-0.03871	0.01120	-0.02748	5.91575
R14	2.16285	-0.00033	-0.00007	-0.00009	-0.00017	2.16268
R15	2.16290	-0.00042	-0.00012	-0.00012	-0.00025	2.16265
A1	1.89009	0.00001	-0.00114	-0.00045	-0.00164	1.88846
A2	1.91595	-0.00031	0.00054	-0.00090	-0.00029	1.91565
A3	1.91597	-0.00031	0.00051	-0.00089	-0.00033	1.91564
A4	1.91527	-0.00011	0.00023	-0.00036	-0.00007	1.91520
A5	1.91524	-0.00011	0.00022	-0.00034	-0.00006	1.91518
A6	1.91122	0.00081	-0.00036	0.00290	0.00233	1.91355
A7	2.50124	-0.00047	0.00074	-0.00194	-0.00135	2.49989
A8	2.18531	-0.00041	0.00052	-0.00148	-0.00105	2.18427
A9	1.86919	-0.00034	0.00030	-0.00098	-0.00072	1.86847
A10	1.87044	-0.00035	0.00032	-0.00098	-0.00072	1.86972
A11	2.18642	-0.00040	0.00046	-0.00144	-0.00107	2.18535
A12	2.50256	-0.00047	0.00067	-0.00196	-0.00142	2.50115
A13	0.63215	-0.00012	0.00024	-0.00096	-0.00072	0.63143
A14	0.75555	-0.00014	-0.00409	-0.00094	-0.00497	0.75058
A15	0.74352	-0.00012	0.00497	-0.00131	0.00373	0.74724
A16	0.74312	0.00020	0.00087	-0.00086	-0.00020	0.74292
A17	0.81670	0.00020	0.00159	-0.00130	0.00004	0.81674
A18	0.74344	0.00020	0.00092	-0.00097	-0.00023	0.74321
A19	3.08039	-0.00005	-0.00226	0.00032	-0.00194	3.07845
A20	3.21528	0.00006	0.00169	-0.00028	0.00140	3.21668
D1	-1.42101	0.00001	0.00545	-0.00196	0.00344	-1.41757
D2	1.42801	-0.00004	-0.00672	-0.00054	-0.00721	1.42080
D3	1.41240	-0.00001	0.00469	-0.00091	0.00381	1.41620
D4	-1.40611	0.00000	-0.00621	-0.00135	-0.00759	-1.41370

Item	Value	Threshold	Converged?
Maximum Force	0.001012	0.000450	NO

RMS Force 0.000355 0.000300 NO
 Maximum Displacement 0.034297 0.001800 NO
 RMS Displacement 0.008608 0.001200 NO

Predicted change in Energy=-1.044201D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.144018	0.126502	0.000341
2	9	0	1.540865	0.029125	0.002765
3	9	0	-0.199965	1.484636	-0.001901
4	9	0	-0.372263	-0.487029	1.137523
5	9	0	-0.368492	-0.489788	-1.137050
6	8	0	2.406627	2.798239	-1.140275
7	6	0	2.366206	2.756784	0.002698
8	8	0	2.397980	2.801198	1.145820

Distance matrix (angstroms):

		1	2	3	4	5
1	B	0.000000				
2	F	1.400239	0.000000			
3	F	1.401020	2.269146	0.000000		
4	F	1.391455	2.283451	2.283732	0.000000	
5	F	1.391452	2.283439	2.283707	2.274578	0.000000
6	O	3.682198	3.118345	3.133013	4.868632	4.302606
7	C	3.443328	2.849791	2.864196	4.394242	4.395206
8	O	3.680552	3.118591	3.130482	4.299622	4.867798
		6	7	8		
6	O	0.000000				
7	C	1.144439	0.000000			
8	O	2.286114	1.144425	0.000000		

Stoichiometry CBF402(1-)

Framework group C1[X(CBF402)]

Deg. of freedom 18

Full point group

C1

Largest Abelian subgroup

C1

NOp 1

Largest concise Abelian subgroup

C1

NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.222273	-0.000120	-0.000298
2	9	0	0.395149	-0.002374	-1.130135
3	9	0	0.406856	0.001384	1.138978
4	9	0	2.023454	1.137519	-0.006117
5	9	0	2.024466	-1.137055	-0.002342
6	8	0	-2.278135	-1.142803	-0.000070
7	6	0	-2.221055	0.000212	-0.000189
8	8	0	-2.276160	1.143310	-0.000035

Rotational constants (GHZ): 3.6135928 1.1183072 1.0231467

Standard basis: 6-31+G(d) (6D, 7F)
 There are 152 symmetry adapted basis functions of A symmetry.
 Integral buffers will be 262144 words long.
 Raffenetti 1 integral format.
 Two-electron integral symmetry is turned on.
 152 basis functions, 256 primitive gaussians, 152 cartesian basis
 functions
 32 alpha electrons 32 beta electrons
 nuclear repulsion energy 371.5055233343 Hartrees.
 NAToms= 8 NActive= 8 NUniq= 8 SFac= 7.50D-01 NATFMM= 80 NAOKFM=F
 Big=F
 One-electron integrals computed using PRISM.
 NBasis= 152 RedAO= T NBF= 152
 NBsUse= 152 1.00D-06 NBFU= 152
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
 Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor= 205 diagonalized for initial guess.
 ExpMin= 3.15D-02 ExpMax= 7.00D+03 ExpMxC= 1.05D+03 IAcc=3 IRadAn= 5
 AccDes= 0.00D+00
 HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 5 IDoV=1
 ScaDFX= 1.000000 1.000000 1.000000 1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 SCF Done: E(RHF) = -610.408999452 A.U. after 8 cycles
 Conv = 0.8563D-08 -V/T = 2.0028
 S**2 = 0.0000
 ***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	5	-0.001505630	-0.001130167	-0.000001657
2	9	0.000566089	-0.000192584	0.000005882
3	9	-0.000092326	0.000145186	-0.000006851
4	9	0.000513306	0.000566747	0.000046981
5	9	0.000511315	0.000562586	-0.000050648
6	8	-0.000170401	-0.000175120	0.000129804
7	6	0.000327614	0.000394662	0.000015783
8	8	-0.000149968	-0.000171310	-0.000139294

Cartesian Forces: Max 0.001505630 RMS 0.000479147

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Internal Forces: Max 0.000616039 RMS 0.000216300

Search for a local minimum.

Step number 14 out of a maximum of 49

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Update second derivatives using D2CorX and points 10 11 12 13 14

Trust test= 1.37D+00 RLast= 8.45D-02 DXMaxT set to 1.00D+00

Eigenvalues --- 0.00061 0.00098 0.00547 0.00954 0.06792

Eigenvalues --- 0.09568 0.16406 0.20427 0.21647 0.25000

Eigenvalues --- 0.25000 0.25102 0.38651 0.44454 0.46136

Eigenvalues --- 0.46211 1.14947 1.375101000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.00000

RFO step: Lambda=-5.01079502D-06.

Quartic linear search produced a step of 0.65502.

Iteration 1 RMS(Cart)= 0.00415119 RMS(Int)= 0.00002993

Iteration 2 RMS(Cart)= 0.00000789 RMS(Int)= 0.00002849

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002849

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.64607	0.00053	0.00145	0.00073	0.00221	2.64828
R2	2.64754	0.00010	0.00103	0.00000	0.00106	2.64861
R3	2.62947	-0.00040	-0.00129	-0.00042	-0.00171	2.62776
R4	2.62946	-0.00040	-0.00128	-0.00042	-0.00169	2.62777
R5	6.95835	-0.00005	0.00433	0.00283	0.00713	6.96547
R6	6.50695	0.00015	0.00297	0.00529	0.00824	6.51519
R7	6.95524	-0.00004	0.00429	0.00359	0.00786	6.96309
R8	5.89282	-0.00005	0.02472	-0.00345	0.02128	5.91410
R9	5.38533	0.00013	0.02420	-0.00201	0.02220	5.40753
R10	5.89328	-0.00005	0.02244	-0.00331	0.01914	5.91242
R11	5.92054	-0.00008	-0.02025	0.00935	-0.01088	5.90965
R12	5.41255	0.00011	-0.02222	0.01256	-0.00966	5.40289
R13	5.91575	-0.00007	-0.01800	0.01056	-0.00743	5.90833
R14	2.16268	-0.00006	-0.00011	-0.00003	-0.00015	2.16253
R15	2.16265	-0.00008	-0.00016	-0.00001	-0.00018	2.16247
A1	1.88846	0.00004	-0.00107	0.00037	-0.00071	1.88774
A2	1.91565	-0.00021	-0.00019	-0.00074	-0.00091	1.91474
A3	1.91564	-0.00021	-0.00021	-0.00072	-0.00091	1.91472
A4	1.91520	-0.00013	-0.00004	-0.00051	-0.00054	1.91467
A5	1.91518	-0.00012	-0.00004	-0.00049	-0.00052	1.91466
A6	1.91355	0.00062	0.00153	0.00205	0.00352	1.91707
A7	2.49989	-0.00032	-0.00088	-0.00117	-0.00211	2.49779
A8	2.18427	-0.00031	-0.00068	-0.00105	-0.00176	2.18251
A9	1.86847	-0.00030	-0.00047	-0.00089	-0.00137	1.86710
A10	1.86972	-0.00030	-0.00047	-0.00090	-0.00139	1.86833
A11	2.18535	-0.00031	-0.00070	-0.00102	-0.00174	2.18361
A12	2.50115	-0.00032	-0.00093	-0.00118	-0.00214	2.49901
A13	0.63143	-0.00001	-0.00047	-0.00028	-0.00075	0.63068
A14	0.75058	-0.00002	-0.00325	0.00048	-0.00275	0.74784

A15	0.74724	-0.00001	0.00244	-0.00129	0.00116	0.74841
A16	0.74292	0.00011	-0.00013	-0.00019	-0.00039	0.74253
A17	0.81674	0.00010	0.00003	-0.00063	-0.00068	0.81606
A18	0.74321	0.00011	-0.00015	-0.00028	-0.00048	0.74273
A19	3.07845	0.00011	-0.00127	0.00131	0.00004	3.07849
A20	3.21668	-0.00012	0.00092	-0.00125	-0.00033	3.21635
D1	-1.41757	0.00002	0.00225	-0.00162	0.00061	-1.41696
D2	1.42080	-0.00003	-0.00472	0.00092	-0.00378	1.41702
D3	1.41620	-0.00002	0.00249	-0.00121	0.00128	1.41749
D4	-1.41370	0.00002	-0.00497	0.00074	-0.00423	-1.41793

Item	Value	Threshold	Converged?
Maximum Force	0.000616	0.000450	NO
RMS Force	0.000216	0.000300	YES
Maximum Displacement	0.017750	0.001800	NO
RMS Displacement	0.004150	0.001200	NO

Predicted change in Energy=-5.118040D-06

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Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.143382	0.123829	0.000322
2	9	0	1.540917	0.019732	0.003443
3	9	0	-0.193309	1.484368	-0.002571
4	9	0	-0.374699	-0.484907	1.138152
5	9	0	-0.369868	-0.488540	-1.137758
6	8	0	2.404708	2.801896	-1.140177
7	6	0	2.365470	2.759900	0.002740
8	8	0	2.398376	2.803387	1.145771

Distance matrix (angstroms):

		1	2	3	4	5
1	B	0.000000				
2	F	1.401411	0.000000			
3	F	1.401583	2.269964	0.000000		
4	F	1.390548	2.282939	2.283023	0.000000	
5	F	1.390557	2.282933	2.283022	2.275918	0.000000
6	O	3.685970	3.129606	3.127254	4.870212	4.304096
7	C	3.447688	2.861539	2.859084	4.396187	4.397178
8	O	3.684709	3.128719	3.126553	4.301498	4.869750
		6	7	8		
6	O	0.000000				
7	C	1.144361	0.000000			
8	O	2.285957	1.144331	0.000000		

Stoichiometry CBF402(1-)

Framework group C1[X(CBF402)]

Deg. of freedom 18

Full point group C1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)
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Number	Number	Type	X	Y	Z
1	5	0	-1.224736	-0.000087	0.000040
2	9	0	-0.403574	-0.000367	1.135666
3	9	0	-0.401502	-0.000614	-1.134297
4	9	0	-2.023367	1.138250	-0.000835
5	9	0	-2.024459	-1.137668	-0.000583
6	8	0	2.279634	-1.142789	0.000016
7	6	0	2.222952	0.000167	-0.000012
8	8	0	2.278128	1.143167	0.000023

Rotational constants (GHZ): 3.6113366 1.1170882 1.0220908
 Standard basis: 6-31+G(d) (6D, 7F)
 There are 152 symmetry adapted basis functions of A symmetry.
 Integral buffers will be 262144 words long.
 Raffanetti 1 integral format.
 Two-electron integral symmetry is turned on.
 152 basis functions, 256 primitive gaussians, 152 cartesian basis functions
 32 alpha electrons 32 beta electrons
 nuclear repulsion energy 371.4071915849 Hartrees.
 NAToms= 8 NActive= 8 NUniq= 8 SFac= 7.50D-01 NATFMM= 80 NAOKFM=F
 Big=F
 One-electron integrals computed using PRISM.
 NBasis= 152 RedAO= T NBF= 152
 NBsUse= 152 1.00D-06 NBFU= 152
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
 Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 SCF Done: E(RHF) = -610.409005894 A.U. after 12 cycles
 Convrg = 0.4829D-08 -V/T = 2.0028
 S**2 = 0.0000
 ***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	5	-0.000293678	-0.000271615	-0.000004410
2	9	0.000097698	-0.000100193	-0.000000487

3	9	-0.000108940	0.000010575	-0.000000726
4	9	0.000155195	0.000186734	0.000137495
5	9	0.000155999	0.000187215	-0.000135843
6	8	-0.000142396	-0.000172724	-0.000064344
7	6	0.000271579	0.000322625	-0.000029181
8	8	-0.000135457	-0.000162617	0.000097495

Cartesian Forces: Max 0.000322625 RMS 0.000162602

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Internal Forces: Max 0.000260404 RMS 0.000089750
 Search for a local minimum.
 Step number 15 out of a maximum of 49
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points 10 11 12 13 14
 15

Trust test= 1.26D+00 RLast= 4.30D-02 DXMaxT set to 1.00D+00

Eigenvalues ---	0.00056	0.00099	0.00547	0.00954	0.07215
Eigenvalues ---	0.09953	0.13410	0.16420	0.20503	0.25000
Eigenvalues ---	0.25000	0.25096	0.39386	0.45078	0.46111
Eigenvalues ---	0.46211	1.16378	1.37538	1000.00000	1000.00000
Eigenvalues ---	1000.00000	1000.00000	1000.00000	1000.00000	1000.00000
Eigenvalues ---	1000.00000	1000.00000	1000.00000	1000.00000	1000.00000
Eigenvalues ---	1000.00000	1000.00000	1000.00000	1000.00000	1000.00000
Eigenvalues ---	1000.00000	1000.00000	1000.00000	1000.00000	1000.00000

RFO step: Lambda=-1.30792918D-06.
 Quartic linear search produced a step of 0.33979.
 Iteration 1 RMS(Cart)= 0.00059243 RMS(Int)= 0.00000237
 Iteration 2 RMS(Cart)= 0.00000033 RMS(Int)= 0.00000235

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.64828	0.00010	0.00075	-0.00003	0.00072	2.64901
R2	2.64861	0.00003	0.00036	-0.00015	0.00021	2.64882
R3	2.62776	-0.00003	-0.00058	0.00015	-0.00044	2.62732
R4	2.62777	-0.00003	-0.00058	0.00014	-0.00044	2.62733
R5	6.96547	-0.00008	0.00242	-0.00223	0.00018	6.96566
R6	6.51519	0.00007	0.00280	-0.00073	0.00207	6.51725
R7	6.96309	-0.00008	0.00267	-0.00180	0.00087	6.96396
R8	5.91410	-0.00003	0.00723	-0.00746	-0.00023	5.91387
R9	5.40753	0.00010	0.00754	-0.00637	0.00117	5.40870
R10	5.91242	-0.00003	0.00650	-0.00663	-0.00012	5.91230
R11	5.90965	-0.00003	-0.00370	0.00476	0.00106	5.91071
R12	5.40289	0.00011	-0.00328	0.00644	0.00316	5.40604
R13	5.90833	-0.00002	-0.00252	0.00470	0.00218	5.91050
R14	2.16253	0.00008	-0.00005	0.00002	-0.00003	2.16250
R15	2.16247	0.00011	-0.00006	0.00005	-0.00001	2.16246
A1	1.88774	0.00004	-0.00024	0.00053	0.00028	1.88803
A2	1.91474	-0.00008	-0.00031	-0.00031	-0.00062	1.91412
A3	1.91472	-0.00007	-0.00031	-0.00030	-0.00061	1.91412
A4	1.91467	-0.00008	-0.00018	-0.00030	-0.00048	1.91419
A5	1.91466	-0.00008	-0.00018	-0.00030	-0.00047	1.91419
A6	1.91707	0.00026	0.00120	0.00067	0.00186	1.91893
A7	2.49779	-0.00011	-0.00072	-0.00022	-0.00094	2.49685
A8	2.18251	-0.00013	-0.00060	-0.00034	-0.00094	2.18156

A9	1.86710	-0.00015	-0.00046	-0.00044	-0.00091	1.86619
A10	1.86833	-0.00015	-0.00047	-0.00045	-0.00092	1.86741
A11	2.18361	-0.00013	-0.00059	-0.00033	-0.00092	2.18269
A12	2.49901	-0.00011	-0.00073	-0.00023	-0.00095	2.49806
A13	0.63068	0.00004	-0.00025	0.00022	-0.00003	0.63065
A14	0.74784	0.00004	-0.00093	0.00097	0.00004	0.74788
A15	0.74841	0.00004	0.00039	-0.00059	-0.00019	0.74821
A16	0.74253	0.00003	-0.00013	0.00030	0.00016	0.74270
A17	0.81606	0.00002	-0.00023	0.00013	-0.00010	0.81596
A18	0.74273	0.00003	-0.00016	0.00025	0.00008	0.74281
A19	3.07849	0.00012	0.00001	0.00095	0.00096	3.07946
A20	3.21635	-0.00014	-0.00011	-0.00093	-0.00105	3.21530
D1	-1.41696	0.00002	0.00021	-0.00067	-0.00047	-1.41743
D2	1.41702	-0.00002	-0.00129	0.00110	-0.00019	1.41683
D3	1.41749	-0.00002	0.00044	-0.00082	-0.00039	1.41710
D4	-1.41793	0.00002	-0.00144	0.00137	-0.00006	-1.41799

Item	Value	Threshold	Converged?
Maximum Force	0.000260	0.000450	YES
RMS Force	0.000090	0.000300	YES
Maximum Displacement	0.001952	0.001800	NO
RMS Displacement	0.000592	0.001200	YES

Predicted change in Energy=-1.099954D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.142925	0.123558	0.000298
2	9	0	1.540856	0.019602	0.003558
3	9	0	-0.194342	1.484069	-0.002705
4	9	0	-0.374244	-0.484397	1.138678
5	9	0	-0.369211	-0.488180	-1.138341
6	8	0	2.404373	2.801668	-1.140175
7	6	0	2.365983	2.760243	0.002776
8	8	0	2.398637	2.803105	1.145833

Distance matrix (angstroms):

		1	2	3	4	5
1	B	0.000000				
2	F	1.401794	0.000000			
3	F	1.401695	2.270597	0.000000		
4	F	1.390318	2.282569	2.282538	0.000000	
5	F	1.390325	2.282571	2.282545	2.277028	0.000000
6	O	3.686068	3.129485	3.127815	4.869508	4.303007
7	C	3.448783	2.862158	2.860754	4.396227	4.397237
8	O	3.685167	3.128653	3.127704	4.300767	4.869393
		6	7	8		
6	O	0.000000				
7	C	1.144346	0.000000			
8	O	2.286016	1.144326	0.000000		

Stoichiometry CBF402(1-)

Framework group C1[X(CBF402)]

Deg. of freedom 18

Full point group C1
 Largest Abelian subgroup C1 NOp 1
 Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-1.225248	-0.000062	-0.000042
2	9	0	-0.403641	0.000005	1.135734
3	9	0	-0.402491	-0.000969	-1.134862
4	9	0	-2.022651	1.138855	-0.000905
5	9	0	-2.023816	-1.138172	0.000077
6	8	0	2.279189	-1.142874	-0.000017
7	6	0	2.223534	0.000118	-0.000003
8	8	0	2.278114	1.143142	-0.000004

Rotational constants (GHZ): 3.6093387 1.1172110 1.0221465

Standard basis: 6-31+G(d) (6D, 7F)

There are 152 symmetry adapted basis functions of A symmetry.

Integral buffers will be 262144 words long.

Raffenetti 1 integral format.

Two-electron integral symmetry is turned on.

152 basis functions, 256 primitive gaussians, 152 cartesian basis functions

32 alpha electrons 32 beta electrons

nuclear repulsion energy 371.3954195878 Hartrees.

NAtoms= 8 NActive= 8 NUniq= 8 SFac= 7.50D-01 NATFMM= 80 NAOKFM=F
 Big=F

One-electron integrals computed using PRISM.

NBasis= 152 RedAO= T NBF= 152

NBsUse= 152 1.00D-06 NBFU= 152

Initial guess read from the read-write file:

Initial guess orbital symmetries:

Occupied	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
Virtual	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RHF) = -610.409007223 A.U. after 7 cycles

Convrg = 0.7902D-08 -V/T = 2.0028

S**2 = 0.0000

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	5	0.000080304	0.000013747	-0.000002438
2	9	-0.000039305	-0.000032943	-0.000002056
3	9	-0.000048728	0.000000392	0.000000567
4	9	0.000007370	0.000015431	0.000074844
5	9	0.000009028	0.000017509	-0.000072883
6	8	-0.000047441	-0.000065956	-0.000059210
7	6	0.000084256	0.000110036	-0.000022339
8	8	-0.000045484	-0.000058216	0.000083514

Cartesian Forces: Max 0.000110036 RMS 0.000052238

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Berny optimization.

Internal Forces: Max 0.000078951 RMS 0.000031430

Search for a local minimum.

Step number 16 out of a maximum of 49

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Update second derivatives using D2CorX and points 10 11 12 13 14

15 16

Trust test= 1.21D+00 RLast= 5.98D-03 DXMaxT set to 1.00D+00

Eigenvalues --- 0.00058 0.00096 0.00549 0.00952 0.07157

Eigenvalues --- 0.08564 0.12516 0.16424 0.20497 0.25000

Eigenvalues --- 0.25000 0.25080 0.39592 0.45387 0.46138

Eigenvalues --- 0.46212 1.15611 1.375301000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.00000

RFO step: Lambda=-1.38365614D-07.

Quartic linear search produced a step of 0.26288.

Iteration 1 RMS(Cart)= 0.00060664 RMS(Int)= 0.00000015

Iteration 2 RMS(Cart)= 0.00000012 RMS(Int)= 0.00000007

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.64901	-0.00003	0.00019	-0.00022	-0.00003	2.64898
R2	2.64882	0.00002	0.00006	-0.00006	0.00000	2.64882
R3	2.62732	0.00005	-0.00011	0.00019	0.00008	2.62740
R4	2.62733	0.00005	-0.00011	0.00018	0.00007	2.62740
R5	6.96566	-0.00004	0.00005	-0.00237	-0.00232	6.96333
R6	6.51725	0.00001	0.00054	-0.00210	-0.00156	6.51569
R7	6.96396	-0.00004	0.00023	-0.00220	-0.00197	6.96199
R8	5.91387	-0.00001	-0.00006	-0.00317	-0.00323	5.91064
R9	5.40870	0.00004	0.00031	-0.00280	-0.00249	5.40620
R10	5.91230	0.00000	-0.00003	-0.00256	-0.00259	5.90971
R11	5.91071	0.00000	0.00028	-0.00046	-0.00018	5.91053
R12	5.40604	0.00004	0.00083	-0.00038	0.00045	5.40650
R13	5.91050	0.00000	0.00057	-0.00076	-0.00019	5.91031
R14	2.16250	0.00006	-0.00001	0.00002	0.00002	2.16252
R15	2.16246	0.00008	0.00000	0.00004	0.00003	2.16250
A1	1.88803	0.00002	0.00007	0.00024	0.00032	1.88834
A2	1.91412	-0.00001	-0.00016	-0.00001	-0.00018	1.91395

A3	1.91412	-0.00001	-0.00016	-0.00001	-0.00017	1.91395
A4	1.91419	-0.00002	-0.00013	-0.00005	-0.00018	1.91400
A5	1.91419	-0.00003	-0.00012	-0.00006	-0.00018	1.91401
A6	1.91893	0.00005	0.00049	-0.00010	0.00039	1.91932
A7	2.49685	-0.00001	-0.00025	0.00017	-0.00008	2.49677
A8	2.18156	-0.00002	-0.00025	0.00005	-0.00020	2.18137
A9	1.86619	-0.00004	-0.00024	-0.00006	-0.00030	1.86590
A10	1.86741	-0.00004	-0.00024	-0.00007	-0.00031	1.86710
A11	2.18269	-0.00003	-0.00024	0.00005	-0.00019	2.18250
A12	2.49806	-0.00001	-0.00025	0.00016	-0.00009	2.49797
A13	0.63065	0.00003	-0.00001	0.00023	0.00022	0.63087
A14	0.74788	0.00003	0.00001	0.00040	0.00041	0.74829
A15	0.74821	0.00003	-0.00005	0.00010	0.00005	0.74826
A16	0.74270	0.00000	0.00004	0.00027	0.00031	0.74300
A17	0.81596	0.00000	-0.00003	0.00028	0.00026	0.81622
A18	0.74281	0.00000	0.00002	0.00025	0.00027	0.74308
A19	3.07946	0.00004	0.00025	0.00018	0.00044	3.07989
A20	3.21530	-0.00006	-0.00028	-0.00023	-0.00050	3.21480
D1	-1.41743	0.00001	-0.00012	0.00016	0.00004	-1.41739
D2	1.41683	-0.00001	-0.00005	0.00031	0.00026	1.41709
D3	1.41710	-0.00001	-0.00010	-0.00004	-0.00014	1.41696
D4	-1.41799	0.00001	-0.00002	0.00057	0.00055	-1.41744

Item	Value	Threshold	Converged?
Maximum Force	0.000079	0.000450	YES
RMS Force	0.000031	0.000300	YES
Maximum Displacement	0.001765	0.001800	YES
RMS Displacement	0.000607	0.001200	YES

Predicted change in Energy=-1.293979D-07

Optimization completed.

-- Stationary point found.

! Optimized Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.
! R1	R(1,2)	1.4018	-DE/DX = 0.0
! R2	R(1,3)	1.4017	-DE/DX = 0.0
! R3	R(1,4)	1.3903	-DE/DX = 0.0001
! R4	R(1,5)	1.3903	-DE/DX = 0.0
! R5	R(1,6)	3.6861	-DE/DX = 0.0
! R6	R(1,7)	3.4488	-DE/DX = 0.0
! R7	R(1,8)	3.6852	-DE/DX = 0.0
! R8	R(2,6)	3.1295	-DE/DX = 0.0

!	R9	R(2, 7)	2.8622	-DE/DX =	0.0
!					
!	R10	R(2, 8)	3.1287	-DE/DX =	0.0
!					
!	R11	R(3, 6)	3.1278	-DE/DX =	0.0
!					
!	R12	R(3, 7)	2.8608	-DE/DX =	0.0
!					
!	R13	R(3, 8)	3.1277	-DE/DX =	0.0
!					
!	R14	R(6, 7)	1.1443	-DE/DX =	0.0001
!					
!	R15	R(7, 8)	1.1443	-DE/DX =	0.0001
!					
!	A1	A(2, 1, 3)	108.1759	-DE/DX =	0.0
!					
!	A2	A(2, 1, 4)	109.6712	-DE/DX =	0.0
!					
!	A3	A(2, 1, 5)	109.6709	-DE/DX =	0.0
!					
!	A4	A(3, 1, 4)	109.6747	-DE/DX =	0.0
!					
!	A5	A(3, 1, 5)	109.6749	-DE/DX =	0.0
!					
!	A6	A(4, 1, 5)	109.9467	-DE/DX =	0.0001
!					
!	A7	A(4, 1, 6)	143.0588	-DE/DX =	0.0
!					
!	A8	A(4, 1, 7)	124.9944	-DE/DX =	0.0
!					
!	A9	A(4, 1, 8)	106.9251	-DE/DX =	0.0
!					
!	A10	A(5, 1, 6)	106.9945	-DE/DX =	0.0
!					
!	A11	A(5, 1, 7)	125.0588	-DE/DX =	0.0
!					
!	A12	A(5, 1, 8)	143.1282	-DE/DX =	0.0
!					
!	A13	A(6, 1, 8)	36.1337	-DE/DX =	0.0
!					
!	A14	A(6, 2, 8)	42.8505	-DE/DX =	0.0
!					
!	A15	A(6, 3, 8)	42.8693	-DE/DX =	0.0
!					
!	A16	A(2, 6, 3)	42.5533	-DE/DX =	0.0
!					
!	A17	A(2, 7, 3)	46.751	-DE/DX =	0.0
!					
!	A18	A(2, 8, 3)	42.56	-DE/DX =	0.0
!					
!	A19	L(6, 7, 8, -2, -1)	176.4399	-DE/DX =	0.0
!					
!	A20	L(6, 7, 8, -1, -2)	184.2231	-DE/DX =	-0.0001
!					

```

! D1      D(8,2,6,3)          -81.2126          -DE/DX =    0.0
!
! D2      D(6,2,8,3)           81.1783           -DE/DX =    0.0
!
! D3      D(8,3,6,2)           81.1938           -DE/DX =    0.0
!
! D4      D(6,3,8,2)          -81.2449           -DE/DX =    0.0
!

```


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Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.142925	0.123558	0.000298
2	9	0	1.540856	0.019602	0.003558
3	9	0	-0.194342	1.484069	-0.002705
4	9	0	-0.374244	-0.484397	1.138678
5	9	0	-0.369211	-0.488180	-1.138341
6	8	0	2.404373	2.801668	-1.140175
7	6	0	2.365983	2.760243	0.002776
8	8	0	2.398637	2.803105	1.145833

Distance matrix (angstroms):

		1	2	3	4	5
1	B	0.000000				
2	F	1.401794	0.000000			
3	F	1.401695	2.270597	0.000000		
4	F	1.390318	2.282569	2.282538	0.000000	
5	F	1.390325	2.282571	2.282545	2.277028	0.000000
6	O	3.686068	3.129485	3.127815	4.869508	4.303007
7	C	3.448783	2.862158	2.860754	4.396227	4.397237
8	O	3.685167	3.128653	3.127704	4.300767	4.869393
		6	7	8		
6	O	0.000000				
7	C	1.144346	0.000000			
8	O	2.286016	1.144326	0.000000		

Stoichiometry CBF402(1-)

Framework group C1[X(CBF402)]

Deg. of freedom 18

Full point group C1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-1.225248	-0.000062	-0.000042
2	9	0	-0.403641	0.000005	1.135734
3	9	0	-0.402491	-0.000969	-1.134862
4	9	0	-2.022651	1.138855	-0.000905

5	9	0	-2.023816	-1.138172	0.000077
6	8	0	2.279189	-1.142874	-0.000017
7	6	0	2.223534	0.000118	-0.000003
8	8	0	2.278114	1.143142	-0.000004

 Rotational constants (GHZ): 3.6093387 1.1172110 1.0221465

Population analysis using the SCF density.

Orbital symmetries:

Occupied	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)				
Virtual	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)

The electronic state is 1-A.

Alpha occ. eigenvalues	--	-26.08039	-26.08035	-26.07642	-26.07641	-
20.52095						
Alpha occ. eigenvalues	--	-20.52093	-11.32658	-7.52435	-1.42168	-
1.40403						
Alpha occ. eigenvalues	--	-1.35977	-1.35972	-1.35770	-1.34896	-
0.65741						
Alpha occ. eigenvalues	--	-0.61149	-0.60458	-0.58142	-0.58066	-
0.54059						
Alpha occ. eigenvalues	--	-0.54009	-0.53997	-0.45842	-0.45732	-
0.42226						
Alpha occ. eigenvalues	--	-0.42018	-0.41872	-0.40400	-0.40242	-
0.39482						
Alpha occ. eigenvalues	--	-0.39245	-0.39086			
Alpha virt. eigenvalues	--	0.16915	0.20846	0.21169	0.21195	
0.22875						
Alpha virt. eigenvalues	--	0.22973	0.23966	0.28056	0.36201	
0.36302						
Alpha virt. eigenvalues	--	0.37894	0.40971	0.41694	0.42522	
0.46453						
Alpha virt. eigenvalues	--	0.47895	0.48773	0.49625	0.50921	
0.51157						
Alpha virt. eigenvalues	--	0.53679	0.53836	0.54612	0.55084	
0.58167						
Alpha virt. eigenvalues	--	0.58937	0.59664	0.62714	0.62764	
0.62923						
Alpha virt. eigenvalues	--	0.66229	0.71224	0.72801	0.74495	
0.75306						

Alpha virt. eigenvalues --	0.75732	0.79446	0.79840	0.86886
1.01591				
Alpha virt. eigenvalues --	1.02732	1.07557	1.10258	1.10423
1.12587				
Alpha virt. eigenvalues --	1.35063	1.38596	1.48993	1.52828
1.56350				
Alpha virt. eigenvalues --	1.59912	1.60496	1.62081	1.65283
1.69091				
Alpha virt. eigenvalues --	1.74621	1.80577	1.80883	1.84489
1.86703				
Alpha virt. eigenvalues --	1.90694	2.02925	2.04309	2.05807
2.06048				
Alpha virt. eigenvalues --	2.08119	2.09673	2.12104	2.12105
2.13127				
Alpha virt. eigenvalues --	2.14960	2.16543	2.18081	2.18438
2.24753				
Alpha virt. eigenvalues --	2.26360	2.26998	2.28662	2.34215
2.34430				
Alpha virt. eigenvalues --	2.34555	2.37064	2.39575	2.45197
2.47294				
Alpha virt. eigenvalues --	2.48348	2.48540	2.49057	2.51627
2.51846				
Alpha virt. eigenvalues --	2.52126	2.52203	2.55131	2.57652
2.62189				
Alpha virt. eigenvalues --	2.64383	2.71606	2.82824	3.06382
3.06737				
Alpha virt. eigenvalues --	3.08932	3.32121	3.34202	3.41690
3.50948				
Alpha virt. eigenvalues --	3.51410	3.62681	3.63301	3.63957
3.81404				
Alpha virt. eigenvalues --	3.90282	3.92335	4.37233	4.69179
5.20406				
Alpha virt. eigenvalues --	5.42403	5.93054	5.95449	6.10086
6.54131				

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	B	2.571850	0.122690	0.122684	0.157189	0.157148	-0.000394
2	F	0.122690	9.612146	0.015781	-0.003760	-0.003747	-0.001872
3	F	0.122684	0.015781	9.612124	-0.003749	-0.003725	-0.001886
4	F	0.157189	-0.003760	-0.003749	9.545541	-0.010068	-0.000080
5	F	0.157148	-0.003747	-0.003725	-0.010068	9.545578	-0.001191
6	O	-0.000394	-0.001872	-0.001886	-0.000080	-0.001191	8.016598
7	C	-0.014577	0.002222	0.002169	0.002551	0.002560	0.526452
8	O	-0.000378	-0.001881	-0.001888	-0.001189	-0.000081	-0.105072
		7	8				
1	B	-0.014577	-0.000378				
2	F	0.002222	-0.001881				
3	F	0.002169	-0.001888				
4	F	0.002551	-0.001189				
5	F	0.002560	-0.000081				
6	O	0.526452	-0.105072				
7	C	4.114877	0.526486				
8	O	0.526486	8.016495				

Mulliken atomic charges:

1

```

1 B    1.883788
2 F    -0.741579
3 F    -0.741511
4 F    -0.686435
5 F    -0.686475
6 O    -0.432554
7 C     0.837259
8 O    -0.432493
Sum of Mulliken charges= -1.00000
Atomic charges with hydrogens summed into heavy atoms:
      1
1 B    1.883788
2 F    -0.741579
3 F    -0.741511
4 F    -0.686435
5 F    -0.686475
6 O    -0.432554
7 C     0.837259
8 O    -0.432493
Sum of Mulliken charges= -1.00000
Electronic spatial extent (au): <R**2>= 1058.2475
Charge= -1.0000 electrons
Dipole moment (field-independent basis, Debye):
  X=    4.8593    Y=    0.0006    Z=   -0.0007    Tot=    4.8593
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=   -55.8016  YY=   -52.0215  ZZ=   -46.1207
  XY=    0.0024  XZ=    0.0002  YZ=    0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=   -4.4870  YY=   -0.7069  ZZ=    5.1939
  XY=    0.0024  XZ=    0.0002  YZ=    0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=   11.4316  YYY=   -0.0086  ZZZ=   -0.0096  XYY=   -4.3745
  XXY=    0.0192  XXZ=    0.0048  XZZ=   -0.9411  YZZ=    0.0031
  YYZ=    0.0024  XYZ=   -0.0045
Hexadecapole moment (field-independent basis, Debye-Ang**3):
  XXXX=  -894.1357  YYYY=  -214.2033  ZZZZ=  -121.2904  XXXY=    0.0218
  XXXZ=   -0.0163  YYYY=    0.0071  YYYZ=    0.0030  ZZZX=    0.0083
  ZZZY=   -0.0028  XXYY=  -223.7974  XXZZ=  -151.8146  YYZZ=  -53.3540
  XXYZ=    0.0108  YXXZ=   -0.0052  ZZXY=   -0.0006
N-N= 3.713954195878D+02 E-N=-2.209783673543D+03 KE= 6.087265832957D+02
1|1|UNPC-UNK|FOpt|RHF|6-31+G(d)|C1B1F402(1-)|PCUSER|11-Apr-2008|0||# o
pt freq=raman hf/6-31+g(d) geom=connectivity|BC_HF631+G(d)||-1,1|B,0.
1429253057,0.1235578352,0.0002977042|F,1.5408555403,0.019602051,0.0035
575438|F,-0.1943418183,1.4840686308,-0.0027046663|F,-0.3742444306,-0.4
843972277,1.1386782263|F,-0.3692113513,-0.4881799099,-1.1383408375|0,2
.404373025,2.8016677221,-1.1401752996|C,2.365983095,2.7602431581,0.002
7763631|0,2.3986369343,2.8031049604,1.1458329172||Version=IA32W-G03Rev
D.01|State=1-A|HF=-610.4090072|RMSD=7.902e-009|RMSF=5.224e-005|Thermal
=0.|Dipole=1.2320845,1.4618042,0.0015119|PG=C01 [X(C1B1F402)]||@

```

TOWERING GENIUS DISDAINS A BEATEN PATH. IT SEEKS
REGIONS HITHERTO UNEXPLORED.

-- ABRAHAM LINCOLN

Job cpu time: 0 days 0 hours 28 minutes 15.0 seconds.
 File lengths (MBytes): RWF= 21 Int= 0 D2E= 0 Chk= 5
 Scr= 1

Normal termination of Gaussian 03 at Fri Apr 11 22:02:49 2008.
 Link1: Proceeding to internal job step number 2.

 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31+G(d) Freq

1/10=4, 29=7, 30=1, 38=1, 40=1, 46=1/1, 3;
 2/40=1/2;
 3/5=1, 6=6, 7=11, 11=1, 16=1, 25=1, 30=1, 70=2, 71=2/1, 2, 3;
 4/5=1, 7=1/1;
 5/5=2, 38=6/2;
 8/6=4, 10=90, 11=11/1;
 10/13=10/2;
 11/6=2, 8=1, 9=11, 15=111, 16=1/1, 2, 10;
 10/6=1/2;
 6/7=2, 8=2, 9=2, 10=2, 18=1, 28=1/1;
 7/8=1, 10=1, 25=1/1, 2, 3, 16;
 1/10=4, 30=1, 46=1/3;
 99//99;

BC_HF631+G(d)

Redundant internal coordinates taken from checkpoint file:

BC_HF631+G(d).chk

Charge = -1 Multiplicity = 1

B, 0, 0.1429253057, 0.1235578352, 0.0002977042
 F, 0, 1.5408555403, 0.019602051, 0.0035575438
 F, 0, -0.1943418183, 1.4840686308, -0.0027046663
 F, 0, -0.3742444306, -0.4843972277, 1.1386782263
 F, 0, -0.3692113513, -0.4881799099, -1.1383408375
 O, 0, 2.404373025, 2.8016677221, -1.1401752996
 C, 0, 2.365983095, 2.7602431581, 0.0027763631
 O, 0, 2.3986369343, 2.8031049604, 1.1458329172
 Recover connectivity data from disk.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Initialization pass.

 ! Initial Parameters !
 ! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.
! R1	R(1,2)	1.4018	calculate D2E/DX2
analytically !			
! R2	R(1,3)	1.4017	calculate D2E/DX2
analytically !			
! R3	R(1,4)	1.3903	calculate D2E/DX2
analytically !			

! R4 R(1,5)	1.3903	calculate D2E/DX2
analytically !		
! R5 R(1,6)	3.6861	calculate D2E/DX2
analytically !		
! R6 R(1,7)	3.4488	calculate D2E/DX2
analytically !		
! R7 R(1,8)	3.6852	calculate D2E/DX2
analytically !		
! R8 R(2,6)	3.1295	calculate D2E/DX2
analytically !		
! R9 R(2,7)	2.8622	calculate D2E/DX2
analytically !		
! R10 R(2,8)	3.1287	calculate D2E/DX2
analytically !		
! R11 R(3,6)	3.1278	calculate D2E/DX2
analytically !		
! R12 R(3,7)	2.8608	calculate D2E/DX2
analytically !		
! R13 R(3,8)	3.1277	calculate D2E/DX2
analytically !		
! R14 R(6,7)	1.1443	calculate D2E/DX2
analytically !		
! R15 R(7,8)	1.1443	calculate D2E/DX2
analytically !		
! A1 A(2,1,3)	108.1759	calculate D2E/DX2
analytically !		
! A2 A(2,1,4)	109.6712	calculate D2E/DX2
analytically !		
! A3 A(2,1,5)	109.6709	calculate D2E/DX2
analytically !		
! A4 A(3,1,4)	109.6747	calculate D2E/DX2
analytically !		
! A5 A(3,1,5)	109.6749	calculate D2E/DX2
analytically !		
! A6 A(4,1,5)	109.9467	calculate D2E/DX2
analytically !		
! A7 A(4,1,6)	143.0588	calculate D2E/DX2
analytically !		
! A8 A(4,1,7)	124.9944	calculate D2E/DX2
analytically !		
! A9 A(4,1,8)	106.9251	calculate D2E/DX2
analytically !		
! A10 A(5,1,6)	106.9945	calculate D2E/DX2
analytically !		
! A11 A(5,1,7)	125.0588	calculate D2E/DX2
analytically !		
! A12 A(5,1,8)	143.1282	calculate D2E/DX2
analytically !		
! A13 A(6,1,8)	36.1337	calculate D2E/DX2
analytically !		
! A14 A(6,2,8)	42.8505	calculate D2E/DX2
analytically !		
! A15 A(6,3,8)	42.8693	calculate D2E/DX2
analytically !		

```

! A16  A(2,6,3)          42.5533      calculate D2E/DX2
analytically !
! A17  A(2,7,3)          46.751       calculate D2E/DX2
analytically !
! A18  A(2,8,3)          42.56        calculate D2E/DX2
analytically !
! A19  L(6,7,8,-2,-1)    176.4399    calculate D2E/DX2
analytically !
! A20  L(6,7,8,-1,-2)    184.2231    calculate D2E/DX2
analytically !
! D1    D(8,2,6,3)       -81.2126    calculate D2E/DX2
analytically !
! D2    D(6,2,8,3)       81.1783     calculate D2E/DX2
analytically !
! D3    D(8,3,6,2)       81.1938     calculate D2E/DX2
analytically !
! D4    D(6,3,8,2)       -81.2449    calculate D2E/DX2
analytically !

```

```

-----
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run= 2 maximum allowed number of steps= 2.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

```

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.142925	0.123558	0.000298
2	9	0	1.540856	0.019602	0.003558
3	9	0	-0.194342	1.484069	-0.002705
4	9	0	-0.374244	-0.484397	1.138678
5	9	0	-0.369211	-0.488180	-1.138341
6	8	0	2.404373	2.801668	-1.140175
7	6	0	2.365983	2.760243	0.002776
8	8	0	2.398637	2.803105	1.145833

Distance matrix (angstroms):

		1	2	3	4	5
1	B	0.000000				
2	F	1.401794	0.000000			
3	F	1.401695	2.270597	0.000000		
4	F	1.390318	2.282569	2.282538	0.000000	
5	F	1.390325	2.282571	2.282545	2.277028	0.000000
6	O	3.686068	3.129485	3.127815	4.869508	4.303007
7	C	3.448783	2.862158	2.860754	4.396227	4.397237
8	O	3.685167	3.128653	3.127704	4.300767	4.869393
		6	7	8		
6	O	0.000000				
7	C	1.144346	0.000000			
8	O	2.286016	1.144326	0.000000		

```

Stoichiometry CBF402(1-)
Framework group C1[X(CBF402)]
Deg. of freedom 18

```

Full point group C1
 Largest Abelian subgroup C1 NOp 1
 Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-1.225248	-0.000062	-0.000042
2	9	0	-0.403641	0.000005	1.135734
3	9	0	-0.402491	-0.000969	-1.134862
4	9	0	-2.022651	1.138855	-0.000905
5	9	0	-2.023816	-1.138172	0.000077
6	8	0	2.279189	-1.142874	-0.000017
7	6	0	2.223534	0.000118	-0.000003
8	8	0	2.278114	1.143142	-0.000004

Rotational constants (GHZ): 3.6093387 1.1172110 1.0221465

Standard basis: 6-31+G(d) (6D, 7F)

There are 152 symmetry adapted basis functions of A symmetry.

Integral buffers will be 262144 words long.

Raffenetti 1 integral format.

Two-electron integral symmetry is turned on.

152 basis functions, 256 primitive gaussians, 152 cartesian basis functions

32 alpha electrons 32 beta electrons

nuclear repulsion energy 371.3954195878 Hartrees.

NAtoms= 8 NActive= 8 NUniq= 8 SFac= 7.50D-01 NATFMM= 80 NAOKFM=F

Big=F

One-electron integrals computed using PRISM.

NBasis= 152 RedAO= T NBF= 152

NBsUse= 152 1.00D-06 NBFU= 152

Initial guess read from the checkpoint file:

BC_HF631+G(d).chk

Initial guess orbital symmetries:

Occupied	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)				
Virtual	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RHF) = -610.409007223 A.U. after 1 cycles

Convrg = 0.2147D-08 -V/T = 2.0028

S**2 = 0.0000

Range of M.O.s used for correlation: 1 152
 NBasis= 152 NAE= 32 NBE= 32 NFC= 0 NFV= 0
 NR0rb= 152 NOA= 32 NOB= 32 NVA= 120 NVB= 120

**** Warning!!: The largest alpha MO coefficient is 0.13672931D+02

Differentiating once with respect to electric field.
 with respect to dipole field.

Electric field/nuclear overlap derivatives assumed to be zero.

Integrals replicated using symmetry in FoFDir.

MinBra= 0 MaxBra= 2 Meth= 1.

IRaf= 0 NMat= 3 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2

JSym2E=2.

There are 3 degrees of freedom in the 1st order CPHF.

3 vectors were produced by pass 0.

AX will form 3 A0 Fock derivatives at one time.

3 vectors were produced by pass 1.

3 vectors were produced by pass 2.

3 vectors were produced by pass 3.

3 vectors were produced by pass 4.

3 vectors were produced by pass 5.

3 vectors were produced by pass 6.

3 vectors were produced by pass 7.

3 vectors were produced by pass 8.

3 vectors were produced by pass 9.

2 vectors were produced by pass 10.

2 vectors were produced by pass 11.

Inv2: IOpt= 1 Iter= 1 AM= 8.91D-16 Conv= 1.00D-12.

Inverted reduced A of dimension 34 with in-core refinement.

End of Minotr Frequency-dependent properties file 721 does not exist.

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

G2DrvN: will do 9 centers at a time, making 1 passes doing MaxLOS=2.

FoFDir/FoFCou used for L=0 through L=2.

DoAtom=TTTTTTTT

Differentiating once with respect to electric field.
 with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Integrals replicated using symmetry in FoFDir.

MinBra= 0 MaxBra= 2 Meth= 1.

IRaf= 0 NMat= 27 IRICut= 27 DoRegI=T DoRafI=T ISym2E= 2

JSym2E=2.

There are 27 degrees of freedom in the 1st order CPHF.

24 vectors were produced by pass 0.

AX will form 24 A0 Fock derivatives at one time.

24 vectors were produced by pass 1.

24 vectors were produced by pass 2.

24 vectors were produced by pass 3.

24 vectors were produced by pass 4.

24 vectors were produced by pass 5.

24 vectors were produced by pass 6.

13 vectors were produced by pass 7.

3 vectors were produced by pass 8.

1 vectors were produced by pass 9.

Inv2: IOpt= 1 Iter= 1 AM= 2.36D-15 Conv= 1.00D-12.

Inverted reduced A of dimension 185 with in-core refinement.
 Isotropic polarizability for W= 0.000000 30.50 Bohr**3.
 End of Minotr Frequency-dependent properties file 721 does not exist.

Population analysis using the SCF density.

Orbital symmetries:

Occupied	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)				
Virtual	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)
	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)	(A)

The electronic state is 1-A.

Alpha occ. eigenvalues	--	-26.08039	-26.08035	-26.07642	-26.07641	-
20.52095						
Alpha occ. eigenvalues	--	-20.52092	-11.32658	-7.52435	-1.42168	-
1.40403						
Alpha occ. eigenvalues	--	-1.35977	-1.35972	-1.35770	-1.34896	-
0.65741						
Alpha occ. eigenvalues	--	-0.61149	-0.60458	-0.58142	-0.58066	-
0.54059						
Alpha occ. eigenvalues	--	-0.54009	-0.53997	-0.45842	-0.45732	-
0.42226						
Alpha occ. eigenvalues	--	-0.42018	-0.41872	-0.40400	-0.40242	-
0.39482						
Alpha occ. eigenvalues	--	-0.39245	-0.39086			
Alpha virt. eigenvalues	--	0.16915	0.20846	0.21169	0.21195	
0.22875						
Alpha virt. eigenvalues	--	0.22973	0.23966	0.28056	0.36201	
0.36302						
Alpha virt. eigenvalues	--	0.37894	0.40971	0.41694	0.42522	
0.46453						
Alpha virt. eigenvalues	--	0.47895	0.48773	0.49625	0.50921	
0.51157						
Alpha virt. eigenvalues	--	0.53679	0.53836	0.54612	0.55084	
0.58167						
Alpha virt. eigenvalues	--	0.58937	0.59664	0.62714	0.62764	
0.62923						
Alpha virt. eigenvalues	--	0.66229	0.71224	0.72801	0.74495	
0.75306						
Alpha virt. eigenvalues	--	0.75732	0.79446	0.79840	0.86886	
1.01591						

Alpha virt. eigenvalues --	1.02732	1.07557	1.10258	1.10423
1.12587				
Alpha virt. eigenvalues --	1.35063	1.38596	1.48993	1.52828
1.56350				
Alpha virt. eigenvalues --	1.59912	1.60496	1.62081	1.65283
1.69091				
Alpha virt. eigenvalues --	1.74621	1.80577	1.80883	1.84489
1.86703				
Alpha virt. eigenvalues --	1.90694	2.02925	2.04309	2.05807
2.06048				
Alpha virt. eigenvalues --	2.08119	2.09673	2.12104	2.12105
2.13127				
Alpha virt. eigenvalues --	2.14960	2.16543	2.18081	2.18438
2.24753				
Alpha virt. eigenvalues --	2.26360	2.26998	2.28662	2.34215
2.34430				
Alpha virt. eigenvalues --	2.34555	2.37064	2.39575	2.45197
2.47294				
Alpha virt. eigenvalues --	2.48348	2.48540	2.49057	2.51627
2.51846				
Alpha virt. eigenvalues --	2.52126	2.52203	2.55131	2.57652
2.62189				
Alpha virt. eigenvalues --	2.64383	2.71606	2.82824	3.06382
3.06737				
Alpha virt. eigenvalues --	3.08932	3.32121	3.34202	3.41690
3.50948				
Alpha virt. eigenvalues --	3.51410	3.62681	3.63301	3.63957
3.81404				
Alpha virt. eigenvalues --	3.90282	3.92335	4.37233	4.69179
5.20406				
Alpha virt. eigenvalues --	5.42403	5.93054	5.95449	6.10086
6.54131				

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1 B	2.571850	0.122690	0.122684	0.157189	0.157148	-0.000394	
2 F	0.122690	9.612146	0.015781	-0.003760	-0.003747	-0.001872	
3 F	0.122684	0.015781	9.612124	-0.003749	-0.003725	-0.001886	
4 F	0.157189	-0.003760	-0.003749	9.545541	-0.010068	-0.000080	
5 F	0.157148	-0.003747	-0.003725	-0.010068	9.545578	-0.001191	
6 O	-0.000394	-0.001872	-0.001886	-0.000080	-0.001191	8.016598	
7 C	-0.014577	0.002222	0.002169	0.002551	0.002560	0.526452	
8 O	-0.000378	-0.001881	-0.001888	-0.001189	-0.000081	-0.105072	
	7	8					
1 B	-0.014577	-0.000378					
2 F	0.002222	-0.001881					
3 F	0.002169	-0.001888					
4 F	0.002551	-0.001189					
5 F	0.002560	-0.000081					
6 O	0.526452	-0.105072					
7 C	4.114877	0.526486					
8 O	0.526486	8.016495					

Mulliken atomic charges:

	1
1 B	1.883788
2 F	-0.741579

```

3 F -0.741511
4 F -0.686435
5 F -0.686475
6 O -0.432554
7 C 0.837259
8 O -0.432493
Sum of Mulliken charges= -1.00000
Atomic charges with hydrogens summed into heavy atoms:
1
1 B 1.883788
2 F -0.741579
3 F -0.741511
4 F -0.686435
5 F -0.686475
6 O -0.432554
7 C 0.837259
8 O -0.432493
Sum of Mulliken charges= -1.00000
APT atomic charges:
1
1 B 2.078265
2 F -0.771404
3 F -0.771415
4 F -0.763487
5 F -0.763507
6 O -0.805038
7 C 1.601568
8 O -0.804982
Sum of APT charges= -1.00000
APT Atomic charges with hydrogens summed into heavy atoms:
1
1 B 2.078265
2 F -0.771404
3 F -0.771415
4 F -0.763487
5 F -0.763507
6 O -0.805038
7 C 1.601568
8 O -0.804982
Sum of APT charges= -1.00000
Electronic spatial extent (au): <R**2>= 1058.2475
Charge= -1.0000 electrons
Dipole moment (field-independent basis, Debye):
X= 4.8593 Y= 0.0006 Z= -0.0007 Tot= 4.8593
Quadrupole moment (field-independent basis, Debye-Ang):
XX= -55.8016 YY= -52.0215 ZZ= -46.1207
XY= 0.0024 XZ= 0.0002 YZ= 0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
XX= -4.4870 YY= -0.7069 ZZ= 5.1939
XY= 0.0024 XZ= 0.0002 YZ= 0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
XXX= 11.4316 YYY= -0.0086 ZZZ= -0.0096 XYY= -4.3745
XXY= 0.0192 XXZ= 0.0048 XZZ= -0.9411 YZZ= 0.0031
YYZ= 0.0024 XYZ= -0.0045
Hexadecapole moment (field-independent basis, Debye-Ang**3):

```

```

XXXX= -894.1357 YYYY= -214.2033 ZZZZ= -121.2904 XXXY= 0.0218
XXXZ= -0.0163 YYYY= 0.0071 YYYZ= 0.0030 ZZZX= 0.0083
ZZZY= -0.0028 XXYY= -223.7973 XXZZ= -151.8146 YYZZ= -53.3540
XXYZ= 0.0108 YYXZ= -0.0052 ZZXY= -0.0006
N-N= 3.713954195878D+02 E-N=-2.209783673517D+03 KE= 6.087265832346D+02
Exact polarizability: 27.805 -0.006 38.379 0.001 0.000 25.326
Approx polarizability: 22.764 -0.007 36.733 0.000 0.000 22.621
Full mass-weighted force constant matrix:
Low frequencies --- -6.0394 -2.1919 -0.0005 0.0007 0.0008
1.9900
Low frequencies --- 26.7550 51.4827 62.3135
Diagonal vibrational polarizability:
52.8262779 27.6775101 22.2203981
Diagonal vibrational hyperpolarizability:
-72.2516207 -0.2761557 -0.0129554
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering
activities (A**4/AMU), depolarization ratios for plane and unpolarized
incident light, reduced masses (AMU), force constants (mDyne/A),
and normal coordinates:

```

		1 A			2 A			3 A		
Frequencies	--	26.7547			51.4827			62.3133		
Red. masses	--	18.1117			18.0681			16.7877		
Frc consts	--	0.0076			0.0282			0.0384		
IR Inten	--	0.3639			0.8935			0.0000		
Raman Activ	--	0.2030			0.0007			1.1980		
Depolar (P)	--	0.7500			0.7500			0.7500		
Depolar (U)	--	0.8571			0.8571			0.8571		
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	5	0.00	0.09	0.00	0.00	0.00	0.13	0.00	0.00	0.00
2	9	0.00	0.39	0.00	-0.43	0.00	0.43	0.00	-0.25	0.00
3	9	0.00	0.39	0.00	0.43	0.00	0.43	0.00	0.25	0.00
4	9	-0.42	-0.21	0.00	0.00	0.00	-0.19	0.00	0.00	0.26
5	9	0.42	-0.21	0.00	0.00	0.00	-0.18	0.00	0.00	-0.27
6	8	-0.27	-0.18	0.00	0.00	0.00	-0.24	0.00	0.00	0.61
7	6	0.00	-0.17	0.00	0.00	0.00	-0.25	0.00	0.00	0.00
8	8	0.27	-0.18	0.00	0.00	0.00	-0.24	0.00	0.00	-0.61

		4 A			5 A			6 A		
Frequencies	--	76.3790			116.5706			366.5290		
Red. masses	--	15.4586			15.9756			18.9976		
Frc consts	--	0.0531			0.1279			1.5037		
IR Inten	--	7.4947			0.0527			0.0000		
Raman Activ	--	0.0255			1.7736			0.2382		
Depolar (P)	--	0.6321			0.7500			0.7500		
Depolar (U)	--	0.7746			0.8571			0.8571		
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	5	0.24	0.00	0.00	0.00	0.11	0.00	0.00	0.00	0.00
2	9	0.24	0.00	0.00	0.00	0.16	0.00	0.00	-0.51	0.00
3	9	0.24	0.00	0.00	0.00	0.16	0.00	0.00	0.51	0.00
4	9	0.25	0.00	0.00	-0.10	0.04	0.00	0.00	0.00	-0.49
5	9	0.25	0.00	0.00	0.10	0.04	0.00	0.00	0.00	0.49
6	8	-0.48	0.00	0.00	0.63	-0.20	0.00	0.00	0.00	0.01
7	6	-0.50	0.00	0.00	0.00	-0.22	0.00	0.00	0.00	0.00
8	8	-0.48	0.00	0.00	-0.63	-0.20	0.00	0.00	0.00	-0.01

		A			A			A		
Frequencies	--	1168.0666			1508.5677			2554.4672		
Red. masses	--	12.0261			15.9704			12.8700		
Frc consts	--	9.6674			21.4139			49.4801		
IR Inten	--	462.4592			1.7968			1062.5113		
Raman Activ	--	0.2668			14.2753			0.2143		
Depolar (P)	--	0.7500			0.1097			0.7500		
Depolar (U)	--	0.8571			0.1978			0.8571		
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1 5		0.00	0.93	0.00	-0.01	0.00	0.00	0.00	0.01	0.00
2 9		0.00	-0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3 9		0.00	-0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4 9		0.12	-0.22	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5 9		-0.12	-0.22	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6 8		0.00	0.00	0.00	-0.03	0.70	0.00	0.01	-0.33	0.00
7 6		0.00	-0.01	0.00	0.08	0.00	0.00	0.00	0.88	0.00
8 8		0.00	0.00	0.00	-0.03	-0.70	0.00	-0.01	-0.33	0.00

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Atom 1 has atomic number 5 and mass 11.00931

Atom 2 has atomic number 9 and mass 18.99840

Atom 3 has atomic number 9 and mass 18.99840

Atom 4 has atomic number 9 and mass 18.99840

Atom 5 has atomic number 9 and mass 18.99840

Atom 6 has atomic number 8 and mass 15.99491

Atom 7 has atomic number 6 and mass 12.00000

Atom 8 has atomic number 8 and mass 15.99491

Molecular mass: 130.99275 amu.

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	500.019911615	3.398691765	6.63855
X	1.00000	0.00000	0.00000
Y	0.00000	1.00000	0.00000
Z	0.00000	0.00000	1.00000

This molecule is an asymmetric top.

Rotational symmetry number 1.

Warning -- assumption of classical behavior for rotation
may cause significant error

Rotational temperatures (Kelvin) 0.17322 0.05362 0.04906

Rotational constants (GHZ): 3.60934 1.11721 1.02215

Zero-point vibrational energy 74845.5 (Joules/Mol)

17.88850 (Kcal/Mol)

Warning -- explicit consideration of 10 degrees of freedom as
vibrations may cause significant error

Vibrational temperatures: 38.49 74.07 89.65 109.89 167.72
(Kelvin) 527.35 537.86 781.31 781.59 790.03

1067.46 1087.33 1152.61 1614.45 1657.46

1680.59 2170.49 3675.30

Zero-point correction= 0.028507 (Hartree/Particle)

Thermal correction to Energy= 0.036941

Thermal correction to Enthalpy= 0.037885

Thermal correction to Gibbs Free Energy= -0.007873
 Sum of electronic and zero-point Energies= -610.380500
 Sum of electronic and thermal Energies= -610.372066
 Sum of electronic and thermal Enthalpies= -610.371122
 Sum of electronic and thermal Free Energies= -610.416880

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	23.181	25.241	96.307
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.523
Rotational	0.889	2.981	28.746
Vibrational	21.404	19.280	27.038
Vibration 1	0.593	1.984	6.057
Vibration 2	0.596	1.977	4.760
Vibration 3	0.597	1.972	4.383
Vibration 4	0.599	1.965	3.982
Vibration 5	0.608	1.936	3.156
Vibration 6	0.739	1.541	1.094
Vibration 7	0.745	1.526	1.064
Vibration 8	0.898	1.155	0.559
Vibration 9	0.898	1.155	0.558
Vibration 10	0.904	1.142	0.546

	Q	Log10(Q)	Ln(Q)
Total Bot	0.418134D+04	3.621316	8.338388
Total V=0	0.541584D+17	16.733666	38.530689
Vib (Bot)	0.165981D-09	-9.779941	-22.519147
Vib (Bot) 1	0.773998D+01	0.888740	2.046399
Vib (Bot) 2	0.401481D+01	0.603665	1.389989
Vib (Bot) 3	0.331304D+01	0.520226	1.197866
Vib (Bot) 4	0.269782D+01	0.431013	0.992443
Vib (Bot) 5	0.175445D+01	0.244142	0.562157
Vib (Bot) 6	0.497884D+00	-0.302871	-0.697387
Vib (Bot) 7	0.485725D+00	-0.313610	-0.722114
Vib (Bot) 8	0.290919D+00	-0.536228	-1.234711
Vib (Bot) 9	0.290759D+00	-0.536466	-1.235260
Vib (Bot) 10	0.286045D+00	-0.543566	-1.251606
Vib (V=0)	0.214985D+04	3.332409	7.673155
Vib (V=0) 1	0.825611D+01	0.916776	2.110954
Vib (V=0) 2	0.454582D+01	0.657612	1.514208
Vib (V=0) 3	0.385056D+01	0.585523	1.348217
Vib (V=0) 4	0.324376D+01	0.511049	1.176733
Vib (V=0) 5	0.232431D+01	0.366294	0.843423
Vib (V=0) 6	0.120561D+01	0.081208	0.186988
Vib (V=0) 7	0.119709D+01	0.078125	0.179890
Vib (V=0) 8	0.107848D+01	0.032810	0.075548
Vib (V=0) 9	0.107840D+01	0.032778	0.075474
Vib (V=0) 10	0.107604D+01	0.031828	0.073287
Electronic	0.100000D+01	0.000000	0.000000
Translational	0.589286D+08	7.770326	17.891837
Rotational	0.427495D+06	5.630931	12.965697

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z

1	5	0.000080299	0.000013742	-0.000002438
2	9	-0.000039301	-0.000032943	-0.000002054
3	9	-0.000048731	0.000000393	0.000000567
4	9	0.000007372	0.000015434	0.000074842
5	9	0.000009030	0.000017510	-0.000072881
6	8	-0.000047444	-0.000065960	-0.000059257
7	6	0.000084246	0.000110025	-0.000022260
8	8	-0.000045471	-0.000058201	0.000083482

 Cartesian Forces: Max 0.000110025 RMS 0.000052234

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.

Internal Forces: Max 0.000078915 RMS 0.000031429

Search for a local minimum.

Step number 1 out of a maximum of 2

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Second derivative matrix not updated -- analytic derivatives used.

Eigenvalues --- 0.00075 0.00086 0.00119 0.00291 0.00305

Eigenvalues --- 0.06407 0.07388 0.11338 0.17713 0.18208

Eigenvalues --- 0.20940 0.22247 0.28099 0.34963 0.41165

Eigenvalues --- 0.43294 1.06622 1.077091000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

Eigenvalues --- 1000.000001000.000001000.000001000.00000

Angle between quadratic step and forces= 76.06 degrees.

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.00075090 RMS(Int)= 0.00000031

Iteration 2 RMS(Cart)= 0.00000025 RMS(Int)= 0.00000010

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.64901	-0.00003	0.00000	-0.00018	-0.00018	2.64883
R2	2.64882	0.00002	0.00000	0.00001	0.00001	2.64883
R3	2.62732	0.00005	0.00000	0.00016	0.00016	2.62748
R4	2.62733	0.00005	0.00000	0.00015	0.00015	2.62748
R5	6.96566	-0.00004	0.00000	-0.00312	-0.00312	6.96254
R6	6.51725	0.00001	0.00000	-0.00163	-0.00163	6.51563
R7	6.96396	-0.00004	0.00000	-0.00143	-0.00143	6.96253
R8	5.91387	-0.00001	0.00000	-0.00357	-0.00357	5.91030
R9	5.40870	0.00004	0.00000	-0.00228	-0.00228	5.40641
R10	5.91230	0.00000	0.00000	-0.00199	-0.00199	5.91031
R11	5.91071	0.00000	0.00000	-0.00040	-0.00040	5.91031
R12	5.40604	0.00004	0.00000	0.00038	0.00038	5.40642
R13	5.91050	0.00000	0.00000	-0.00020	-0.00020	5.91031
R14	2.16250	0.00006	0.00000	0.00002	0.00002	2.16252
R15	2.16246	0.00008	0.00000	0.00006	0.00006	2.16252
A1	1.88803	0.00002	0.00000	0.00041	0.00041	1.88843
A2	1.91412	-0.00001	0.00000	-0.00017	-0.00017	1.91395
A3	1.91412	-0.00001	0.00000	-0.00016	-0.00016	1.91395
A4	1.91419	-0.00002	0.00000	-0.00023	-0.00023	1.91395
A5	1.91419	-0.00003	0.00000	-0.00023	-0.00023	1.91395
A6	1.91893	0.00005	0.00000	0.00039	0.00039	1.91932
A7	2.49685	-0.00001	0.00000	0.00052	0.00052	2.49737

A8	2.18156	-0.00002	0.00000	0.00036	0.00036	2.18192
A9	1.86619	-0.00004	0.00000	0.00028	0.00028	1.86648
A10	1.86741	-0.00004	0.00000	-0.00091	-0.00091	1.86650
A11	2.18269	-0.00003	0.00000	-0.00075	-0.00075	2.18194
A12	2.49806	-0.00001	0.00000	-0.00067	-0.00067	2.49739
A13	0.63065	0.00003	0.00000	0.00024	0.00024	0.63089
A14	0.74788	0.00003	0.00000	0.00040	0.00040	0.74828
A15	0.74821	0.00003	0.00000	0.00007	0.00007	0.74828
A16	0.74270	0.00000	0.00000	0.00035	0.00035	0.74305
A17	0.81596	0.00000	0.00000	0.00025	0.00025	0.81621
A18	0.74281	0.00000	0.00000	0.00023	0.00023	0.74305
A19	3.07946	0.00004	0.00000	0.00046	0.00046	3.07991
A20	3.21530	-0.00006	0.00000	-0.00057	-0.00057	3.21473
D1	-1.41743	0.00001	0.00000	0.00021	0.00021	-1.41722
D2	1.41683	-0.00001	0.00000	0.00039	0.00039	1.41722
D3	1.41710	-0.00001	0.00000	0.00012	0.00012	1.41722
D4	-1.41799	0.00001	0.00000	0.00078	0.00078	-1.41721

Item	Value	Threshold	Converged?
Maximum Force	0.000079	0.000450	YES
RMS Force	0.000031	0.000300	YES
Maximum Displacement	0.002644	0.001800	NO
RMS Displacement	0.000751	0.001200	YES

Predicted change in Energy=-1.520050D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

1|1|UNPC-UNK|Freq|RHF|6-31+G(d)|C1B1F402(1-)|PCUSER|11-Apr-2008|0||#N
 Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31+G(d) Freq||BC_HF63
 1+G(d)||-1,1|B,0.1429253057,0.1235578352,0.0002977042|F,1.5408555403,0.
 019602051,0.0035575438|F,-0.1943418183,1.4840686308,-0.0027046663|F,-
 0.3742444306,-0.4843972277,1.1386782263|F,-0.3692113513,-0.4881799099,
 -1.1383408375|0,2.404373025,2.8016677221,-1.1401752996|C,2.365983095,2.
 7602431581,0.0027763631|0,2.3986369343,2.8031049604,1.1458329172||Ver
 sion=IA32W-G03RevD.01|State=1-A|HF=-610.4090072|RMSD=2.147e-009|RMSF=5.
 223e-005|ZeroPoint=0.0285071|Thermal=0.0369412|Dipole=1.2320845,1.461
 8042,0.0015121|DipoleDeriv=2.0908554,0.1066574,0.0000219,0.1067544,2.1
 274434,0.0001644,0.0000532,0.0001603,2.0164964,-1.1659506,-0.0120583,-
 0.0014501,0.0037589,-0.6335658,0.0001309,-0.0014814,0.0000743,-0.51469
 5,-0.6471746,0.0920267,-0.0005032,0.0761808,-1.1524718,0.0011305,-0.00
 04889,0.001192,-0.5145981,-0.651705,-0.1213097,0.1869504,-0.1212779,-0.
 6914091,0.2198083,0.1990854,0.2341748,-0.9473462,-0.6500069,-0.120883
 5,-0.1852458,-0.1209567,-0.6929222,-0.2212269,-0.1974026,-0.2356156,-0.
 9475934,-0.4198837,-0.0297217,0.0785788,-0.029826,-0.4296246,0.088968
 ,0.0465264,0.0509132,-1.5656068,0.8631033,0.1148628,-0.0055837,0.11481
 6,0.9023119,0.0015747,-0.0056131,0.0015551,3.0392897,-0.4192381,-0.029
 5736,-0.0727683,-0.0294494,-0.4297618,-0.0905498,-0.040679,-0.0524542,
 -1.5659466|Polar=26.3567238,1.221724,26.7745647,-0.0317547,0.0096508,3
 8.379388|PolarDeriv=-0.7168998,0.1291874,0.1097463,-0.0036015,-0.00030
 71,0.4291913,-0.0778205,0.2836096,-0.6408683,-0.0012139,0.0032675,0.50
 89634,-0.0032471,-0.0004539,0.0031123,0.4184099,0.4960681,0.0002054,3.
 9124114,-0.0521167,1.0043031,0.0054467,-0.0005285,0.5444082,0.0250849,
 1.2570629,0.0341389,0.0000659,0.0030321,-0.0756521,0.0045125,-0.000317
 3,0.0025206,0.9770231,-0.0135422,0.005516,-0.5622781,1.2600038,-0.2041
 241,-0.0023534,0.0011745,-0.1659817,1.0241415,-0.3224733,3.8334916,0.0
 016669,-0.0041195,0.5236422,-0.0019387,0.0011158,-0.0034651,-0.1774196
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 9, -0.2948526, -0.7231498, -0.7674971, -0.9172887, -3.0410484, 0.401144, 0.27
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 74, 0.4550773, 0.5240666, -9.5996096, -0.8340247, -0.7396524, -0.5129195, 0.0
 000387, 0.0002901, 0.061612, -0.4233356, -0.7795736, -1.1734334, -0.0008899,
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 08, -0.0173912, 0.2421264, 0.4730131, 0.1138267, 3.073581, 0.1512624, 2.57951
 65, 0.3192122, 2.6903204, 0.4340854, 0.5306085, 9.6033563|HyperPolar=1.5546
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 035, 3.7180555, 0.0083922|PG=C01 [X(C1B1F402)]|NImag=0|0.43996481, 0.011
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 , -0.00360925, -0.02999741, -0.00550987, -0.00329532, -0.00424248, -0.066184
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 , 0.04998924, 0.00458846, 0.00064819, -0.00073793, -0.00315117, -0.00285934,
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 , 0.00749223, 0.00002108, 0.00020512, 0.00244544, -0.00155911, 0.00019823, 0.
 00245064, 0.00157357, -0.09394935, 0.00049975, 0.03000182, 0.18744533, -0.01
 340709, -0.00333335, -0.00001455, 0.00643933, 0.00406845, 0.00000111, 0.0039
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 -0.00995080, 0.00002485, 0.00001794, -0.00996389, 0.00001289, 0.00000729, -0.
 00424957, -0.00000188, -0.00000958, -0.00424163, 0.02536583, 0.02657020, -1.
 07369334, -0.00494361, 0.00124678, 2.16126065, -0.00093250, 0.00459473, 0.0
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LENDING MONEY TO FRIENDS CAUSES THEM TO LOSE THEIR MEMORIES.

-- PETER'S THEORY OF RECIPROCAL INHIBITION OF FISCAL RECALL

Job cpu time: 0 days 0 hours 11 minutes 8.0 seconds.

File lengths (MBytes): RWF= 42 Int= 0 D2E= 0 Chk= 5 Scr=

1

Normal termination of Gaussian 03 at Fri Apr 11 22:13:57 2008.