Investigating 3,4-bis(3-nitrofurazan-4-yl)furoxan Detonation with a Rapidly Tuned Density Functional Tight Binding Model

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We describe a machine learning approach to rapidly tune density functional tight binding models for description of detonation chemistry in organic molecular materials. Resulting models enable simulations on the several 10s of ps scales characteristic to these processes, with "quantum-accuracy." We use this approach to investigate early shock chemistry in 3,4-bis(3-nitrofurazan-4-yl)furoxan, a hydrogen-free energetic material known to form onion-like nanocarbon particulates following detonation. We find that the ensuing chemistry is significantly characterized by formation of large $C_xN_yO_z$ species, which are likely precursors to the experimentally observed carbon condensates. Beyond utility as a means of investigating detonation chemistry, the present approach can be used to generate quantum-based reference data for development of full machine-learned interatomic potentials capable of simulation on even greater time and length scales, i.e. for applications where characteristics timescales exceed the reach of methods including Kohn-Sham density functional theory which are commonly used for reference data generation.

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I. INTRODUCTION

Evolution of organic molecular materials under extreme conditions (e.g. 1000s of K and 10s of GPa) is central to research spanning from astrochemistry¹⁻³ to nanomaterial fabrication⁴⁻⁶. However, a confluence of challenges including complicated physical and chemical processes exhibiting a broad range of characteristic time and length scales have made a clear picture elusive^{4,5,7-11}. For example, materials lacking sufficient oxygen to undergo complete combustion are known to form carbon condensates (e.g. nanodiamond, graphitic nano-onions and nano-ribbons, etc.) when driven to high temperature and pressure (e.g. via shockwaves), where resulting condensate size, composition, and allotrope are governed by the starting material’s chemical composition, the thermodynamic pathway through which it is heated, compressed, and eventually expanded and cooled, and the associated chemistry and kinetics⁴. Ultimately, this process involves phenomena occurring on both nanometer length scales over 10s of picoseconds (e.g. chemistry mediated condensate formation), as well as those occurring on scales approaching microns and microseconds (e.g. condensate growth and aggregation)^{6,12-14}. Material evolution under extreme conditions is often studied through detonation or shock experiments, where the resulting dynamic and transient conditions can make determination of fundamental properties like system temperature exceedingly challenging and ultimately preclude elucidating early time chemistry driving carbon cluster formation.

Atomistic simulations excel at probing sub-micron and -microsecond scales and can provide complementary insights (e.g. determining phase boundaries,¹⁵ assigning temperature for shock experiments^{16,17}, investigating thermal decomposition¹⁸, etc.); however, this approach hinges upon the underlying interatomic model. Quantum mechanical methods including Kohn-Sham density functional theory¹⁹ (DFT) have been shown to be well suited for studying materials under extreme conditions^{17,20,21}, but high associated computational cost precludes access to timescales relevant to shockwave-driven chemistry (e.g. several 10s of picoseconds to microseconds). Molecular mechanics-based simulations can overcome this difficulty and enable access to much larger time and length scales; however, models capable of accurately describing system structure, dynamics, speciation, and kinetics under extreme conditions are scarce, and generating new parameter sets remains a significant undertaking. Density functional theory tight binding with self-consistent-charges²² (DFTB-SCC) is a

FIG. 1. Snapshot of a thermalized DNTF crystal. Atoms in cyan, blue, and red correspond to carbon, nitrogen, and oxygen, respectively.

practical alternative, exhibiting substantially improved predictive power over molecular mechanic approaches, and a 3-orders-of-magnitude increase in simulation efficiency over DFT. However, this approximate quantum-mechanical method utilizes parameter sets that are not generally designed for application to organic molecular materials under extreme conditions.

In this paper, we show how machine learning (ML) can be used to generate corrections to standard DFTB models enabling quantum-accurate simulations for shock compressed materials on timescales substantially greater than those accessible to DFT. We focus here on developing a model for the energetic material 3,4-bis(3-nitrofurazan-4-yl)furoxan (i.e. $\text{C}_6\text{N}_8\text{O}_8$, often referred to as DNTF or BNFF), shown in figure 1. DNTF exhibits an usually high detonation temperature and has been recently shown to produce liquid carbon nanodroplets upon detonation, which subsequently solidify into graphitic nano-onions⁶. Using the developed model, we investigate early decomposition chemistry under conditions of pressure and temperature typical of strong shocks. Results are compared with predictions from thermochemical calculations, and are discussed in the context of studies probing the relationship between chemical kinetics, thermodynamics, oxygen balance and carbon condensation in shock compressed organic molecular materials. Specifically, we aim to shed light on: (1) what are the major chemical kinetics steps associated with shock decomposition of DNTF? (2) what is the equation of state of the shocked material? (3) how do these results compare with those for other carbon-rich compounds? and (4) what are the implications of the present results for nanocarbon formation mechanisms in DNTF and in general? In the following sections we provide a high-level overview of DFTB-SCC, describe

the ML approach used to generate a model tuned for DNTF, and validate it by comparing model-predicted DNTF structure, equation of state, speciation, and kinetics with that from DFT. Following, speciation, kinetics, and the shock Hugoniot equation of state are explored and compared with existing thermochemical models. Ultimately, we find that our ML-tuned DFTB approach is well suited for the study of organic molecular materials subject to extreme temperature and pressure conditions and can provide important insights into the early chemistry and kinetics.

II. COMPUTATIONAL METHODS

All DFT simulations were performed for systems of 264 atoms using the VASP^{23–26} package with a planewave cutoff of 1000 eV, the Perdew-Burke-Ernzerhof generalized gradient approximation functional^{27,28} (PBE), projector-augmented wave pseudopotentials^{29,30} (PAW), the DFT-D2 method³¹ for description of dispersion interactions, and a 0.5 fs time-step. Simulations in the canonical (i.e. *NVT*) ensemble used a Nose-Hoover thermostat^{32,33}. DNTF density at the melting point was approximated through a 6 ps isobaric-isothermal (i.e. *NpT*) ensemble simulation using Langevin dynamics with a Parrinello-Rahman barostat^{34,35}.

DFTB forces, stresses, and energies were evaluated with self-consistent charges (SCC), using the DFTB+ package³⁶ with the the Mio-1-1 parameter set (available at <http://www.dftb.org>), unless otherwise stated. The SCC convergence criteria was set to 10^{-6} au and the Universal Force Field³⁷ (UFF) was used as a dispersion correction. A timestep of 0.5 fs was used for systems at or below the DNTF melting point and a value of 0.2 fs was used otherwise. DFTB calculations in the canonical ensemble were performed with a Nose-Hoover thermostat, for systems of 264 atoms, while shock simulations were run for 176-atom systems. DFTB-ChIMES model simulation results are presented as averages across eight independent simulations. A locally modified version of DFTB+ was used for ML-corrected DFTB calculations; a library for computing ChIMES interactions, which also contains all published parameter sets, is available at https://github.com/rk-lindsey/chimes_calculator. We note that simulations using the Mio+ChIMES model are of approximately the same efficiency as those using Mio-1-1 alone (i.e. ChIMES evaluations take < 0.1 s/ionic-step compared to ≈ 13 s/ionic-step for Mio-1-1 alone), and that in general, the present DFTB simulations provide a $> 2.5 \times 10^3$ increase in steps/CPU-hr relative to DFT.

A. DFTB Overview

The DFTB-SCC formalism has been discussed in detail elsewhere^{22,36,38,39}. Briefly, the method assumes neutral, spherically symmetric charge densities on the atoms and expands the DFT Hamiltonian to second-order in charge fluctuations. The DFTB total energy is expressed as

$$E_{\text{DFTB}} = E_{\text{BS}} + E_{\text{Coul}} + E_{\text{disp}} + E_{\text{rep}} \quad (1)$$

where E_{BS} corresponds to the band structure energy, E_{Coul} is a self-consistently computed charge fluctuation term, E_{disp} is an empirical dispersion correction, and E_{rep} is an empirical term accounting for ion-ion repulsions and Hartree and exchange-correlation double counting terms. The computational efficiency of DFTB is primarily realized through E_{BS} , which is taken as a sum over occupied electronic states from the approximate DFTB Hamiltonian. E_{BS} is usually computed from pre-tabulated Slater-Koster tables derived from DFT calculations with a minimal basis set, giving rise to an orders-of-magnitude increase in computational efficiency for a given system size, relative to DFT. Numerous DFTB Slater-Koster and E_{rep} parameter sets are available (i.e. at <http://www.dftb.org>), but these models are typically intended for biological systems (i.e. ambient T and p) or inorganic materials. Below, we will describe how the Chebyshev Interaction model for Efficient Simulation (ChIMES) can be used to introduce a correction term (E_{corr}) to an existing DFTB model (Mio-1-1) for description of DNTF under extreme T and p . We note that, for the remainder of this work, the resulting model will be referred to as Mio+ChIMES.

B. ChIMES Overview

ChIMES^{40–44} is a machine learned (ML) reactive interatomic interaction potential (IAP) explicitly describing many-body interactions through linear combinations of Chebyshev polynomials. Though ChIMES has been applied as a standalone IAP to systems spanning ambient water⁴² to molten carbon⁴⁰ and shocked carbon monoxide⁹, it has only been used as a DFTB correction for description of non-organic materials⁴¹, to date. The ChIMES total energy is given by

$$E_{n_{\text{B}}} = \sum_{i_1}^{n_{\text{a}}} {}^1E_{i_1} + \sum_{i_1 > i_2}^{n_{\text{a}}} {}^2E_{i_1 i_2} + \sum_{i_1 > i_2 > i_3}^{n_{\text{a}}} {}^3E_{i_1 i_2 i_3} + \cdots + \sum_{i_1 > i_2 \dots i_{n_{\text{B}}-1} > i_{n_{\text{B}}}}^{n_{\text{a}}} {}^{n_{\text{B}}}E_{i_1 i_2 \dots i_{n_{\text{B}}}}, \quad (2)$$

where E_{n_B} is the total ChIMES system energy, n_B is the maximum bodiedness, ${}^n E_{i_1 i_2 \dots i_n}$ is the n -body ChIMES energy for a given set of n atoms with indices $i = i_1, i_2, \dots, i_n$, and n_a is the total number of atoms in the system. We note that ChIMES takes the single body interactions as constant values. ChIMES models developed in the present work include 1-through-3-body interactions, with 2-body interactions are given by

$${}^2 E_{ij} = f_p(r_{ij}) + f_s^{e_i e_j}(r_{ij}) \sum_{n=1}^{\mathcal{O}_{2B}} c_n^{e_i e_j} T_n(s_{ij}^{e_i e_j}), \quad (3)$$

where f_p is a penalty function which discourages sampling of unphysically short pair distances, r_{ij} is the distance between two atoms i and j . The function $f_s^{e_i e_j}(r_{ij})$ ensures the potential energy surface for interactions between atoms i and j , (i.e. which are of element types e_i and e_j , respectively) decays smoothly to zero at the the outer cutoff. The sum over $c_n^{e_i e_j} T_n(s_{ij}^{e_i e_j})$ gives a polynomial series of order $\mathcal{O}_{2B}$, where T_n is an order n Chebyshev polynomial of the first kind, $c_n^{e_i e_j}$ is the corresponding coefficient, and the argument $s_{ij}^{e_i e_j}$ gives a pair distance transformed to span the $[-1,1]$ domain over which Chebyshev polynomials are defined. For a detailed description of $f_p^{e_i e_j}$, $f_s^{e_i e_j}$, and transformation of r_{ij} to $s_{ij}^{e_i e_j}$, the reader is referred to the supporting information and 44.

The ChIMES 3-body energy between atoms i, j, k is constructed from interaction terms for the constituent atom pairs ij, ik, jk , i.e.:

$$E_{ijk} = f_s^{e_i e_j}(r_{ij}) f_s^{e_i e_k}(r_{ik}) f_s^{e_j e_k}(r_{jk}) \times \sum_{m=0}^{\mathcal{O}_{3B}} \sum_{p=0}^{\mathcal{O}_{3B}} \sum_{q=0}^{\mathcal{O}_{3B}} c_{m,p,q}^{e_i e_j, e_i e_k, e_j e_k} T_m(s_{ij}^{e_i e_j}) T_p(s_{ik}^{e_i e_k}) T_q(s_{jk}^{e_j e_k}), \quad (4)$$

*

where $\mathcal{O}_n^*$ is the maximum polynomial order for an n body interactions, and the asterisk indicates a sufficient number of non-zero terms exist that the graph formed by the edges of interacting atoms connects all n atoms, which guarantees a true n -body interaction.

ChIMES coefficients were fit using the following objective function

$$F_{\text{obj}} = \frac{1}{n_f(3n_a + n_t + 1)} \times \sum_{i=1}^{n_f} \left[\sum_{j=1}^{n_a} \sum_{k=1}^3 w_{F_{ijk}}^2 (\Delta F_{ijk})^2 + \sum_{l=1}^{n_t} w_{\sigma_{il}}^2 (\Delta \sigma_{il})^2 + w_{E_i}^2 (\Delta E_i)^2 \right], \quad (5)$$

where $\Delta X = X^{\text{DFT}} - (X^{\text{DFTB,BS}} + X^{\text{DFTB,Coul}} + X^{\text{DFTB,disp}} + X^{\text{ChIMES}\{c\}})$. F_{obj} and $\{c\}$ are the weighted root-mean-squared error and model coefficients, respectively. The number of frames and atoms are given by n_f and n_a , respectively, and the factor of 1 in the denominator arises from inclusion of a single per-configuration energy, E_i . F_{ijk} indicates the k^{th} Cartesian component of the force on atom j in configuration i . Units of $\text{kcal mol}^{-1} \text{\AA}^{-1}$

and kcal mol⁻¹ were used for forces, energies, and stresses respectively. The superscripts “ChIMES,” “DFTB,” and “DFT” indicate forces, energies, or stresses predicted from the present ChIMES correction, DFTB and the DFT molecular dynamics (DFT-MD) training trajectory, respectively.

Because ChIMES models are parameterically linear, coefficients can be rapidly obtained by solving the following overdetermined matrix equation:

$$\mathbf{w}\mathbf{M}\mathbf{c} = \mathbf{w}\mathbf{X}^{\text{DFT}} \quad (6)$$

where $\mathbf{X}^{\text{DFT}}$ is the vector of F_{ijk}^{DFT} , E_i and σ_{il}^{DFT} values, $\mathbf{w}$ is a diagonal matrix of weights to be applied to the elements of $\mathbf{X}^{\text{DFT}}$ and rows of $\mathbf{M}$, and the elements of design matrix $\mathbf{M}$ are given by:

$$M_{ab} = \frac{\partial(X^{\text{DFTB,BS}} + X^{\text{DFTB,Coul}} + X^{\text{DFTB,disp}} + X_a^{\text{ChIMES}\{c\}})}{\partial c_b}, \quad (7)$$

where a represents a combined index over force and energy components, and b is the index over permutationally invariant model parameters. As is described elsewhere⁴⁴, model parameters are obtained via least absolute shrinkage and selection operator⁴⁵ (LASSO) regression, which optimizes a modified objective function (e.g. $F_{\text{LASSO}} = F_{\text{obj}} + 2\lambda \sum |c_i|$) in which the absolute values (L1 norm) have the effect of setting certain ChIMES parameter values, c_i , to 0, and can thus lead to substantial gains in model efficiency. For this work, a regularization parameter of $\lambda = 0.01$ was used and the design matrix was left un-normalized.

C. Initial Training Set Generation

Because our target is a model capable of describing chemistry in shock-compressed DNTF, it is critical that the training set contains data at relevant thermodynamic conditions (e.g. including detonation). However, identifying these states is difficult since the existing experimental data are very limited and previous simulation studies are lacking for this material. To overcome this challenge, thermochemical calculations⁴⁶ were used to predict the reacted shock Hugoniot of DNTF up to approximately 40 GPa, encompassing the range of conditions under which recent experiments studied and characterized the carbon condensation processes⁶. Three state points for generation of DFT-MD training data were identified

TABLE I. Thermodynamic state points for DFT simulations and thermochemical Hugoniot EOS predictions. $t_{\text{sim,DFT}}$ is the total DFT simulation length. $X_{\text{full,EOS}}$ are properties (e.g. temperature, T , or pressure, p) predicted by thermochemical calculations for the fully reacted DNTF systems, where in this context, fully reacted corresponds to chemically equilibrated mixtures of small molecular species and carbon particles.

ρ	T_{DFT}	P_{DFT}	$t_{\text{sim,DFT}}$	$T_{\text{full,EOS}}$	$P_{\text{full,EOS}}$
g cm ⁻³	K	GPa	ps	K	GPa
1.86	300	0.03	5.00	4220	19.7
1.80	383	0.31	5.00		
2.00	2000	5.50	5.00		
2.00	4250	13.6	2.50	4250	20.7
2.25	4440	21.0	2.50	4440	28.3
2.50	4700	28.5	2.50	4700	39.0
2.50	9000	35.6	0.25		

from this Hugoniot; three additional state points were utilized for training data generation, corresponding to the material under ambient conditions, at its melting point, and above its thermal decomposition temperature⁴⁷. Finally, a high temperature training point was added to ensure adequate sampling of close interatomic contacts. These state points along with the DFT-MD simulation length are given in Table I. All simulations were initialized with the material in its molecular crystal state. We note that the DFT trajectories were fairly short and are therefore unlikely to have reached the fully chemically equilibrated state assumed by thermochemical calculations. However, the following section describes how a single iterative fitting step can significantly extend the effective timescale spanned by the training set.

III. RESULTS

In the following section, we discuss development of the Mio+ChIMES model and compare its performance relative to standard DFTB (i.e. Mio-1-1) in terms of recovery of DFT

FIG. 2. Atom force components, frame energies, and frame diagonal stress tensor components predicted by Mio-1-1 (orange) and Mio+ChIMES (blue) relative to DFT, at the DFT thermodynamic state points indicated in Table I. The solid line is drawn as a guide to the eye and provides $x = y$. Forces, energies, and stresses are given in units of $\text{kcal mol}^{-1} \text{\AA}^{-1}$, kcal mol^{-1} , and GPa, respectively, and the thermodynamic state point is given as a temperature in each plot and corresponds to a training state point.

forces, energies, and stresses, and for prediction of physical properties (i.e. pressures, system structure, speciation, and kinetics). The validated model is then used to investigate DNTF decomposition kinetics, generate a “quantum-based” prediction of the material shock Hugoniot, and to explore shockwave-driven chemistry; results are discussed in relation to other carbon-rich organic materials and thermochemical calculations.

A. Model Generation and Validation

The model developed herein used polynomial orders of $\mathcal{O}_{2B}/\mathcal{O}_{3B} = 12/7$, which were found to afford a balance between model complexity and accuracy. Unless otherwise spec-

ified, model hyperparameters (e.g. inner and outer interaction cutoffs, pair Morse-like parameters, etc.) were set using previously described protocols^{42,43} and are given along with the remaining model parameters (e.g. Chebyshev polynomial coefficients) in the supporting information. An initial model was trained to a total of 175 configurations (i.e. 25 at each training state point). The ChIMES interaction for this system was found to be more susceptible to overfitting than standalone ChIMES models because only a very short-ranged portion of the underlying DFTB interaction is being corrected. This can prove problematic when DFT and the base DFTB model yield even small differences in longer-ranged (e.g. dispersion) interactions, since the relatively short-ranged ChIMES model may take on an unphysical form to try to account for these differences. We note that this tendency can be mitigated through weighting. For this work forces, diagonal stress tensor components, and overall system energies were considered in our fits and were assigned fitting weights of 1.0, $20e^{-5\sigma}$, and $0.55e^{(E_{\text{min,DFT}}-E)/2000}$, respectively, where forces, energies, and stresses are in units of kcal mol⁻¹ Å⁻¹, kcal mol⁻¹, and GPa, respectively. The resulting model exhibited excellent recovery of DFT structure, equation of state, and chemical kinetics and was stable when extended out to 10 ps. However, exploratory shock simulations using the MSST technique⁴⁸ indicated that systems sample densities significantly greater than those in the DFT training set (e.g. 3.5-4.0 g cm⁻³), before reaction-driven pressure relaxation to the system’s nominal reacted Hugoniot state. As a consequence, these simulations rapidly became unstable (i.e. substantial deviation in the conserved quantity was observed) due to sampling of these high density configurations which the initial model was unable to describe. The model was refit to remedy this behavior. Rather than generating training configurations at these problematic high density state points from expensive DFT-MD simulations, a single iterative refinement was performed, where approximately 50 configurations from the Mio+ChIMES MSST simulations were sent to DFT for single point evaluation, and combined with the training set from which a new model was generated. This model was found to be stable for the duration of the simulations, and as an added benefit, introduced configurations corresponding to substantially longer simulations (e.g. 10s of picoseconds) than those originally generated via DFT-MD. Figure 2 provides a comparison between forces, energies, and diagonal stress tensor components predicted by DFT, standard (Mio-1-1) DFTB, and Mio+ChIMES. Overall Mio-1-1 performance is good, but we find (1) systematic over-prediction in force magnitudes for $T = 300 - 4250$ and larger residuals com-

FIG. 3. DNTF pressures predicted by DFT, standard DFTB (Mio), and the DFTB-ChIMES model (Mio+ChIMES) at thermodynamic states spanning ambient to shock compressed conditions. Error bars provide standard deviations across independent simulations.

pared to Mio+ChIMES, (2) offsets in energies relative to DFT, particularly at 300, 4250, and 9000 K, and (3) larger stress tensor magnitudes at 300 and 383 K.

Performance of Mio+ChIMES relative to DFT and Mio-1-1 was also benchmarked in terms of physical properties arising from MD simulations at each of the DFT state points and length indicated in Table I. Unsurprisingly, figure 3 shows that pressure recovery at each state point is improved by the Mio+ChIMES model. The radial pair distribution functions arising from these simulations are provided in figure S1 of the supplementary information and show that, in general, Mio-1-1 and Mio+ChIMES are in equivalently excellent agreement with DFT at ambient and moderately extreme conditions (e.g. 2000 K and below), but the ChIMES-corrected model is found to yield significantly improved recovery of DFT structure under extreme conditions (i.e. $T > 4440$ K, $\rho > 2.25$ g cm³).

Model performance was also investigated in terms of speciation. Figure 4 compares evolution of instantaneous bond-type counts between the DFT, Mio-1-1, and Mio+ChIMES. For this analysis, two atoms were considered bonded if their distance fell below 1.90, 1.80, 1.80, 1.75, 1.65, or 1.70 Å for C–C, C–N, C–O, N–N, N–O, and O–O atom pairs, respectively. Of course, resulting bond counts will vary depending on choice of criteria; however, for the present analysis we simply aim to establish a consistent metric to compare chemistry across

FIG. 4. Time evolution of bond counts in DNTF. DFT and Mio-1-1 predictions are given in solid and dashed lines, respectively, while shaded curves provide the spread about the Mio+ChIMES prediction in terms of 1st and 3rd quartiles. Bond types are indicated by the line colors, as given in the figure legend.

each of the three simulation methods. Slow reaction kinetics at 2000 K and the single independent simulation run for Mio-1-1 and DFT preclude conclusive remarks on suitability

FIG. 5. Comparison of mole fractions (top) and lifetimes (bottom) for small species formed in DNTF over the range of training thermodynamic conditions, predicted by DFT, standard DFTB (Mio), and the DFTB-ChIMES model (Mio+ChIMES). Boxplots are used to convey the DFTB-ChIMES data, and provide the max/min values (indicated by the error bars), 1st and 3rd quartiles (indicated by the range of the shaded box), and the average value (indicated by the horizontal line within each box)

of Mio-1-1 and Mio+ChIMES for description of chemistry at this state point. However, we find that above 2000 K, Mio-1-1 significantly over-predicts the number of O-N bonds and under-predicts both C-O and N-N bond counts at any given time. In contrast, Mio+ChIMES predictions are found to be in excellent agreement with DFT at all state points.

Chemistry was also evaluated in terms of predicted small molecule mole fractions and

FIG. 6. Time resolved evolution of small molecule mass fractions during Mio+ChIMES *NVT* simulations. Solid lines provide average values across 8-independent simulations and the shaded region gives the corresponding 1st and 3rd quartiles.

lifetimes, where a species was said to exist if all atoms remained within the cutoffs provided above for 50 fs (i.e. long enough to observe one or two bond vibrations). The results, plotted in figure 5, compare mole fractions and lifetimes for CO, CO₂, N₂, NO, N₂O, and O₂, (i.e. small molecules characteristic to decomposition of DNTF) at each of the DFT state points

indicated in Table I. Once again, we find that the Mio+ChIMES model yields enhanced recovery of DFT chemistry over Mio-1-1, though both are found to yield reasonable lifetime predictions. Overall, we find the present Mio+ChIMES model highly suited for studying DNTF under extreme conditions.

B. Decomposition Kinetics

We begin the study of DNTF subject to extreme conditions by investigating chemical decomposition kinetics at the three previously identified Hugoniot state points. For these simulations, systems were initialized in the molecular crystal state at the target density and temperature, and left to evolve over 10 ps. Experimentally, this would approximately correspond to single crystal DNTF suddenly heated under constant volume conditions, e.g. in a diamond anvil cell. We find that small molecule chemistry is similar across all three state points, with N_xO_y species dominating at early times, and CO_x and N_2 at late times. We note that other larger species with $C_xN_yO_z$ stoichiometry are also present in the Mio+ChIMES simulations (see Table II); hence, mass fractions in each plot do not sum to unity. From the relatively flat shape of each speciation trajectory, we conclude that the highest temperature state point in Figure 6 is closest to reaching what is likely to be a metastable state; the two lower-temperature systems appear to still be relaxing. Earlier work investigating the influence of oxygen balance on shockwave-driven chemical kinetics showed that in N-containing organic materials formation of equilibrium molecular products N_2 and CO_2 is significantly retarded in the presence of excess oxygen (i.e. in positive oxygen balance systems) due to formation of the “oxygen trapping” ion NO_3 ⁴⁹. Given that DNTF exhibits a negative oxygen balance, it is thus unsurprising that a lack of NO_3 and generally uninhibited N_2 and CO_2 formation are observed; this is also in agreement with DFTB simulations for other materials with similar oxygen balance⁵⁰. At the same time, we note that the speciation displays considerable complexity, with large $C_xN_yO_z$ products constituting a sizable mass fraction of the system at the end of the simulations, ranging from approximately 25 to 40% across the investigated densities. It is likely that these are the kinetic precursors to the carbon precipitates observed experimentally⁶, and therefore significant chemistry coupled with growth will occur on larger time scales. A similar effect was observed in high pressure and temperature simulations of carbon monoxide (CO)⁵¹, where large C_xO_y clusters were found to play an

TABLE II. Average overall mass fraction of large $C_xN_yO_z$ species at the end of each set of simulations, and average mass fraction of each constituent atom type.

Simulation	x_{other}	%C _{other}	%N _{other}	%O _{other}
8.25 km/s	0.54	29	30	41
8.50 km/s	0.63	28	31	41
8.75 km/s	0.77	26	32	42
9.00 km/s	0.76	26	34	40
9.50 km/s	0.84	26	33	42
2.00 g cm ⁻³ / 4250 K	0.25	33	38	29
2.25 g cm ⁻³ / 4440 K	0.28	33	33	34
2.50 g cm ⁻³ / 4700 K	0.40	31	34	35

important role in early carbon condensation kinetics.

Thermochemical calculations⁴⁶ at the simulated thermodynamic states (i.e. listed in Table I) indicate that the fully chemically equilibrated system corresponds to a mixture of small, stable molecules (e.g. N_2 , CO_2 , CO , NO , NO_2 , etc.) and carbon nanocondensates^{11,52}. Indeed, experiments indicate that DNTF produces a significant amount of carbon particles with sizes from a few to 10s of nanometers⁶. However, these are outside the length scales accessible to the current DFTB simulations, and therefore direct speciation comparisons between simulations and chemical equilibrium calculations are not necessarily edifying. A partially equilibrated calculation may be a better approximation of the simulated end states, but unfortunately the complex $C_xN_yO_z$ species identified in the simulations are difficult to capture in a thermochemical framework. Instead, we performed constrained thermochemical calculations in which a fraction of DNTF equal with the observed $C_xN_yO_z$ species mass fraction remains unreacted while the rest is a chemically equilibrated mixture of molecular products alone, without condensed carbon. These calculations are henceforth referred to as “partially-reacted” and should provide a chemistry picture somewhat closer to that observed at the present simulation scale. Consistent with the Mio+ChIMES calculations, these show that CO , CO_2 , and N_2 are the dominant species formed (see table III. In

TABLE III. Small molecule mass fractions predicted via thermochemical calculation for the “partially reacted” system.

Simulation	x_{CO_2}	x_{CO}	x_{N_2}
2.00 g cm ⁻³ / 4250 K	0.24	0.31	0.31
2.25 g cm ⁻³ / 4440 K	0.22	0.29	0.29
2.50 g cm ⁻³ / 4700 K	0.18	0.23	0.23

particular, the calculated N₂ mass fractions of 0.31, 0.29 and 0.23 at the 4250, 4440, and 4700 K state points, respectively, appear to match reasonably well the simulation values at the three thermodynamic points; CO₂ fractions on the other hand are approximately 25% smaller and those for CO are roughly double the simulated results. Overall, the agreement is therefore only qualitative, likely due to the unfolding slow carbon kinetics signaled by the presence of large C_xN_yO_z species, and the crude approximation used to capture their effect in the thermochemical estimates. Nevertheless, such comparisons bridging exceedingly different modeling methodologies can help translate insights and quantitative observations from atomistic simulations into equation of state and kinetic models applicable on much larger scales.

C. Hugoniot Equation of State and Shock-Driven Chemistry

In this section, we discuss prediction of the DNTF detonation state. For this work, we employed the extended Lagrangian Multiscale Shock Technique (MSST), which constrains the thermodynamic states of a MD simulation to those for a steady planar shockwave within continuum theory (i.e. simulating steady shock waves by constraining the stress and energy of a MD simulation to the Rayleigh line and the Hugoniot energy relations). This approach, which is discussed in greater detail elsewhere^{48,53,54}, has been used to study shock properties of numerous materials, and here is used to estimate the DFT Chapman-Jouguet (C-J) detonation state, Hugoniot curve, and shockwave-driven chemistry through our presently developed Mio+ChIMES proxy.

MSST simulations were run with a version of the LAMMPS software package locally

FIG. 7. Sample temperature, pressure, and density trajectories for MSST simulations.

modified to use DFTB+ for evaluation of force, energy, and stress with the presently developed Mio+ChIMES model. These simulations comprised 176 atom systems initialized at a density of 1.86 g cm^{-3} and MSST cell-mass-like parameter and macroscopic explicit viscosity parameters of $Q = 2.76 \times 10^{-13} \text{ kg}^2 \text{ m}^{-4}$ and $m = 0.02 \text{ kg m}^{-1} \text{ s}^{-1}$, respectively. Temperature, pressure, and density trajectories for simulations using shock velocities of 8.00 to 9.50 km s^{-1} are given in Figure 7.

The C-J detonation velocity (i.e. the speed with which a steady state unsupported shock wave propagates through the material) establishes a lower limit on shock velocities for

FIG. 8. DNTF shock Hugoniot states (reacted and unreacted) determined from the Mio+ChIMES MSST simulations compared with thermochemical estimates for a fully- and partially- chemically equilibrated system (see text), along with an analytic unreacted EOS based on high pressure experimental and simulation data.

which steady state solutions to the MSST equations exist. In the present work, we use this to estimate a lower-bound C-J velocity of at least 8.25 km s^{-1} for DNTF, since temperature, pressure, and density trajectories are found to diverge at 8.00 km s^{-1} , and the latter is the lowest explored value for which stable simulations were obtained; the experimentally measured DNTF C-J detonation velocity⁵⁵ at this density is 8.9 km s^{-1} . We note that at shock velocities near but below the C-J points, MSST trajectory divergence can be slow, thus it is possible that the present trajectories at 8.50 and 8.75 could ultimately prove unstable if extended to substantially longer time scales (i.e. by orders of magnitude).

For shock velocities exhibiting steady solutions, the trajectories in Figure 7 indicate 3 distinct phases. The shockwave first drives the unreacted system to high density and pressure and intermediate temperature, corresponding to an unreacted shock Hugoniot point. Systems then begin to undergo decomposition chemistry, which drives expansion and an increase in temperature due to energy release. Finally, systems appear to relax to a quasi equilibrium state, corresponding to an incompletely reacted shock Hugoniot point. Figure 8 provides unreacted and reacted Hugoniot data resulting from these simulations in the classical P vs

V representation. MSST simulations at a given shock velocity contribute a maximum of two data points (though unreacted points for shock velocities of 9.00 and 9.50 km s⁻¹ could not be uniquely determined from the MSST trajectories due to rapid onset of reaction) and system evolution occurs along the Rayleigh line connecting the unreacted, reacted and initial states. Figure 9 provides the corresponding chemical evolution, and indicates a number of features common across all shock velocities. Similar to the NVT decomposition kinetics study, we find that NO and NO₂ are the primary small molecules formed at early times, followed by CO₂ and N₂; interestingly, NO concentrations settle to progressively larger values for systems subjected to stronger shocks, possibly indicative of impeded chemistry at high densities. The kinetic time-scales of CO₂ and N₂ release are summarized in Table IV. These were obtained by fitting the CO₂ and N₂ trajectories to a rate equation of the form $x_{i,t} = x_{i,\infty}(1 - e^{-k_i\Delta t})$, where $x_{i,t}$ and $x_{i,\infty}$ are the mass fraction of species i at time t and at nominal equilibrium, k_i is the effective rate constant, $\Delta t = t - t_0$, and t_0 is the time point during the MSST trajectory at which chemistry begins. We note that at low shock velocities these rates are consistent with those reported from simulation studies of 1,3,5,7-Tetranitro-1,3,5,7-tetrazoctan (i.e. HMX) under similar conditions⁵⁰. Although the reacted states reached at the end of the shock simulations yield similar speciation to those from the NVT runs, they contain a significantly larger fraction of C _{x} N _{y} O _{z} species, varying from approximately 55% at the lowest shock velocity to 85% at the largest one. Table II also indicates that carbon concentration in the C _{x} N _{y} O _{z} material generated by shock compression is slightly enhanced relative to that of the DNTF molecule (e.g. 26-29% compared to 23%), while N concentration is reduced, and O concentration remains relatively unchanged (e.g. 30-33 compared to 36% and 40-42 compared to 41%, respectively). In contrast, the NVT simulations exhibit greater enhancements in C concentration in the material (e.g. 31-33%), and N and O concentrations which are relatively unchanged and decreased, respectively. To highlight the impact of C _{x} N _{y} O _{z} on the predicted shock Hugoniot, we also show in Fig. 8 both fully chemically equilibrated and 25% “partially reacted” thermochemical calculations (see previous description). The comparison between simulation results and thermochemical estimates illustrates the different stages of reactivity reached by the end of the simulations at different shock speeds, and suggests that the large C _{x} N _{y} O _{z} species occurring after the break-up of the DNTF molecules likely hinder the advance of the system toward chemical equilibrium. High densities appear to play an especially important role in these initial pro-

TABLE IV. Kinetics for N_2 and CO_2 formation (i.e. dominant small molecule species) from shock compressed DNTF predicted from Mio+ChIMES MSST simulations. Values for HMX⁵⁰, which were obtained from previous simulation studies, are provided for comparison.

	N_2		CO_2	
u_s (km s ⁻¹)	x_∞	k (ps ⁻¹)	x_∞	k (ps ⁻¹)
8.25	0.206	0.09	0.264	0.09
8.50	0.141	0.18	0.164	0.19
8.75	0.102	0.24	0.114	0.25
9.00	0.076	0.35	0.087	0.35
9.50	0.076	0.39	0.065	0.57
HMX	–	0.08	–	0.05

cesses, which we believe precede the ultimate formation of carbon (likely liquid) clusters via densification, “impurity” (N and O) elimination and growth from these $\text{C}_x\text{N}_y\text{O}_z$ kinetic precursors. The relatively rapid release of CO_2 compared to N_2 appears consistent with the hypothesis⁶ that nitrogen is likelier than oxygen to become trapped in condensates formed from detonation of DNTF. In light of the previous discussion and the finite size effects further precluding the physical and chemical relaxation of the system into the fully reacted state containing a mixture of carbon particle and small molecular species, it is not surprising that Mio+ChIMES simulations yield reacted temperatures that are significantly lower than the thermochemical results - see Fig. 8(inset). (Differences in the unreacted temperatures are likely due to uncertainties in the thermal properties of DNTF.) It is clear that much larger length and time-scale simulations are necessary to capture the full system evolution and provide a clear picture of the dominant physicochemical mechanisms accompanying the shockwave compression of DNTF, and likely other carbon-rich energetic materials. Nevertheless, the current simulations yield the initial kinetic steps along the shock-constrained trajectory leading to the final chemical equilibrium state and can serve as checks for future studies employing efficient classical interatomic potentials.

Previous small-scale quantum-based studies have addressed the decomposition of other

FIG. 9. Time resolved evolution of small molecule mass fractions during Mio+ChIMES MSST simulations. Solid lines provide average values across 8-independent simulations and the shaded region gives the corresponding 1st and 3rd quartiles. Mass fractions for small molecules and other material are given on the left and right y -axis, respectively.

energetic materials such as 1,3,5,7-tetranitro-1,3,5,7-tetrazoctane (HMX)⁵⁰, which has a negative oxygen balance close to that of the DNTF studied here, and 2,4,6-triamino-1,3,5-trinitrobenzene (TATB)⁵⁶, with a substantially larger magnitude oxygen balance. HMX de-

composition at high density and temperature appears dominated by the production of small molecular species, while TATB was found to form very large, relatively stable C- and N-containing heterocyclic clusters. We learn here that sizable $C_xN_yO_z$ species are likely to be the kinetic precursors to the carbon particles that condense out of detonating DNTF⁶. We have also previously investigated reactivity in a CO fluid^{9,43,51}, where carbon condensation at high pressures and temperatures proceeds through a reaction-driven phase separation mechanism^{43,51,57}). Given that DNTF reaches detonation conditions similar to those yielding carbon condensates in CO (i.e. well into the liquid region of the carbon phase diagram), but it has a smaller (absolute) oxygen balance and also contains nitrogen, we believe that its study can shed further light on the complex interplay between carbon content, chemistry and thermodynamics in shocked energetic materials. Using relatively small system sizes we captured relevant early chemistry effects in DNTF; substantially larger scale simulations will be the subject of future work. We also note that expansion from the high pressure states studied here is likely to be a fruitful future direction, as the thermodynamic pathway along which the system is quenched can significantly impact carbon condensate size, chemistry and allotrope⁶.

IV. CONCLUSIONS

In this work we demonstrate an effective ML approach in which ChIMES, a many-body reactive ML-IAP, is used to tune an approximate quantum mechanical model (i.e. the DFTB Mio-1-1 model) for description of reactivity in organic molecular materials under extreme conditions. We employ thermochemical calculations to guide generation of an initial training set through prediction of shock Hugoniot state points, and adopt an iterative approach wherein configurations from MSST simulations with the resulting Mio+ChIMES models are added to the training set to improve description of shock conditions and relaxation to the reacted states. Resulting models, which were shown to maintain DFT-accuracy for description of system forces, energies, and stresses as well as structure, chemistry, and kinetics, were used to investigate decomposition and early shockwave driven chemistry in DNTF, a CNO energetic material known to form liquid carbon and nano-onion carbon condensates.

We find that, on the DFTB accessible time scales, an important aspect of DNTF chem-

istry is the formation of CO_2 , N_2 and CO . Following DNTF decomposition and significant production of these molecular products, the system appears to reach a metastable state earlier than other energetic materials with comparable oxygen balance such as HMX. This may be related to the absence of H_2O as an available product, which mediates carbon and nitrogen chemistry at extreme conditions⁵⁸. Though NO and NO_2 formation delays CO_2 , N_2 and CO production to some extent, NO_3 does not appear to play any role in inhibiting the chemistry, as it does in oxygen-rich and oxygen balanced materials. Crucially, we find that the occurrence and slow evolution of large $\text{C}_x\text{N}_y\text{O}_z$ species, which are likely precursors to the carbon condensates observed in experiments, is a major feature of shock-driven DNTF chemistry. Their detailed kinetics can only be characterized by simulations on time and length-scales larger than those accessible to DFTB. Nevertheless, the Mio+ChIMES MSST simulations yield a lower-bound for the C—J detonation velocity and shock Hugoniot curves that are consistent with experiment and thermochemical estimates.

Ultimately, we find that the present Mio+ChIMES approach is well suited for the study of organic molecular materials under extreme conditions (i.e. where existing DFTB parameter sets are generally not applicable). Beyond providing a means of achieving long-timescale simulation with DFT-accuracy, this approach can greatly enhance efficiency in developing standalone ML-IAP (e.g. ChIMES) models, by serving as an effective (and rapid) means of generating DFT-quality data in cases where experimental results are scarce. Future work will focus on use of the present Mio+ChIMES DNTF model to generate reference data for development of a full ChIMES ML-IAP that can be leveraged in large scale (i.e. millions-of atoms) simulations and further extend simulation timescales to enable direct investigation of carbon condensation processes in carbon-rich organic materials.

V. SUPPLEMENTARY MATERIAL

The following files are available free of charge.

- SI.pdf: Additional discussion of the ChIMES model form and validation
- ChIMES_DNTF.2+3b.DFTB.params.txt: ChIMES parameters for the DFTB (Mio-1-1) E_{corr} developed in this work

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The data that supports the findings of this study are available within the article and its supplementary material..

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Supplementary Information: Investigating 3,4-bis(3-nitrofurazan-4-yl)furoxan Detonation with a Rapidly Tuned Density Functional Tight Binding Model

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Additional ChIMES Details

The Chebyshev polynomials comprising ChIMES interactions take a transformed pair distance, i.e. $s_{ij}^{e_i e_j}$, as their argument. In contrast to a “standard” pair distance (e.g. r_{ij} , which gives the distance between two atoms i and j), $s_{ij}^{e_i e_j}$ gives a pair distance transformed to span the [-1,1] domain over which Chebyshev polynomials are defined, and is obtained through:¹

$$x_{ij}^{e_i e_j} = \exp(-r_{ij}^{e_i e_j} / \lambda^{e_i e_j}) \quad (1)$$

$$x_{\text{avg}}^{e_i e_j} = 0.5(x_{\text{c,out}}^{e_i e_j} + x_{\text{c,in}}^{e_i e_j}) \quad (2)$$

$$x_{\text{diff}}^{e_i e_j} = 0.5|x_{\text{c,out}}^{e_i e_j} - x_{\text{c,in}}^{e_i e_j}| \quad (3)$$

$$s_{ij}^{e_i e_j} = (x_{ij}^{e_i e_j} - x_{\text{avg}}^{e_i e_j}) / x_{\text{diff}}^{e_i e_j} \quad (4)$$

where e_i is the element type of atom i , $s_{ij}^{e_i e_j}$ is the pair distance and $\lambda^{e_i e_j}$ can be considered a characteristic bonding distance, typically set to the location of the first peak in the DFT radial distribution function for the $e_i e_j$ atom pair type, and $r_{\text{c,in}}^{e_i e_j} / r_{\text{c,out}}^{e_i e_j}$ are the corresponding inner/outer cutoff radii. We note that Eq. 1 enforces a natural decrease in interaction strength as distance is increased, and increasing $\lambda^{e_i e_j}$ has the effect of decreasing the rate of interaction decay as $r_{\text{c,out}}^{e_i e_j}$ is approached, in a Morse-like¹ fashion.

As described in the main text, ChIMES interactions also include a smoothing function (i.e. $f_s^{e_i e_j}$) which ensures each term in the polynomial series decays to zero at the outer cutoff, without any discontinuities. The smoothing function takes on the form:

$$f_s^{e_i e_j}(r_{ij}) = \begin{cases} 0, & \text{if } r_{ij} > r_{\text{c,out}}^{e_i e_j} \\ 1, & \text{if } r_{ij} < d_t \\ \frac{1}{2} + \frac{1}{2} \sin \left(\pi \left[\frac{r_{ij} - d_t}{r_{\text{c,out}}^{e_i e_j} - d_t} \right] + \frac{\pi}{2} \right), & \text{otherwise} \end{cases} \quad (5)$$

where the threshold distance is given by $d_t = r_{\text{c,out}}^{m_1(y)} (1 - f_O)$, and f_O is a value in [0,1] taken to be 0.5, here. This function exhibits a smooth step, allowing the interaction energy to remain unmodified by the smoothing function for all $r_{ij} < d_t$. We note that this smoothing function is particularly useful for many-body interactions of large n , where the product of $\binom{n}{2} f_s^{e_i e_j}(r_{ij})$ factors is used, and can otherwise severely reduce energy contributions to the total energy for $n > 2$.

Finally, ChIMES two-body interactions include a penalty function which discourages the system from sampling pair distances below the inner cutoffs. The penalty function is given by:

$$f_p^{e_i e_j}(r_{ij}) = \begin{cases} A_p^{e_i e_j} (r_{\text{c,in}}^{e_i e_j} + d_p^{e_i e_j} - r_{ij})^3, & \text{if } r_{ij} < r_{\text{c,in}}^{e_i e_j} + d_p \\ 0, & \text{otherwise} \end{cases} \quad (6)$$

where $A_p^{e_i e_j}$, $d_p^{e_i e_j}$, and $r_{\text{c,in}}^{e_i e_j}$ are the penalty function strength, kick-in distance, and the inner cutoff for atom types e_i and e_j , respectively.

Additional Validation Data

The ChIMES-corrected DFTB model (i.e. Mio+ChIMES) discussed in the main text evaluated in terms of the radial pair distribution functions (RDFs) for each atom pair type at each training thermodynamic state point. Figure 1 provides RDFs for DNTF predicted by DFT, “standard” DFTB (i.e. Mio-1-1), and the presently developed Mio+ChIMES model. In general, we find both DFTB models in good agreement with DFT, though the Mio+ChIMES model tends to yield better performance under more extreme conditions (e.g. $T \geq 4440$).

Figure 1: Radial pair distribution functions predicted by DFT, Mio-1-1 (“Mio”), and the presently developed Mio+ChIMES models.

References

- (1) Braams, B. J.; Bowman, J. M. Permutationally invariant potential energy surfaces in high dimensionality. *Int. Rev. Phys. Chem.* **2009**, *28*, 577–606.

! This model is only intended for DNTF from approximately 300 to 9000 K and 1.86 to 3.4 gcc

! This model is not applicable to other atom type ratios

!

!

USECOUL: false

FITCOUL: false

USEPOVR: false

FITPOVR: false

USE3BCH: true

USE4BCH: false

PAIRTYPE: CHEBYSHEV 12 8 0 -1 1

ATOM TYPES: 3

# TYPEIDX #	# ATM_TYP #	# ATMCHRG #	# ATMMASS #
0	C	0	12.0107
1	N	0	14.0067
2	O	0	15.999

ATOM PAIRS: 6

# PAIRIDX #	# ATM_TY1 #	# ATM_TY2 #	# S_MINIM #	# S_MAXIM #	# S_DELTA #	#
CHBDIST #	# MORSE_LAMBDA #					
0	C	C	1.080	3.0	0.01	MORSE 1.40
1	N	N	0.935	3.0	0.01	MORSE 1.13
2	O	O	1.080	3.0	0.01	MORSE 2.35
3	C	N	0.995	3.0	0.01	MORSE 1.30
4	C	O	0.955	3.0	0.01	MORSE 1.20
5	N	O	0.960	3.0	0.01	MORSE 1.15

FCUT TYPE: TERSOFF 0.5

PAIR CHEBYSHEV PENALTY DIST: 0.02

PAIR CHEBYSHEV PENALTY SCALING: 1000000.0

SPECIAL 3B S_MAXIM: SPECIFIC 10

CCCCC CC CC CC 3.00000 3.00000 3.00000
CCCNCN CC CN CN 3.00000 3.00000 3.00000
CCCOCO CC CO CO 3.00000 3.00000 3.00000
CNCNNN CN CN NN 3.00000 3.00000 3.00000
CNCONO CN CO NO 3.00000 3.00000 3.00000
COCOOO CO CO OO 3.00000 3.00000 3.00000
NNNNNN NN NN NN 3.00000 3.00000 3.00000
NNNONO NN NO NO 3.00000 3.00000 3.00000
NONOOO NO NO OO 3.00000 3.00000 3.00000
OOOOOO OO OO OO 3.00000 3.00000 3.00000

ATOM PAIR TRIPLETS: 10

ATOM PAIR QUADRUPLTS: 0

PAIR CHEBYSHEV PARAMS

PAIRTYPE PARAMS: 0 C C

0 -22.3416405279
1 9.991423956054
2 -6.975426943187
3 1.522138916278
4 -0.8607258377407
5 2.107066974107
6 -2.450494382222
7 0.6075393845831
8 -0.4032939229531
9 0.5770468647435
10 -0.6855333350413

11 0.5254109036754

PAIRTYPE PARAMS: 1 N N

0 6.032592456936
1 11.57081911618
2 2.614242090383
3 -7.917005724114
4 8.229418287383
5 0.2224753695561
6 0.9239671094822
7 -1.174713847289
8 3.24614691441
9 -2.296458575943
10 0.887089625148
11 -0.0009331334258886

PAIRTYPE PARAMS: 2 O O

0 -31.68506413688
1 18.21328634329
2 -5.928017516687
3 13.15602372867
4 -11.6648020585
5 7.949578712528
6 -3.487756504078
7 3.502174389637
8 -3.171502434946
9 1.322516316714
10 -0.6397425233484
11 0.3873698922037

PAIRTYPE PARAMS: 3 C N

0 -3.032288794861
1 11.85464638299
2 3.689531382371
3 -3.000940965044
4 1.175906583971
5 1.275267355812
6 -0.2233697483747
7 -0.4256839494941
8 0.5948275266625
9 0.08631529090629
10 -0.1971497557096
11 0.2147071116057

PAIRTYPE PARAMS: 4 C O

0 -9.091927806649
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2 3.969231583633
3 3.169556820228
4 -1.213055631955
5 2.831566572585
6 -1.065828659787
7 1.499037708973
8 0.5663897970059
9 0.2767692441393
10 -0.1790891237699
11 0.4422505706705

PAIRTYPE PARAMS: 5 N O

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2 11.62532499841
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4 4.27521556458
5 -0.5978367075403
6 -0.01153016949812
7 -0.646879800712
8 1.16573947956
9 -0.1781964321031
10 -0.5267877128879
11 0.5429088039348

TRIPLET CHEBYSHEV PARAMS

TRIPLETTYPE PARAMS:

INDEX: 0 ATOMS: C C C

PAIRS: CC CC CC UNIQUE: -1 TOTAL: 423

index | powers | equiv index | param index | parameter

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4 1 0 2 3 1 -3.022816795842
5 0 2 1 3 1 -3.022816795842
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7 1 2 0 3 1 -3.022816795842
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QUADRUPLLET CHEBYSHEV PARAMS

PAIRMAPS: 9

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3 CN
4 CO
3 NC
1 NN
5 NO
4 OC
5 ON
2 OO

TRIPMAPS: 27

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1 CCCNCN
2 CCCOCO
1 CNCCCN
1 CNCNCC
3 CNCNNN
4 CNCONO
3 CNNNCN
4 CNNOCO
2 COCCCO
4 COCNNO
2 COCOCC
5 COCOOO
4 CONOCN
5 COOOCO
3 NNCNCN
6 NNNNNN
7 NNNONO
4 NOCNCO
4 NOCOCN
7 NONNNO
7 NONONN
8 NONOOO
8 NOOONO
5 OOCOCO
8 OONONO
9 OOOOOO

NO ENERGY OFFSETS: 3

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ENERGY OFFSET 2 3908.19887304
ENERGY OFFSET 3 0.0
ENDFILE