

Supporting information for the article “Development of the ReaxFF Reactive Force Field for the Y-doped BaZrO<sub>3</sub> Proton Conductor” by Adri C.T. van Duin, Boris V. Merinov, Sang Soo Han, Claudio O. Dorso, and William A. Goddard III.

## **ReaxFF reactive force field potential functions**

This document contains all the general ReaxFF-potential functions. In the current ReaxFF code all the energy contributions in this document are calculated regardless of system composition. All parameters that do not bear a direct physical meaning are named after the partial energy contribution that they appear in. For example,  $p_{val1}$  and  $p_{val2}$  are parameters in the valence angle potential function. Parameters with a more direct physical meaning, like the torsional rotational barriers ( $V_1, V_2, V_3$ ) bear their more recognizable names.

### **1. Overall system energy**

Equation (1) describes the ReaxFF overall system energy.

$$E_{system} = E_{bond} + E_{lp} + E_{over} + E_{under} + E_{val} + E_{pen} + E_{coa} + E_{C2} + E_{triple} + E_{tors} + E_{conj} + E_{H-bond} + E_{vdWaals} + E_{Coulomb} \quad (1)$$

Below follows a description of the partial energies introduced in equation (1).

### **2. Bond Order and Bond Energy**

A fundamental assumption of ReaxFF is that the bond order  $BO'_{ij}$  between a pair of atoms can be obtained directly from the interatomic distance  $r_{ij}$  as given in Equation (2). In calculating the bond orders, ReaxFF distinguishes between contributions from sigma bonds, pi-bonds and double pi bonds.

$$BO'_{ij} = BO_{ij}^{\sigma} + BO_{ij}^{\pi} + BO_{ij}^{\pi\pi} = \exp \left[ p_{bo1} \cdot \left( \frac{r_{ij}}{r_o^{\sigma}} \right)^{p_{bo2}} \right] + \exp \left[ p_{bo3} \cdot \left( \frac{r_{ij}}{r_o^{\pi}} \right)^{p_{bo4}} \right] + \exp \left[ p_{bo5} \cdot \left( \frac{r_{ij}}{r_o^{\pi\pi}} \right)^{p_{bo6}} \right] \quad (2)$$

Based on the uncorrected bond orders  $BO'$ , derived from Equation 1, an uncorrected overcoordination  $\Delta'$  can be defined for the atoms as the difference between the total bond order around the atom and the number of its bonding electrons  $Val$ .

$$\Delta'_i = -Val_i + \sum_{j=1}^{neighbours(i)} BO'_{ij} \quad (3a)$$

ReaxFF then uses these uncorrected overcoordination definitions to correct the bond orders  $BO'_{ij}$  using the scheme described in Equations (4a-f). To soften the correction for atoms bearing lone electron pairs a second overcoordination definition  $\Delta'^{boc}$  (equation 3b) is used in equations 4e and 4f. This allows atoms like nitrogen and oxygen, which bear lone electron pairs after filling their valence, to break up these electron pairs and involve them in bonding without obtaining a full bond order correction.

$$\Delta_i^{'boc} = -Val_i^{'boc} + \sum_{j=1}^{neighbours(i)} BO_{ij}' \quad (3b)$$

$$\begin{aligned} BO_{ij}^{\sigma} &= BO_{ij}'^{\sigma} \cdot f_1(\Delta_i', \Delta_j') \cdot f_4(\Delta_i', BO_{ij}') \cdot f_5(\Delta_j', BO_{ij}') \\ BO_{ij}^{\pi} &= BO_{ij}'^{\pi} \cdot f_1(\Delta_i', \Delta_j') \cdot f_1(\Delta_i', \Delta_j') \cdot f_4(\Delta_i', BO_{ij}') \cdot f_5(\Delta_j', BO_{ij}') \\ BO_{ij}^{\pi\pi} &= BO_{ij}'^{\pi\pi} \cdot f_1(\Delta_i', \Delta_j') \cdot f_1(\Delta_i', \Delta_j') \cdot f_4(\Delta_i', BO_{ij}') \cdot f_5(\Delta_j', BO_{ij}') \\ BO_{ij} &= BO_{ij}^{\sigma} + BO_{ij}^{\pi} + BO_{ij}^{\pi\pi} \end{aligned} \quad (4a)$$

$$f_1(\Delta_i', \Delta_j') = \frac{1}{2} \cdot \left( \frac{Val_i + f_2(\Delta_i', \Delta_j')}{Val_i + f_2(\Delta_i', \Delta_j') + f_3(\Delta_i', \Delta_j')} + \frac{Val_j + f_2(\Delta_i', \Delta_j')}{Val_j + f_2(\Delta_i', \Delta_j') + f_3(\Delta_i', \Delta_j')} \right) \quad (4b)$$

$$f_2(\Delta_i', \Delta_j') = \exp(-p_{boc1} \cdot \Delta_i') + \exp(-p_{boc1} \cdot \Delta_j') \quad (4c)$$

$$f_3(\Delta_i', \Delta_j') = -\frac{1}{p_{boc2}} \cdot \ln \left\{ \frac{1}{2} \cdot \left[ \exp(-p_{boc2} \cdot \Delta_i') + \exp(-p_{boc2} \cdot \Delta_j') \right] \right\} \quad (4d)$$

$$f_4(\Delta_i', BO_{ij}') = \frac{1}{1 + \exp(-p_{boc3} \cdot (p_{boc4} \cdot BO_{ij}' \cdot BO_{ij}' - \Delta_i^{'boc}) + p_{boc5})} \quad (4e)$$

$$f_5(\Delta_j', BO_{ij}') = \frac{1}{1 + \exp(-p_{boc3} \cdot (p_{boc4} \cdot BO_{ij}' \cdot BO_{ij}' - \Delta_j^{'boc}) + p_{boc5})} \quad (4f)$$

A corrected overcoordination  $\Delta_i$  can be derived from the corrected bond orders using equation (5).

$$\Delta_i = -Val_i + \sum_{j=1}^{neighbours(i)} BO_{ij} \quad (5)$$

Equation (6) is used to calculate the bond energies from the corrected bond orders  $BO_{ij}$ .

$$E_{bond} = -D_e^{\sigma} \cdot BO_{ij}^{\sigma} \cdot \exp \left[ p_{bel} \left( 1 - (BO_{ij}^{\sigma})^{p_{be2}} \right) \right] - D_e^{\pi} \cdot BO_{ij}^{\pi} - D_e^{\pi\pi} \cdot BO_{ij}^{\pi\pi} \quad (6)$$

### 3. Lone pair energy

Equation (8) is used to determine the number of lone pairs around an atom.  $\Delta_i^e$  is determined in Equation (7) and describes the difference between the total number of outer shell electrons (6 for oxygen, 4 for silicon, 1 for hydrogen) and the sum of bond orders around an atomic center.

$$\Delta_i^e = -Val_i^e + \sum_{j=1}^{neighbours(i)} BO_{ij} \quad (7)$$

$$n_{lp,i} = \text{int}\left(\frac{\Delta_i^e}{2}\right) + \exp\left[-p_{lp1} \cdot \left(2 + \Delta_i^e - 2 \cdot \text{int}\left\{\frac{\Delta_i^e}{2}\right\}\right)^2\right] \quad (8)$$

For oxygen with normal coordination (total bond order=2,  $\Delta_i^e=4$ ), equation (8) leads to 2 lone pairs. As the total bond order associated with a particular O starts to exceed 2, equation (8) causes a lone pair to gradually break up, causing a deviation  $\Delta_i^{lp}$ , defined in equation (9), from the optimal number of lone pairs  $n_{lp,opt}$  (e.g. 2 for oxygen, 0 for silicon and hydrogen).

$$\Delta_i^{lp} = n_{lp,opt} - n_{lp,i} \quad (9)$$

This is accompanied by an energy penalty, as calculated by equation (10).

$$E_{lp} = \frac{p_{lp2} \cdot \Delta_i^{lp}}{1 + \exp(-75 \cdot \Delta_i^{lp})} \quad (10)$$

#### 4. Overcoordination

For an overcoordinated atom ( $\Delta_i > 0$ ), equations (11a-b) impose an energy penalty on the system. The degree of overcoordination  $\Delta$  is decreased if the atom contains a broken-up lone electron pair. This is done by calculating a corrected overcoordination (equation 11b), taking the deviation from the optimal number of lone pairs, as calculated in equation (9), into account.

$$E_{over} = \frac{\sum_{j=1}^{nbond} p_{ovun1} \cdot D_e^\sigma \cdot BO_{ij}}{\Delta_i^{lpcorr} + Val_i} \cdot \Delta_i^{lpcorr} \cdot \left[ \frac{1}{1 + \exp(p_{ovun2} \cdot \Delta_i^{lpcorr})} \right] \quad (11a)$$

$$\Delta_i^{lpcorr} = \Delta_i - \frac{\Delta_i^{lp}}{1 + p_{ovun3} \cdot \exp\left(p_{ovun4} \cdot \left\{ \sum_{j=1}^{neighbours(i)} (\Delta_j - \Delta_j^{lp}) \cdot (BO_{ij}^\pi + BO_{ij}^{\pi\pi}) \right\}\right)} \quad (11b)$$

#### 5. Undercoordination

For an undercoordinated atom ( $\Delta_i < 0$ ), we want to take into account the energy contribution for the resonance of the  $\pi$ -electron between attached under-coordinated atomic centers. This is done by equations 12 where  $E_{under}$  is only important if the bonds between under-coordinated atom  $i$  and its under-coordinated neighbors  $j$  partly have  $\pi$ -bond character.

$$E_{under} = -p_{ovun5} \cdot \frac{1 - \exp(p_{ovun6} \cdot \Delta_i^{lpcor})}{1 + \exp(-p_{ovun2} \cdot \Delta_i^{lpcor})} \cdot \frac{1}{1 + p_{ovun7} \cdot \exp \left[ p_{ovun8} \cdot \left\{ \sum_{j=1}^{neighbours(i)} (\Delta_j - \Delta_j^{lp}) \cdot (BO_{ij}^\pi + BO_{ij}^{\pi\pi}) \right\} \right]} \quad (12)$$

## 6. Valence Angle Terms

**6.1 Angle energy.** Just as for bond terms, it is important that the energy contribution from valence angle terms goes to zero as the bond orders in the valence angle goes to zero. Equations (13a-g) are used to calculate the valence angle energy contribution. The equilibrium angle  $\Theta_0$  for  $\Theta_{ijk}$  depends on the sum of  $\pi$ -bond orders ( $SBO$ ) around the central atom  $j$  as described in Equation (13d). Thus, the equilibrium angle changes from around 109.47 for  $sp^3$  hybridization ( $\pi$ -bond=0) to 120 for  $sp^2$  ( $\pi$ -bond=1) to 180 for  $sp$  ( $\pi$ -bond=2) based on the geometry of the central atom  $j$  and its neighbors. In addition to including the effects of  $\pi$ -bonds on the central atom  $j$ , Equation (13d) also takes into account the effects of over- and under-coordination in central atom  $j$ , as determined by equation (13e), on the equilibrium valency angle, including the influence of a lone electron pair.  $Val^{angle}$  is the valency of the atom used in the valency and torsion angle evaluation.  $Val^{angle}$  is the same as  $Val^{boc}$  used in equation (3c) for non-metals. The functional form of Equation (13f) is designed to avoid singularities when  $SBO=0$  and  $SBO=2$ . The angles in Equations (13a)-(13g) are in radians.

$$E_{val} = f_7(BO_{ij}) \cdot f_7(BO_{jk}) \cdot f_8(\Delta_j) \cdot \left\{ p_{val1} - p_{val1} \exp \left[ -p_{val2} (\Theta_0(BO) - \Theta_{ijk})^2 \right] \right\} \quad (13a)$$

$$f_7(BO_{ij}) = 1 - \exp(-p_{val3} \cdot BO_{ij}^{p_{val4}}) \quad (13b)$$

$$f_8(\Delta_j) = p_{val5} - (p_{val5} - 1) \cdot \frac{2 + \exp(p_{val6} \cdot \Delta_j^{angle})}{1 + \exp(p_{val6} \cdot \Delta_j^{angle}) + \exp(-p_{val7} \cdot \Delta_j^{angle})} \quad (13c)$$

$$SBO = \sum_{n=1}^{neighbours(j)} (BO_{jn}^\pi + BO_{jn}^{\pi\pi}) + \left[ 1 - \prod_{n=1}^{neighbours(j)} \exp(-BO_{jn}^8) \right] \cdot (-\Delta_j^{angle} - p_{val8} \cdot n_{lp,j}) \quad (13d)$$

$$\Delta_j^{angle} = -Val_j^{angle} + \sum_{n=1}^{neighbours(j)} BO_{jn} \quad (13e)$$

$$SBO2 = 0 \text{ if } SBO \leq 0$$

$$SBO2 = SBO^{p_{val9}} \text{ if } 0 < SBO < 1 \quad (13f)$$

$$SBO2 = 2 - (2 - SBO)^{p_{val9}} \text{ if } 1 < SBO < 2$$

$$SBO2 = 2 \text{ if } SBO > 2$$

$$\Theta_0(BO) = \pi - \Theta_{0,0} \cdot \left\{ 1 - \exp[-p_{val10} \cdot (2 - SBO2)] \right\} \quad (13g)$$

**6.2 Penalty energy.** To reproduce the stability of systems with two double bonds sharing an atom in a valency angle, like allene, an additional energy penalty, as described in Equations (14a) and

(14b), is imposed for such systems. Equation (9b) deals with the effects of over/undercoordination in central atom  $j$  on the penalty energy.

$$E_{pen} = p_{pen1} \cdot f_9(\Delta_j) \cdot \exp\left[-p_{pen2} \cdot (BO_{ij} - 2)^2\right] \exp\left[-p_{pen2} \cdot (BO_{jk} - 2)^2\right] \quad (14a)$$

$$f_9(\Delta_j) = \frac{2 + \exp(-p_{pen3} \cdot \Delta_j)}{1 + \exp(-p_{pen3} \cdot \Delta_j) + \exp(p_{pen4} \cdot \Delta_j)} \quad (14b)$$

**6.3 Three-body conjugation term.** The hydrocarbon ReaxFF potential contained only a four-body conjugation term (see section 7.2), which was sufficient to describe most conjugated hydrocarbon systems. However, this term failed to describe the stability obtained from conjugation by the  $-\text{NO}_2$ -group. To describe the stability of such groups a three-body conjugation term is included (equation 15).

$$E_{coa} = p_{coa1} \cdot \frac{1}{1 + \exp(p_{coa2} \cdot \Delta_j^{val})} \cdot \exp\left[-p_{coa3} \cdot \left(-BO_{ij} + \sum_{n=1}^{neighbours(i)} BO_{in}\right)^2\right] \cdot \exp\left[-p_{coa3} \cdot \left(-BO_{jk} + \sum_{n=1}^{neighbours(i)} BO_{kn}\right)^2\right] \cdot \exp\left[-p_{coa4} \cdot (BO_{ij} - 1.5)^2\right] \cdot \exp\left[-p_{coa4} \cdot (BO_{jk} - 1.5)^2\right] \quad (15)$$

## 7. Torsion angle terms

**7.1 Torsion rotation barriers.** Just as with angle terms we need to ensure that dependence of the energy of torsion angle  $\omega_{ijkl}$  accounts properly for  $\text{BO} \rightarrow 0$  and for  $\text{BO}$  greater than 1. This is done by Equations (16a)-(16c).

$$E_{tors} = f_{10}(BO_{ij}, BO_{jk}, BO_{kl}) \cdot \sin \Theta_{ijk} \cdot \sin \Theta_{jkl} \cdot \left[ \frac{1}{2} V_1 \cdot (1 + \cos \omega_{ijkl}) + \frac{1}{2} V_2 \cdot \exp\left\{p_{tor1} \cdot (BO_{jk}^\pi - 1 + f_{11}(\Delta_j, \Delta_k))^2\right\} \cdot (1 - \cos 2\omega_{ijkl}) + \frac{1}{2} V_3 \cdot (1 + \cos 3\omega_{ijkl}) \right] \quad (16a)$$

$$f_{10}(BO_{ij}, BO_{jk}, BO_{kl}) = \left[1 - \exp(-p_{tor2} \cdot BO_{ij})\right] \cdot \left[1 - \exp(-p_{tor2} \cdot BO_{jk})\right] \cdot \left[1 - \exp(-p_{tor2} \cdot BO_{kl})\right] \quad (16b)$$

$$f_{11}(\Delta_j, \Delta_k) = \frac{2 + \exp\left[-p_{tor3} \cdot (\Delta_j^{angle} + \Delta_k^{angle})\right]}{1 + \exp\left[-p_{tor3} \cdot (\Delta_j^{angle} + \Delta_k^{angle})\right] + \exp\left[p_{tor4} \cdot (\Delta_j^{angle} + \Delta_k^{angle})\right]} \quad (16c)$$

**7.2 Four body conjugation term.** Equations (17a-b) describe the contribution of conjugation effects to the molecular energy. A maximum contribution of conjugation energy is obtained when successive bonds have bond order values of 1.5 as in benzene and other aromatics.

$$E_{conj} = f_{12}(BO_{ij}, BO_{jk}, BO_{kl}) \cdot p_{cot1} \cdot \left[1 + (\cos^2 \omega_{ijkl} - 1) \cdot \sin \Theta_{ijk} \cdot \sin \Theta_{jkl}\right] \quad (17a)$$

$$f_{12}(BO_{ij}, BO_{jk}, BO_{kl}) = \exp\left[-p_{cot2} \cdot \left(BO_{ij} - 1\frac{1}{2}\right)^2\right] \cdot \exp\left[-p_{cot2} \cdot \left(BO_{jk} - 1\frac{1}{2}\right)^2\right] \cdot \exp\left[-p_{cot2} \cdot \left(BO_{kl} - 1\frac{1}{2}\right)^2\right] \quad (17b)$$

## 8. Hydrogen bond interactions

Equation (18) described the bond-order dependent hydrogen bond term for a X-H—Z system as incorporated in ReaxFF.

$$E_{Hbond} = p_{hb1} \cdot \left[1 - \exp(p_{hb2} \cdot BO_{XH})\right] \cdot \exp\left[p_{hb3} \cdot \left(\frac{r_{hb}^o}{r_{HZ}} + \frac{r_{HZ}}{r_{hb}^o} - 2\right)\right] \cdot \sin^8\left(\frac{\Theta_{XHZ}}{2}\right) \quad (18)$$

## 9. Correction for C<sub>2</sub>

ReaxFF erroneously predicts that two carbons in the C<sub>2</sub>-molecule form a very strong (triple) bond, while in fact the triple bond would get de-stabilized by terminal radical electrons, and for that reason the carbon-carbon bond is not any stronger than a double bond. To capture the stability of C<sub>2</sub> we introduced a new partial energy contribution (E<sub>C2</sub>). Equation (19) shows the potential function used to de-stabilize the C<sub>2</sub> molecule:

$$E_{C_2} = k_{c_2} \cdot (BO_{ij} - \Delta_i - 0.04 \cdot \Delta_i^4 - 3)^2 \quad \text{if } BO_{ij} - \Delta_i - 0.04 \cdot \Delta_i^4 > 3$$

$$E_{C_2} = 0 \quad \text{if } BO_{ij} - \Delta_i - 0.04 \cdot \Delta_i^4 \leq 3 \quad (19)$$

where  $\Delta_i$  is the level of under/overcoordination on atom  $i$  as obtained from subtracting the valency of the atom (4 for carbon) from the sum of the bond orders around that atom and  $k_{c_2}$  the force field parameter associated with this partial energy contribution.

## 11. Triple bond energy correction.

To describe the triple bond in carbon monoxide a triple bond stabilization energy is used, making CO both stable and inert. This energy term only affects C-O bonded pairs. Equation (20) shows the energy function used to describe the triple bond stabilization energy.

$$E_{trip} = p_{trip1} \exp[-p_{trip2} (BO_{ij} - 2.5)^2] \cdot \frac{\exp[-p_{trip4} \cdot (\sum_{k=1}^{neighbours(i)} BO_{ik} - BO_{ij})] + \exp[-p_{trip4} \cdot (\sum_{k=1}^{neighbours(j)} BO_{jk} - BO_{ij})]}{1 + 25 \cdot \exp[p_{trip3} (\Delta_i + \Delta_j)]}$$

## 12. Nonbonded interactions

In addition to valence interactions which depend on overlap, there are repulsive interactions at short interatomic distances due to Pauli principle orthogonalization and attraction energies at long distances due to dispersion. These interactions, comprised of van der Waals and Coulomb forces, are included for *all* atom pairs, thus avoiding awkward alterations in the energy description during bond dissociation.

**12.1 Taper correction.** To avoid energy discontinuities when charged species move in and out of the non-bonded cutoff radius ReaxFF employs a Taper correction, as developed by de Vos Burchart (1995). Each nonbonded energy and derivative is multiplied by a Taper-term, which is taken from a distance-dependent 7<sup>th</sup> order polynomial (equation 21)).

$$Tap = Tap_7 \cdot r_{ij}^7 + Tap_6 \cdot r_{ij}^6 + Tap_5 \cdot r_{ij}^5 + Tap_4 \cdot r_{ij}^4 + Tap_3 \cdot r_{ij}^3 + Tap_2 \cdot r_{ij}^2 + Tap_1 \cdot r_{ij} + Tap_0 \quad (21)$$

The terms in this polynomial are chosen to ensure that all 1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> derivatives of the non-bonded interactions to the distance are continuous and go to zero at the cutoff boundary. To that end, the terms Tap<sub>0</sub> to Tap<sub>7</sub> in equation (21) are calculated by the scheme in equation (22), where R<sub>cut</sub> is the non-bonded cutoff radius.

$$\begin{aligned}
Tap_7 &= 20/R_{cut}^7 \\
Tap_6 &= -70/R_{cut}^6 \\
Tap_5 &= 84/R_{cut}^5 \\
Tap_4 &= -35/R_{cut}^4 \quad (22) \\
Tap_3 &= 0 \\
Tap_2 &= 0 \\
Tap_1 &= 0 \\
Tap_0 &= 1
\end{aligned}$$

**12.2 van der Waals interactions.** To account for the van der Waals interactions we use a distance-corrected Morse-potential (Equations. 23a-b). By including a shielded interaction (Equation 23b) excessively high repulsions between bonded atoms (1-2 interactions) and atoms sharing a valence angle (1-3 interactions) are avoided.

$$E_{vdWaal} = Tap \cdot D_{ij} \cdot \left\{ \exp \left[ \alpha_{ij} \cdot \left( 1 - \frac{f_{13}(r_{ij})}{r_{vdW}} \right) \right] - 2 \cdot \exp \left[ \frac{1}{2} \cdot \alpha_{ij} \cdot \left( 1 - \frac{f_{13}(r_{ij})}{r_{vdW}} \right) \right] \right\} \quad (23a)$$

$$f_{13}(r_{ij}) = \left[ r_{ij}^{p_{vdW1}} + \left( \frac{1}{\gamma_w} \right)^{p_{vdW1}} \right]^{\frac{1}{p_{vdW1}}} \quad (23b)$$

### 12.3 Coulomb Interactions

As with the van der Waals-interactions, Coulomb interactions are taken into account between *all* atom pairs. To adjust for orbital overlap between atoms at close distances a shielded Coulomb-potential is used (Equation 24).

$$E_{coulomb} = Tap \cdot C \cdot \frac{q_i \cdot q_j}{\left[ r_{ij}^3 + \left( 1/\gamma_{ij} \right)^3 \right]^{1/3}} \quad (24)$$

Atomic charges are calculated using the Electron Equilibration Method (EEM)-approach. The EEM charge derivation method is similar to the QEq-scheme; the only differences, apart from parameter definitions, are that EEM does not use an iterative scheme for hydrogen charges (as in QEq) and that QEq uses a more rigorous Slater orbital approach to account for charge overlap.

### Reactive MD-force field: BaZrYOH fuel cells March 2007.

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39      ! Number of general parameters
50.0000 !p(boc1)
9.5469  !p(boc2)
26.5405 !p(coa2)
3.0000  !p(trip4)
6.5000  !p(trip3)
0.0000  !kc2
1.0588  !p(ovun6)
9.0000  !p(trip2)
12.1176 !p(ovun7)
13.3056 !p(ovun8)

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0.0000 !p(tripl)
0.0000 !Lower Taper-radius
10.0000 !Upper Taper-radius
0.0000 !Not used (n.u.)
33.8667 !p(val7)
6.0891 !p(lp1)
1.0563 !p(val9)
2.0384 !p(val10)
0.0000 !n.u.
6.9290 !p(pen2)
0.3989 !p(pen3)
3.9954 !p(pen4)
0.0000 !n.u.
5.7796 !p(tor2)
10.0000 !p(tor3)
1.9487 !p(tor4)
0.0000 !n.u.
2.1645 !p(cot2)
1.5591 !p(vdW1)
0.0100 !Cutoff for bond order (*100)
2.1365 !p(coa4)
2.0000 !p(ovun4)
3.0000 !p(ovun3)
1.8512 !p(val8)
0.0000 !n.u.
0.0000 !n.u.
0.0000 !Molecular energy (not used)
0.0000 !Molecular energy (not used)
2.6962 !p(coa3)
8      ! Nr of atoms; atomID;ro(sigma);Val;mass;Rvdw;Dij;gamma;ro(pi);Val(e)
      alfa;gamma(w);Val(angle);p(ovun5);n.u.;chiEEM;etaEEM;n.u.
      ro(pipi);p(lp2);Heat increment;p(boc4);p(boc3);p(boc5),n.u.;n.u.
      p(ovun2);p(val3);n.u.;Val(boc);p(val5);n.u.;n.u.;n.u.
C      1.3644   4.0000  12.0000   1.9803   0.1720   0.8712   1.2395   4.0000
      9.4734   2.1241   4.0000  31.8793  79.5548   5.7254   6.9235   0.0000
      1.2636   0.0000  -0.0537   5.7133  33.5629  11.9957   0.8563   0.0000
      -2.8983   4.7820   1.0564   4.0000   2.9663   0.0000   0.0000   0.0000
H      0.6853   1.0000   1.0080   1.3588   0.0622   0.7625  -0.1000   1.0000
      9.3992   5.0518   1.0000   0.0000 121.1250   3.8520   9.3303   1.0000
      -0.1000   0.0000  -0.1609   3.9714   3.2094   0.9031   1.0698   0.0000
      -15.7683   3.3504   1.0338   1.0000   2.8793   0.0000   0.0000   0.0000
O      1.2891   2.0000  15.9990   1.9741   0.0880   0.8659   1.0323   6.0000
      10.2186   7.7719   4.0000  30.8697 116.0768   8.5000   6.9585   2.0000
      0.9456   4.1347  -1.3533  20.7724   3.5512   0.5074   0.9745   0.0000
      -3.6141   2.7025   1.0493   4.0000   2.9225   0.0000   0.0000   0.0000
N      1.2333   3.0000  14.0000   1.9324   0.1376   0.8596   1.1748   5.0000
      10.0667   7.8431   4.0000  32.2482 100.0000   6.8418   6.3404   2.0000
      1.0433  13.7673  -1.1806   2.1961   3.0696   2.7683   0.9745   0.0000
      -4.3875   2.6192   1.0183   4.0000   2.8793   0.0000   0.0000   0.0000
Zr     2.6383   4.0000  91.2240   2.2842   0.2481   0.5792  -1.0000   4.0000
      11.6632  48.5301   4.0000  -5.0000   0.0000  -1.5489   6.1282   0.0000
      -1.0000   0.0000 143.1770  48.2657   0.2144   0.0000   0.8563   0.0000
      -4.3695   3.3675   1.0338   8.0000   2.2632   0.0000   0.0000   0.0000
Y      2.7973   3.0000  88.9052   2.4630   0.2892   0.4474  -1.0000   3.0000
      11.9899  50.0000   3.0000  -5.0000   0.0000  -7.2157   7.8528   0.0000
      -1.0000   0.0000 143.1770 127.9235  78.0398   0.0000   0.8563   0.0000
      -2.5000   2.9867   1.0338   3.0000   2.5791   0.0000   0.0000   0.0000

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Ba  2.5456   2.0000 137.3270   2.7000   0.2962   0.6301  -1.0000   2.0000
    10.3042  47.4978   2.0000  -5.0000   0.0000  -2.4182   5.5000   0.0000
    -1.0000   0.0000 143.1770 109.4891   9.4011   0.0147   0.8563   0.0000
    -7.5000   2.9867   1.0338   2.0000   2.5791   0.0000   0.0000   0.0000
X   -0.1000   2.0000   1.0080   2.0000   0.0000   1.0000  -0.1000   6.0000
    10.0000   2.5000   4.0000   0.0000   0.0000   8.5000   1.5000   0.0000
    -0.1000   0.0000  -2.3700   8.7410  13.3640   0.6690   0.9745   0.0000
   -11.0000   2.7466   1.0338   6.2998   2.8793   0.0000   0.0000   0.0000
22  !Bonds; at1;at2;De(sigma);De(pi);De(pipi);p(bo1);p(bo5);l3corr;p(bo6),
p(ovun)
      p(be2);p(bo3);p(bo4);n.u.;p(bo1);p(bo2);n.u.;n.u.
1  1 139.8093 110.6913  77.2102   0.2737  -0.7584   1.0000  38.4226   0.3288
    0.1235  -0.2010   8.6973   1.0000  -0.1042   6.1688   1.0000   0.0000
1  2 159.8520   0.0000   0.0000  -0.4646   0.0000   1.0000   6.0000   0.6170
    12.3878   1.0000   0.0000   1.0000  -0.0098   8.5954   0.0000   0.0000
2  2 170.0433   0.0000   0.0000  -0.3573   0.0000   1.0000   6.0000   0.7489
    9.6471   1.0000   0.0000   1.0000  -0.0169   5.8818   0.0000   0.0000
1  3 161.6647  58.4169 126.5609   0.2952  -0.1638   1.0000  12.1551   0.4055
    0.3211  -0.2388   7.5568   1.0000  -0.1729   4.9857   0.0000   0.0000
3  3  87.8137 171.0665  40.0000   0.9810  -0.2106   1.0000  29.4721   1.0000
    0.8827  -0.1679   7.7980   1.0000  -0.1290   7.0000   1.0000   0.0000
1  4 134.4562 139.7869  80.3761   0.0334  -0.1113   1.0000  27.0713   0.2076
    0.1315  -0.3049   7.0000   1.0000  -0.1355   5.2219   1.0000   0.0000
3  4 130.8596 169.4551  40.0000   0.3837  -0.1639   1.0000  35.0000   0.2000
    1.0000  -0.3579   7.0004   1.0000  -0.1193   6.8773   1.0000   0.0000
4  4 157.9384  82.5526 152.5336   0.4010  -0.1034   1.0000  12.4261   0.5828
    0.1578  -0.1509  11.9186   1.0000  -0.0861   5.4271   1.0000   0.0000
2  3 198.1847   0.0000   0.0000  -0.4899   0.0000   1.0000   6.0000   0.3987
    2.4577   1.0000   0.0000   1.0000  -0.0549   5.6546   0.0000   0.0000
2  4 231.8173   0.0000   0.0000  -0.3364   0.0000   1.0000   6.0000   0.4402
    8.8910   1.0000   0.0000   1.0000  -0.0327   6.5754   0.0000   0.0000
5  5  74.5027   0.0000   0.0000  -0.2541  -0.2000   0.0000  16.0000   0.3564
    0.5882  -0.2000  15.0000   1.0000  -0.1315   6.4024   0.0000   0.0000
3  5 112.4500   0.0000   0.0000   0.3505  -0.3000   1.0000  36.0000   0.4053
    0.1765  -0.2000  15.0000   1.0000  -0.1300  10.6008   1.0000   0.0000
2  5  38.8626   0.0000   0.0000  -0.1577   0.0000   1.0000   6.0000   0.5000
    17.8821   1.0000   0.0000   1.0000  -0.2095   6.3931   0.0000   0.0000
6  6  64.9243   0.0000   0.0000  -0.2933  -0.2000   0.0000  16.0000   0.3630
    1.3309  -0.2000  15.0000   1.0000  -0.0513   7.1116   0.0000   0.0000
3  6 146.8558   0.0000   0.0000  -0.0215  -0.3000   1.0000  36.0000   0.8913
    0.0564  -0.2000  15.0000   1.0000  -0.1659   7.0537   1.0000   0.0000
2  6  38.8626   0.0000   0.0000  -0.1577   0.0000   1.0000   6.0000   0.2901
    17.8821   1.0000   0.0000   1.0000  -0.2095   6.3931   0.0000   0.0000
5  6  63.5575   0.0000   0.0000  -0.1255  -0.2000   0.0000  16.0000   0.4238
    0.5959  -0.2000  15.0000   1.0000  -0.0923   7.4284   0.0000   0.0000
3  7  29.1935   0.0000   0.0000  -0.1434  -0.3000   1.0000  36.0000   0.2069
    0.5062  -0.2000  15.0000   1.0000  -0.0559   7.0193   1.0000   0.0000
2  7  38.8626   0.0000   0.0000  -0.1577   0.0000   1.0000   6.0000   0.2901
    17.8821   1.0000   0.0000   1.0000  -0.2095   6.3931   0.0000   0.0000
5  7  87.4453   0.0000   0.0000   0.0004  -0.2000   0.0000  16.0000   0.2593
    1.0000  -0.2000  15.0000   1.0000  -0.0864   5.4765   0.0000   0.0000
6  7  21.0000   0.0000   0.0000   0.0004  -0.2000   0.0000  16.0000   0.6594
    1.0000  -0.2000  15.0000   1.0000  -0.1155   9.0213   0.0000   0.0000
7  7  30.1404   0.0000   0.0000   0.0004  -0.2000   0.0000  16.0000   0.4086
    1.0000  -0.2000  15.0000   1.0000  -0.0439   5.2951   0.0000   0.0000
15  ! Off-diagonal terms.at1;at2;Dij;RvdW;alfa;ro(sigma);ro(pi);ro(pipi)
1  2   0.0431   1.7204  10.3632   1.0386  -1.0000  -1.0000

```

2	3	0.0468	1.9998	10.2265	0.9368	-1.0000	-1.0000
2	4	0.1059	1.8290	9.7818	0.9598	-1.0000	-1.0000
1	3	0.1142	1.9602	9.4709	1.3065	1.1260	1.0865
1	4	0.1445	1.8771	10.0000	1.7000	1.1885	1.1363
3	4	0.1058	2.0043	10.1244	1.7000	1.1096	1.0206
3	5	0.1473	1.7130	12.0284	1.9555	-1.0000	-1.0000
3	6	0.1114	1.7581	13.0000	1.7808	-1.0000	-1.0000
3	7	0.2824	1.7518	13.0000	2.1585	-1.0000	-1.0000
5	7	0.2904	2.5610	12.9818	2.4596	-1.0000	-1.0000
6	7	0.2079	2.1282	11.3529	2.4769	-1.0000	-1.0000
5	6	0.2936	2.2035	12.2199	2.5822	-1.0000	-1.0000
2	5	0.1000	1.7610	10.4809	0.1000	-1.0000	-1.0000
2	6	0.1000	1.7610	10.4809	0.1000	-1.0000	-1.0000
2	7	0.1000	1.7610	10.4809	0.1000	-1.0000	-1.0000

56 Angles: .at1;at2;at3;Thetao,o;p(val1);p(val2);p(coal);p(val7);p(pen1);p(val4)

1	1	1	75.8304	33.9168	0.8043	0.0000	0.1780	10.5736	1.0400
1	1	2	69.6421	9.2578	3.6521	0.0000	0.0058	0.0000	1.0400
2	1	2	75.4958	14.5436	2.7438	0.0000	0.0127	0.0000	1.0400
1	2	2	0.0000	0.0000	6.0000	0.0000	0.0000	0.0000	1.0400
1	2	1	0.0000	3.4110	7.7350	0.0000	0.0000	0.0000	1.0400
2	2	2	0.0000	27.9213	5.8635	0.0000	0.0000	0.0000	1.0400
1	1	3	78.2305	16.3043	3.3209	0.0000	1.1127	0.0000	1.1880
3	1	3	80.2229	45.0000	2.6995	0.0000	1.1127	0.0000	1.1880
1	1	4	66.1305	41.9072	1.4346	0.0000	1.1127	0.0000	1.1880
3	1	4	73.9544	45.0000	1.5778	0.0000	1.1127	0.0000	1.1880
4	1	4	64.1581	45.0000	0.6370	0.0000	1.1127	0.0000	1.1880
2	1	3	66.0941	11.3875	3.9388	0.0000	0.0755	0.0000	1.0500
2	1	4	74.2929	10.7059	6.3074	0.0000	0.0755	0.0000	1.0500
1	2	4	0.0000	0.0019	6.3000	0.0000	0.0000	0.0000	1.0400
1	3	1	72.6402	38.4252	1.3200	0.0000	0.6142	0.0000	1.0783
1	3	3	88.5142	45.0000	0.7808	0.0000	0.6142	0.0000	1.0783
1	3	4	82.4890	43.2625	1.1759	0.0000	0.6142	0.0000	1.0783
3	3	3	80.7324	35.1410	1.4999	0.0000	0.6142	0.0000	1.0783
3	3	4	84.3637	25.1714	2.5361	0.0000	0.6142	0.0000	1.0783
4	3	4	89.7071	45.0000	1.2301	0.0000	0.6142	0.0000	1.0783
1	3	2	77.4332	39.5610	1.3429	0.0000	0.1218	0.0000	1.0500
2	3	3	85.7907	10.5506	6.2301	0.0000	0.1218	0.0000	1.0500
2	3	4	75.6201	45.0000	2.5874	0.0000	0.1218	0.0000	1.0500
2	3	2	78.9033	33.3823	1.7364	0.0000	0.1218	0.0000	1.0500
1	4	1	66.0330	22.0295	1.4442	0.0000	1.6777	0.0000	1.0500
1	4	3	103.3204	33.0381	0.5787	0.0000	1.6777	0.0000	1.0500
1	4	4	104.1335	8.6043	1.6495	0.0000	1.6777	0.0000	1.0500
3	4	3	74.1978	42.1786	1.7845	-18.0069	1.6777	0.0000	1.0500
3	4	4	74.8600	43.7354	1.1572	-0.9193	1.6777	0.0000	1.0500
4	4	4	75.0538	14.8267	5.2794	0.0000	1.6777	0.0000	1.0500
1	4	2	69.1106	25.5067	1.1003	0.0000	0.0222	0.0000	1.0369
2	4	3	81.3686	40.0712	2.2396	0.0000	0.0222	0.0000	1.0369
2	4	4	83.0104	43.4766	1.5328	0.0000	0.0222	0.0000	1.0500
2	4	2	70.8687	12.0168	5.0132	0.0000	0.0222	0.0000	1.1243
1	2	3	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
1	2	4	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
1	2	5	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
3	2	4	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
4	2	4	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
2	2	3	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
2	2	4	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
3	2	3	0.0000	5.0000	3.0000	0.0000	0.0000	0.0000	1.0400

2	3	5	42.5058	10.0776	5.0000	0.0000	0.9289	0.0000	1.1912
2	3	6	50.0000	4.9111	1.0014	0.0000	1.0000	0.0000	1.1000
2	3	7	90.0000	4.4647	1.6312	0.0000	1.0000	0.0000	1.1000
3	5	3	55.8643	20.0000	0.3771	0.0000	0.1000	0.0000	1.4634
3	6	3	50.0000	20.0000	4.0000	0.0000	1.8576	0.0000	2.8010
3	7	3	90.0000	1.9850	5.0000	0.0000	0.2383	0.0000	1.2332
5	3	5	5.9871	8.9966	0.2147	0.0000	2.7977	0.0000	3.0000
5	3	6	8.1047	0.0887	0.1451	0.0000	0.1000	0.0000	2.8519
5	3	7	62.7913	3.1555	2.9321	0.0000	1.8172	0.0000	1.4679
6	3	6	3.0435	5.9522	9.0000	0.0000	1.6570	0.0000	1.1000
6	3	7	79.3434	1.5639	1.7219	0.0000	1.3741	0.0000	2.3497
7	3	7	54.7688	2.3715	3.0312	0.0000	1.6441	0.0000	1.4931
3	3	5	80.0000	10.0000	1.2500	0.0000	0.5554	0.0000	1.2000
3	3	6	80.0000	15.0000	1.2500	0.0000	0.5554	0.0000	1.2000

14 ! Torsions. at1;at2;at3;at4;;V1;V2;V3;p(tor1);p(cot1);n.u;n.u.

1	1	1	1	0.0000	38.9174	0.3649	-8.2931	-2.0127	0.0000	0.0000
1	1	1	2	0.0000	49.1001	0.2713	-8.5284	-1.5309	0.0000	0.0000
2	1	1	2	0.0000	34.0265	0.3804	-6.3917	-0.9965	0.0000	0.0000
0	1	2	0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0	2	2	0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0	1	3	0	3.9830	13.0320	0.4739	-1.9813	-2.0000	0.0000	0.0000
0	2	3	0	0.0000	0.1000	0.0200	-2.5415	0.0000	0.0000	0.0000
0	3	3	0	0.0318	23.1045	1.2614	-12.3670	0.0000	0.0000	0.0000
0	1	4	0	-2.4242	128.1636	0.3739	-6.6098	-2.0000	0.0000	0.0000
0	2	4	0	0.0000	0.1000	0.0200	-2.5415	0.0000	0.0000	0.0000
0	3	4	0	1.4816	55.6641	0.0004	-7.0465	-2.0000	0.0000	0.0000
0	4	4	0	-0.3244	27.7086	0.0039	-2.8272	-2.0000	0.0000	0.0000
0	1	1	0	0.0000	0.6675	0.0000	-8.2352	0.0000	0.0000	0.0000
4	1	4	4	-5.5181	8.9706	0.0004	-6.1782	-2.0000	0.0000	0.0000

4 ! Nr of hydrogen bonds. at1;at2;at3;r(hb);p(hb1);p(hb2);p(hb3)

3	2	3	1.4000	-1.7731	1.4695	3.5257				
3	2	4	1.6337	-11.7496	1.4695	3.5257				
4	2	3	1.3999	-9.6921	1.4695	3.5257				
4	2	4	1.7514	-7.5768	1.4695	3.5257				

**Coordinates of 10 structures shown in Figure 4.**

**Structure 1**

a = 8.84 b = 4.45 c = 4.28  $\alpha = 90.76$   $\beta = 90.00$   $\gamma = 90.00$

Ba 0.29206 -0.28916 0.23814  
Zr 2.21049 1.83524 2.38354  
O 2.20355 1.58037 0.26788  
O 2.23335 -0.51655 2.28905  
O 0.17084 1.53763 2.60861  
Ba 4.11905 -0.29204 0.23309  
Y 6.63500 1.64621 2.48976  
O 6.64714 1.53197 0.34715  
O 6.63454 -0.58548 2.41803  
O 4.25249 1.53578 2.60348  
H 6.62499 3.80390 1.29899

**Structure 2**

a = 8.84 b = 4.33 c = 4.33  $\alpha = 90.28$   $\beta = 90.00$   $\gamma = 90.00$

Ba 0.14540 0.08715 0.10486  
Zr 2.12670 2.18416 2.20864  
O 2.13571 1.91458 0.03192  
O 2.13193 -0.02122 1.93040  
O 0.01330 2.26364 2.44504  
Ba 4.12511 0.07822 0.08742  
Y 6.54889 2.35798 2.28542  
O 6.12959 1.74940 -0.00577  
O 6.87986 0.01088 1.39439  
O 4.22962 2.25639 2.41396  
H 6.54294 0.85486 0.64555

**Structure 3**

a = 8.96 b = 4.24 c = 4.38  $\alpha = 90.00$   $\beta = 90.00$   $\gamma = 91.40$

Ba 0.14138 -0.24077 -0.00679  
Zr 2.24924 2.06237 2.17078  
O 2.40418 2.05016 -0.01597  
O 2.49284 -0.03852 2.18436  
O 0.21004 2.52565 2.18940  
Ba 4.19326 0.07353 -0.03107  
Y 6.93115 1.64925 2.21591  
O 7.25342 1.49510 0.04718  
O 6.00924 -0.49458 2.52577  
O 4.39563 2.01070 2.15912  
H 5.21014 2.87562 2.29752

**Structure 4**

a = 8.98 b = 4.24 c = 4.38  $\alpha = 89.98$   $\beta = 89.98.00$   $\gamma = 91.31$

Ba 0.21251 -0.12886 -0.01407

Zr	2.32567	2.17771	2.15991
O	2.47959	2.15927	-0.02809
O	2.56773	0.07410	2.17415
O	0.28386	2.64006	2.17779
Ba	4.27344	0.18749	-0.04172
Y	7.01927	1.77322	2.21156
O	7.33679	1.61995	0.04413
O	6.09209	-0.38065	2.51386
O	4.48009	2.12371	2.14703
H	5.29589	2.98886	2.28444

### Structure 5

a = 8.88 b = 4.31 c = 4.38  $\alpha = 90.00$   $\beta = 90.00$   $\gamma = 90.00$

Ba	0.28775	0.05517	-0.01432
Zr	2.26223	2.22409	2.18934
O	2.15114	2.13957	0.01878
O	2.39968	-0.01615	2.31100
O	0.19474	2.03019	2.17334
Ba	4.25615	0.23735	-0.01039
Y	6.73292	1.94355	2.18009
O	6.67248	1.78602	-0.00822
O	6.55559	-0.21724	2.17716
O	4.29427	1.79093	2.16337
H	5.49655	3.98623	2.17650

### Structure 6

a = 8.88 b = 4.33 c = 4.46  $\alpha = 89.55$   $\beta = 89.68$   $\gamma = 86.27$

Ba	0.13947	-0.17647	-0.10062
Zr	2.00398	2.07725	2.18931
O	1.94210	1.92523	0.01450
O	-0.11703	2.13263	2.12996
Ba	3.97191	0.18052	-0.12398
Y	6.59867	2.02588	2.23234
O	6.69527	1.82268	0.02626
O	5.68636	-0.29830	2.55483
O	4.11788	2.19723	2.13929
O	2.09075	-0.09741	2.45802
H	4.88799	3.12946	2.31907

### Structure 7

a = 8.81 b = 4.37 c = 4.42  $\alpha = 90.00$   $\beta = 90.00$   $\gamma = 90.00$

Ba	-0.09372	0.04558	0.07373
Zr	2.16657	2.33772	2.21526
O	2.26460	2.22906	-0.21182
O	2.09542	0.09935	1.77846
O	0.12833	2.22629	2.42273

Ba	4.54307	-0.03827	0.03483
Y	6.58873	2.16076	2.22518
O	6.44700	2.11308	0.00849
O	6.65222	-0.02653	2.02537
O	4.21142	2.14362	2.37045
H	2.65479	1.47341	0.42095

**Structure a**

a = 8.58 b = 8.57 c = 8.49  $\alpha = 90.00$   $\beta = 90.00$   $\gamma = 90.00$

Ba	-0.05372	-0.05103	-0.11967
Zr	2.14253	2.08944	2.09894
O	1.52098	1.90417	-0.01755
O	2.23449	0.01642	2.71111
O	-0.04855	2.05168	2.61752
Ba	4.38070	-0.00907	-0.11593
Zr	6.41534	2.10191	2.07393
O	6.82209	2.60302	-0.02939
O	6.49514	0.00770	1.53601
O	4.25061	2.04292	1.55435
Ba	0.12778	4.21305	-0.04116
Zr	2.14261	6.46497	2.11196
O	2.25442	7.13129	0.05848
O	2.14369	4.32291	1.61583
O	0.02186	6.39965	2.21433
Ba	4.19772	4.22037	0.06533
Y	6.43623	6.41030	2.09648
O	6.08064	5.92271	-0.02393
O	6.41209	4.22111	2.45948
O	4.25278	6.38044	2.51859
H	6.67040	8.08695	5.84771
Ba	0.03259	0.03364	4.21459
Zr	2.15241	2.15609	6.30848
O	2.39497	2.72014	4.20122
O	2.10269	0.02598	5.83108
O	-0.01246	2.34395	5.92641
Ba	4.33301	-0.13561	4.28873
Zr	6.40607	2.31229	6.33391
O	5.81067	1.87663	4.17562
O	6.51890	0.28055	6.56094
O	4.26216	2.17341	6.88792
Ba	0.00676	4.23279	4.11311
Zr	2.13269	6.43492	6.37560
O	1.92545	5.90747	4.30439
O	2.26287	4.33967	6.90269
O	-0.04075	6.36497	6.89285
Ba	4.30117	4.32623	4.15688

Zr	6.44508	6.20880	6.38080
O	6.60689	6.92922	4.30707
O	6.36464	4.29480	5.66367
O	4.31630	6.68101	6.23700

**Structure b**

a = 8.58 b = 8.55 c = 8.50  $\alpha = 90.00$   $\beta = 90.00$   $\gamma = 90.00$

Ba	0.05140	0.01518	0.00749
Zr	2.15252	2.10735	2.16443
O	2.27119	1.59314	0.07338
O	2.30383	-0.04514	2.80312
O	-0.01526	1.58817	2.10485
Ba	4.27438	-0.06271	-0.15520
Zr	6.49694	2.24177	2.18936
O	6.44857	2.66150	0.05103
O	5.96372	-0.09929	1.67526
O	4.32412	2.47617	2.34180
Ba	0.00429	4.29633	-0.01123
Zr	2.14982	6.42329	2.12000
O	2.22093	6.98311	-0.02410
O	1.83049	4.22925	1.74212
O	0.04437	6.62560	1.76488
Ba	4.29458	4.22705	0.10442
Y	6.45931	6.32582	2.11210
O	6.40371	5.79219	-0.09018
O	6.87882	4.24395	2.61945
O	4.25988	6.16575	1.81119
H	5.09504	8.76222	2.22036
Ba	-0.01767	0.06536	4.21193
Zr	2.13533	2.12318	6.43165
O	2.15459	2.66923	4.31677
O	1.66092	-0.03572	6.07234
O	-0.01765	2.39178	6.32968
Ba	4.29025	0.04933	4.34579
Zr	6.42595	2.12853	6.41799
O	6.47142	1.54206	4.27899
O	6.60394	-0.06690	6.99378
O	4.27092	1.64273	6.37261
Ba	0.08375	4.27808	4.35170
Zr	2.12353	6.38396	6.37773
O	2.17483	5.85270	4.22433
O	2.36103	4.25014	6.99921
O	-0.00119	5.87555	6.37038
Ba	4.21883	4.22490	4.29510
Zr	6.44036	6.37113	6.34565
O	6.66205	6.84406	4.26387

O 6.09728 4.21325 5.88175  
O 4.27310 6.74172 6.18947

### Structure c

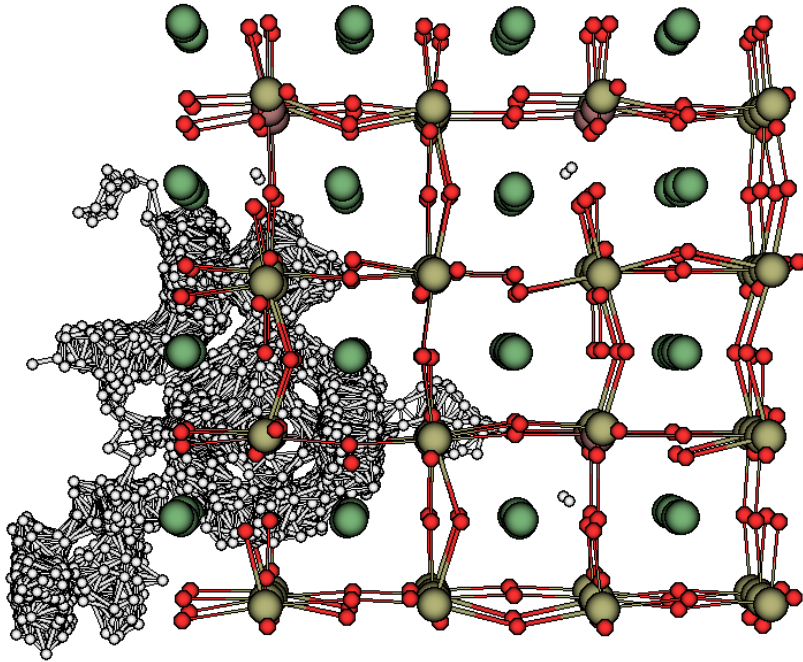
a = 8.58 b = 8.57 c = 8.51  $\alpha = 90.00$   $\beta = 90.00$   $\gamma = 90.00$

Ba -0.01901 0.02070 0.01346  
Zr 2.19692 1.96713 2.13114  
O 2.05562 1.52090 -0.05539  
O 2.37267 -0.00838 2.85579  
O 0.01425 1.58265 2.11231  
Ba 4.32896 -0.01849 -0.05504  
Zr 6.43805 2.09565 2.09101  
O 6.61504 2.71302 -0.05036  
O 6.30818 -0.06271 1.66032  
O 4.31239 2.09623 1.63822  
Ba -0.00904 4.32136 0.00107  
Zr 2.16317 6.60613 2.19580  
O 2.15519 7.00976 0.06540  
O 1.92103 3.98289 1.79427  
O 0.04859 6.28030 2.14912  
Ba 4.27608 4.29178 0.13018  
Y 6.43760 6.36164 2.17939  
O 6.34441 5.93774 -0.00192  
O 6.56801 4.16641 2.67161  
O 4.22939 6.02679 2.16566  
H 1.20154 4.70222 2.11499  
Ba -0.04685 0.09729 4.27746  
Zr 2.14004 2.15870 6.37614  
O 2.27510 2.67585 4.21419  
O 1.88921 -0.04508 5.95695  
O -0.01057 2.25242 5.95007  
Ba 4.32678 -0.02361 4.40535  
Zr 6.42272 2.18346 6.35784  
O 6.33778 1.56302 4.19459  
O 6.54586 -0.00042 6.93742  
O 4.27614 1.90010 6.21610  
Ba 0.05064 4.31203 4.30439  
Zr 2.11942 6.40834 6.43270  
O 2.10798 5.88876 4.28554  
O 2.26568 4.24642 7.06373  
O -0.01560 5.93494 6.44958  
Ba 4.21629 4.33206 4.21586  
Zr 6.44300 6.38671 6.40018  
O 6.55095 6.96927 4.31804  
O 6.17903 4.28120 5.81840  
O 4.27125 6.60396 6.25329

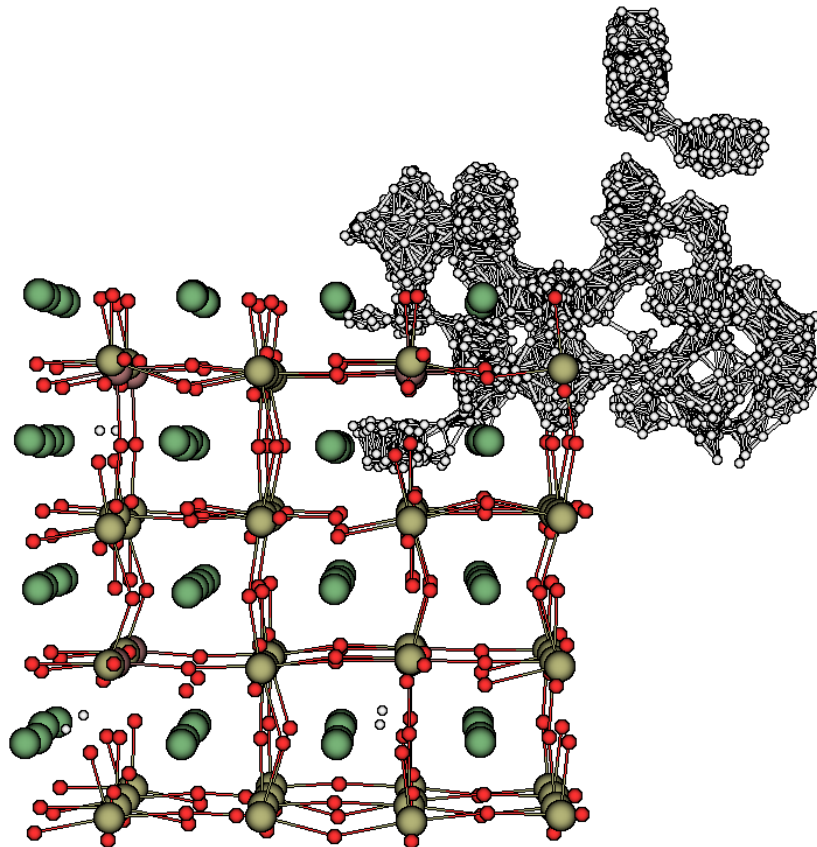


## Trajectories for the mobile hydrogen atoms

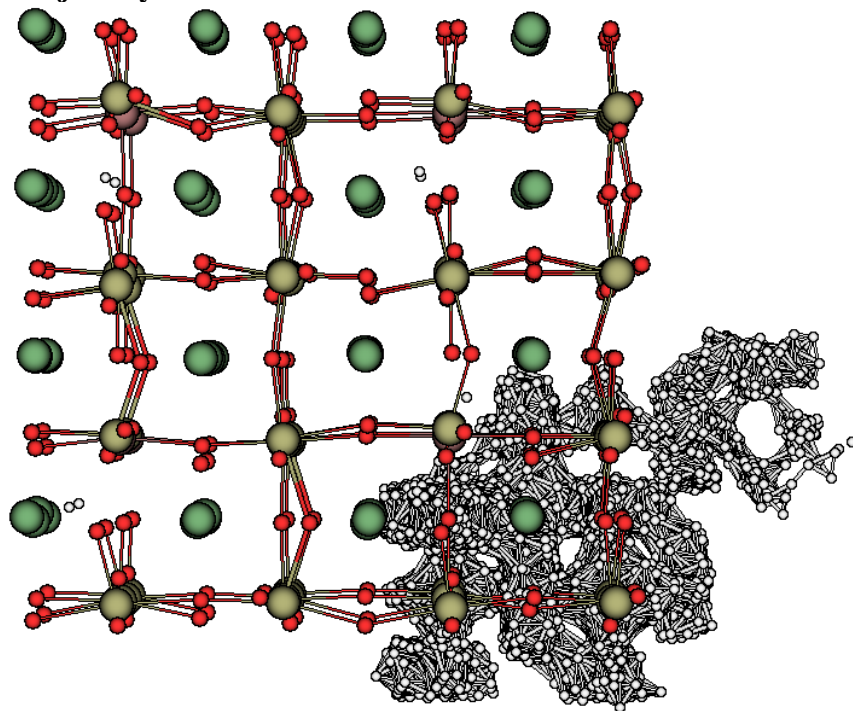
### Trajectory 2



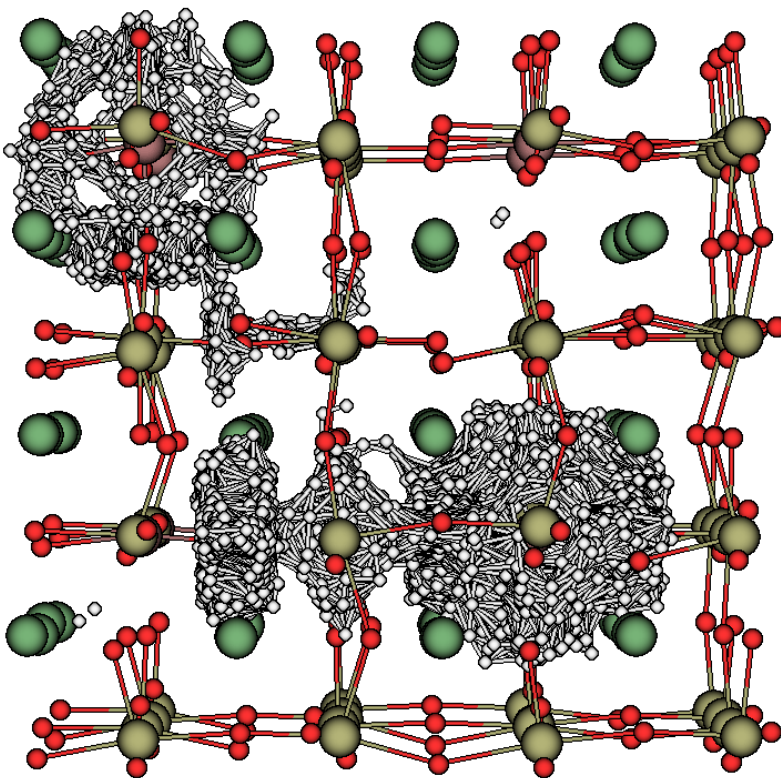
### Trajectory 3



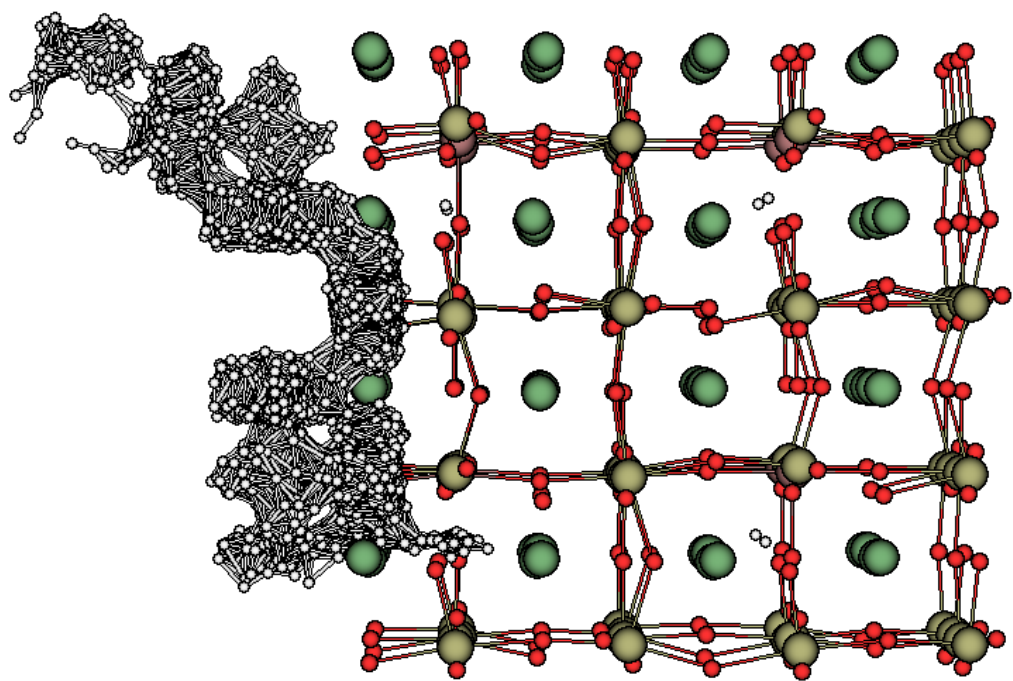
Trajectory 4



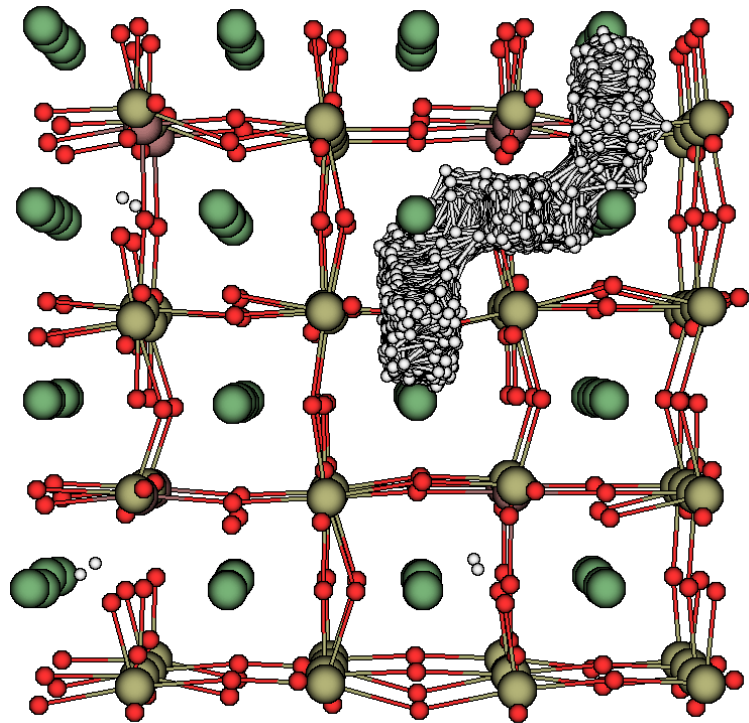
Trajectory 5



### Trajectory 6



### Trajectory 7



### Trajectory 8

