

Electronic Supplementary Information

Reactive Force Fields for Modeling Oxidative Degradation of Organic Matter in Geological Formations

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● Bond formation energies used in the new ReaxFF and DFT calculations

Bond formation energies calculated in the new ReaxFF against DFT energies for a variety of conformational structures in total 70 H/C/O/Cl components are summarized in Table S1.

Table S1. Comparison of bond formation energies of total 70 H/C/O/Cl compounds in the fitting data set and the validation data set, as calculated with the new ReaxFF, compared to DFT energies.

Species	$E_f(eV)^*$		Error (%)
	B3LYP/ 6-31G(d)	new ReaxFF	
Acetyl chloride, chloro- (C ₂ H ₂ Cl ₂ O)	-34.10	-34.87	2.3
Acetyl chloride (C ₂ H ₃ ClO)	-35.45	-35.93	1.4
Acetaldehyde, chloro- (C ₂ H ₃ ClO)	-34.72	-34.18	1.6
Methyl chloroformate (C ₂ H ₃ ClO ₂)	-42.51	-41.21	3.1
2-Chloroethanol (C ₂ H ₅ ClO)	-40.46	-41.31	2.1
Ethyl hypochlorite (C ₂ H ₅ ClO)	-38.99	-38.98	0.0
Methane, chloromethoxy- (C ₂ H ₅ ClO)	-40.43	-41.14	1.8
Acetyl chloride, dichloro- (C ₂ HCl ₃ O)	-32.61	-32.71	0.3
Chloral (C ₂ HCl ₃ O)	-31.95	-31.18	2.4
2-Chloro-2-propen-1-ol (C ₃ H ₅ ClO)	-48.80	-49.97	2.4
2-Propanone, 1-chloro- (C ₃ H ₅ ClO)	-49.70	-49.67	0.1
3-Chloro-2-propen-1-ol (C ₃ H ₅ ClO)	-48.72	-49.63	1.9
Oxirane, (chloromethyl)- (C ₃ H ₅ ClO)	-48.55	-48.42	0.3
Oxirane, (chloromethyl)-, (R)- (C ₃ H ₅ ClO)	-48.55	-48.41	0.3
Propanoyl chloride (C ₃ H ₅ ClO)	-50.15	-51.25	2.2
Furan, 3-chloro- (C ₄ H ₃ ClO)	-52.20	-52.22	0.0
Furan, 2-chloro- (C ₄ H ₃ ClO)	-52.19	-52.23	0.1
3-chlorofuran (C ₄ H ₃ ClO)	-52.20	-52.40	0.4
tert-butyl-hypochlorite (C ₄ H ₉ ClO)	-68.66	-71.38	4.0
Methyl hypochlorite (CH ₃ ClO)	-24.14	-23.14	4.2
Formyl chloride (CHOCl)	-20.35	-19.94	2.1
Chloromethyl chloroformate (C ₂ H ₂ Cl ₂ O ₂)	-41.29	-40.10	2.9
Formic acid dichloromethyl ester (C ₂ H ₂ Cl ₂ O ₂)	-41.03	-38.06	7.2
Chloro 2-chloroacetate (C ₂ H ₂ Cl ₂ O ₂)	-39.72	-38.97	1.9
2,2,2-Trichloroethanol (C ₂ H ₃ Cl ₃ O)	-37.89	-38.66	2.0
1,2,2-Trichloroethanol (C ₂ H ₃ Cl ₃ O)	-38.17	-38.82	1.7
Ether chloromethyl dichloromethyl (C ₂ H ₃ Cl ₃ O)	-38.12	-38.25	0.3
Methyltrichloromethyl ether (C ₂ H ₃ Cl ₃ O)	-37.79	-39.47	4.4
1,1,2-Trichloroethanol (C ₂ H ₃ Cl ₃ O)	-38.37	-39.40	2.7
Acetoxyacetyl chloride (C ₄ H ₅ ClO ₃)	-73.71	-70.47	4.4
Epichlorohydrin carbonate (C ₄ H ₅ ClO ₃)	-73.45	-67.86	7.6
Ethyl chloroglyoxylate (C ₄ H ₅ ClO ₃)	-73.38	-69.56	5.2
Butyl chloroformate (C ₅ H ₉ ClO ₂)	-86.78	-88.13	1.5
Ethyl 2-chloropropionate (C ₅ H ₉ ClO ₂)	-86.87	-86.52	0.4
Ethyl 3-chloropropionate (C ₅ H ₉ ClO ₂)	-86.95	-86.74	0.2
Isopropyl chloroacetate (C ₅ H ₉ ClO ₂)	-86.86	-85.50	1.6
2-Chlorophenol (C ₆ H ₅ ClO)	-76.74	-77.50	1.0
3-Chlorophenol (C ₆ H ₅ ClO)	-76.69	-78.24	2.0
4-Chlorophenol (C ₆ H ₅ ClO)	-76.68	-78.42	2.3
2-Chloromethyl-5-methoxy-4H-pyran-4-one (C ₇ H ₇ ClO ₃)	-104.85	-102.48	2.3
3-Chloro-5-hydroxymethyl benzene-1,2-diol (C ₇ H ₇ ClO ₃)	-105.42	-104.11	1.2
Benzyl alcohol 3-chloro-2,5-dihydroxy (C ₇ H ₇ ClO ₃)	-105.03	-103.95	1.0
Methyl 5-chloromethyl-2-furoate (C ₇ H ₇ ClO ₃)	-105.72	-103.00	2.6
2-Chloro-4-methoxybenzene-1,3-diol (C ₇ H ₇ ClO ₃)	-105.09	-103.58	1.4
3-Chlorophenylacetic acid (C ₈ H ₇ ClO ₂)	-108.30	-107.47	0.8
4-Chlorophenylacetic acid (C ₈ H ₇ ClO ₂)	-108.30	-107.58	0.7
4-Methoxybenzoyl chloride (C ₈ H ₇ ClO ₂)	-107.88	-109.55	1.5
Benzyl chloroformate (C ₈ H ₇ ClO ₂)	-107.99	-110.14	2.0
3-Chloro-4-hydroxy-8-oxabicyclo (C ₇ H ₇ ClO ₃)	-103.90	-101.58	2.2
5-Chloro-2,2-hydroxyethyl furan-3-carbaldehyde (C ₇ H ₇ ClO ₃)	-104.29	-101.57	2.6
4-Chloro-2-hydroxyphenyl methanediol (C ₇ H ₇ ClO ₃)	-104.74	-101.74	2.9
4-Chloro-3-hydroxymethyl benzene-1,2-diol (C ₇ H ₇ ClO ₃)	-104.77	-103.82	0.9

3-Chloro-2-hydroxy-2,3,3a,6a-tetrahydrocyclopenta[b]turan-4-one (C ₇ H ₇ ClO ₃)	-104.71	-101.94	2.6
Methyl 2-chlorobenzoate (C ₈ H ₇ ClO ₂)	-107.57	-107.85	0.3
Phenoxyacetyl chloride (C ₈ H ₇ ClO ₂)	-107.09	-109.14	1.9
3-chloro-4,1-methyl-2-propenyl 3-cyclobutene-1,2-dione (C ₈ H ₇ ClO ₂)	-105.25	-104.81	0.4
5-chloromethyl-2-hydroxycyclohepta 2,4,6-trien-1-one (C ₈ H ₇ ClO ₂)	-106.78	-107.85	1.0
E-3-chloro-1-2-methylfuran-3-yl, prop-2-en-1-one (C ₈ H ₇ ClO ₂)	-106.39	-105.94	0.4
5-1-chlorovinyl 1,3-benzodioxole (C ₉ H ₇ ClO ₂)	-115.22	-115.92	0.6
4-2-chlorophenyl oxetane-2-one (C ₉ H ₇ ClO ₂)	-116.13	-115.97	0.1
1-(5-chlorofuran-2-yl) pent-4-yn-1-one (C ₉ H ₇ ClO ₂)	-113.70	-114.45	0.7
2-chloro-3-hydroxy-2,3-dihydroinden-1-one (C ₉ H ₇ ClO ₂)	-116.23	-117.02	0.7
2-2-furanyl-3-chloro-4-methylfuran (C ₉ H ₇ ClO ₂)	-115.18	-116.06	0.8
(4S)-4-[(1E)-4,4-dichlorobuta-1,3-dienyl]-2,2-dimethyl-1,3-dioxolane (C ₉ H ₁₂ Cl ₂ O ₂)	-130.63	-132.52	1.4
2-(4-Dichlorophenoxy) propan-1-ol (C ₉ H ₁₀ Cl ₂ O ₂)	-125.80	-127.56	1.4
2-hydroxypentanoyl chloride (C ₅ H ₉ ClO ₂)	-86.03	-87.54	1.7
5-chloropentanoic acid (C ₅ H ₉ ClO ₂)	-86.69	-87.13	0.5
2-chloropentanoic acid (C ₅ H ₉ ClO ₂)	-86.48	-86.51	0.0
R-3-Methoxybutanoic acid chloride (C ₅ H ₉ ClO ₂)	-85.91	-85.94	0.0
2S-2-Chloro-2-methylbutanoic acid (C ₅ H ₉ ClO ₂)	-86.53	-86.68	0.2
	RMS error (eV)	1.57	avgError %
			1.7

* $E_f = E_{complex} - n_C E_C - n_H E_H - n_O E_O - n_{Cl} E_{Cl}$, where n is the number of atoms for each element composed of all the 70 molecules.

● PES using the new ReaxFF for reactive bonding interactions

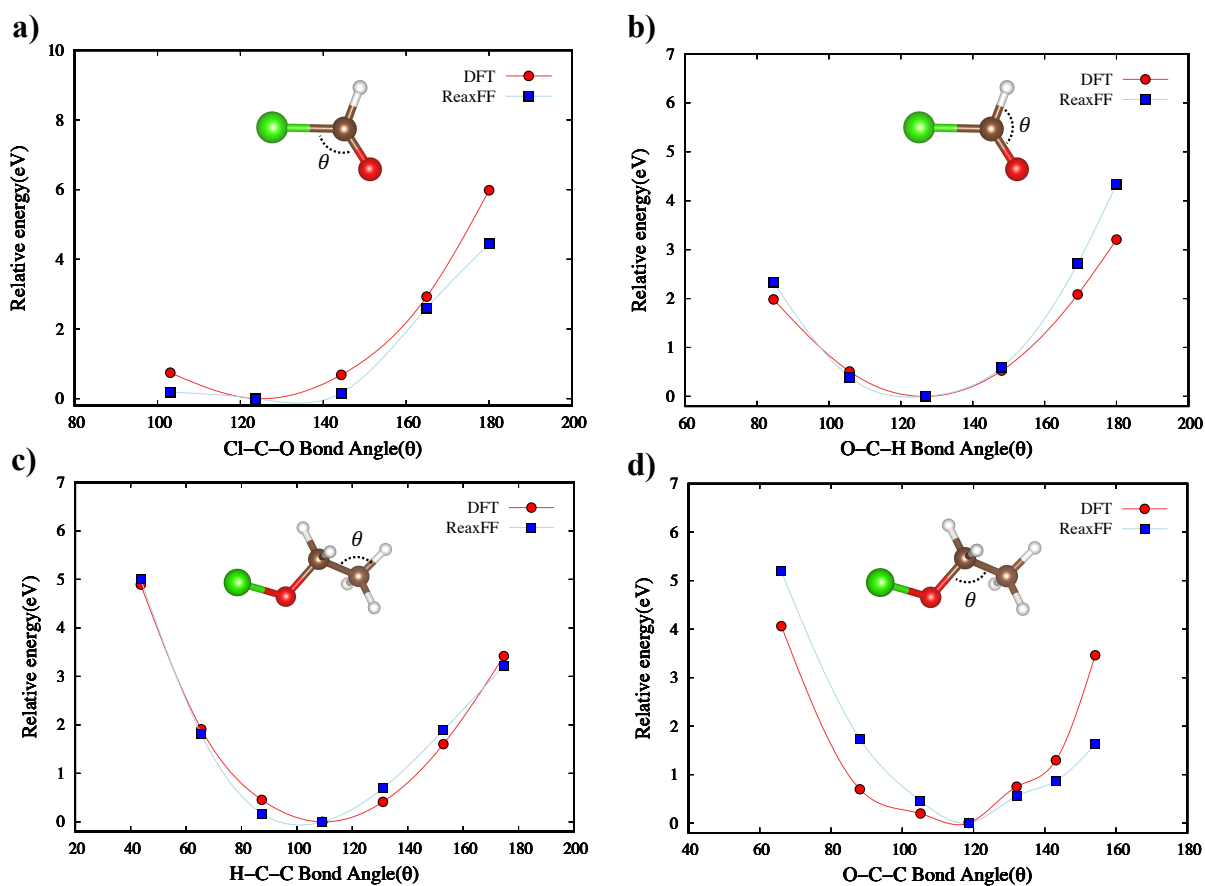


Fig. S1 Relative energies comparison of DFT and the new ReaxFF calculations for a) Cl-C-O and b) O-C-H bond angles in CHClO as well as for c) H-C-C and O-C-C bond angles in C₂H₅ClO.

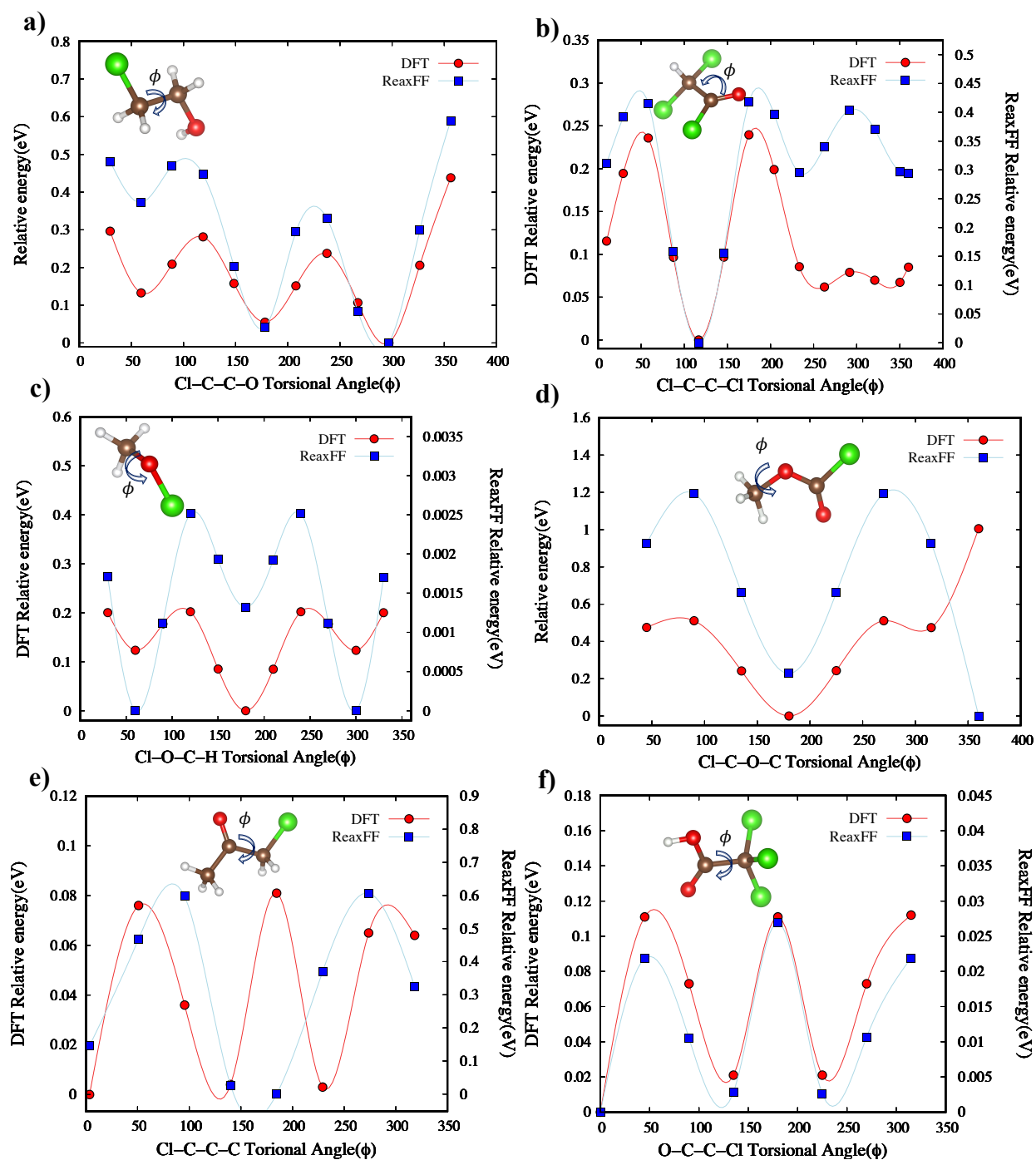


Fig. S2 Relative energies comparison of DFT and the new ReaxFF calculations for a) Cl-C-C-O, b) Cl-C-C-Cl, c) Cl-O-C-H, and d) Cl-C-O-C, e) Cl-C-C-C, and f) O-C-C-Cl torsional angles in $C_2H_3Cl_3$, C_2HCl_3O , CH_3ClO , $C_2H_3ClO_2$, C_3H_5ClO , and $C_2HCl_3O_2$, respectively. These different conformational structures show $sp-sp^2$, and $sp-sp^3$, sp^2-sp^3 , and sp^3-sp^3 hybridized configurations.

● PES using the new ReaxFF for non-reactive bonding interactions

- Charge distributions

In the cases of c) formic acid, dichloromethyl ester ($C_2H_2Cl_2O_2$) and h) methyltrichloromethyl ether ($C_2H_3Cl_3O$), the charges of the chlorine atom and its immediate carbon atom calculated in the new ReaxFF differ from those of the DFT (B3LYP/6-31G**) method. This discrepancy can be justified on the basis of electronegativity, $\chi_O = 3.44 > \chi_{Cl} = 3.16 > \chi_C = 2.55 > \chi_H = 2.20$, meaning that because chlorine has a stronger electronegativity than that of carbon, it should be more negatively charged compared to its immediate carbon atom, which is in good agreement with the new ReaxFF predictions whose values are well consistent with the pattern of Bader atomic charge¹ values calculated by Bader analysis with PBE functional².

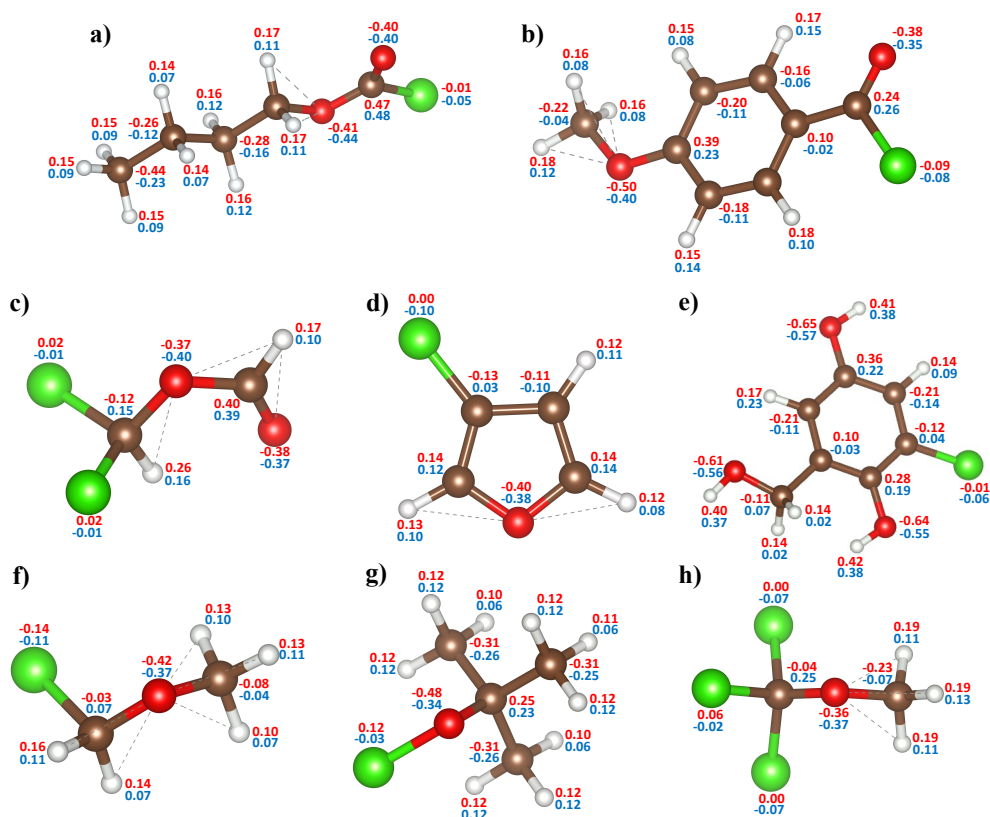


Fig. S3 Charge distributions comparison of DFT and the new ReaxFF calculations in a) $C_3H_9ClO_2$, b) $C_8H_7ClO_2$, c) $C_2H_2Cl_2O_2$, d) C_4H_3ClO , e) $C_7H_7ClO_3$ f) C_2H_5ClO , g) C_4H_9ClO , and h) $C_2H_3Cl_3O$ molecules, respectively.

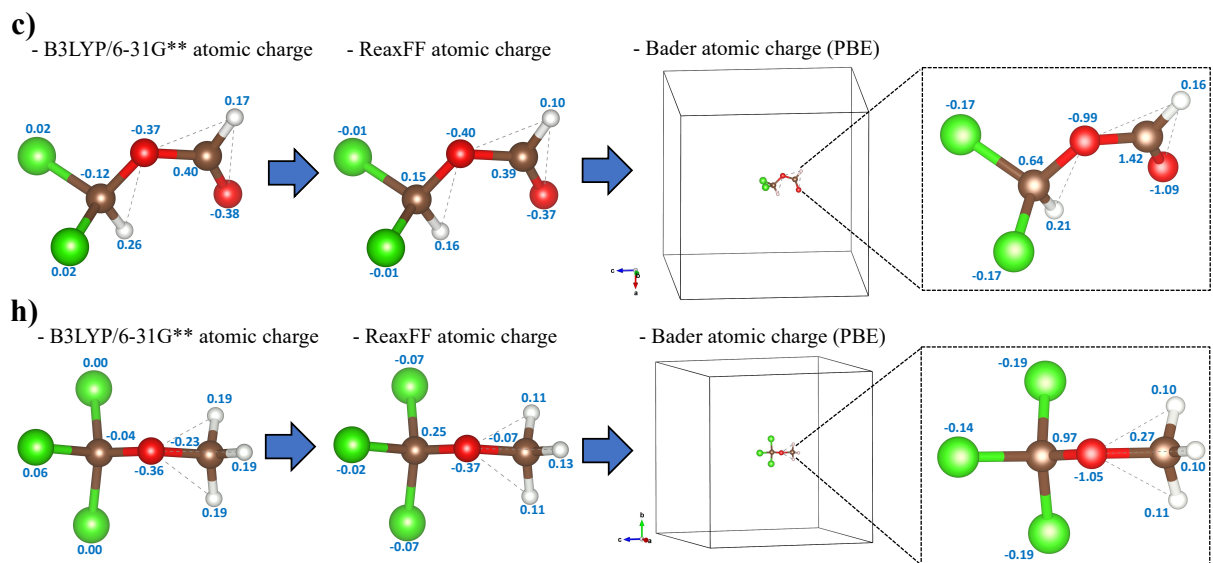


Fig. S4 Bader charge analysis of the atomic charge interpretations, shown Fig. S3, whose patterns are well consistent with the new ReaxFF atomic charges, whereas there is the discrepancy in atomic charges between B3LYP and the new ReaxFF.

- Non-bonding dispersions

To show the quality of our parametrization for dispersion interactions, we compare the non-bonded energies between a water molecule and hydrogen-terminated ClO_n^- oxidizers in DFT and ReaxFF calculations, displayed in Fig. S5. In general, DFT calculations show no cohesive attraction between $HClO_n$ ($n:1 \sim 4$) and water, except for a slight attraction of 0.1 eV in the case of $HClO_4$, shown in Fig. S5 (a) This can be rationalized in terms of charge electrostatic potential multipole expansion in terms of charge-dipole, dipole-dipole, and dipole-quadrupole interactions. H-terminated ClO_n^- oxidizers are charge-neutral. Since their dipoles are smaller than that of water, the cohesive energies are not present. We confirm this by calculating non-bonded energies between a water molecule and ClO_n^- oxidizers, inset of Fig. S5 (a), which is roughly 0.2 eV due to arising from charge-dipole interactions. Our ReaxFF parametrization, however, shows an attractive potential between a water molecule and H-terminated ClO_n^- oxidizers. The depth of the non-bonded attractive energy well is roughly 0.7 eV, Fig. S5 (b). We believe that the majority of this attractive potential is arising from coulombic interactions, as shown in the inset of Fig. S5 (b). Such discrepancy is, in parts, due to the previous C/H/O parameterization dataset by van Duin and Goddard³ that we based our C/H/O/Cl parameter set on.

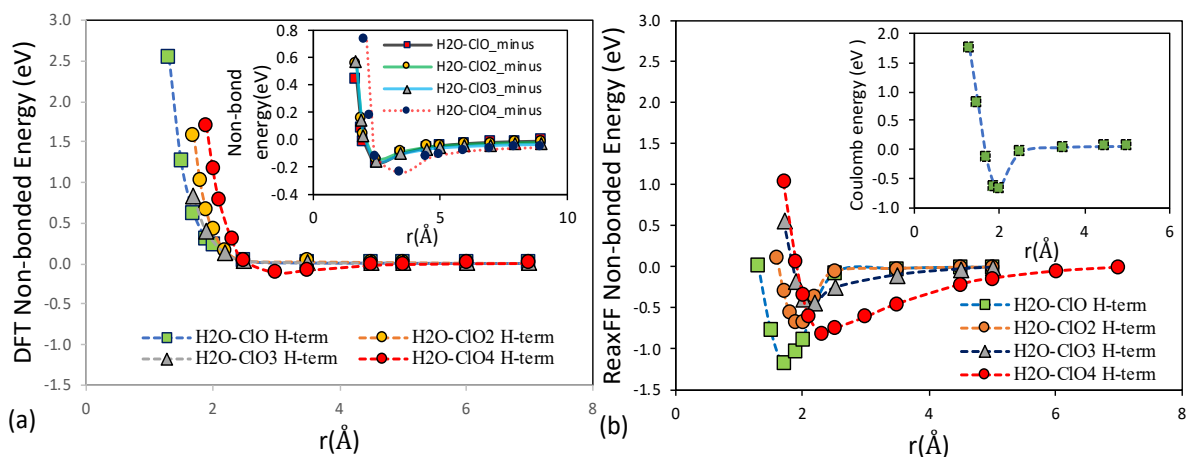
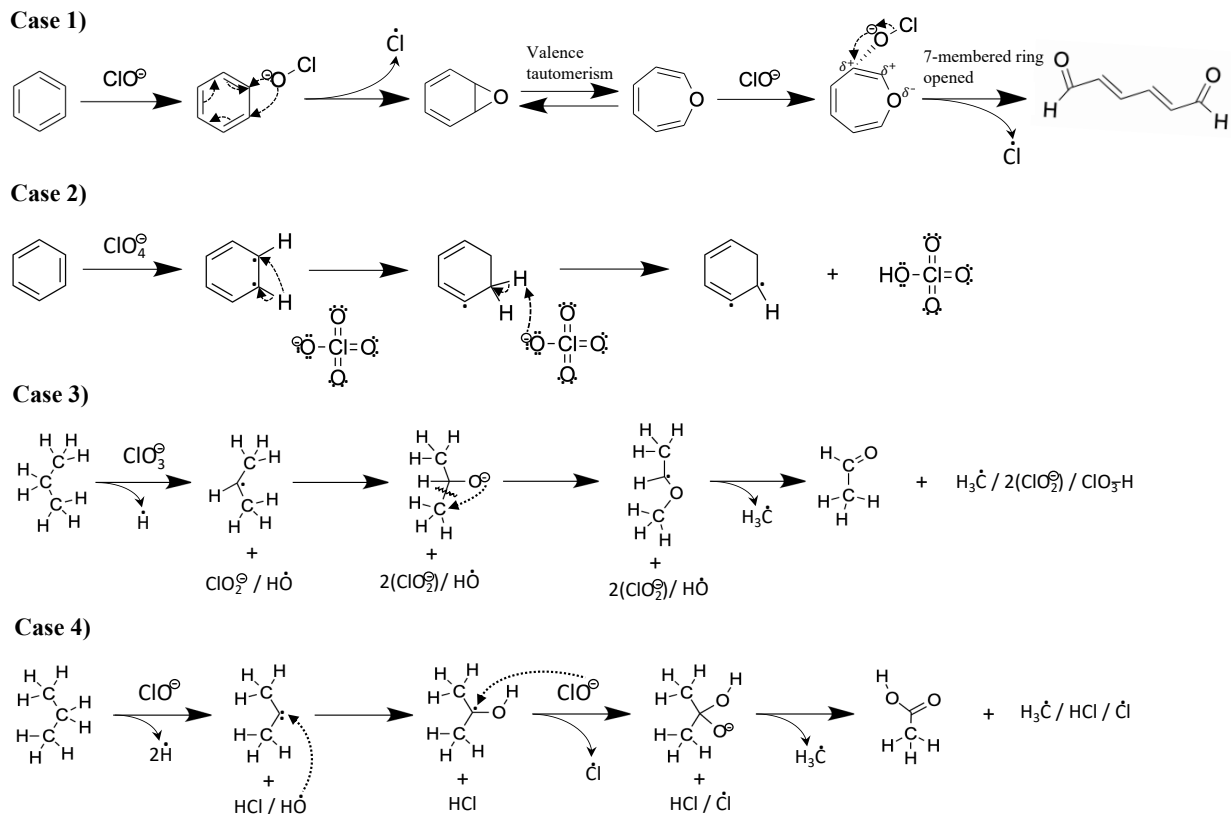


Fig. S5 The comparison between a) DFT and b) ReaxFF non-bonded energies for water and hydrogen-terminated ClO_n^- oxidizers. The inset in graph a) shows the non-bonded energy between water and ClO_n^- oxidizers at the DFT (B3LYP/6-31++G**(D3)). The inset in part b) shows the coulombic contributions to non-bonded interactions in ClO_n^- oxidizer.

● Transition state (TS) simulations of hydrocarbon oxidation

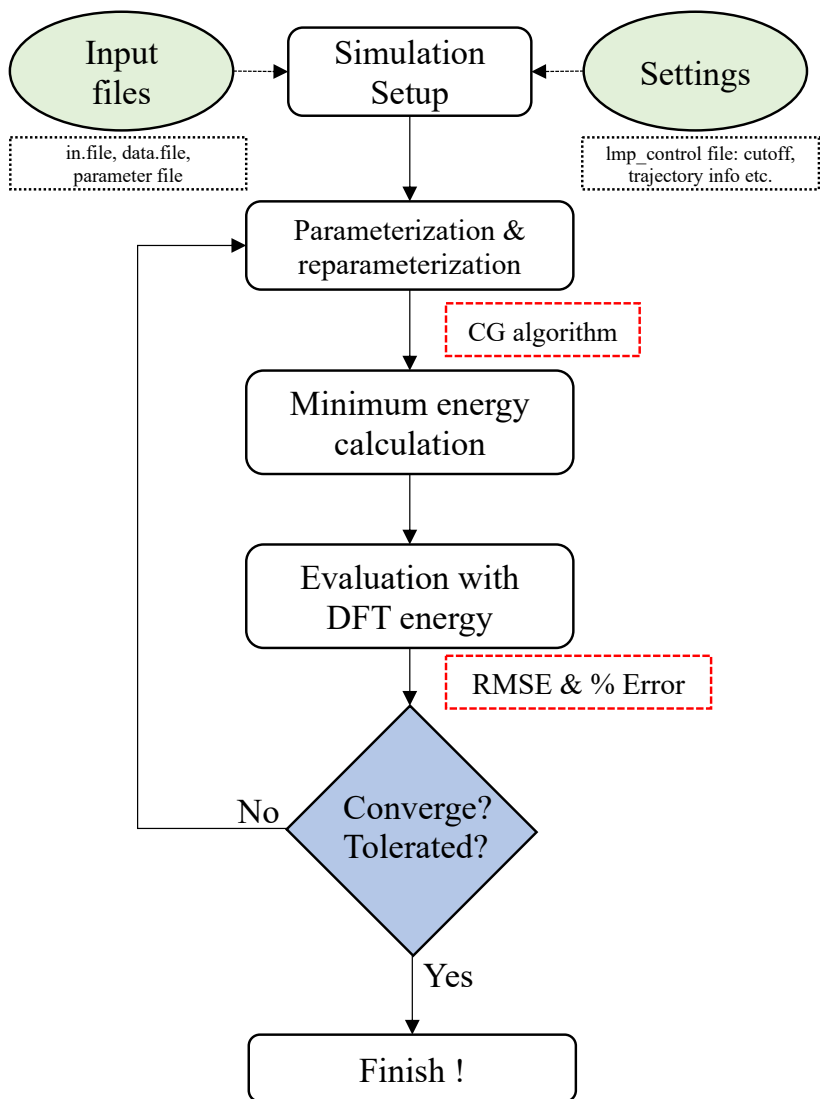
The reasonable reaction paths defined by *ab-initio* MD simulations for an oxidation of a small hydrocarbon using chlorate oxidizers (ClO_n^- ; $1 \leq n \leq 4$) were proposed and validated for the new ReaxFF force field. In Case 1) reaction path, benzene oxygenation begins with causing epoxidation on the C-C bridge, and thus the benzene becomes a linear-like hydrocarbon with CHO hydrophilic ends. Case 2) mainly shows proton transfers within the benzene structure itself and then, its transfer to the oxygen of ClO_4^- . In Case 3), proton transfer from propane by the presence of ClO_3^- oxidizer, C-O bond formation on carbon radical of isopropyl backbone, and the generation of an acetaldehyde containing a CHO hydrophilic polar end are observed. Case 4) shows radical-radical combination of $\cdot\text{H}$ and $\cdot\text{Cl}$ to make HCl, and also acetic acid as the final product is produced in the reaction profile.



Scheme 1. Four reasonable oxidative reaction pathways of small aromatic and aliphatic hydrocarbons, determined by *ab-initio* MD simulations with NVT ensemble, and used for the new ReaxFF force field validations based on the *ab-initio* MD trajectories.

- **Flow chart of the new ReaxFF parameterization**

To ensure proper parametrization, the new ReaxFF parametrization scheme follows a relaxed optimization. This means that we optimize each molecule with the current ReaxFF parameters during each optimization cycle before comparing its corresponding energy with DFT results. The relaxed optimization process will ensure that not only the formation energy but also the equilibrium shape and connectivity of molecules remains the same in the parametrized ReaxFF potential.



Scheme 2. Optimization flowchart for calibration of the C/H/O/Cl ReaxFF parameter.

● The new ReaxFF parameters

39 ! Number of general parameters
50.0000 !Overcoordination parameter
9.5469 !Overcoordination parameter
26.5405 !Valency angle conjugation parameter
1.5105 !Triple bond stabilisation parameter
6.6630 !Triple bond stabilisation parameter
70.0000 !C2-correction
1.0588 !Undercoordination parameter
4.6000 !Triple bond stabilisation parameter
12.1176 !Undercoordination parameter
13.3056 !Undercoordination parameter
-70.1292 !Triple bond stabilization energy
0.0000 !Lower Taper-radius
10.0000 !Upper Taper-radius
0.0000 !Not used
33.8667 !Valency undercoordination
6.0891 !Valency angle/lone pair parameter
1.0563 !Valency angle
2.0384 !Valency angle parameter
6.1431 !Not used
6.9290 !Double bond/angle parameter
0.3989 !Double bond/angle parameter: overcoord
3.9954 !Double bond/angle parameter: overcoord
0.0000 !Not used
5.7796 !Torsion/BO parameter
10.0000 !Torsion overcoordination
1.9487 !Torsion overcoordination
0.0000 !Conjugation 0 (not used)
0.8645 !Conjugation
1.5591 !vdWaals shielding
0.1000 !Cutoff for bond order (*100)
0.0045 !Valency angle conjugation parameter
0.6991 !Overcoordination parameter
50.0000 !Overcoordination parameter
1.8512 !Valency/lone pair parameter
0.0000 !Not used
0.0000 !Not used
0.0000 !Molecular energy (not used)
0.0000 !Molecular energy (not used)
2.6962 !Valency angle conjugation parameter
5 ! Nr of atoms; atomID;ro(sigma); Val;atom 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 1.3817 4.0000 12.0000 1.9333 0.1838 0.9000 1.1341 4.0000
9.7602 1.3346 4.0000 34.9350 79.5548 5.9966 7.2000 0.0000
1.2114 0.0000 202.5551 8.9539 34.9289 13.5366 0.8563 0.0000
-2.8983 2.5000 1.0564 4.0000 2.9663 0.0000 0.0000 0.0000
H 0.7853 1.0000 1.0080 1.5904 0.0419 1.0206 -0.1000 1.0000
9.3557 5.0518 1.0000 0.0000 121.1250 5.1900 7.8366 1.0000
-0.1000 0.0000 62.4879 1.9771 3.3517 0.7571 1.0698 0.0000
-15.7683 2.1488 1.0338 1.0000 2.8793 0.0000 0.0000 0.0000
O 1.2477 2.0000 15.9990 2.3890 0.1000 1.0898 1.0548 6.0000
9.7300 3.7719 4.0000 37.5000 116.0768 9.6000 8.9922 2.0000
0.9049 0.4056 59.0626 3.5027 0.7640 0.0021 0.9745 0.0000
-3.5500 2.9000 1.0493 4.0000 2.9225 0.0000 0.0000 0.0000
Cl 1.7140 1.0000 35.4500 1.8139 0.1000 0.3500 -1.0000 7.0000
9.5345 10.2330 1.0000 0.0000 0.0000 6.7204 6.1703 0.0000
-1.0000 1.2769 143.1770 6.2293 5.2294 5.1542 0.8563 0.0000
-3.4980 2.9867 1.0338 6.2998 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 127.6226 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

10 ! Nr of bonds; at1;at2;De(sigma);De(pi);De(pipi);p(be1);p(bo5);13corr;n.u.;p(bo6),p(ovun1)
p(be2);p(bo3);p(bo4);n.u.;p(bo1);p(bo2)

1 1 156.5953 101.0397 80.0000 -0.8157 -0.4591 1.0000 37.7369 0.4235
0.4527 -0.1000 9.2605 1.0000 -0.0750 6.8316 1.0000 0.0000

1 2 170.2316 0.0000 0.0000 -0.5931 0.0000 1.0000 6.0000 0.7340
4.2267 1.0000 0.0000 1.0000 -0.0500 6.8315 0.0000 0.0000

2 2 156.0973 0.0000 0.0000 -0.1377 0.0000 1.0000 6.0000 0.8240
2.9907 1.0000 0.0000 1.0000 -0.0593 4.8358 0.0000 0.0000

1 3 160.4802 105.1693 23.3059 -0.3873 -0.1613 1.0000 10.8851 1.0000
0.5341 -0.3174 7.0303 1.0000 -0.1463 5.2913 0.0000 0.0000

3 3 53.1463 178.6202 51.1430 -0.2902 -0.1244 1.0000 29.6439 0.9114
0.2441 -0.1239 7.6487 1.0000 -0.1302 6.2919 1.0000 0.0000

2 3 180.4373 0.0000 0.0000 -0.8074 0.0000 1.0000 6.0000 0.5514
1.2490 1.0000 0.0000 1.0000 -0.0657 5.0451 0.0000 0.0000

1 4 100.2833 0.0000 0.0000 -0.1200 -0.1100 0.0000 16.0000 0.4950
1.3214 -0.1000 15.0000 1.0000 -0.1121 5.5000 0.0000 0.0000

2 4 103.2500 0.0000 0.0000 0.3457 -0.2000 0.0000 16.0000 1.2500
2.5963 -0.2000 15.0000 1.0000 -0.1251 5.2687 0.0000 0.0000

3 4 58.0784 0.0000 0.0000 0.5000 -0.2000 0.0000 16.0000 0.5000
1.0001 -0.2000 15.0000 1.0000 -0.1000 10.0000 0.0000 0.0000

4 4 57.3614 0.0000 0.0000 -0.0803 -0.2000 0.0000 16.0000 1.2356
1.0338 -0.2000 15.0000 1.0000 -0.1188 5.6715 0.0000 0.0000

7 ! Nr of off-diagonal terms. at1;at2;Dij;RvdW;alfa;ro(sigma);ro(pi);ro(pipi)

1 2 0.1219 1.4000 9.8442 1.1203 -1.0000 -1.0000

2 3 0.0344 1.6800 10.3247 0.9013 -1.0000 -1.0000

1 3 0.1031 1.8523 9.8442 1.2775 1.1342 1.0621

1 4 0.0051 1.9015 10.7291 1.8029 -1.0000 -1.0000

2 4 0.0068 1.8740 10.6297 1.2200 -1.0000 -1.0000

3 4 0.0227 1.8551 9.2308 1.3000 -1.0000 -1.0000

4 4 0.1145 1.9102 10.9874 1.7095 -1.0000 -1.0000

26 ! Nr of angles. at1;at2;at3;Theta,o;p(val1);p(val2);p(coa1);p(val7);p(pen1);p(val4)

1 1 1 67.2326 22.0695 1.6286 0.0000 1.7959 15.4141 1.8089

1 1 2 65.2527 14.3185 6.2977 0.0000 0.5645 0.0000 1.1530

2 1 2 70.0840 25.3540 3.4508 0.0000 0.0050 0.0000 3.0000

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 49.5561 7.3771 4.9568 0.0000 0.7533 15.9906 1.0010

3 1 3 70.1171 39.8746 2.5403 -24.3902 1.7740 -42.9758 2.1240

2 1 3 65.0000 14.2057 4.8649 0.0000 0.3504 0.0000 1.7185

1 3 1 74.3994 44.7500 0.7982 0.0000 3.0000 0.0000 1.0528

1 3 3 80.9854 36.6201 2.0201 0.0000 0.7434 67.0264 3.0000

3 3 3 80.7324 30.4554 0.9953 0.0000 1.6310 50.0000 1.0783

1 3 2 71.5018 21.7062 0.4735 0.0000 0.5186 0.0000 1.1793

2 3 3 84.9468 23.3540 1.5057 0.0000 2.6374 0.0000 1.3023

2 3 2 77.0645 10.4737 1.2895 0.0000 0.9924 0.0000 1.1043

1 2 3 0.0000 25.0000 3.0000 0.0000 1.0000 0.0000 1.0400

3 2 3 0.0000 0.0148 6.0000 0.0000 0.0000 0.0000 1.0400

2 2 3 0.0000 9.7025 6.0000 0.0000 0.0000 0.0000 1.0400

4 1 1 10.0000 0.5000 1.4000 0.0000 0.9000 0.0000 0.5201

4 1 2 15.0000 15.0000 0.1000 0.0000 0.0010 0.0000 0.1100

4 1 4 10.0000 1.1000 1.0000 0.0000 1.0000 0.0000 1.0000

2 1 4 63.9629 41.6246 1.4921 0.0000 0.2000 0.0000 2.8070

1 1 4 55.8437 45.0000 1.2491 0.0000 1.1825 0.0000 3.0000

3 1 4 10.0000 0.0015 1.0000 -41.0000 1.0000 0.0000 1.0000

1 3 4 75.5983 53.0000 1.6248 0.0000 0.4000 0.0000 0.4286

4 1 3 8.1000 10.0000 1.0000 0.0000 0.0000 0.0000 1.0500

39 ! Nr of torsions. at1;at2;at3;at4;;V1;V2;V3;p(tor1);p(cot1);n.u.;n.u.

1 1 1 1 -0.2500 11.5822 0.1879 -4.7057 -2.2047 0.0000 0.0000

1 1 1 2 -0.2500 31.2596 0.1709 -4.6391 -1.9002 0.0000 0.0000

2 1 1 2 -0.1770 30.0252 0.4340 -5.0019 -2.0697 0.0000 0.0000

1 1 1 3 -0.7098 22.2951 0.0060 -2.5000 -2.1688 0.0000 0.0000

2 1 1 3 -0.3568 22.6472 0.6045 -4.0088 -1.0000 0.0000 0.0000

3 1 1 3 -0.0528 6.8150 0.7498 -5.0913 -1.0000 0.0000 0.0000

1 1 3 1 2.0007 25.5641 -0.0608 -2.6456 -1.1766 0.0000 0.0000

1 1 3 2 -1.1953 42.1545 -1.0000 -8.0821 -1.0000 0.0000 0.0000

2 1 3 1 -0.9284 34.3952 0.7285 -2.5440 -2.4641 0.0000 0.0000

2	1	3	2	-2.5000	79.6980	1.0000	-3.5697	-2.7501	0.0000	0.0000
1	1	3	3	-0.0179	5.0603	-0.1894	-2.5000	-2.0399	0.0000	0.0000
2	1	3	3	-0.5583	80.0000	1.0000	-4.4000	-3.0000	0.0000	0.0000
3	1	3	1	-2.5000	76.0427	-0.0141	-3.7586	-2.9000	0.0000	0.0000
3	1	3	2	0.0345	78.9586	-0.6810	-4.1777	-3.0000	0.0000	0.0000
3	1	3	3	-2.5000	66.3525	0.3986	-3.0293	-3.0000	0.0000	0.0000
1	3	3	1	2.5000	-0.5332	1.0000	-3.5096	-2.9000	0.0000	0.0000
1	3	3	2	-2.5000	3.3219	0.7180	-5.2021	-2.9330	0.0000	0.0000
2	3	3	2	2.2500	-6.2288	1.0000	-2.6189	-1.0000	0.0000	0.0000
1	3	3	3	0.0531	-17.3983	1.0000	-2.5000	-2.1584	0.0000	0.0000
2	3	3	3	0.4723	-12.4144	-1.0000	-2.5000	-1.0000	0.0000	0.0000
3	3	3	3	-2.5000	-25.0000	1.0000	-2.5000	-1.0000	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	2	3	0	0.0000	0.1000	0.0200	-2.5415	0.0000	0.0000	0.0000
0	1	1	0	0.0000	50.0000	0.3000	-4.0000	-2.0000	0.0000	0.0000
0	3	3	0	0.5511	25.4150	1.1330	-5.1903	-1.0000	0.0000	0.0000
1	1	3	3	-2.0000	73.0530	1.5000	-9.0000	-2.0000	0.0000	0.0000
1	3	3	1	0.0002	80.0000	-1.5000	-2.5000	-2.0000	0.0000	0.0000
3	1	3	3	-1.8835	20.0000	1.5000	-9.0000	-2.0000	0.0000	0.0000
2	3	4	3	1.6439	21.4220	-0.6344	-1.1422	0.0000	0.0000	0.0000
1	3	4	3	-0.7000	26.4579	-1.0000	-8.1063	0.0000	0.0000	0.0000
1	1	3	4	-0.2000	5.9300	-1.0000	-4.1028	0.0000	0.0000	0.0000
2	1	3	4	1.5000	13.6826	0.1478	-1.9478	0.0000	0.0000	0.0000
4	3	3	4	-0.0641	59.7588	-1.0000	-0.5975	0.0000	0.0000	0.0000
3	3	4	3	1.5000	50.0000	0.3000	-5.5000	0.0000	0.0000	0.0000
3	1	1	4	1.0000	25.3373	1.0000	-4.1453	-0.9511	0.0000	0.0000
4	1	1	4	-0.9000	20.8427	1.0000	-4.0186	-1.7241	0.0000	0.0000
2	1	1	4	-3.5000	-35.8297	0.6745	-1.9954	-3.9000	0.0000	0.0000
1	1	1	4	1.0000	20.0000	-1.0000	-4.5000	-1.0000	0.0000	0.0000
3	! Nr of hydrogen bonds. at1;at2;at3;r(hb);p(hb1);p(hb2);p(hb3)									
3	2	3	1.9682	-4.4628	1.7976	3.0000				
3	2	5	1.8833	-3.6250	1.4500	19.5000				
5	2	3	1.8487	-0.0100	1.4500	19.5000				

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