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TITLE:

Vibrational Spectra of a N719-Chromophore/Titania Interface from Empirical-Potential Molecular-Dynamics Simulation, Solvated by a Room Temperature Ionic Liquid

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SUMMARY:
A dye-sensitized solar cell was solvated by RTILs; using optimized empirical potentials, a molecular dynamics simulation was applied to compute vibrational properties. The obtained vibrational spectra were compared with experiment and ab initio molecular dynamics; various empirical potential spectra show how partial-charge charge parameterization of the ionic liquid affects vibrational spectra prediction.

ABSTRACT:
The accurate molecular simulation prediction of vibrational spectra, and other structural, energetic and spectral characteristics, of photo-active metal-oxide surfaces in contact with light-absorbing dyes is an ongoing thorny and elusive challenge in physical chemistry. With this in mind, a molecular-dynamics (MD) simulation were performed by using optimized empirical potentials for a well-representative and prototypical dye-sensitized solar cell (DSC) solvated by a widely-studied room temperature ionic liquid (RTIL), in the guise of a $[bmim]^+[NTf2]^-$ RTIL solvating an N719-sensitizing dye adsorbed onto 101 anatase-titania. In doing so, important insights were gleaned into how using a RTIL as the electrolytic hole acceptor modulates the dynamical and vibrational properties of a N719 dye, estimating the spectra for the DSC photo-active interface via Fourier transformation of mass-weighted velocity autocorrelation functions from MD. The acquired vibrational spectra were compared with the experiment spectra and those sampled from ab initio molecular dynamics (AIMD); in particular, various empirical-potential spectra generated from MD provide insight into how partial-charge charge parameterization of the ionic liquid affects vibrational spectra prediction. In any event, careful fitting of empirical force-field models has been shown to be an effective tool in handling DSC vibrational properties, when validated by AIMD and an experiment.

INTRODUCTION:

In dye-sensitized solar cells (DSCs), the optical band gap of semiconductors is bridged by a light-absorbing, or sensitizing, dye. DSCs require continual recharging: therefore, a redox electrolyte is essential to foster this constant supply of charge (typically in the form of an I^-/I^{3-}, in an organic solvent). This facilitates the passage of holes from the sensitizing dye to the electrolyte, with injected photo-excited electrons into the metal-oxide substrate passing through to an external circuit, with eventual recombination taking place at the cathode[1]. A crucial aspect underpinning DSCs' positive outlook for a wide variety of real world applications originates in their straightforward manufacture, without the need for raw materials high in purity; this is in stark contrast with the high capital cost and ultra-purity required for silicon-based photovoltaics. In any event, the prospect of significantly improving the working-life timescales of DSCs by swapping less stable electrolytes with room-temperature ionic liquids (RTILs) having low volatility shows significant promise. The solid-like physical properties of RTILs combined with their liquid-like electrical properties (such as low toxicity, flammability, and volatility)[1] lead these to constitute rather excellent candidate electrolytes for usage in DSC applications.

Given such prospects for RTILs in DSCs, it is hardly surprising that, in recent years, there has been a substantial boost of activity in studying DSC-prototype N719-chromophore/titania interfaces with RTILs. In particular, important work on such systems has been performed[2-5], which consider a broad suite of physico-chemical processes, including the charge-replenishment kinetics in dyes[2,5], the mechanistic steps of electron-hole dynamics and transfer[3], and, of course, the effects of titania substrates' nanoscale nature upon these, and other, processes[4].

Now, bearing in mind impressive advances in DFT-based molecular simulation, particularly AIMD[6], as a highly useful prototypical design tool in materials science and particularly for DSCs[7-11], with critical assessment of optimal functional selection being vital[8,9], AIMD techniques have proven very useful previously in scrutinizing rather significant dispersion and explicit-RTIL solvation effects on dye structure, adsorption modes and vibrational properties at DSC-semiconductor surfaces. In particular, the adoption of AIMD had led to some success in attaining reasonable, semi-quantitative capture and prediction of important electronic properties, such as band gap, as well as structural binding[13] and vibrational spectra[14] In refs. 12-14, AIMD simulations were performed extensively on the photo-active N719-chromophore dye bound to (101) anatase-titania surface, assessing both electronic properties and structural properties in the presence of both $[bmim]^+[NTf2]^-$ [12,13] and $[bmim]^+[I]^-$ [14] RTILs, in addition to vibrational spectra for the case of $[bmim]^+[I]^-$[14]. In particular, the rigidity of the semiconductor's surface[15], apart from its inherent comparative photo-activity, led the surface to slightly alter within the AIMD simulation, which makes (101) anatase interfaces[12-14] a suitable choice. As ref. 12 shows, the mean distance between the cations and the surface dropped by about 0.5 Å, the average separation between the cations and anions decreased by 0.6 Å, and the noticeable altering of the RTILs in the first layer around the dye, where the cation was on average 1.5 Å further from the center of the dye, were directly caused by explicit dispersion interactions in RTIL-solvated systems. Unphysical kinking of the adsorbed N719 dye's configuration was also a result of the introduction of explicit dispersion effects in vacuo. In ref. 13, analysis was conducted on whether these structural effects of explicit RTIL solvation and functional selection affected the behavior of the DSSCs, concluding that both explicit solvation and treatment of dispersion is very important. In ref. 14, with high-quality experimental vibrational-spectral data of other groups on hand, the particular effects were benchmarked systematically on both explicit $[bmim]^+[I]^-$ solvation and accurate handling of dispersion established in refs. 12 & 13 on the reproduction of salient spectral-mode features; this led to the conclusion that explicit solvation is important, alongside accurate treatment of dispersion interactions, echoing earlier findings for both structural and dynamical properties in the case of AIMD modeling of catalysts in explicit solvent[16]. Indeed, Mosconi et al. have also performed an impressive assessment of explicit-solvation effects on DFT treatment of DSC simulation[17]. Bahers et al.[18] studied experimental absorption spectra for dyes along with the related spectra at the TD-DFT level; these TD-DFT spectra agreed very well in terms of their computed transitions with their experimental counterparts. In addition, absorption spectra of pyrrolidine (PYR) derivatives were studied by Preat et al. in several solvents[19], providing significant insights into the dyes' geometrical and electronic structures, and evincing adequate structural modifications that serve to optimize the properties of the PYR-based DSSCs – a spirit of simulation-led/rationalized 'molecular design', indeed.

Having clearly established the important contribution of both DFT and AIMD towards accurate modelling of DSCs' properties and function, including such important technical matters like explicit solvation and appropriate treatment of dispersion interactions from structural, electronic and vibrational standpoints[7-14], now – in the present work - the focus turns towards the pragmatic question of how well empirical-potential approaches can be tailored to address the apposite and reasonable prediction of structural and vibrational properties of such prototypical DSC systems, taking the N719 dye adsorbed on anatase (101) in the $[bmim]^+[NTf2]^-$ RTIL as a case in point. This is important, not only because of the large corpus of forcefield-based molecular-simulation activities and methodological machinery available to tackle DSC simulation[7], and metal-oxide surfaces more widely, but also because of their staggeringly reduced computational cost vis-à-vis DFT-based approaches, together with the possibility of very efficient coupling to biased-sampling approaches to capture more efficiently phase space and structural evolution in highly viscous RTIL solvents, dominated by solid-like physical properties at ambient temperatures. Therefore, motivated by this open question of gauging and optimizing forcefield approaches, informed by both DFT and AIMD as well as experimental data for vibrational spectra[14], we turn to the pressing task of assessing empirical-potential performance at vibrational-spectra prediction from MD, using mass-weighted Fourier transforms of the N719 dye's atomic velocity autocorrelation function (VACF). One key concern is how different partial-charge parameterizations of the RTIL may affect vibrational-spectra prediction, and particular attention was given to this point, as well as the wider task of tailoring forcefields for optimal spectral-mode prediction relative to experiment and AIMD[20].

PROTOCOL:

1. Performing MD Simulation using DL_POLY

1.1 Construct the DSC-systems initial structure of the N719-dye adsorbed to an anatase-titania (101) surface solvated by $[bmim]+[NTf2]^-$ taken from previous work[12,13]. Draw the required structure using VESTA software.

1.2 Choose the N719 cis-di(thiocyanato)-bis (2,2'-bipyridl-4-carboxylate-4'-carboxylic acid)-ruthenium (II)-sensitizing dye with no counterions and ensure the presence of two surface-bound protons to provide for overall-system charge neutrality.

NOTE: Indeed, in depth studies by De Angelis et al. have established this to constitute a realistic representation of N719 adsorbed to anatase-titania.[21] This is because in ref. 21, there was the most convincing level of agreement with experimental results for a number of properties; in experimental systems, the *de-facto* surface protonation is thought to emerge from ILs' cations and anions leading to some degree of charge transfer with the surface[21].

1.3 Ensure that the dye is adsorbed chemically to the TiO_2 surface through two carboxylate groups (i.e., bidentate). This initial adsorbed dye configuration is similar to that denoted as I1 and found by Schiffman et al.,[22] which was determined to be the most stable with surface protonation taken into account. Consult refs. 12 & 13 for a detailed account of how this is done, including chemical-adsorption coordinates.

1.4 Ensure that the sensitizing dye N719 (cis-di(thiocyanato)-bis(2,20-bipyridl-4-carboxylate-40-carboxylic acid)-ruthenium(II)) has no counterions. Add two surface-bound protons for charge neutrality, as in ref. 12 & 13.

1.5 Select 12 cation-anion pairs of 1-butyl-3 methylimidazolium bis(trifluoromethyl sulfonyl)imide, comprising 480 atoms[12,13]. These were taken from refs. 12 & 13.

1.6 Relax the RTIL configuration via empirical-potentials, using the well-validated forcefield of Lopes et al.[23]. Model anatase using the Matsui-Akaogi (MA) force-field and include the mobility of the titania in the relaxation process. Using the DL-POLY details in step 2.1 below, perform a geometry-optimization in DL-POLY, rather than MD, with a conjugate-gradient-minimization relative termination gradient of 0.001. Here, specify optimization in the FIELD file, rather than dynamics.

1.7 For the anatase surface, $(TiO2)_{96}$, consisting of 288 atoms, ensure it is periodic along x- and y- laboratory axes, projecting to the RTIL a pair of parallel (101) surfaces; the dimensions in x-axis 23 Å and y-axis to 21 Å. This was taken from refs. 12 & 13.

1.8 Ensure that the entire DSC system with an explicit solvent is composed of 827 atoms[12,13]; For the 'in-vacuo' case, bereft of RTIL solvation, there should be 347 atoms in the system.

2 Performing forcefield-based MD Simulation using DL_POLY

2.1 Perform MD using DL-POLY with various different partial-charge sets (vide infra) for 15 ps with a 1 fs time-step and at 300 K in an NVT ensemble[24,25], using the Lopes et al.[23] forcefield parameters for the RTIL and general-purpose OPLS model for the dye[26], with the well-studied and reliable Matsui-Akaogi potential acting for titania[27] force-field. To run DL-POLY on the terminal, type **DLPOLY.X** & where the input files are located.

2.2 Perform classical MD via these above-specified empirical force-fields, as implemented in DL_POLY[28]. Here, there is no need to use a graphical user interface (GUI) in the software, so it is recommended to input the details using the comprehensive, and easy-to-follow software manual[29]. Here, in the CONTROL file (check Supplemental Information for the input files), specify 'Nose-Hoover' for NVT, and opt for position-velocity trajectory printing every 1 fs.

2.3 In the FIELD file, for Lennard-Jones parameters, apply Lorentz-Berthelot combining rules[25]. Taking the arithmetic mean of the Lennard-Jones (LJ) radii and the geometric mean of the LJ well-depths, for the empirical force-fields, as detailed in ref. 25, and enter this in the bottom section of the FIELD file under the non-bonded-interactions tab.

2.4 To handle long-range electrostatics, apply the Ewald method[25]; use a non-bonded cut-off length of r_{cut} = 10 Å. Consult refs. 25 & 30 for precise details as to how to optimize electrostatic parameters. Set the real-space decay parameter for the Ewald method in the CONTROL file to be ~3.14 / r_{cut} , and choose the number of Ewald wave-vectors to ensure a relative tolerance in the Ewald evaluation of 1E-5; specify that in the CONTROL file.

2.5 Ensure, in the CONTROL file, state that r_{cut} = 10 Å; carry out a series of potential-energy evaluations with a REVCON file (renamed as CONFIG) until the system pressure in OUTPUT converges to within a few percent to choose r_{cut}, but avoid any r_{cut} below ~2.5 times the largest LJ distance[25,30].

NOTE: This short 15 ps MD-propagation timescale is chosen to be similar to that of ~8.5 ps Born-Oppenheimer-MD (BOMD) simulations with an identical starting configuration of refs. 9, 10 & 17, so as to allow for direct comparison vibrational-spectra prediction afforded by both AI-[20] and forcefield-based MD (with comparison and validation against experiment also).

2.6 From the HISTORY file (into which both velocities and positions have been printed at each time step, as directed from the CONTROL file), extract the x-, y-, z-velocities by using python **dye_atom_velocity_seperate.py** (see Supplemental Information) in the terminal. It will separate the velocities at each step.

2.7 Compute the VACF by using **vacf151005.py** (see Supplemental Information). In the terminal, type **./classical_dye_autocorr.sh**; it will compute the VACF of all dye atoms. Compute spectra from MD (whether AIMD[14,20] or forcefield-based) using mass-weighted Fourier transforms of the dye's atomic velocity autocorrelation function (VACF)[31-33] by using python **MWPS.py** (see Supplemental Information). In the terminal, type **./run_all_4.sh**; it will compute the mass weighted power spectra.

2.8 Perform a Fourier transform on these VACFs using commonly available software.

2.9 Bear in mind that the best-quality DFT treatment in AIMD (e.g., use of explicit solvation and accurate treatment of dispersion, alongside a canny choice of functional) is important to use for benchmarking against experimental data[12,13,20] and gauging/tailoring the comparative performance of empirical-potential MD, in particular, the large influence of electrostatics and choices for partial charges[16]. See refs. 12 and 13 and study these to gain an in-depth appreciation, and, if intending to do AIMD (which is not the case in the present study), act accordingly in such a situation in the future, should the need to conduct AIMD arise.

3 Comparing results of each of the force-fields

NOTE: It is important to assess partial-charge sets for the RTIL for empirical-potential-based MD simulation in step 2, for ready comparison against each other, experiment and ab initio-MD results in explicit RTIL solvent (using the PBE functional with Grimme-D3 dispersion, given its superior performance for prediction of vibrational spectra)[20]; these were as follows:

3.1 Note that in the case of literature-derived RTIL charges, the anion charges are to be found from Extended Hückel Theory,[34,35] based on AIMD trajectories[23], owing to the absence of anion-charge parameterisation in ref. 20, with cation charges to be taken from Lopes et al.[23] Prepare a table of the literature charges, and put into FIELD-file format for DL-POLY.

3.2 Note that Mulliken RTIL charges are to be calculated via Mulliken population analysis. Perform the Mulliken analysis by averaging over four points of the ab initio MD trajectory[20], renormalize and prepare a table of the literature charges, and put into FIELD-file format for DL-POLY.

3.3 Note that Extended Hückel Theory (EHT) charges are to be fitted from the final configuration of AIMD trajectories,[20] using EHT, applied to both RTIL anions and cations. Perform the EHT analysis by averaging over four points of the ab initio MD trajectory[20], as implemented in the MOE software package (by selecting 'Charge Analysis' menu after reading in the configuration file),[35] renormalize and prepare a table of the literature charges, and put into FIELD-file format for DL-POLY.

3.4 Note that Hirshfeld RTIL charges are to be calculated from Hirshfeld-charge analysis by averaging over four points of the ab initio MD trajectory[20], for anions and cations,[20] as implemented in the MOE software package (by selecting 'Charge Analysis' menu after reading in the configuration file)[35]. From renormalization of these so-obtained charges, tabulate these in the appropriate format in the DL-POLY FIELD file.

3.5 Bear in mind that the different charge sets for the $[bmim]^+[NTf2]^-$ atoms are presented in **Table 1 & Table 2**, which also show the mean amount by which some of the atomic charges needed to be modified, so as to take symmetry and overall charge conservation into account.

3.7 Note that the final charge sets are to have the sum of charges adding up to +1 on the cation and -1 on the anion. The cation and anion are shown in **Figure 1a** and **Figure 1b**, respectively. The underlying DFT-sampled spectra, from which these charge sets were inspired, by and large, have implicit charge transfer and tend to lead to charges closer to ±1.

REPRESENTATIVE RESULTS:

Structural Properties of Binding Motifs

Representative binding motifs for the four different partial-charge sets are depicted in **Figure 2**, after 15 ps of MD. In **Figure 2a**, for the (above-described) literature-derived charges, it can be seen that there is a prominent hydrogen-bonding interaction with a surface proton. From careful analyses of the trajectory, the hydrogen bonds are mostly surface-proton-bound whilst the other three (AIMD-derived)[20] charge sets do not feature such a strong Coulombic interaction with a surface proton. Referring to Figure 1f of ref. 20, which depicts the AIMD-relaxed dye-binding configuration after ~8.5 ps, there is also less evidence of strong hydrogen-bonding with a surface proton, so this is qualitatively consistent in tailoring the present forcefield-based MD with AIMD-based charge sets to achieve qualitatively similar substrate-binding arrangements (**Figure 2b**-**2d**). Indeed, the smaller magnitude of the partial charges in the literature-derived case vis-à-vis those sampled in various ways from AIMD (**Table 1** & **Table 2**) leads to a lesser extent of charge shielding in comparison to larger-magnitude partial RTIL charges, which serves to emphasize more the electrostatic (hydrogen-bond) interaction with the surface proton evident in **Figure 2a**. In any event, interestingly, the Mulliken-derived charge set shows a certain sustained ‘kinking’ of the dye to have a prominent hydrogen bond with a bridging oxygen atom at the anatase surface (**Figure 2b**), which is redolent of the PBE system of ref. 15 without Grimme dispersion (**Figure 2d** therein): the generally-recognized inferior quality of Mulliken charges leads to this less physical, persistent kinking, which has been studied in more detail in refs. 12, 13 & 20. Tellingly, the better-quality charge fits (EHT and Hückel) from AIMD[20] lead to more realistic N719-binding motifs in **Figure 2c,2d**, which are in accord with PBE-based BOMD featuring Grimmer-D3 dispersion in ref. 20 (cf. Figure 1f therein); comparison of motifs with ref. 20 shows this is somewhat more the case for Hirshfeld charges.

Empirical-Potential Spectra

Having established at gross structural level already the clear influence of RTIL partial-charge sets in parameterizing and tailoring pragmatically the efficacy of forcefield-based MD vis-à-vis the best-quality AIMD data available, we now turn to considering empirical-potential-based MD for replication of N719 vibrational spectra. The mass-weighted VACF spectra for the four different parametrized charge sets are shown in **Figure 3**; as mentioned previously, although all four MD-generated spectra have the same forcefields for their dyes and surfaces, they differ in the partial charges applied to the RTIL cations and anions.

Now, prior to discussing the MD-predicted vibrational spectra, let us make some brief explanatory comments about their more fundamental nature and higher-level interpretation. The continuous colored lines in **Figure 3** denote the (empirical-potential) MD-based spectra in the range from 0 to 2500 cm^{-1}, for all four RTIL partial-charge sets. The dashed vertical gray lines are established experimental modes for the N719 dye and are at the frequencies 1230, 1380, 1450, 1540, 1600, 1720 and 2100 cm^{-1}, respectively[36]. The two grey spectral insets are experimental ATR-FTIR results from ref. 37, with the topmost one being the spectra for unsolvated N719 powder and the bottom one that for unsolvated N719 powder adsorbed on anatase. These experimental results are intended as a guide only, in that the spectra are slightly different in other studies and the two experimental insets are themselves somewhat different due to adsorption to anatase. A solvent's presence would be expected to alter the spectra, whether it be an RTIL or the more traditional acetonitrile. Also, it must be noted that the experimental spectra have a reduced frequency window available, and are in effect denoting a mixture of dynamical properties of multiple dyes in various geometries; in contrast, it ought to be borne in mind that the results are for a single N719 molecule adsorbed to the anatase substrate, therefore leading to an inevitably more sharp signal.

Now, the modes themselves are discussed more in refs. 14 & 18; the present discussion focusses more on fidelity of each technique in reproducing these, as opposed to their underlying nature.

0-500 cm^{-1}: The previous AIMD results (i.e., PBE-based BOMD with Grimme-D3 dispersion and explicit RTIL solvation)[20] show a cluster of spectroscopic peaks in the 300-400 cm^{-1} region. In terms of closeness to the ab initio spectra, the classical charge sets were ranked in order from closest to furthest away as EHT, Hirshfeld, literature-based and Mulliken.

500-1000 cm^{-1}: The ab initio MD spectra[20] display prominent vibrational peaks at 625, 750 and 825 cm^{-1}; the main peaks present in the classical spectra are at 600 and 800 cm^{-1} for the literature-derived charges, 525 and 800 cm^{-1} for the Mulliken charges, 675, 810, and 900 cm^{-1} for the EHT charges and 650,800 and 900 cm^{-1} for the Hirshfeld charge set. Although the literature and Mulliken charge sets reproduce grosso modo some of the features of the ab initio spectra, both the EHT and Hirshfeld-derived charge sets generate spectra which have their main peaks only 25-75 cm^{-1} above those of the ab initio ones. Given the much closer structural resemblance of the binding motif in **Figure 2c,2d** relative to Figure 1f of ref. 20, this excellent, semi-quantitative agreement is encouraging for tailoring and optimising pragmatically forcefields using high-quality AIMD.

1000-1500 cm^{-1}: The BOMD spectra evince strong peaks at 1000, 1300, and 1400 cm^{-1},[20] whereas the main peaks present in the forcefield-based spectra are at 1075 and 1200 cm-1 for the literature-derived charges, 1080, 1350 and 1450 cm^{-1} for Mulliken charges, 1075 and 1200 cm^{-1} for the EHT charges and 1075 and 1250 cm^{-1} for the Hirshfeld charge set. Although the forcefield-based RTIL-charge sets produce results close to those of AIMD simulation,[20] a key difference between these and BOMD lies in the important fact that the present empirical-potential simulations allow only for physical adsorption rather than also for the possibility of chemical adsorption. Clearly, this will have a particularly strong effect in this vibrational-bending spectral region and serves to explain a good deal of the altering of vibrational modes related to surface binding.

1500+ cm^{-1}: In the stretch-dominated frequency range above 1500 cm^{-1}, the solvated ab initio spectra[20] exhibit modes at 1525, 1575, 1600, 1700 and 2075 cm^{-1}. All four forcefield-based spectra have modes in the region of 1525 cm^{-1}, whilst none capture the thiocyano mode around 2075 cm^{-1}. The literature-derived charge set produces spectra which shows vibrational modes at 1625 and 1700 cm^{-1}, whereas spectra derived from the use of Mulliken charges result in modes at 1600, 1675 and 1775 cm^{-1}. The EHT-generated spectra have a mode at 1700 cm^{-1}, and the

Hirshfeld-generated spectra does a rather excellent job of reproducing DFT-based MD results with modes at 1575, 1600 and 1700 cm^{-1}. It is clear that the greater sophistication of the Hirshfeld charge fitting does pay important dividends with respect to basic qualitative reproduction of salient spectral features, showcasing further the important effect of RTILs and suitable treatment of their electrostatics on capturing the essential details of N719 vibrational properties.

FIGURE AND TABLE LEGENDS:

Figure 1. Cation and anion images of the considered system. Carbon is shown in cyan, nitrogen in blue, oxygen in red, hydrogen in white, sulphur in yellow, and fluorine in pink.

Figure 2. Frontal view showing the relaxed geometries of the systems under consideration, after 15 ps of MD. Carbon is shown in grey, nitrogen in blue, oxygen in red, hydrogen in white, titanium in silver, Sulphur in yellow and ruthenium in light green. The explicitly solvated systems are shown without RTIL ions for ease of viewing.

Figure 3. Vibrational Spectra for adsorbed-N719 from MD; the forcefield-based MD simulations differ from each other only in their partial-charge parametrization of the RTIL. Within each plot the grey (lower) / (upper) inset corresponds to the experimental ATR-FTIR signal from León[37], for (dry-N719 adsorbed onto anatase) / (dry-N719 powder). The dashed lines indicate established vibrational modes[30]. **a**) Literature-derived RTIL Charges, **b**) Mulliken RTIL Charges, **c**) Extended-Huckel-Theory Charges, and **d**) Hirshfeld RTIL Charges.

Table 1. Different parametrized charge sets for the atomic partial charges of the cation. Mean modification is the per atom alteration of charge necessary to achieve overall charge neutrality.

Table 2. The different parameterized charge sets for the atomic partial charges of the anion. Mean modification is the per atom alteration of charge necessary to achieve overall charge neutrality.

DISCUSSION:

Ab initio simulation techniques are expensive to perform and hence to perform simulation on much longer timescales would require the use of empirical forcefields for at least some of the DSC system. Towards this end, an equivalent atomistic model was created of the [bmim]+[NTf2]- solvated interface, using an empirical, classical-simulation forcefield for MD. The anatase was modeled using the Matsui-Akaogi (MA) forcefield, whilst the dye structure was handled using OPLS parameters. For the RTIL, four different forcefields were employed to determine the importance of the charge of the RTIL on the dyes's vibrational dynamics. The force-field parameters were the same for each, and only the charge parameterization was varied, with the forcefield parameters generated from an automatic-fitting procedure utilizing extended Huckel theory (EHT), as implemented in the MOE software package and fitted against the ab initio trajectories.

The ab initio results show a cluster of spectroscopic peaks in the region of 300-400, 625, 750, 825, 1000, 1300, 1400, 1500, 1525, 1575, 1600, 1700 and 2075 cm^{-1}. In terms of closeness to the ab initio spectra, the classical charge sets were ranked, in order from closest to farther away, as EHT, Hirshfeld, Literature, and Mulliken. The main peaks present in the classical spectra are at 600, 800, 1075, 1200, 1525 cm^{-1} for literature-derived charges. The peaks, using Mulliken charges, arise at 525, 800, 1080, 1350, 1450, 1525, 1625, 1700 cm^{-1}. The EHT charges lead to peaks in the region of 675, 810, 900, 1075, 1200, 1525 cm^{-1}. Finally, the Hirshfeld charge evinces peaks at 650, 800, 900, 1075, 1250 and 1525 cm^{-1}.

Lest the reasonably-superior Hirshfeld-charge performance (both structurally and vibrationally), lead one to suspect those forcefield methods, when tailored pragmatically for charges informed by good-quality DFT and AIMD, may invariably serve as a reasonable substitute for AIMD in prototypical DSC design, this rather optimistic picture does not always hold. Indeed, where the empirical-potential models do fail in the present N719 scenario – somewhat spectacularly, it must be admitted - is in the spectral region between 1800 and 2000 cm^{-1}. Both the PBE-Grimme-BOMD[20] and experimental results[37] show little activity in this region, whereas all classical-charge parametrizations show, erroneously and misleadingly, strong modes. This, and the already-mentioned lack of the thiocyano mode is most likely due to the forcefield model of the dye (OPLS, in the present case) being unable to capture properly this dynamical behavior. The charge parametrization, in this particular frequency range, would then be of secondary importance compared with the bonding and angular terms in the forcefield. This serves as a 'cautionary tale' that although partial-charge fitting is an important first step, the reparameterization of certain key stretch and bend interactions in the empirical models is likely to be important also.

In closing, vibrational spectra for the photo-active interface in a DSC were reported by means of Fourier transforming mass-weighted VACFs generated from the trajectories of forcefield-based molecular dynamics, using various RTIL-charge parameterizations of increasing complexity and sophistication. In addition, gross structural binding modes have also been considered (**Figure 2**), together with the sensitivity thereof to partial-charge sets. It has been found that the EHT, and Hirshfeld charge sets, performed reasonably well with respect to reproduction of gross binding motifs vis-à-vis high-quality AIMD, and also reproduction of salient ATR-FTIR vibrational-spectra features (as well as relative to AIMD spectra). However, a salutary and important lesson is that the lack of prediction of thiocyano mode as well as artificial modes in the 1800 - 2000 cm^{-1} range shows the limits of simplistic forcefields to reproduce good-accuracy AIMD and experiment, and signals the need to reparametrize selected bonded-interaction aspects of subsets of the forcefields. In this respect, force-matching to AIMD is an effective and promising strategy, whilst the use of tight-binding MD with good training sets for parameterization is also likely to be a very important future direction in simulation-enabled DSC-prototype design. Still, the present study has still underlined the effectiveness and importance of pragmatic usage of good-quality AIMD and DFT in guiding the tailoring of effective partial-charge sets for forcefield-based MD, as well as showing the limits of fitting partial charges alone. Nevertheless, using increasingly popular charge-scaling approaches, which yield charges of around ± 0.8 on the anions and cations, is a good direction for future potential work by the community in terms of the development of appropriate partial-charge sets for use with empirical force-fields.

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DISCLOSURES:
The authors have nothing to disclose.

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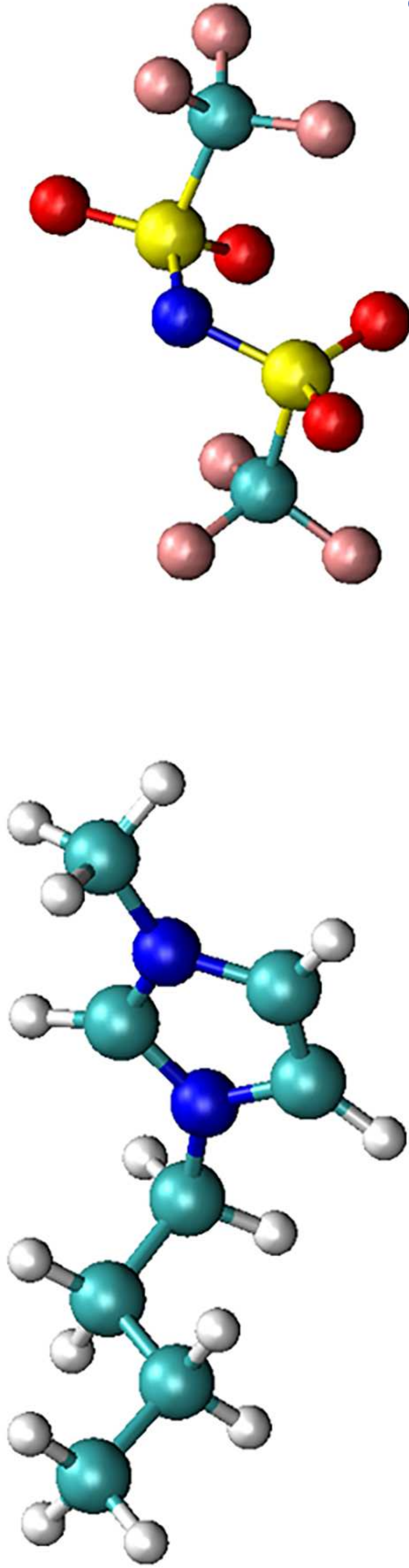

a) cation

b) anion

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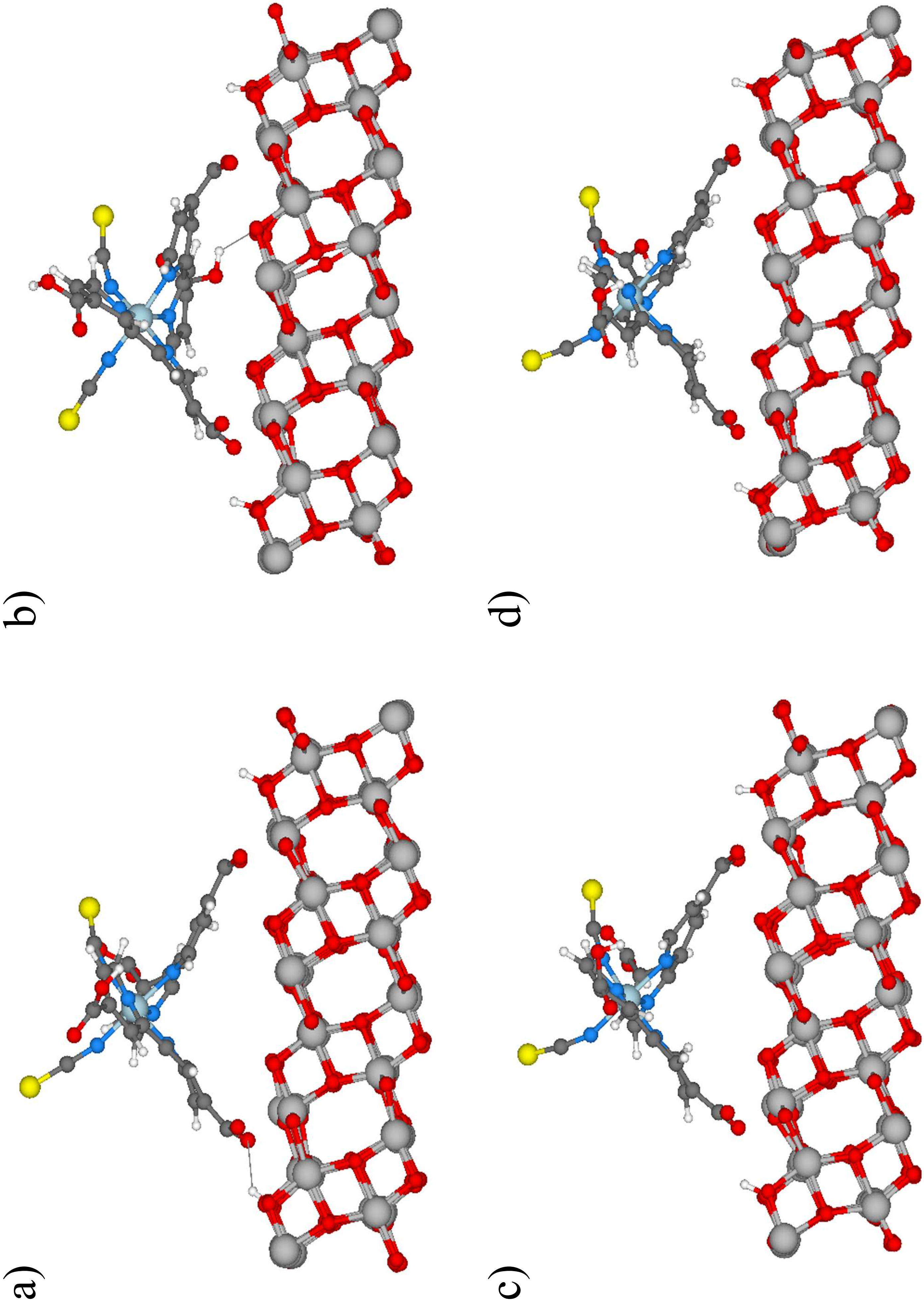

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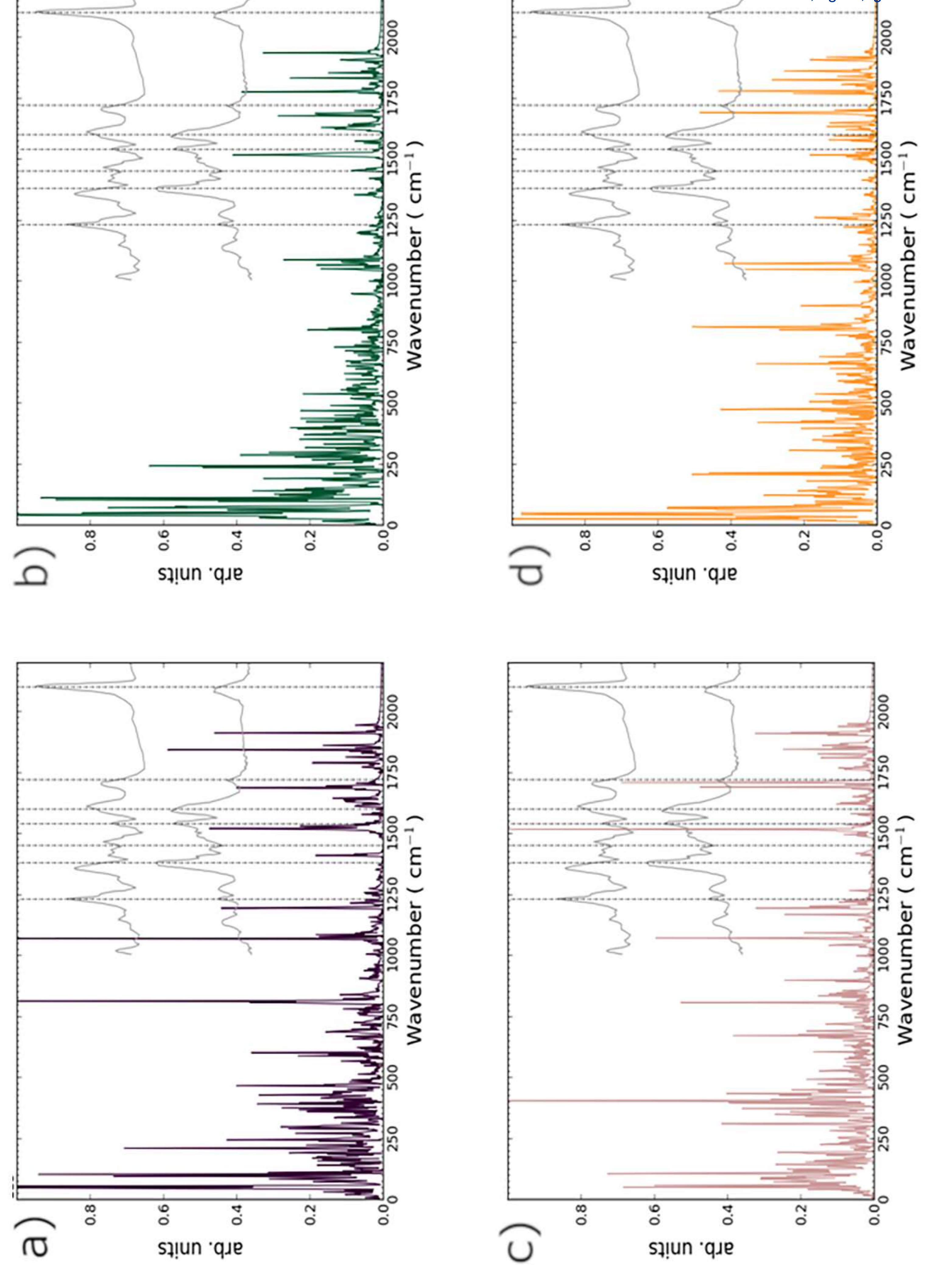

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Atom	Cation			
	Literature	Mulliken	EHT	Hirshfeld
N	0.15	0.005	-0.76	-0.1
C	-0.11	-0.06	0.65	0.14
N	0.15	0.005	-0.76	-0.1
C	-0.13	-0.06	0.2	0.14
C	-0.13	-0.06	0.2	0.14
C	-0.17	-0.34	0.274	0
H	0.21	0.2	0.15	0.11
C	-0.17	-0.34	0.354	0
H	0.21	0.18	0.15	0.09
H	0.21	0.18	0.15	0.09
H	0.13	0.18	0.08	0.08
H	0.13	0.18	0.08	0.08
H	0.13	0.18	0.08	0.08
C	0	-0.25	-0.16	0
H	0.13	0.18	0.08	0.08
H	0.13	0.18	0.08	0.08
C	0	-0.25	-0.16	0
H	0.045	0.151	0.08	0.04
H	0.045	0.151	0.08	0.04
C	-0.17	-0.34	-0.24	0
H	0.045	0.151	0.08	0.04
H	0.045	0.151	0.08	0.04
H	0.045	0.151	0.08	0.04
H	0.045	0.151	0.08	0.04
H	0.045	0.151	0.08	0.04
mean modification	0.0062	0.0159	———	0.0195

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Atom	Anion			
	Literature	Mulliken	EHT	Hirshfeld
N	-0.368	-0.44	-0.368	-0.62
S	1.311	0.5	1.311	1.41
O	-0.717	-0.3	-0.717	-0.64
C	1.09	0.25	1.09	0.8
mean modification	———	0.0062	———	0.0045

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Name of Material/Equipment	Company	Catalog Number	Comments/Description
This was molecular simulation, so no experimental equipment was used. The name of the software was DL-POLY (the 'Classic' version of which is available under GnuPublic Licence, via sourceforge)			

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TITLE:
Vibrational Spectra of an N719-chromophore/titania interface from empirical-potential molecular-dynamics simulation, solvated by a room-temperature ionic liquid

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Supporting Information

To run the DL-POLY program, three input files are needed - namely CONTROL, FIELD and CONFIG. The contents of these files are given below. To run MPI-enabled DL-POLY on terminal, please use **nohup mpirun -np # DL_POLY.X &** on a terminal.

is the number of processors required.

1. CONTROL file

```
DL_POLY DSSC with RTIL bmim[I]

##l_scr
##nfold 1 1 1
# Define the State Point
temperature        3.00E+02
pressure           1.00E-03
#pressure is in kbar
#temperature is in kelvin

# Simulation Timesteps and Equilibration
steps                  200000000       #total number of steps e.g
120000
equilibration          100000        #equilibrate for this many
scale               5        #rescale atomic velocities every m steps
variable timestep          1.000E-03        #in ps
#mult               1      #multi-step interval


restart


# Ensemble Options
ensemble nvt hoover   1.0
#                  thermostat   barostat relaxation time in ps
```

```
# Specify Cut-Offs
cutoff           1.000E+01          #angstrom forces cutoff e.g 9A
cutoff
rvdw             0.9000E+01          #short range cutoff (A)
delr             5.0000E-01           #verlet neighbour list shell
(A)

# RDF Options
print                   1000          #print system data every n
timesteps
rdf 100000         #calculate rdf every n steps
zden
                   #calculate zdensity profile
print rdf                            #print radial dist. function

job time           259200           #wall time
close time         3.0000E+02       #job closure time


# Forces Options
spme precision    1.0000E-06
#smooth particle mesh ewald precision

# Statistics Options
stats                   1000000      #colect stats every n
timesteps
stack                   1000000      #rolling average stack

shake            0.0001     #shake tolerance   (default 1.000E-8)


steps 200000000
#no vdw
#no elec



# Trajectory Controls
trajectory 1 100000 2
#start at 1,   1 between,
#keytraj   -- file output type 1 = coord only, 2=coord +vel,
3=coord+vel+force



finish
```

1. FIELD file

```
bmim [NTf2] with anatase (MA) surface and N719 dye (GAFF & AMBER99)
+ two surface protons
UNITS kcal
molecules 6
Titanium
  nummols 96
  atoms  1
  Ti  47.8670  2.196    1       0       1       1       TI      Ti
und
FINISH
Oxygen
  nummols 190
  atoms  1
  O   15.9994  -1.098   1       0       1       1       O       O
und
FINISH
N719
   nummols 1
   atoms 57
O1      16.0000 -0.6164 1      0       1       1       O1      O
und
HO      1.0080  0.4536  1      0       1       2       HO      H
und
C       12.0010 0.5874  1      0       1       3       C       C
und
OH      16.0000 -0.6964 1      0       1       4       OH      O
und
CA      12.0010 0.0398  1      0       1       5       CA      C
und
CA      12.0010 -0.1964 1      0       1       6       CA      C
und
HA      1.0080  0.1036  1      0       1       7       HA      H
und
CA      12.0010 0.1136  1      0       1       8       CA      C
und
H6      1.0080  0.1036  1      0       1       9       H6      H
und
NC      14.0100 -0.6664 1      0       1       10      NC      N
und
CA      12.0010 0.2636  1      0       1       11      CA      C
und
CA      12.0010 -0.1964 1      0       1       12      CA      C
und
HA      1.0080  0.1036  1      0       1       13      HA      H
und
CA      12.0010 0.2636  1      0       1       14      CA      C
und
CA      12.0010 -0.1964 1      0       1       15      CA      C
und
HA      1.0080  0.1036  1      0       1       16      HA      H
und
CA      12.0010 -0.2254 1      0       1       17      CA      C
und
C       12.0010 0.9326  1      0       1       18      C       C
und
```

O2	16.0000	-0.9464	1	0	1	19	O2	O	und
O2	16.0000	-0.9464	1	0	1	20	O2	O	und
CA	12.0010	-0.1964	1	0	1	21	CA	C	und
HA	1.0080	0.1036	1	0	1	22	HA	H	und
CA	12.0010	0.1136	1	0	1	23	CA	C	und
H6	1.0080	0.1036	1	0	1	24	H6	H	und
NC	14.0100	-0.6664	1	0	1	25	NC	N	und
Ru	101.07	2.0000	1	0	1	26	Ru	Ru	und
N2	14.0100	-0.0994	1	0	1	27	N2	N	und
CZ	12.0010	0.8866	1	0	1	28	CZ	C	und
SH	32.0600	0.0736	1	0	1	29	SH	S	und
N2	14.0100	-0.0994	1	0	1	30	N2	N	und
CZ	12.0010	0.8866	1	0	1	31	CZ	C	und
SH	32.0600	0.0736	1	0	1	32	SH	S	und
NC	14.0100	-0.6664	1	0	1	33	NC	N	und
CA	12.0010	0.1136	1	0	1	34	CA	C	und
H6	1.0080	0.1036	1	0	1	35	H6	H	und
CA	12.0010	-0.1964	1	0	1	36	CA	C	und
HA	1.0080	0.1036	1	0	1	37	HA	H	und
CA	12.0010	-0.2254	1	0	1	38	CA	C	und
C	12.0010	0.9326	1	0	1	39	C	C	und
O2	16.0000	-0.9464	1	0	1	40	O2	O	und
HO	1.0080	0.4536	1	0	1	41	HO	H	und
O2	16.0000	-0.9464	1	0	1	42	O2	O	und
CA	12.0010	-0.1964	1	0	1	43	CA	C	und
HA	1.0080	0.1036	1	0	1	44	HA	H	und
CA	12.0010	0.2636	1	0	1	45	CA	C	und
CA	12.0010	0.2636	1	0	1	46	CA	C	und

```
CA       12.0010 -0.1964 1       0         1        47       CA       C
und
HA       1.0080  0.1036  1       0         1        48       HA       H
und
CA       12.0010 0.0398  1       0         1        49       CA       C
und
C        12.0010 0.5874  1       0         1        50       C        C
und
O1       16.0000 -0.6164 1       0         1        51       O1       O
und
OH       16.0000 -0.6964 1       0         1        52       OH       O
und
CA       12.0010 -0.1964 1       0         1        53       CA       C
und
HA       1.0080  0.1036  1       0         1        54       HA       H
und
CA       12.0010 0.1136  1       0         1        55       CA       C
und
H6       1.0080  0.1036  1       0         1        56       H6       H
und
NC       14.0100 -0.6664 1       0         1        57       NC       N
und
 bonds 62
harm     1       3       1140    1.229   1
harm     3       5       938     1.409   2
harm     3       4       900     1.364   3
harm     5       6       938     1.4     4
harm     5       12      938     1.4     5
harm     6       8       938     1.4     6
harm     8       10      880     1.34    7
harm     10      11      880     1.34    8
harm     11      12      938     1.4     9
harm     11      14      938     1.4     10
harm     14      15      938     1.4     11
harm     14      25      880     1.34    12
harm     15      17      938     1.4     13
harm     17      21      938     1.4     14
harm     17      18      938     1.409   15
harm     18      19      1312    1.25    16
harm     18      20      1312    1.25    17
harm     21      23      938     1.4     18
harm     23      25      880     1.34    19
harm     27      28      923.036 1.359   20
harm     28      29      727.824 1.642   21
harm     30      31      923.036 1.359   22
harm     31      32      727.824 1.642   23
harm     33      34      880     1.34    24
harm     33      45      880     1.34    25
harm     34      36      938     1.4     26
harm     36      38      938     1.4     27
harm     38      43      938     1.4     28
harm     38      39      938     1.409   29
harm     39      42      1312    1.25    30
harm     39      40      1312    1.25    31
harm     43      45      938     1.4     32
harm     45      46      938     1.4     33
```

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harm    46      47      938     1.4     34
harm    46      57      880     1.34    35
harm    47      49      938     1.4     36
harm    49      53      938     1.4     37
harm    49      50      938     1.409   38
harm    50      52      900     1.364   39
harm    50      51      1140    1.229   40
harm    53      55      938     1.4     41
harm    55      57      880     1.34    42
harm    26      10      360     1.96    43
harm    26      25      360     1.96    44
harm    26      27      360     1.96    45
harm    26      30      360     1.96    46
harm    26      33      360     1.96    47
harm    26      57      360     1.96    48
harm    2       4       1106    0.96    49
harm    6       7       734     1.08    50
harm    8       9       734     1.08    51
harm    12      13      734     1.08    52
harm    15      16      734     1.08    53
harm    21      22      734     1.08    54
harm    23      24      734     1.08    55
harm    34      35      734     1.08    56
harm    36      37      734     1.08    57
harm    41      52      1106    0.96    58
harm    43      44      734     1.08    59
harm    47      48      734     1.08    60
harm    53      54      734     1.08    61
harm    55      56      734     1.08    62
  angles 98
harm    4       3       5       140     120.00  1
harm    1       3       5       140     120.00  2
harm    1       3       4       160     120.00  3
harm    2       4       3       100     113.00  4
harm    6       5       12      126     120.00  5
harm    3       5       6       126     120.00  6
harm    3       5       12      126     120.00  7
harm    7       6       8       100     120.00  8
harm    5       6       7       100     120.00  9
harm    5       6       8       126     120.00  10
harm    9       8       10      140     120.00  11
harm    6       8       9       100     120.00  12
harm    6       8       10      140     120.00  13
harm    8       10      11      140     120.00  14
harm    12      11      14      126     120.00  15
harm    10      11      12      140     120.00  16
harm    10      11      14      140     120.00  17
harm    5       12      13      100     120.00  18
harm    5       12      11      126     120.00  19
harm    11      12      13      100     120.00  20
harm    15      14      25      140     120.00  21
harm    11      14      15      126     120.00  22
harm    11      14      25      140     120.00  23
harm    16      15      17      100     120.00  24
harm    14      15      16      100     120.00  25
harm    14      15      17      126     120.00  26
```

harm	15	17	21	126	120.00	27
harm	15	17	18	126	120.00	28
harm	18	17	21	126	120.00	29
harm	17	18	19	140	120.00	30
harm	17	18	20	140	120.00	31
harm	19	18	20	160	126.00	32
harm	22	21	23	100	120.00	33
harm	17	21	22	100	120.00	34
harm	17	21	23	126	120.00	35
harm	24	23	25	140	120.00	36
harm	21	23	24	100	120.00	37
harm	21	23	25	140	120.00	38
harm	14	25	23	140	120.00	39
harm	27	28	29	34.902	180.00	40
harm	30	31	32	34.902	180.00	41
harm	34	33	45	140	120.00	42
harm	35	34	36	100	120.00	43
harm	33	34	35	140	120.00	44
harm	33	34	36	140	120.00	45
harm	37	36	38	100	120.00	46
harm	34	36	37	100	120.00	47
harm	34	36	38	126	120.00	48
harm	36	38	43	126	120.00	49
harm	36	38	39	126	120.00	50
harm	39	38	43	126	120.00	51
harm	38	39	42	140	120.00	52
harm	38	39	40	140	120.00	53
harm	40	39	42	160	126.00	54
harm	44	43	45	100	120.00	55
harm	38	43	44	100	120.00	56
harm	38	43	45	126	120.00	57
harm	43	45	46	126	120.00	58
harm	33	45	43	140	120.00	59
harm	33	45	46	140	120.00	60
harm	47	46	57	140	120.00	61
harm	45	46	47	126	120.00	62
harm	45	46	57	140	120.00	63
harm	48	47	49	100	120.00	64
harm	46	47	48	100	120.00	65
harm	46	47	49	126	120.00	66
harm	47	49	53	126	120.00	67
harm	47	49	50	126	120.00	68
harm	50	49	53	126	120.00	69
harm	49	50	52	140	120.00	70
harm	49	50	51	140	120.00	71
harm	51	50	52	160	120.00	72
harm	41	52	50	100	113.00	73
harm	54	53	55	100	120.00	74
harm	49	53	54	100	120.00	75
harm	49	53	55	126	120.00	76
harm	56	55	57	140	120.00	77
harm	53	55	56	100	120.00	78
harm	53	55	57	140	120.00	79
harm	46	57	55	140	120.00	80
harm	33	26	30	32.8	180.00	81
harm	25	26	27	32.8	180.00	82

```
harm    57      26      10      32.8    180.00  83
harm    33      26      10      104.8   91.00   84
harm    33      26      25      104.8   91.00   85
harm    57      26      25      104.8   91.00   87
harm    10      26      30      104.8   91.00   88
harm    25      26      30      104.8   91.00   89
harm    33      26      27      104.8   91.00   90
harm    37      26      27      104.8   91.00   91
harm    26      10      8       133.8   123.00  92
harm    26      10      11      133.8   123.00  93
harm    26      25      23      133.8   123.00  94
harm    26      25      14      133.8   123.00  95
harm    26      33      45      133.8   123.00  96
harm    26      33      34      133.8   123.00  97
harm    26      57      55      133.8   123.00  98
harm    26      57      46      133.8   123.00  99
  dihedrals 176
cos     4       3       5       6       3.63    180     1.00    0.50
0.50
cos     4       3       5       12      3.63    180     1.00    0.50
0.50
cos     1       3       5       6       3.63    180     1.00    0.50
0.50
cos     1       3       5       12      3.63    180     1.00    0.50
0.50
cos     5       3       4       2       2.3     180     1.00    0.50
0.50
cos     1       3       4       2       2.3     180     1.00    0.50
0.50
cos     12      5       6       7       3.63    180     1.00    0.50
0.50
cos     12      5       6       8       3.63    180     1.00    0.50
0.50
cos     3       5       6       7       3.63    180     1.00    0.50
0.50
cos     3       5       6       8       3.63    180     1.00    0.50
0.50
cos     6       5       12      13      3.63    180     1.00    0.50
0.50
cos     6       5       12      11      3.63    180     1.00    0.00
0.00
cos     3       5       12      13      3.63    180     1.00    0.50
0.50
cos     3       5       12      11      3.63    180     1.00    0.50
0.50
cos     7       6       8       9       3.63    180     1.00    0.50
0.50
cos     7       6       8       10      3.63    180     1.00    0.50
0.50
cos     5       6       8       9       3.63    180     1.00    0.50
0.50
cos     5       6       8       10      3.63    180     1.00    0.50
0.50
cos     9       8       10      11      4.8     180     1.00    0.50
0.50
```

cos	6	8	10	11	4.8	180	1.00	0.00	0.00
cos	8	10	11	12	4.8	180	1.00	0.00	0.00
cos	8	10	11	14	4.8	180	1.00	0.50	0.50
cos	14	11	12	13	3.63	180	1.00	0.50	0.50
cos	14	11	12	5	3.63	180	1.00	0.50	0.50
cos	10	11	12	13	3.63	180	1.00	0.50	0.50
cos	10	11	12	5	3.63	180	1.00	0.00	0.00
cos	12	11	14	15	3.63	180	1.00	0.50	0.50
cos	12	11	14	25	3.63	180	1.00	0.50	0.50
cos	10	11	14	15	3.63	180	1.00	0.50	0.50
cos	10	11	14	25	3.63	180	1.00	0.50	0.50
cos	11	14	15	16	3.63	180	1.00	0.50	0.50
cos	11	14	15	17	3.63	180	1.00	0.50	0.50
cos	25	14	15	16	3.63	180	1.00	0.50	0.50
cos	25	14	15	17	3.63	180	1.00	0.50	0.50
cos	15	14	25	23	4.8	180	1.00	0.00	0.00
cos	11	14	25	23	4.8	180	1.00	0.50	0.50
cos	16	15	17	21	3.63	180	1.00	0.50	0.50
cos	16	15	17	18	3.63	180	1.00	0.50	0.50
cos	14	15	17	21	3.63	180	1.00	0.50	0.50
cos	14	15	17	18	3.63	180	1.00	0.50	0.50
cos	15	17	21	22	3.63	180	1.00	0.50	0.50
cos	15	17	21	23	3.63	180	1.00	0.00	0.00
cos	18	17	21	22	3.63	180	1.00	0.50	0.50
cos	18	17	21	23	3.63	180	1.00	0.50	0.50
cos	21	17	18	19	3.63	180	1.00	0.50	0.50
cos	21	17	18	20	3.63	180	1.00	0.50	0.50
cos	15	17	18	19	3.63	180	1.00	0.50	0.50

cos	15	17	18	20	3.63	180	1.00	0.50	0.50
cos	22	21	23	24	3.63	180	1.00	0.50	0.50
cos	22	21	23	25	3.63	180	1.00	0.50	0.50
cos	17	21	23	24	3.63	180	1.00	0.50	0.50
cos	17	21	23	25	3.63	180	1.00	0.00	0.00
cos	24	23	25	14	4.8	180	1.00	0.50	0.50
cos	21	23	25	14	4.8	180	1.00	0.00	0.00
cos	45	33	34	35	4.8	180	1.00	0.50	0.50
cos	45	33	34	36	4.8	180	1.00	0.50	0.50
cos	34	33	45	43	4.8	180	1.00	0.50	0.50
cos	34	33	45	46	4.8	180	1.00	0.50	0.50
cos	35	34	36	37	3.63	180	1.00	0.50	0.50
cos	35	34	36	38	3.63	180	1.00	0.50	0.50
cos	33	34	36	37	3.63	180	1.00	0.50	0.50
cos	33	34	36	38	3.63	180	1.00	0.50	0.50
cos	37	36	38	43	3.63	180	1.00	0.50	0.50
cos	37	36	38	39	3.63	180	1.00	0.50	0.50
cos	34	36	38	43	3.63	180	1.00	0.00	0.00
cos	34	36	38	39	3.63	180	1.00	0.50	0.50
cos	36	38	43	44	3.63	180	1.00	0.50	0.50
cos	36	38	43	45	3.63	180	1.00	0.00	0.00
cos	39	38	43	44	3.63	180	1.00	0.50	0.50
cos	39	38	43	45	3.63	180	1.00	0.50	0.50
cos	36	38	39	42	3.63	180	1.00	0.50	0.50
cos	36	38	39	40	3.63	180	1.00	0.50	0.50
cos	43	38	39	42	3.63	180	1.00	0.50	0.50
cos	43	38	39	40	3.63	180	1.00	0.50	0.50
cos	44	43	45	46	3.63	180	1.00	0.50	0.50

cos	44	43	45	33	3.63	180	1.00	0.50	0.50
cos	38	43	45	46	3.63	180	1.00	0.50	0.50
cos	38	43	45	33	3.63	180	1.00	0.00	0.00
cos	43	45	46	47	3.63	180	1.00	0.50	0.50
cos	43	45	46	57	3.63	180	1.00	0.50	0.50
cos	33	45	46	47	3.63	180	1.00	0.50	0.50
cos	33	45	46	57	3.63	180	1.00	0.50	0.50
cos	45	46	47	48	3.63	180	1.00	0.50	0.50
cos	45	46	47	49	3.63	180	1.00	0.50	0.50
cos	57	46	47	48	3.63	180	1.00	0.50	0.50
cos	57	46	47	49	3.63	180	1.00	0.50	0.50
cos	47	46	57	55	4.8	180	1.00	0.50	0.50
cos	45	46	57	55	4.8	180	1.00	0.50	0.50
cos	48	47	49	53	3.63	180	1.00	0.50	0.50
cos	48	47	49	50	3.63	180	1.00	0.50	0.50
cos	46	47	49	53	3.63	180	1.00	0.50	0.50
cos	46	47	49	50	3.63	180	1.00	0.50	0.50
cos	47	49	53	54	3.63	180	1.00	0.50	0.50
cos	47	49	53	55	3.63	180	1.00	0.00	0.00
cos	50	49	53	54	3.63	180	1.00	0.50	0.50
cos	50	49	53	55	3.63	180	1.00	0.50	0.50
cos	53	49	50	52	3.63	180	1.00	0.50	0.50
cos	53	49	50	51	3.63	180	1.00	0.50	0.50
cos	47	49	50	52	3.63	180	1.00	0.50	0.50
cos	47	49	50	51	3.63	180	1.00	0.50	0.50
cos	49	50	52	41	2.3	180	1.00	0.50	0.50
cos	51	50	52	41	2.3	180	1.00	0.50	0.50
cos	54	53	55	56	3.63	180	1.00	0.50	0.50

cos	54	53	55	57	3.63	180	1.00	0.50	0.50
cos	49	53	55	56	3.63	180	1.00	0.50	0.50
cos	49	53	55	57	3.63	180	1.00	0.00	0.00
cos	56	55	57	46	4.8	180	1.00	0.50	0.50
cos	53	55	57	46	4.8	180	1.00	0.00	0.00
cos	26	27	28	29	2.41	180	1.00	0.50	0.50
cos	26	30	31	32	2.41	180	1.00	0.50	0.50
cos	26	10	8	6	2.81	180	1.00	0.50	0.50
cos	26	10	11	12	2.81	180	1.00	0.50	0.50
cos	26	25	23	21	2.81	180	1.00	0.50	0.50
cos	26	25	14	15	2.81	180	1.00	0.50	0.50
cos	26	33	45	43	2.81	180	1.00	0.50	0.50
cos	26	33	34	36	2.81	180	1.00	0.50	0.50
cos	26	57	55	53	2.81	180	1.00	0.50	0.50
cos	26	57	46	47	2.81	180	1.00	0.50	0.50
cos	26	10	8	9	0.00	180	1.00	0.00	0.00
cos	26	10	11	14	0.00	180	1.00	0.00	0.00
cos	26	25	14	11	0.00	180	1.00	0.00	0.00
cos	26	25	23	24	0.00	180	1.00	0.00	0.00
cos	26	57	55	56	0.00	180	1.00	0.00	0.00
cos	26	57	46	45	0.00	180	1.00	0.00	0.00
cos	26	33	45	46	0.00	180	1.00	0.00	0.00
cos	26	33	34	35	0.00	180	1.00	0.00	0.00
cos	10	26	27	28	0.00	90	1.00	0.00	0.00
cos	10	26	25	14	0.00	180	1.00	0.00	0.00
cos	10	26	25	23	0.00	180	1.00	0.00	0.00
cos	10	26	30	31	0.00	90	1.00	0.00	0.00
cos	10	26	33	45	0.00	90	1.00	0.00	0.00

cos	10	26	33	34	0.00	90	1.00	0.00	0.00
cos	10	26	57	55	0.00	90	1.00	0.00	0.00
cos	10	26	57	46	0.00	90	1.00	0.00	0.00
cos	25	26	27	28	0.00	180	1.00	0.00	0.00
cos	25	26	30	31	0.00	90	1.00	0.00	0.00
cos	25	26	10	11	0.00	180	1.00	0.00	0.00
cos	25	26	10	8	0.00	180	1.00	0.00	0.00
cos	25	26	57	46	0.00	90	1.00	0.00	0.00
cos	25	26	57	55	0.00	90	1.00	0.00	0.00
cos	25	26	33	34	0.00	90	1.00	0.00	0.00
cos	25	26	33	45	0.00	90	1.00	0.00	0.00
cos	33	26	30	31	0.00	180	1.00	0.00	0.00
cos	33	26	27	28	0.00	90	1.00	0.00	0.00
cos	33	26	57	55	0.00	180	1.00	0.00	0.00
cos	33	26	57	46	0.00	180	1.00	0.00	0.00
cos	33	26	10	8	0.00	90	1.00	0.00	0.00
cos	33	26	10	11	0.00	90	1.00	0.00	0.00
cos	33	26	25	14	0.00	90	1.00	0.00	0.00
cos	33	26	25	23	0.00	90	1.00	0.00	0.00
cos	57	26	30	31	0.00	180	1.00	0.00	0.00
cos	57	26	27	28	0.00	90	1.00	0.00	0.00
cos	57	26	10	8	0.00	90	1.00	0.00	0.00
cos	57	26	10	11	0.00	90	1.00	0.00	0.00
cos	57	26	25	23	0.00	90	1.00	0.00	0.00
cos	57	26	25	14	0.00	90	1.00	0.00	0.00
cos	57	26	33	45	0.00	180	1.00	0.00	0.00
cos	57	26	33	34	0.00	180	1.00	0.00	0.00
cos	30	26	27	28	0.00	90	1.00	0.00	0.00

```
cos     30      26      25      14      0.00    90      1.00    0.00
0.00
cos     30      26      25      23      0.00    90      1.00    0.00
0.00
cos     30      26      33      34      0.00    180     1.00    0.00
0.00
cos     30      26      33      45      0.00    180     1.00    0.00
0.00
cos     30      26      57      55      0.00    180     1.00    0.00
0.00
cos     30      26      57      46      0.00    180     1.00    0.00
0.00
cos     30      26      10      11      0.00    90      1.00    0.00
0.00
cos     30      26      10      8       0.00    90      1.00    0.00
0.00
cos     27      26      30      31      0.00    90      1.00    0.00
0.00
cos     27      26      25      14      0.00    180     1.00    0.00
0.00
cos     27      26      25      23      0.00    180     1.00    0.00
0.00
cos     27      26      33      34      0.00    90      1.00    0.00
0.00
cos     27      26      33      45      0.00    90      1.00    0.00
0.00
cos     27      26      57      55      0.00    90      1.00    0.00
0.00
cos     27      26      57      46      0.00    90      1.00    0.00
0.00
cos     27      26      10      8       0.00    180     1.00    0.00
0.00
cos     27      26      10      11      0.00    180     1.00    0.00
0.00
INVERSIONS   24
plan 5 6 10 26      40.000000 0.00000000
plan 34 36 33 26      40.000000 0.00000000
plan 6 5 8 3      40.000000 0.00000000
plan 36 34 38 35      40.000000 0.00000000
plan 8 6 11 7      40.000000 0.00000000
plan 38 36 43 37      40.000000 0.00000000
plan 11 8 12 14      40.000000 0.00000000
plan 43 38 48 46      40.000000 0.00000000
plan 12 11 10 9      40.000000 0.00000000
plan 48 43 33 39      40.000000 0.00000000
plan 10 12 5 13      40.000000 0.00000000
plan 33 48 34 44      40.000000 0.00000000
plan 14 15 11 25       40.000000 0.00000000
plan 46 47 43 57      40.000000 0.00000000
plan 15 14 17 16      40.000000 0.00000000
plan 47 46 49 48      40.000000 0.00000000
plan 17 15 21 18      40.000000 0.00000000
plan 49 47 53 50      40.000000 0.00000000
plan 21 17 23 22      40.000000 0.00000000
plan 53 49 55 54      40.000000 0.00000000
plan 23 21 25 24      40.000000 0.00000000
```

```
plan 55 53 57 56      40.000000 0.00000000
plan 25 23 14 26      40.000000 0.00000000
plan 57 55 46 26      40.000000 0.00000000
FINISH
Protons
  nummols 2
  atoms 2
  HS  1.0080  0.2992       1       0       1       1       HS      H
und
  OS  15.9994  -1.098   1       0       1       2       OS      O
und
constraints 1
1       2       0.96
FINISH
bmim
 nummols  12
 atoms  25
 N*     14.01   -0.764  1       0       1       1       N*      N
und
 c2     12.001  0.65    1       0       1       2       c2      C
und
 N*     14.01   -0.764  1       0       1       3       N*      N
und
 c2     12.001  0.2     1       0       1       4       c2      C
und
 c2     12.001  0.2     1       0       1       5       c2      C
und
 CT     12.001  0.274   1       0       1       6       CT      C
und
 H5     1.008   0.15    1       0       1       7       H5      H
und
 CT     12.001  0.354   1       0       1       8       CT      C
und
 H4     1.008   0.15    1       0       1       9       H4      H
und
 H4     1.008   0.15    1       0       1       10      H4      H
und
 H1     1.008   0.08    1       0       1       11      H1      H
und
 H1     1.008   0.08    1       0       1       12      H1      H
und
 H1     1.008   0.08    1       0       1       13      H1      H
und
 2C     12.001  -0.16   1       0       1       14      2C      C
und
 H1     1.008   0.08    1       0       1       15      H1      H
und
 H1     1.008   0.08    1       0       1       16      H1      H
und
 2C     12.001  -0.16   1       0       1       17      2C      C
und
 HC     1.008   0.08    1       0       1       18      HC      H
und
 HC     1.008   0.08    1       0       1       19      HC      H
und
```

```
 CT     12.001  -0.24   1       0       1       20      CT      C
und
 HC     1.008   0.08    1       0       1       21      HC      H
und
 HC     1.008   0.08    1       0       1       22      HC      H
und
 HC     1.008   0.08    1       0       1       23      HC      H
und
 HC     1.008   0.08    1       0       1       24      HC      H
und
 HC     1.008   0.08    1       0       1       25      HC      H
und
 bonds  25
harm    1       6       674     1.475   1
harm    1       5       613.69  1.385   2
harm    1       2       700.762 1.345   3
harm    2       3       700.83  1.345   4
harm    3       8       674     1.475   5
harm    3       4       613.706 1.385   6
harm    4       5       736.148 1.33    7
harm    8       14      620     1.526   8
harm    14      17      620     1.526   9
harm    17      20      620     1.526   10
harm    2       7       659     1.09    11
harm    4       9       659     1.09    12
harm    5       10      659     1.09    13
harm    6       11      659     1.09    14
harm    6       12      659     1.09    15
harm    6       13      659     1.09    16
harm    8       15      659     1.09    17
harm    8       16      659     1.09    18
harm    14      18      659     1.09    19
harm    14      19      659     1.09    20
harm    17      21      659     1.09    21
harm    17      22      659     1.09    22
harm    20      23      659     1.09    23
harm    20      24      659     1.09    24
harm    20      25      659     1.09    25
 angles  45
harm    5       1       6       112.296 119.881 1
harm    2       1       6       130.654 118.729 2
harm    2       1       5       164.162 121.39  3
harm    1       2       7       130.654 121.401 4
harm    1       2       3       182.526 117.199 5
harm    3       2       7       130.66  121.4   6
harm    4       3       8       112.298 119.881 7
harm    2       3       8       130.66  118.729 8
harm    2       3       4       164.17  121.39  9
harm    5       4       9       146.448 125.52  10
harm    3       4       9       112.298 114.326 11
harm    3       4       5       179.96  120.154 12
harm    4       5       10      146.448 125.52  13
harm    1       5       10      112.296 114.326 14
harm    1       5       4       179.958 120.154 15
harm    11      6       12      70      109.5   16
harm    11      6       13      70      109.5   17
```

```
harm    12      6       13      70      109.5   18
harm    1       6       11      100     109.5   19
harm    1       6       12      100     109.5   20
harm    1       6       13      100     109.5   21
harm    15      8       16      70      109.5   22
harm    14      8       15      103.41  109.471 23
harm    14      8       16      103.41  109.471 24
harm    3       8       15      100     109.5   25
harm    3       8       16      100     109.5   26
harm    3       8       14      157.916 104.954 27
harm    18      14      19      70      109.5   28
harm    17      14      18      100     109.5   29
harm    17      14      19      100     109.5   30
harm    8       14      18      100     109.5   31
harm    8       14      19      100     109.5   32
harm    8       14      17      143.156 104.954 33
harm    21      17      22      70      109.5   34
harm    20      17      21      100     109.5   35
harm    20      17      22      100     109.5   36
harm    14      17      21      100     109.5   37
harm    14      17      22      100     109.5   38
harm    14      17      20      143.792 104.954 39
harm    23      20      24      70      109.5   40
harm    23      20      25      70      109.5   41
harm    24      20      25      70      109.5   42
harm    17      20      23      100     109.5   43
harm    17      20      24      100     109.5   44
harm    17      20      25      100     109.5   45
 dihedrals  59
cos3    7       4       5       9       0       10.75   0       0.5
0.5
cos3    7       4       5       3       0       10.75   0       0.0
0.0
cos3    1       4       5       9       0       10.75   0       0.5
0.5
cos3    1       4       5       3       0       10.75   0       0.0
0.0
cos3    7       4       1       6       0       3       0       0.5
0.5
cos3    7       4       1       2       0       3       0       0.0
0.0
cos3    5       4       1       6       0       3       0       0.0
0.0
cos3    5       4       1       2       0       3       0       0.0
0.0
cos3    9       5       3       8       0       3       0       0.5
0.5
cos3    9       5       3       2       0       3       0       0.5
0.5
cos3    4       5       3       8       0       3       0       0.0
0.0
cos3    4       5       3       2       0       3       0       0.0
0.0
cos3    4       1       6       11      0       0       0.1314  0.5
0.5
```

cos3	4	1	6	12	0	0	0.1314	0.5	0.5
cos3	4	1	6	13	0	0	0.1314	0.5	0.5
cos3	2	1	6	11	0	0	0	0.5	0.5
cos3	2	1	6	12	0	0	0	0.5	0.5
cos3	2	1	6	13	0	0	0	0.5	0.5
cos3	6	1	2	10	0	4.649	0	0.5	0.5
cos3	6	1	2	3	0	4.649	0	0.5	0.5
cos3	4	1	2	10	0	4.649	0	0.0	0.0
cos3	4	1	2	3	0	4.649	0	0.0	0.0
cos3	5	3	8	15	0	0	0.1314	0.5	0.5
cos3	5	3	8	16	0	0	0.1314	0.5	0.5
cos3	5	3	8	14	-1.3758	1.0581	0.2095	0.5	0.5
cos3	2	3	8	15	0	0	0	0.5	0.5
cos3	2	3	8	16	0	0	0	0.5	0.5
cos3	2	3	8	14	-0.7715	0	0	0.5	0.5
cos3	8	3	2	10	0	4.649	0	0.5	0.5
cos3	8	3	2	1	0	4.649	0	0.5	0.5
cos3	5	3	2	10	0	4.649	0	0.0	0.0
cos3	5	3	2	1	0	4.649	0	0.0	0.0
cos3	15	8	14	23	0	0	0.3179	0.5	0.5
cos3	15	8	14	25	0	0	0.3179	0.5	0.5
cos3	15	8	14	17	0	0	0.3657	0.5	0.5
cos3	16	8	14	24	0	0	0.3179	0.5	0.5
cos3	16	8	14	25	0	0	0.3179	0.5	0.5
cos3	16	8	14	17	0	0	0.3657	0.5	0.5
cos3	3	8	14	24	0	0	0	0.5	0.5
cos3	3	8	14	25	0	0	0	0.5	0.5
cos3	3	8	14	17	0.1763	-0.16265	0.24362	0.5	0.5

```
cos3    24      14      17      22      0       0       0.3179  0.5
0.5
cos3    24      14      17      23      0       0       0.3179  0.0
0.0
cos3    24      14      17      20      0       0       0.3657  0.0
0.0
cos3    25      14      17      22      0       0       0.3179  0.5
0.5
cos3    25      14      17      23      0       0       0.3179  0.0
0.0
cos3    25      14      17      20      0       0       0.3657  0.0
0.0
cos3    8       14      17      22      0       0       0.3657  0.5
0.5
cos3    8       14      17      23      0       0       0.3657  0.0
0.0
cos3    8       14      17      20      0.1738  0.1569  0.2787  0.5
0.5
cos3    22      17      20      18      0       0       0.3179  0.5
0.5
cos3    22      17      20      19      0       0       0.3179  0.5
0.5
cos3    22      17      20      21      0       0       0.3179  0.0
0.0
cos3    23      17      20      18      0       0       0.3179  0.5
0.5
cos3    23      17      20      19      0       0       0.3179  0.5
0.5
cos3    23      17      20      21      0       0       0.3179  0.5
0.5
cos3    14      17      20      18      0       0       0.3657  0.0
0.0
cos3    14      17      20      19      0       0       0.3657  0.0
0.0
cos3    14      17      20      21      0       0       0.3657  0.0
0.0
INVERSIONS   5
plan   1   2   5   6    40.000000 0.00000000
plan   2   3   1   7    40.000000 0.00000000
plan   3   4   2   8    40.000000 0.00000000
plan   4   3   5   9    40.000000 0.00000000
plan   5   1   4   10   40.000000 0.00000000
finish
NTf2
nummols  12
atoms  15
 n      14.01   -0.368  1       0       1       1        n      N
und
 s      32.06   1.3113  1       0       1       2        s      S
und
 o=     16      -0.717  1       0       1       3        o=     O
und
 o=     16      -0.717  1       0       1       4        o=     O
und
 c3     12.001  1.0898  1       0       1       5        c3     C
und
```

```
 F      19      -0.4277 1       0       1       6        F      F
und
 F      19      -0.4277 1       0       1       7        F      F
und
 F      19      -0.4277 1       0       1       8        F      F
und
 s      32.06   1.3113  1       0       1       9        s      S
und
 o=     16      -0.717  1       0       1       10       o=     O
und
 o=     16      -0.717  1       0       1       11       o=     O
und
 c3     12.001  1.0898  1       0       1       12       c3     C
und
 F      19      -0.4277 1       0       1       13       F      F
und
 F      19      -0.4277 1       0       1       14       F      F
und
 F      19      -0.4277 1       0       1       15       F      F
und
 bonds  14
harm    1       2       449.074 1.596   1                224.537
harm    1       9       449.074 1.596   2                224.537
harm    2       5       285.92  1.764   3                142.96
harm    2       3       731.254 1.432   4                365.627
harm    2       4       731.254 1.432   5                365.627
harm    5       6       659.596 1.363   6                329.798
harm    5       7       659.596 1.363   7                329.798
harm    5       8       659.596 1.363   8                329.798
harm    9       12      285.92  1.764   9                142.96
harm    9       10      731.254 1.432   10               365.627
harm    9       11      731.254 1.432   11               365.627
harm    12      13      659.596 1.363   12               329.798
harm    12      14      659.596 1.363   13               329.798
harm    12      15      659.596 1.363   14               329.798
 angles  25
harm    2    1          9       136.424 119.753 1
harm    1    2          5       177.112 112.27  2
harm    1    2          3       249.56  117.054 3
harm    1    2          4       249.56  117.054 4
harm    3    2          5       198.624 115.756 5
harm    3    2          4       280.48  122.877 6
harm    4    2          5       198.624 115.756 7
harm    6    5          7       225.98  110.826 8
harm    6    5          8       225.98  110.826 9
harm    7    5          8       225.98  110.826 10
harm    2    5          6       140.968 119.923 11
harm    2    5          7       140.968 119.923 12
harm    2    5          8       140.968 119.923 13
harm    1    9          12      177.112 112.27  14
harm    1    9          10      249.56  117.054 15
harm    1    9          11      249.56  117.054 16
harm    10   9          12      198.624 115.756 17
harm    10   9          11      280.48  122.877 18
harm    11   9          12      198.624 115.756 19
harm    13   12         14      225.98  110.826 20
```

```
harm    13   12          15       225.98  110.826 21
harm    14   12          15       225.98  110.826 22
harm    9    12          13       140.968 119.923 23
harm    9    12          14       140.968 119.923 24
harm    9    12          15       140.968 119.923 25
  dihedrals 24
cos     9       1       2       5       4.57    0       1.00    0.50
0.50
cos     9       1       2       3       7.12    180     1.00    0.50
0.50
cos     9       1       2       4       7.12    180     1.00    0.50
0.50
cos     2       1       9       12      4.57    0       1.00    0.50
0.50
cos     2       1       9       10      7.12    180     1.00    0.50
0.50
cos     2       1       9       11      7.12    180     1.00    0.50
0.50
cos     1       2       5       6       0.49    0       1.00    0.50
0.50
cos     1       2       5       7       0.49    0       1.00    0.50
0.50
cos     1       2       5       8       0.49    0       1.00    0.50
0.50
cos     3       2       5       6       0.64    0       1.00    0.50
0.50
cos     3       2       5       7       0.64    0       1.00    0.50
0.50
cos     3       2       5       8       0.64    0       1.00    0.50
0.50
cos     4       2       5       6       0.64    0       1.00    0.50
0.50
cos     4       2       5       7       0.64    0       1.00    0.50
0.50
cos     4       2       5       8       0.64    0       1.00    0.50
0.50
cos     1       9       12      13      0.49    0       1.00    0.50
0.50
cos     1       9       12      14      0.49    0       1.00    0.50
0.50
cos     1       9       12      15      0.49    0       1.00    0.50
0.50
cos     10      9       12      13      0.64    0       1.00    0.50
0.50
cos     10      9       12      14      0.64    0       1.00    0.50
0.50
cos     10      9       12      15      0.64    0       1.00    0.50
0.50
cos     11      9       12      13      0.64    0       1.00    0.50
0.50
cos     11      9       12      14      0.64    0       1.00    0.50
0.50
cos     11      9       12      15      0.64    0       1.00    0.50
0.50
 finish
vdw 465
```

n	n	lj	0.17	3.257142883
n	s	lj	0.206155281	3.414285742
n	o=	lj	0.188944436	3.111785739
n	c3	lj	0.136374484	3.332142884
n	F	lj	0.101833197	3.191071454
n	N*	lj	0.17	3.257142883
n	c2	lj	0.120913192	3.332142884
n	CT	lj	0.136374484	3.332142884
n	H5	lj	0.050497525	2.841964308
n	H4	lj	0.050497525	2.886607166
n	H1	lj	0.051662365	3.214928592
n	2C	lj	0.136374484	3.332142884
n	HC	lj	0.051662365	2.956250024
s	s	lj	0.25	3.5714286
s	o=	lj	0.229128785	3.268928598
s	c3	lj	0.165378354	3.489285742
s	F	lj	0.12349089	3.348214313
s	N*	lj	0.206155281	3.414285742
s	c2	lj	0.146628783	3.489285742
s	CT	lj	0.165378354	3.489285742
s	H5	lj	0.061237244	2.999107167
s	H4	lj	0.061237244	3.043750024
s	H1	lj	0.06264982	3.37207145
s	2C	lj	0.165378354	3.489285742
s	HC	lj	0.06264982	3.113392882
o=	o=	lj	0.21	2.966428595
o=	c3	lj	0.151571765	3.18678574
o=	F	lj	0.113181271	3.04571431
o=	N*	lj	0.188944436	3.111785739
o=	c2	lj	0.134387499	3.18678574
o=	CT	lj	0.151571765	3.18678574
o=	H5	lj	0.056124861	2.696607164
o=	H4	lj	0.056124861	2.741250022
o=	H1	lj	0.057419509	3.069571448
o=	2C	lj	0.151571765	3.18678574
o=	HC	lj	0.057419509	2.81089288
c3	c3	lj	0.1094	3.407142884
c3	F	lj	0.081690881	3.266071455
c3	N*	lj	0.136374484	3.332142884
c3	c2	lj	0.096996907	3.407142884
c3	CT	lj	0.1094	3.407142884
c3	H5	lj	0.040509258	2.916964309
c3	H4	lj	0.040509258	2.961607167
c3	H1	lj	0.041443697	3.289928592
c3	2C	lj	0.1094	3.407142884
c3	HC	lj	0.041443697	3.031250024
F	F	lj	0.061	3.125000025
F	N*	lj	0.101833197	3.191071454
F	c2	lj	0.072429276	3.266071455
F	CT	lj	0.081690881	3.266071455
F	H5	lj	0.030248967	2.775892879
F	H4	lj	0.030248967	2.820535737
F	H1	lj	0.030946728	3.148857163
F	2C	lj	0.081690881	3.266071455
F	HC	lj	0.030946728	2.890178595
N*	N*	lj	0.17	3.257142883

N*	c2	lj	0.120913192		3.332142884
N*	CT	lj	0.136374484		3.332142884
N*	H5	lj	0.050497525		2.841964308
N*	H4	lj	0.050497525		2.886607166
N*	H1	lj	0.051662365		3.214928592
N*	2C	lj	0.136374484		3.332142884
N*	HC	lj	0.051662365		2.956250024
c2	c2	lj	0.086		3.407142884
c2	CT	lj	0.096996907		3.407142884
c2	H5	lj	0.03591657		2.916964309
c2	H4	lj	0.03591657		2.961607167
c2	H1	lj	0.036745068		3.289928592
c2	2C	lj	0.096996907		3.407142884
c2	HC	lj	0.036745068		3.031250024
CT	CT	lj	0.1094		3.407142884
CT	H5	lj	0.040509258		2.916964309
CT	H4	lj	0.040509258		2.961607167
CT	H1	lj	0.041443697		3.289928592
CT	2C	lj	0.1094		3.407142884
CT	HC	lj	0.041443697		3.031250024
H5	H5	lj	0.015		2.426785734
H5	H4	lj	0.015		2.471428591
H5	H1	lj	0.015346009		2.799750017
H5	2C	lj	0.040509258		2.916964309
H5	HC	lj	0.015346009		2.541071449
H4	H4	lj	0.015		2.516071449
H4	H1	lj	0.015346009		2.844392874
H4	2C	lj	0.040509258		2.961607167
H4	HC	lj	0.015346009		2.585714306
H1	H1	lj	0.0157		3.1727143
H1	2C	lj	0.041443697		3.289928592
H1	HC	lj	0.0157		2.914035732
2C	2C	lj	0.1094		3.407142884
2C	HC	lj	0.041443697		3.031250024
HC	HC	lj	0.0157		2.655357164
Ti	Ti	buck	717647.4	0.154	121.0676
Ti	O	buck	391049.1	0.194	290.3317
Ti	n	lj	0.3805387		2.5426884
Ti	s	lj	0.461471		2.6998313
Ti	o=	lj	0.4229452		2.3973313
Ti	c3	lj	0.3052693		2.6176884
Ti	F	lj	0.2279499		2.476617
Ti	N*	lj	0.3805387		2.5426884
Ti	c2	lj	0.2706597		2.6176884
Ti	CT	lj	0.3052693		2.6176884
Ti	H5	lj	0.1130369		2.1275099
Ti	H4	lj	0.1130369		2.1721527
Ti	H1	lj	0.1156443		2.5004742
Ti	2C	lj	0.3052693		2.6176884
Ti	HC	lj	0.1156443		2.2417956
O	O	buck	271716.3	0.234	696.8883
O	n	lj	0.2120703		3.0809979
O	s	lj	0.257173		3.2381408
O	o=	lj	0.2357029		2.9356408
O	c3	lj	0.1701234		3.1559979
O	F	lj	0.1270341		3.0149265

O	N*	lj	0.2120703	3.0809979
O	c2	lj	0.1508359	3.1559979
O	CT	lj	0.1701234	3.1559979
O	H5	lj	0.0629943	2.6658194
O	H4	lj	0.0629943	2.7104622
O	H1	lj	0.0644474	3.0387837
O	2C	lj	0.1701234	3.1559979
O	HC	lj	0.0644474	2.7801051
n	O1	lj	0.188944436	3.111785739
s	O1	lj	0.229128785	3.268928598
o=	O1	lj	0.21	2.966428595
c3	O1	lj	0.151571765	3.18678574
F	O1	lj	0.113181271	3.04571431
N*	O1	lj	0.188944436	3.111785739
c2	O1	lj	0.134387499	3.18678574
CT	O1	lj	0.151571765	3.18678574
H5	O1	lj	0.056124861	2.696607164
H4	O1	lj	0.056124861	2.741250022
H1	O1	lj	0.057419509	3.069571448
2C	O1	lj	0.151571765	3.18678574
HC	O1	lj	0.057419509	2.81089288
Ti	O1	lj	0.422945174	2.397331298
O	O1	lj	0.235702944	2.935640798
n	HO	lj	0	2.521428592
s	HO	lj	0	2.67857145
o=	HO	lj	0	2.376071448
c3	HO	lj	0	2.596428592
F	HO	lj	0	2.455357163
N*	HO	lj	0	2.521428592
c2	HO	lj	0	2.596428592
CT	HO	lj	0	2.596428592
H5	HO	lj	0	2.106250017
H4	HO	lj	0	2.150892874
H1	HO	lj	0	2.4792143
2C	HO	lj	0	2.596428592
HC	HO	lj	0	2.220535732
Ti	HO	lj	0	1.80697415
O	HO	lj	0	2.34528365
n	C	lj	0.120913192	3.332142884
s	C	lj	0.146628783	3.489285742
o=	C	lj	0.134387499	3.18678574
c3	C	lj	0.096996907	3.407142884
F	C	lj	0.072429276	3.266071455
N*	C	lj	0.120913192	3.332142884
c2	C	lj	0.086	3.407142884
CT	C	lj	0.096996907	3.407142884
H5	C	lj	0.03591657	2.916964309
H4	C	lj	0.03591657	2.961607167
H1	C	lj	0.036745068	3.289928592
2C	C	lj	0.096996907	3.407142884
HC	C	lj	0.036745068	3.031250024
Ti	C	lj	0.270659735	2.617688442
O	C	lj	0.150835854	3.155997942
n	OH	lj	0.189124298	3.165178597
s	OH	lj	0.229346899	3.322321455
o=	OH	lj	0.210199905	3.019821453

c3	OH	lj	0.151716051	3.240178597
F	OH	lj	0.113289011	3.099107168
N*	OH	lj	0.189124298	3.165178597
c2	OH	lj	0.134515427	3.240178597
CT	OH	lj	0.151716051	3.240178597
H5	OH	lj	0.056178288	2.750000022
H4	OH	lj	0.056178288	2.79464288
H1	OH	lj	0.057474168	3.122964305
2C	OH	lj	0.151716051	3.240178597
HC	OH	lj	0.057474168	2.864285737
Ti	OH	lj	0.423347787	2.450724155
O	OH	lj	0.235927317	2.989033655
n	CA	lj	0.120913192	3.332142884
s	CA	lj	0.146628783	3.489285742
o=	CA	lj	0.134387499	3.18678574
c3	CA	lj	0.096996907	3.407142884
F	CA	lj	0.072429276	3.266071455
N*	CA	lj	0.120913192	3.332142884
c2	CA	lj	0.086	3.407142884
CT	CA	lj	0.096996907	3.407142884
H5	CA	lj	0.03591657	2.916964309
H4	CA	lj	0.03591657	2.961607167
H1	CA	lj	0.036745068	3.289928592
2C	CA	lj	0.096996907	3.407142884
HC	CA	lj	0.036745068	3.031250024
Ti	CA	lj	0.270659735	2.617688442
O	CA	lj	0.150835854	3.155997942
n	HA	lj	0.050497525	2.931250023
s	HA	lj	0.061237244	3.088392882
o=	HA	lj	0.056124861	2.785892879
c3	HA	lj	0.040509258	3.006250024
F	HA	lj	0.030248967	2.865178594
N*	HA	lj	0.050497525	2.931250023
c2	HA	lj	0.03591657	3.006250024
CT	HA	lj	0.040509258	3.006250024
H5	HA	lj	0.015	2.516071449
H4	HA	lj	0.015	2.560714306
H1	HA	lj	0.015346009	2.889035732
2C	HA	lj	0.040509258	3.006250024
HC	HA	lj	0.015346009	2.630357164
Ti	HA	lj	0.113036852	2.216795582
O	HA	lj	0.062994262	2.755105082
n	H6	lj	0.050497525	2.886607166
s	H6	lj	0.061237244	3.043750024
o=	H6	lj	0.056124861	2.741250022
c3	H6	lj	0.040509258	2.961607167
F	H6	lj	0.030248967	2.820535737
N*	H6	lj	0.050497525	2.886607166
c2	H6	lj	0.03591657	2.961607167
CT	H6	lj	0.040509258	2.961607167
H5	H6	lj	0.015	2.471428591
H4	H6	lj	0.015	2.516071449
H1	H6	lj	0.015346009	2.844392874
2C	H6	lj	0.040509258	2.961607167
HC	H6	lj	0.015346009	2.585714306
Ti	H6	lj	0.113036852	2.172152724

O	H6	lj	0.062994262	2.710462224
n	NC	lj	0.17	3.257142883
s	NC	lj	0.206155281	3.414285742
o=	NC	lj	0.188944436	3.111785739
c3	NC	lj	0.136374484	3.332142884
F	NC	lj	0.101833197	3.191071454
N*	NC	lj	0.17	3.257142883
c2	NC	lj	0.120913192	3.332142884
CT	NC	lj	0.136374484	3.332142884
H5	NC	lj	0.050497525	2.841964308
H4	NC	lj	0.050497525	2.886607166
H1	NC	lj	0.051662365	3.214928592
2C	NC	lj	0.136374484	3.332142884
HC	NC	lj	0.051662365	2.956250024
Ti	NC	lj	0.38053875	2.542688442
O	NC	lj	0.212070286	3.080997942
n	Ru	lj	0.272873597	2.798571442
s	Ru	lj	0.330907842	2.9557143
o=	Ru	lj	0.303282047	2.653214298
c3	Ru	lj	0.218899977	2.873571442
F	Ru	lj	0.163456416	2.732500013
N*	Ru	lj	0.272873597	2.798571442
c2	Ru	lj	0.194082457	2.873571442
CT	Ru	lj	0.218899977	2.873571442
H5	Ru	lj	0.081055537	2.383392867
H4	Ru	lj	0.081055537	2.428035724
H1	Ru	lj	0.082925268	2.75635715
2C	Ru	lj	0.218899977	2.873571442
HC	Ru	lj	0.082925268	2.497678582
Ti	Ru	lj	0.610817514	2.084117
O	Ru	lj	0.340402245	2.6224265
n	N2	lj	0.17	3.257142883
s	N2	lj	0.206155281	3.414285742
o=	N2	lj	0.188944436	3.111785739
c3	N2	lj	0.136374484	3.332142884
F	N2	lj	0.101833197	3.191071454
N*	N2	lj	0.17	3.257142883
c2	N2	lj	0.120913192	3.332142884
CT	N2	lj	0.136374484	3.332142884
H5	N2	lj	0.050497525	2.841964308
H4	N2	lj	0.050497525	2.886607166
H1	N2	lj	0.051662365	3.214928592
2C	N2	lj	0.136374484	3.332142884
HC	N2	lj	0.051662365	2.956250024
Ti	N2	lj	0.38053875	2.542688442
O	N2	lj	0.212070286	3.080997942
n	CZ	lj	0.120913192	3.332142884
s	CZ	lj	0.146628783	3.489285742
o=	CZ	lj	0.134387499	3.18678574
c3	CZ	lj	0.096996907	3.407142884
F	CZ	lj	0.072429276	3.266071455
N*	CZ	lj	0.120913192	3.332142884
c2	CZ	lj	0.086	3.407142884
CT	CZ	lj	0.096996907	3.407142884
H5	CZ	lj	0.03591657	2.916964309
H4	CZ	lj	0.03591657	2.961607167

H1	CZ	lj	0.036745068		3.289928592
2C	CZ	lj	0.096996907		3.407142884
HC	CZ	lj	0.036745068		3.031250024
Ti	CZ	lj	0.270659735		2.617688442
O	CZ	lj	0.150835854		3.155997942
n	SH	lj	0.206155281		3.414285742
s	SH	lj	0.25		3.5714286
o=	SH	lj	0.229128785		3.268928598
c3	SH	lj	0.165378354		3.489285742
F	SH	lj	0.12349089		3.348214313
N*	SH	lj	0.206155281		3.414285742
c2	SH	lj	0.146628783		3.489285742
CT	SH	lj	0.165378354		3.489285742
H5	SH	lj	0.061237244		2.999107167
H4	SH	lj	0.061237244		3.043750024
H1	SH	lj	0.06264982		3.37207145
2C	SH	lj	0.165378354		3.489285742
HC	SH	lj	0.06264982		3.113392882
Ti	SH	lj	0.461471018		2.6998313
O	SH	lj	0.257172996		3.2381408
n	O2	lj	0.188944436		3.111785739
s	O2	lj	0.229128785		3.268928598
o=	O2	lj	0.21		2.966428595
c3	O2	lj	0.151571765		3.18678574
F	O2	lj	0.113181271		3.04571431
N*	O2	lj	0.188944436		3.111785739
c2	O2	lj	0.134387499		3.18678574
CT	O2	lj	0.151571765		3.18678574
H5	O2	lj	0.056124861		2.696607164
H4	O2	lj	0.056124861		2.741250022
H1	O2	lj	0.057419509		3.069571448
2C	O2	lj	0.151571765		3.18678574
HC	O2	lj	0.057419509		2.81089288
Ti	O2	lj	0.422945174		2.397331298
O	O2	lj	0.235702944		2.935640798
OS	Ti	buck	391049.1	0.194	290.3317
OS	OS	buck	271716.3	0.234	696.8883
OS	O	buck	271716.3	0.234	696.8883
OS	n	lj	0.2120703		3.0809979
OS	s	lj	0.257173		3.2381408
OS	o=	lj	0.2357029		2.9356408
OS	c3	lj	0.1701234		3.1559979
OS	F	lj	0.1270341		3.0149265
OS	N*	lj	0.2120703		3.0809979
OS	c2	lj	0.1508359		3.1559979
OS	CT	lj	0.1701234		3.1559979
OS	H5	lj	0.0629943		2.6658194
OS	H4	lj	0.0629943		2.7104622
OS	H1	lj	0.0644474		3.0387837
OS	2C	lj	0.1701234		3.1559979
OS	HC	lj	0.0644474		2.7801051
OS	O1	lj	0.235702944		2.935640798
OS	HO	lj	0		2.34528365
OS	C	lj	0.150835854		3.155997942
OS	OH	lj	0.235927317		2.989033655
OS	CA	lj	0.150835854		3.155997942

OS	HA	lj	0.062994262	2.755105082
OS	H6	lj	0.062994262	2.710462224
OS	NC	lj	0.212070286	3.080997942
OS	Ru	lj	0.340402245	2.6224265
OS	N2	lj	0.212070286	3.080997942
OS	CZ	lj	0.150835854	3.155997942
OS	SH	lj	0.257172996	3.2381408
OS	O2	lj	0.235702944	2.935640798
n	HS	lj	0.058309519	2.519471442
s	HS	lj	0.070710678	2.6766143
o=	HS	lj	0.064807407	2.374114298
c3	HS	lj	0.046776062	2.594471442
F	HS	lj	0.034928498	2.453400013
N*	HS	lj	0.058309519	2.519471442
c2	HS	lj	0.041472883	2.594471442
CT	HS	lj	0.046776062	2.594471442
H5	HS	lj	0.017320508	2.104292867
H4	HS	lj	0.017320508	2.148935724
H1	HS	lj	0.017720045	2.47725715
2C	HS	lj	0.046776062	2.594471442
HC	HS	lj	0.017720045	2.218578582
Ti	HS	lj	0.130523714	1.805017
O	HS	lj	0.072739508	2.3433265
O1	HS	lj	0.064807407	2.374114298
HO	HS	lj	0.0	1.78375715
C	HS	lj	0.041472883	2.594471442
OH	HS	lj	0.064869099	2.427507155
CA	HS	lj	0.041472883	2.594471442
HA	HS	lj	0.017320508	2.193578582
H6	HS	lj	0.017320508	2.148935724
NC	HS	lj	0.058309519	2.519471442
Ru	HS	lj	0.093594872	2.0609
N2	HS	lj	0.058309519	2.519471442
CZ	HS	lj	0.041472883	2.594471442
SH	HS	lj	0.070710678	2.6766143
O2	HS	lj	0.064807407	2.374114298
OS	HS	lj	0.072739508	2.3433265
HS	HS	lj	0.02	1.7818
O1	O1	lj	0.21	2.966428595
HO	O1	lj	0	2.376071448
C	O1	lj	0.134387499	3.18678574
OH	O1	lj	0.210199905	3.019821453
CA	O1	lj	0.134387499	3.18678574
HA	O1	lj	0.056124861	2.785892879
H6	O1	lj	0.056124861	2.741250022
NC	O1	lj	0.188944436	3.111785739
Ru	O1	lj	0.303282047	2.653214298
N2	O1	lj	0.188944436	3.111785739
CZ	O1	lj	0.134387499	3.18678574
SH	O1	lj	0.229128785	3.268928598
O2	O1	lj	0.21	2.966428595
HO	HO	lj	0	1.7857143
C	HO	lj	0	2.596428592
OH	HO	lj	0	2.429464305
CA	HO	lj	0	2.596428592
HA	HO	lj	0	2.195535732

H6	HO	lj	0	2.150892874
NC	HO	lj	0	2.521428592
Ru	HO	lj	0	2.06285715
N2	HO	lj	0	2.521428592
CZ	HO	lj	0	2.596428592
SH	HO	lj	0	2.67857145
O2	HO	lj	0	2.376071448
C	C	lj	0.086	3.407142884
OH	C	lj	0.134515427	3.240178597
CA	C	lj	0.086	3.407142884
HA	C	lj	0.03591657	3.006250024
H6	C	lj	0.03591657	2.961607167
NC	C	lj	0.120913192	3.332142884
Ru	C	lj	0.194082457	2.873571442
N2	C	lj	0.120913192	3.332142884
CZ	C	lj	0.086	3.407142884
SH	C	lj	0.146628783	3.489285742
O2	C	lj	0.134387499	3.18678574
OH	OH	lj	0.2104	3.07321431
CA	OH	lj	0.134515427	3.240178597
HA	OH	lj	0.056178288	2.839285737
H6	OH	lj	0.056178288	2.79464288
NC	OH	lj	0.189124298	3.165178597
Ru	OH	lj	0.30357075	2.706607155
N2	OH	lj	0.189124298	3.165178597
CZ	OH	lj	0.134515427	3.240178597
SH	OH	lj	0.229346899	3.322321455
O2	OH	lj	0.210199905	3.019821453
CA	CA	lj	0.086	3.407142884
HA	CA	lj	0.03591657	3.006250024
H6	CA	lj	0.03591657	2.961607167
NC	CA	lj	0.120913192	3.332142884
Ru	CA	lj	0.194082457	2.873571442
N2	CA	lj	0.120913192	3.332142884
CZ	CA	lj	0.086	3.407142884
SH	CA	lj	0.146628783	3.489285742
O2	CA	lj	0.134387499	3.18678574
HA	HA	lj	0.015	2.605357164
H6	HA	lj	0.015	2.560714306
NC	HA	lj	0.050497525	2.931250023
Ru	HA	lj	0.081055537	2.472678582
N2	HA	lj	0.050497525	2.931250023
CZ	HA	lj	0.03591657	3.006250024
SH	HA	lj	0.061237244	3.088392882
O2	HA	lj	0.056124861	2.785892879
H6	H6	lj	0.015	2.516071449
NC	H6	lj	0.050497525	2.886607166
Ru	H6	lj	0.081055537	2.428035724
N2	H6	lj	0.050497525	2.886607166
CZ	H6	lj	0.03591657	2.961607167
SH	H6	lj	0.061237244	3.043750024
O2	H6	lj	0.056124861	2.741250022
NC	NC	lj	0.17	3.257142883
Ru	NC	lj	0.272873597	2.798571442
N2	NC	lj	0.17	3.257142883
CZ	NC	lj	0.120913192	3.332142884

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Ru      Ru      lj      0.438           2.34
N2      Ru      lj      0.272873597     2.798571442
CZ      Ru      lj      0.194082457     2.873571442
SH      Ru      lj      0.330907842     2.9557143
O2      Ru      lj      0.303282047     2.653214298
N2      N2      lj      0.17            3.257142883
CZ      N2      lj      0.120913192     3.332142884
SH      N2      lj      0.206155281     3.414285742
O2      N2      lj      0.188944436     3.111785739
CZ      CZ      lj      0.086           3.407142884
SH      CZ      lj      0.146628783     3.489285742
O2      CZ      lj      0.134387499     3.18678574
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O2      O2      lj      0.21            2.966428595
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2. CONFIG file

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Ti              8
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Ti              9
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Ti             10
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Ti             11
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Ti             13
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Ti             16
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Ti	23		
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Ti	27		
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Ti              50
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Ti              55
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Ti              56
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Ti	71		
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Ti              80
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Ti              81
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Ti              86
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Ti	92		
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	-19250.49228	1481.728861	-3475.493431
O2	305		
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	9.980686578	3.047547492	-3.993402203
	10025.30684	3075.996618	-2824.949648
O2	306		
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	-6.297475252	4.969900958	-0.8176267435
	6078.676035	2735.775277	2244.693604
CA	307		
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	1.625865457	2.277330383	-2.022505467
	9112.834554	-341.4816714	-1832.728132
HA	308		
	9.448150510	6.160291563	4.377825145
	4.531631257	8.553673310	23.62156408
	-4317.789263	-4014.999264	-96.99904146
CA	309		
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	-144.1540004	18866.58267	12710.04851
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	-6145.363093	-6791.921901	-2824.070403
Ru	312		
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CA             320
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CA             322
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CA              329
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CA              331
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CA              333
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CA              335
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C               336
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	-2422.696561	-2793.999631	-2948.310557
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2C	411		
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H1            413
    -2.898372867        -3.241992518        -7.673785408
     2.654882952        18.68538140         10.76117913
     3616.359958        591.9047131         1073.879715
2C            414
    -1.845490347        -0.5253786054       -8.249344402
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     10452.81772        28637.69058         -13920.34206
HC            415
    -3.817279735        -0.9672113155       -7.660649995
     7.563502646        -15.12633894        -16.60981438
    -7859.195225        4705.508903         8122.522845
HC            416
    -3.638024170        -0.7588537659       -9.407993259
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    -229.8747141        1205.187936         -325.0514941
CT            417
    -2.051239076        1.048555322         -8.219380705
     1.109509704        -6.119962628        -0.7183302189
     5214.101418        -16656.30679        -6692.531979
HC            418
    -1.156102431        -0.6358106401       -9.102886461
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    -4388.572740        -6804.519869        953.0521400
HC            419
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     5.419381337        -0.6395748498       -1.920920813
     327.9282967        -6931.569425        12951.95643
HC            420
    -1.305084269        1.561673449         -7.581110847
    -1.941449285        16.75978230         28.08621347
    -1824.062154        -3310.590294        -3746.129948
HC            421
    -3.046469458        1.302042195         -7.858515388
    -3.012110860        -15.62838032        -28.89858312
    -622.4371193        637.1810943         -1634.582393
HC            422
    -1.895392869        1.304823606         -9.305359782
    -18.26982033        -5.331549194        -14.34171653
    -4544.272209        6063.087764         11019.92958
N*            423
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    -2.567105807        0.6415101364        3.925484725
    -3181.084691        -6652.867790        10563.99198
c2            424
    0.2988019157        4.688269984         -9.667249015
    -2.977662234        -0.4029407907       3.998140151
    -7158.879860        8689.358583         -7737.898881
N*            425
   -0.3420923555        3.748796573         -10.45703592
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	-0.5243452846	4.901943194	3.047270016
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CT	428		
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	-1.832514625	3.507548942	-10.77152731
	8024.246119	-2706.088644	1309.452773
H5	429		
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	13.12657150	6.844251734	-13.17711757
	-5042.627274	-10136.33446	-4208.785392
CT	430		
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	9.597448119	1.629553553	1.073968180
	-8228.728310	-11556.71748	-24026.65427
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	-12.17741584	15.42655223	-21.35859451
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H4	432		
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	-6.610000493	23.38664823	4.230275468
	-4190.101277	4174.175624	1337.656575
H1	433		
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H1	434		
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	20.35926776	-3.342197853	13.45237903
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2C	436		
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H1	437		
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	2616.457394	9567.096292	5478.671624
H1	438		
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	16.05125299	-6.227732209	20.55843719
	4893.948599	1712.431187	4538.651849
2C	439		
	1.671485831	2.195521473	12.59921944
	1.308936894	6.471252206	7.647754041
	-10283.85554	-8380.648683	-10584.04149

HC	440		
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	-27.79316322	-7.322329929	-25.76382966
	-4094.649248	-5538.109615	3241.842794
HC	441		
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	19.07219516	3.650712078	-10.04735163
	-5922.132932	-4712.596509	-7811.046455
CT	442		
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	3.524612182	-0.9116670339	-6.459787849
	-3915.436479	812.5866383	8005.222188
HC	443		
	1.283115114	1.222145413	12.27561677
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HC	444		
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	-8.666691687	-20.71698656	-5.822288513
	11178.16486	-888.1228863	6104.059940
HC	445		
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	-6.060546575	6.505406443	-14.37647787
	-3666.608723	-3050.032611	-6271.096461
HC	446		
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	5909.530946	5440.136464	-1063.576222
HC	447		
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N*	448		
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N*	450		
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	-13524.05294	-11400.46510	-305.5849939
c2	451		
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	-13116.08829	6289.331007	6470.432749
c2	452		
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	6.904729293	-2.333773619	0.6097206861
	6698.573208	-14923.05173	-586.7803500
CT	453		
	8.910412735	1.206438292	2.807038568
	-7.669563560	-4.617574683	-5.113683895
	-10645.27323	10993.44791	-2864.757495

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CT	455		
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	11.28166740	-4.104943809	2.561798900
	-1525.703820	17532.44169	-6814.113515
H4	456		
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	25.50893487	-4.330677767	1.302130344
	7173.037453	-8722.073328	-3555.583107
H4	457		
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	-23.36307820	-7.341610187	-10.47372179
	7847.638433	9530.613849	7704.900752
H1	458		
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	4505.719891	-1607.345698	3344.587504
H1	459		
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	10.72753887	-2.992699293	-0.8934535491
	8947.460846	-1361.262721	-1491.915111
H1	460		
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	-6735.728693	4321.429437	-941.0404242
2C	461		
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	11316.31758	-21107.49288	4315.484848
H1	462		
	-8.765325295	1.161766240	2.556290226
	34.21744427	6.425378302	-22.03593883
	4968.631385	1756.500136	-7154.045867
H1	463		
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	-3.547367059	-5.686966007	10.13942619
	5017.406707	-3017.822118	-1091.197338
2C	464		
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	5057.948143	926.1316237	-7899.303029
HC	465		
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	-8.180586885	-2.684895794	-23.38988300
	-10647.38445	1041.307926	-554.0448554
HC	466		
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	2.712404453	17.19753649	17.29035713
	2696.033127	2162.536295	4669.033711
CT	467		
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	12184.44794	-8341.380197	18304.62816

HC	468	
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HC	470	
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N*	475	
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c2	476	
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c2	477	
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CT	478	
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-5162.455135	103.9039974	71.63714542
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H4	481	
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H1	487		
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	3863.359606	-4938.093290	-5364.489053
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HC	490		
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HC	493		
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HC	494		
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CT	505		
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H4	506		
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H1	509		
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H1	510		
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2C	511		
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H1	512		
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H1	513		
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2C	514		
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HC	515		
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	-21.62796943	-4.432230055	-10.84554044
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CT	517		
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	-3.056773167	5.511356382	-1.042933699
	3107.809919	-15672.07618	-14968.22607
HC	518		
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HC	520		
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HC	521		
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	-8.277228483	-4.122711120	6.894011777
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HC	522		
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N*              525
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    -19126.06575         4807.060126         1767.388190
c2              526
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c2              527
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CT              528
    -2.770121754         6.999944101         4.172703332
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H5              529
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     11323.37231         8838.955595        -16454.14397
CT              530
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     2.606624304        -1.675694298         0.3899901938
     9673.572609        -2923.372540        -11313.20178
H4              531
    -2.296104978         2.783147635         6.159402170
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H4              532
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    -2450.572530        -2660.628464        -8790.260344
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2C              536
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H1              537
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HC              540
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HC              541
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HC              545
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HC              546
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HC              547
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CT            553
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H4            556
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H1	588	
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N*              598
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H4              606
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     2828.274423        -384.8715164         -7735.815363
c3               727
    -5.507494284        -5.542748435          9.932867233
    0.4126183611         6.453446281          2.889880908
    -201.3616530         10608.69026         -11305.82346
F                728
    -6.582153912        -4.692543595          10.10751284
    -3.046729084         6.248862063         0.5930201064
     3494.071534         523.1744428         -1191.116030
F                729
    -5.443082853        -6.220106725          11.08665390
    -1.561438726       -0.4055967453        -0.2759598706
     3797.044962        -4727.356170          6270.441985
F                730
    -4.388208725        -4.746517132          9.844119612
    0.7223851046        0.2974689999         -3.639722562
    -4219.439520         849.1093654          4999.595390
s                731
    -3.210330504        -7.656803544          8.279374642
     1.087149007        0.4854422005         -5.277323539
     12157.15952        -10871.87364          3291.763680
o=               732
    -2.521354960        -6.402029706          8.590064960
     3.650022903       -0.5663234804          1.077726877
    -6943.631380        -4556.834631         -1068.892534
o=               733
    -2.560460293        -8.844676684          8.812681064
    -3.070676626         3.454848664         -3.935556518
     3847.417447         3787.293767          1027.005440
```

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c3            734
    -3.286949818      -7.891316696       6.472641235
    -1.155214042      0.5381927113      -0.4602166040
    -11612.63651       4559.701956      -15004.82884
F             735
    -2.415667456      -8.837913017       5.970408609
    0.5335960325       2.870838351       4.831150509
    -2148.193599       1264.504345       2471.819896
F             736
    -2.999329998      -6.756038200       5.778562651
    -1.532752307      0.1328915595      -0.6000719297
     5609.166432       2854.490256       1689.634016
F             737
    -4.530774139      -8.218394987       5.941057738
    0.2016675751      -4.652286745      -3.729381483
     5200.437806      -3176.058553       6083.898816
n             738
     10.28274290      -1.954441668      -7.500749528
    -4.978865521      -4.022315856       4.407072221
    -979.9241772       1682.021285       4750.991285
s             739
     9.142828111      -1.106983361      -8.131007313
     2.740942825     -0.4266720701E-01   -1.955044607
    -3900.859278       14846.01470      -12877.60322
o=            740
     9.603764470     -0.5780432206      -9.425535426
    -6.688103814      -1.738862691       3.136206802
    -1172.942806      -3006.552758       8473.384099
o=            741
     8.735751088     -0.3232545673E-01   -7.167372562
    -3.472794458       2.621376192      0.2765573816
     6217.196589      -11501.28608       936.1654075
c3            742
     7.625078484      -2.203782253      -8.492894690
    -3.979581957      -1.474071228      -3.465117785
     1756.218694       9075.592935      -8686.465157
F             743
     7.533856147      -2.591898944      -9.830595752
    -1.236202905     -0.2914232407      -1.529753996
    -3721.074443       4821.254896       6055.692383
F             744
     7.557578946      -3.351754086      -7.826252814
     4.304352637     -0.8481984769       4.311727775
    -5125.299029      -10181.39930       10017.91767
F             745
     6.419487570      -1.537500016      -8.223354876
     3.709420346       2.422615056       12.02753553
     7523.249445      -5801.246787      -2551.541197
s             746
     10.64253928      -3.386232832      -7.965585812
     4.598892851       1.314580657       2.294049779
    -6801.215341      -9300.250710       158.7688925
o=            747
     9.852627908      -3.789187745      -9.085441377
    0.1774106718      -5.812177015      0.3544059479
     5675.169532      -2506.816641      -4609.949039
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o=	748		
	10.52096282	-4.350026593	-6.849126070
	-1.734291443	-3.985055319	2.188689134
	4385.335577	4881.666409	-1949.124518
c3	749		
	-10.30272351	-3.177553456	-8.483886113
	0.3317370630	4.622314061	-0.2503103434
	1048.349080	-162.5477537	577.3702632
F	750		
	-9.927244483	-1.878540332	-8.466903084
	4.775590553	1.720204675	1.973129946
	4838.240609	4202.553967	-2354.518385
F	751		
	-9.979618437	-3.633456098	-9.719374232
	-0.4672425112	-0.4657789099	5.814345872
	-4999.506371	688.3888940	-6102.036092
F	752		
	-9.398192529	-3.828883986	-7.725215136
	-4.350411602	0.8485570623	-1.423568434
	2880.828144	-3186.914138	9128.390332
n	753		
	3.220705154	-2.521355873	2.241497996
	-0.9822533569	-4.875288889	1.087011918
	6726.221044	3986.862722	4805.939984
s	754		
	4.298337129	-3.345194319	3.040220835
	2.574140245	-1.895882485	-1.328645839
	-13185.58791	-2309.241096	5465.112287
o=	755		
	4.618602920	-4.571717051	2.211520852
	-0.5740967601	4.040510402	4.369224938
	-1206.415237	8289.723922	11909.23150
o=	756		
	3.783888958	-3.563736427	4.431596136
	-0.7174286080	-2.630353472	5.509581981
	5623.726022	-6715.539575	-16217.13988
c3	757		
	5.787981732	-2.266189714	3.200339788
	-0.7961955939	1.806984166	4.039436562
	10870.10095	1044.080107	-29317.22433
F	758		
	6.930629127	-2.877190882	2.657510263
	-1.841725391	0.3302500314	0.7967513270
	-7433.015835	2767.122185	5693.957615
F	759		
	5.760743566	-1.039155035	2.528404281
	-1.896677187	1.349930910	-0.6460371572
	433.2874276	-5631.974122	4743.203920
F	760		
	6.150566549	-1.998912172	4.444065492
	1.470449445	-4.070609707	0.8934596186
	2082.303738	4413.152933	12704.71795
s	761		
	2.799758598	-1.027066768	2.605634202
	-1.189808012	-3.404671070	-0.3643636346
	9838.896623	17395.87892	-2910.642543

o= 762		
3.117153399	-0.1199846692	1.447852016
-2.532506090	-1.309751954	-3.786436678
-4903.372972	-9723.977153	2714.223031
o= 763		
3.345055120	-0.5174834104	3.882914251
-0.1968794397	-4.273972567	-3.199235789
-2892.096233	-9804.825132	-8351.283622
c3 764		
1.004459071	-1.206940444	2.796678014
3.800728630	9.015608560	3.626268422
-12362.14409	-8661.435617	-10179.58664
F 765		
0.2060099729	-0.8344546590	1.711638452
-0.7555837958	4.854059020	4.545797684
10014.56390	629.5603104	3655.151057
F 766		
0.4266238201	-0.5684097996	3.845246046
4.132086087	-2.989468596	-0.2349826177
3100.495110	3238.745141	5320.078387
F 767		
0.7007437087	-2.518285023	3.000351071
-5.426802575	2.527707019	-3.379647879
-5069.987064	-2591.500341	3901.893089
n 768		
-2.800797261	3.210896839	10.78606261
-3.750713381	-1.711160730	-0.3276051569
378.7831742	2387.271665	-7702.586798
s 769		
-3.173835008	2.954530194	9.262447895
-3.078470433	0.3062756044	-0.7706005484
-16935.90943	19436.05501	7322.821053
o= 770		
-2.526164343	1.808362042	8.780795529
-2.080721607	2.228112410	-2.550193857
8816.582019	-11565.67595	-4441.014599
o= 771		
-3.011800436	4.132095199	8.403358345
2.719474221	-3.912342816	5.797673549
4226.314075	-4894.550164	6907.008734
c3 772		
-5.011597205	2.612384660	9.419112228
9.111655956	3.375741565	3.605374845
2331.072103	-3341.888768	-7216.323154
F 773		
-5.782860317	3.696847408	8.981523144
-3.235832826	0.3380640115	2.826461327
-22.11615336	-10747.68685	-1090.188218
F 774		
-5.351234332	1.456704785	8.718606159
-1.481382098	0.8198640601	-0.5956614630
-3410.300825	11632.08357	-3437.686494
F 775		
-5.492574943	2.304453480	10.63555439
-0.8076985739	-2.207281140	4.276898614
2250.617241	4378.091741	9548.222768

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s               776
   -2.826042729          4.655668088          11.41426448
    3.132456483          1.452642930          0.1585355682
    16177.16035        -13353.17689          -9536.891313
o=              777
   -2.618653317          4.488555660          12.75301429
  -0.8410053337         -2.185142623          -6.902890392
    3276.528559         -1891.332940          23744.40446
o=              778
   -3.976513878          5.386011634          11.19217982
   0.8465156851E-01     -3.530427416          -1.558838048
   -15653.25138          7586.754216         -12723.37748
c3              779
   -1.290712489          5.472482055          10.74092715
   0.1421021646          1.916290453          0.3511239485
    4550.169976         -1661.146479          -8749.970739
F               780
   -1.489495028          6.628946801          10.05700120
   -7.720313466         -8.362800402          -9.577350566
   -2917.416548          748.0493388          -1646.910540
F               781
  -0.4655270491          5.857764211          11.77193144
   -1.350551295         -4.747143938           3.579434312
    2012.548575         -6084.562958          -4016.177496
F               782
  -0.5020663266          4.706270291           9.863586207
    7.137017126        -0.3621894428          0.5598544170
   -5542.049678          2735.223697           9255.888670
n               783
   -3.622132467          2.099205130           2.726956871
   -4.075046402         0.9933405997          -1.309156791
   -6097.270913          3327.364374           3724.780737
s               784
   -3.355072628         0.5869181075           2.529179524
   0.6424198519         0.2979886139          -1.317590630
    5911.831099          15732.05135          -8204.128850
o=              785
   -1.980824349         0.5586142336           2.089828667
   -1.574781903         -5.462490386          -2.299823451
   -85.67616085         -6207.943475           2293.435390
o=              786
   -4.245602243         0.7814262336E-02       1.537977694
   0.6298668512         -1.573438521          -1.310048168
   -4654.482489         -951.1571132          -3341.967789
c3              787
   -3.565320480        -0.1656416319           4.229498533
  -0.8420965360         0.2141379279          0.9993355572
   -10563.72482         -653.3529756           5038.527307
F               788
   -4.836249971        -0.2393636815           4.816295678
   0.3994973807        -0.9723964649         -0.4703963601
    4864.610495          2880.976150          -13286.35880
F               789
   -3.201118196         -1.464455650           4.161752182
    7.762300063          1.288455633           6.501248997
    3775.603631         -5402.459601           3765.862013
```

F	790		
	-2.817503251	0.4199638521	5.221621549
	1.445316978	4.351715591	-2.925895072
	3383.202431	-956.8107286	-2858.979373
s	791		
	-5.042996699	2.632381417	3.154530597
	-1.633282132	0.6750828640	-1.123210923
	-7664.039620	-23140.90152	-5044.732198
o=	792		
	-5.096088145	2.657870543	4.575463499
	3.139644400	-1.080728801	6.678594779
	4975.512132	10069.87691	7276.602461
o=	793		
	-6.108327771	1.771445178	2.662667184
	-0.7648344950	2.774093362	-9.292220383
	1577.032285	4289.857600	-2548.881183
c3	794		
	-5.182566563	4.288192304	2.384524348
	2.510328579	0.2998244270	-1.990423090
	17488.55668	6529.673112	-2952.811910
F	795		
	-3.993702251	4.795219682	1.816607152
	2.120159291	-2.100260946	5.958386397
	-4685.876392	-4294.934262	10106.20189
F	796		
	-5.605275985	5.226786522	3.281627913
	-1.377434982	-0.1866929512	-4.298891516
	-320.3181256	398.6815025	157.3415674
F	797		
	-6.033741886	4.392076931	1.342047063
	3.623244408	-0.7031102283	-2.512839819
	-12028.32536	3564.224675	-3930.034909
n	798		
	3.275496247	8.063566080	-7.781947747
	2.104396104	1.885846117	3.249657663
	-2428.582481	4.154117825	297.3226954
s	799		
	3.826413928	9.495792795	-8.232388127
	-1.000289532	0.3958392888	-0.4677708661
	1777.949303	104.9102601	-12175.98763
o=	800		
	4.502914402	9.424339375	-9.508945320
	0.7289552316	0.5846481275	-6.179164107
	-5945.398593	-2910.911516	-374.9508750
o=	801		
	4.686388679	10.13532564	-7.257888467
	-0.9150881836	-0.3808786549	-1.341448577
	-1298.423635	-2208.540030	15733.60000
c3	802		
	2.219782226	-9.912550328	-8.375262422
	0.6350592165	1.441549587	0.7064328985
	11025.24812	495.5426500	249.1868198
F	803		
	2.541463198	-8.579011978	-8.504126679
	2.584513367	0.9021714953	-2.157459181
	-4234.448260	-3192.259552	-3088.257816

F	804		
	1.426932122	-10.21521420	-9.465310657
	-2.483071868	-1.773611717	-1.542826234
	628.9992725	-975.5098395	4235.145480
F	805		
	1.412995911	-9.955024391	-7.252180188
	-4.830183814	2.271401860	3.456326522
	-1134.771621	-1979.767577	-603.6420897
s	806		
	3.869166231	6.587641453	-7.959381685
	-1.945239139	2.947309292	-1.466729940
	-49.02396360	11238.54909	716.2651059
o=	807		
	3.514627311	6.024478709	-9.238799735
	9.807546688	0.3025041966	1.617737569
	-5797.080520	2182.146484	-1675.187440
o=	808		
	3.398598015	5.769947751	-6.850231829
	-1.863599925	-8.744815827	8.052734530
	3099.659287	-5186.343708	4937.321218
c3	809		
	5.726702125	6.701953626	-7.927910971
	-8.766663336	9.093035770	3.418616743
	11434.95627	-452.5300396	-14615.62256
F	810		
	6.252673216	6.251280143	-9.135980357
	-8.954807806	3.933735233	0.8958800086
	-2802.189241	-2329.327004	6786.856514
F	811		
	6.335858987	5.893062479	-6.983454987
	5.235728290	0.9267119355	3.662995633
	-629.8443873	-1387.977332	2683.883459
F	812		
	6.355664203	7.898151399	-7.837181079
	7.584469872	0.8822965660E-01	6.125317535
	-1790.380974	4913.235345	3678.440084
n	813		
	10.89694895	8.784818734	11.11505713
	9.390385543	-2.335336744	-1.837141251
	-1222.231233	-10147.42029	3202.721088
s	814		
	10.18074127	7.688099377	10.27705084
	-2.525080413	-0.8947988204	1.191037564
	38991.04388	127.1214137	-721.2289913
o=	815		
	11.14282851	7.218934300	9.231921089
	-6.053142819	9.684376064	-6.522256199
	-8418.427696	255.6756442	6230.223351
o=	816		
	9.091940835	8.268779848	9.743216557
	3.210039704	-8.466540458	2.187800433
	-27697.48994	1890.633390	-7870.383836
c3	817		
	9.825533505	6.362132899	11.54384222
	1.884094562	4.450811928	-1.735490738
	8254.741073	-6807.175645	-5066.078226

```
F              818
    10.85208137         5.438849269         11.65400403
  -0.4685336015       -0.1741993350       -0.4896900688
   -3189.213930         2282.869730        -3254.055609
F              819
    8.719948456         5.638985392         11.29454756
  -0.6881646404         5.469615036         2.539001172
   -4920.284475        -3348.326391        -3473.069804
F              820
    9.669360384         6.779522203         12.80028101
   -7.384742407         2.348829645        -4.516412311
   -2510.611219         8214.636555         7449.009350
s              821
    11.04961745         10.22463333         10.64664379
   0.8696362515        -1.376455665        -3.968806733
    4521.701772         13183.39234        -5007.646221
o=             822
    11.25302764        -10.03036582         9.215633995
   -1.245125053         5.434890849        -3.205999081
   -1824.874989        -8855.911863        -3303.419847
o=             823
   -10.53614171        -9.637105535         11.37113038
    1.532292365        -2.021256025         1.904443576
   -3508.289908        -97.42818273         521.0601272
c3             824
    9.441564730        -9.421075235         11.10734032
  -0.6409271116E-01     3.284505764         6.729569766
    4587.180394        -392.6159047         214.2952501
F              825
    9.691872368        -8.089327673         11.41283375
    2.671728269         3.803108529         2.943379110
   -7627.732708        -3751.536233        -3423.910669
F              826
    8.963823336        -9.984602122         12.22888461
    2.736176886        0.7272694630         2.433063727
   -5287.533133        -378.5032294         6174.369252
F              827
    8.378709989        -9.466424487         10.18454386
    4.240752613         5.016210896        -4.555295952
    9723.380672         5079.844727         5262.704704
```

VACF Python program

```
#updated velocity autocorrelation function calculation
#only calculate the mass-weighted VACF
#aaron byrne




import sys
import numpy as np
from scipy.fftpack import fft
```

```
import matplotlib.pyplot as plt


file_name_1 = sys.argv[1]
file_name_2 = file_name_1



print 'Analyzing autocorrelation for %s' %(file_name_1)



if 'PBE' in file_name_1:
    repres = 'PBE'
    T = 8501
    max_lag_time = 7500
elif 'BLYP' in file_name_1:
    repres = 'BLYP'
    T = 8501
    max_lag_time = 7500
elif 'mull' in file_name_1:
    repres = 'mull'
    T = 15000
    max_lag_time = 12500
elif 'EHT' in file_name_1:
    repres = 'EHT'
    T = 15000
    max_lag_time = 12500
elif 'lopes' in file_name_1:
    repres = 'lopes'
    T = 15000
    max_lag_time = 12500
elif 'hirsh' in file_name_1:
    repres = 'hirsh'
    T = 15000
    max_lag_time = 12500
else:
    print 'error'
    exit()

header = 2                          #number of header lines in file
step = 1 #1fs


f = file_name_1.split('/')
f1 = f[-1]
f2 = f1.split('.')
f3 = f2[0]
f4 = f3 + '.vacf'

f5 = f[2]


file_name_out = './' + f5 + '/' + f4
```

```
#_____________________________________________________________________
___
xyz1 = open(file_name_1,"r")
line = xyz1.readline()     #1st line of xyz file containing number
of atoms (always 1)
line = xyz1.readline()     #2nd line of xyz file containing time
information

data1=[]


for i in range(0,T):        #different times
    line = xyz1.readline()
    atom, velx , vely, velz = line.split()
    data1.append([i,atom,float(velx), float(vely), float(velz)]) #i
is time index
    for k in range(0,header):  #headers of next timestep
        line = xyz1.readline()

xyz1.close()


#print atom
#should always be the same for each file

#_____________________________________________________________________
___

#_____________________________________________________________________
___
xyz2 = open(file_name_2,"r")
line = xyz2.readline()     #1st line of xyz file containing number
of atoms (always 1)
line = xyz2.readline()     #2nd line of xyz file containing time
information

data2=[]


for i in range(0,T):        #different times
    line = xyz2.readline()

    atom, velx , vely, velz = line.split()
    data2.append([i,atom,float(velx), float(vely), float(velz)]) #i
is time index
    for k in range(0,header):  #headers of next timestep
        line = xyz2.readline()

xyz2.close()

#_____________________________________________________________________
___

n_t0 = T - max_lag_time  #number of different starting points
(T=8500)
```

```
massDict =
{'O':16.0,'H':1.008,'C':12.01,'N':14.01,'Ru':101.07,'S':32.06}
mass = massDict[atom]   #get mass of atom




G = [] #normalised and averaged over three components correlation
vector

for d in range(0,max_lag_time): # different values of lag time

    Cx = 0
    Cy = 0
    Cz = 0

    for t0 in range(0,n_t0): #different starting points t0
        Cx = Cx + float(data1[t0][2])*float(data2[t0+d][2])
#/(float(data1[t0][2])*float(data2[t0][2])) # sum( vx(t0)*vx(t0+d) )
        Cy = Cy + float(data1[t0][3])*float(data2[t0+d][3])
        Cz = Cz + float(data1[t0][4])*float(data2[t0+d][4])

    #average over different starting times
    Cx = Cx/n_t0
    Cy = Cy/n_t0
    Cz = Cz/n_t0


    if d == 0:          #no lag   :     <A(0)B(0)>
        normx = Cx
        normy = Cy
        normz = Cz


    Cx = Cx/normx
    Cy = Cy/normy
    Cz = Cz/normz
    C = (Cx + Cy + Cz )/3.0    #3components averaged s.t.
autocorrellation between -1 and +1
    G.append(C)


#cross correlation can of course be outside the +1  <-->  -1 range
and should be normalised by dividing by the max correlation
G = G/np.amax(np.absolute(G))
#G can be normalised without affecting whether F is normalised or
not?



#F = dct(G)
```

```
#fourier transform
N = G.size
time = [i for i in range(0,N)]
#f_signal = fft(G)
#f_signal = abs(f_signal)**2


##normalize or not
#f_signal = f_signal/np.amax(f_signal)



#freq = np.fft.fftfreq(N, d=step)
#freq = freq*1000.0    #convert from fs^-1 to ps^-1
#freq = freq*33.356    #convert to wavenumbers


##___________________________________________________________________
____
#OUTPUT



cfile = open(file_name_out,"w")


#write output file
for i in range(0,max_lag_time):


    g1 = G[i]*mass
    t = time[i]
    g2 = G[i]

    out = "%16.9f%20.9f%20.9f\n" %(g1,t,g2)
    cfile.write(out)

cfile.close()
```