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 seventy H/C/O/Cl components are summarized in Table S1.

Table S1. Comparison of bond formation energies of total seventy 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- ($C_2H_2Cl_2O$)	-34.10	-34.87	2.3
Acetyl chloride (C_2H_3ClO)	-35.45	-35.93	1.4
Acetaldehyde, chloro- (C_2H_3ClO)	-34.72	-34.18	1.6
Methyl chloroformate ($C_2H_3ClO_2$)	-42.51	-41.21	3.1
2-Chloroethanol (C_2H_5ClO)	-40.46	-41.31	2.1
Ethyl hypochlorite (C_2H_5ClO)	-38.99	-38.98	0.0
Methane, chloromethoxy- (C_2H_5ClO)	-40.43	-41.14	1.8
Acetyl chloride, dichloro- (C_2HCl_3O)	-32.61	-32.71	0.3
Chloral (C_2HCl_3O)	-31.95	-31.18	2.4
2-Chloro-2-propen-1-ol (C_3H_5ClO)	-48.80	-49.97	2.4
2-Propanone, 1-chloro- (C_3H_5ClO)	-49.70	-49.67	0.1
3-Chloro-2-propen-1-ol (C_3H_5ClO)	-48.72	-49.63	1.9
Oxirane, (chloromethyl)- (C_3H_5ClO)	-48.55	-48.42	0.3
Oxirane, (chloromethyl)-, (R)- (C_3H_5ClO)	-48.55	-48.41	0.3
Propanoyl chloride (C_3H_5ClO)	-50.15	-51.25	2.2
Furan, 3-chloro- (C_4H_3ClO)	-52.20	-52.22	0.0
Furan, 2-chloro- (C_4H_3ClO)	-52.19	-52.23	0.1
3-chlorofuran (C_4H_3ClO)	-52.20	-52.40	0.4
tert-butyl-hypochlorite (C_4H_9ClO)	-68.66	-71.38	4.0
Methyl hypochlorite (CH_3ClO)	-24.14	-23.14	4.2
Formyl chloride (CHOCl)	-20.35	-19.94	2.1
Chloromethyl chloroformate ($C_2H_2Cl_2O_2$)	-41.29	-40.10	2.9
Formic acid dichloromethyl ester ($C_2H_2Cl_2O_2$)	-41.03	-38.06	7.2
Chloro 2-chloroacetate ($C_2H_2Cl_2O_2$)	-39.72	-38.97	1.9
2,2,2-Trichloroethanol ($C_2H_3Cl_3O$)	-37.89	-38.66	2.0
1,2,2-Trichloroethanol ($C_2H_3Cl_3O$)	-38.17	-38.82	1.7
Ether chloromethyl dichloromethyl ($C_2H_3Cl_3O$)	-38.12	-38.25	0.3
Methyltrichloromethyl ether ($C_2H_3Cl_3O$)	-37.79	-39.47	4.4
1,1,2-Trichloroethanol ($C_2H_3Cl_3O$)	-38.37	-39.40	2.7
Acetoxyacetyl chloride ($C_4H_5ClO_3$)	-73.71	-70.47	4.4
Epichlorohydrin carbonate ($C_4H_5ClO_3$)	-73.45	-67.86	7.6
Ethyl chloroglyoxylate ($C_4H_5ClO_3$)	-73.38	-69.56	5.2
Butyl chloroformate ($C_5H_9ClO_2$)	-86.78	-88.13	1.5
Ethyl 2-chloropropionate ($C_5H_9ClO_2$)	-86.87	-86.52	0.4
Ethyl 3-chloropropionate ($C_5H_9ClO_2$)	-86.95	-86.74	0.2
Isopropyl chloroacetate ($C_5H_9ClO_2$)	-86.86	-85.50	1.6
2-Chlorophenol (C_6H_5ClO)	-76.74	-77.50	1.0
3-Chlorophenol (C_6H_5ClO)	-76.69	-78.24	2.0
4-Chlorophenol (C_6H_5ClO)	-76.68	-78.42	2.3
2-Chloromethyl-5-methoxy-4H-pyran-4-one ($C_7H_7ClO_3$)	-104.85	-102.48	2.3
3-Chloro-5-hydroxymethyl benzene-1,2-diol ($C_7H_7ClO_3$)	-105.42	-104.11	1.2
Benzyl alcohol 3-chloro-2,5-dihydroxy ($C_7H_7ClO_3$)	-105.03	-103.95	1.0
Methyl 5-chloromethyl-2-furoate ($C_7H_7ClO_3$)	-105.72	-103.00	2.6
2-Chloro-4-methoxybenzene-1,3-diol ($C_7H_7ClO_3$)	-105.09	-103.58	1.4
3-Chlorophenylacetic acid ($C_8H_7ClO_2$)	-108.30	-107.47	0.8
4-Chlorophenylacetic acid ($C_8H_7ClO_2$)	-108.30	-107.58	0.7
4-Methoxybenzoyl chloride ($C_8H_7ClO_2$)	-107.88	-109.55	1.5
Benzyl chloroformate ($C_8H_7ClO_2$)	-107.99	-110.14	2.0
3-Chloro-4-hydroxy-8-oxabicyclo ($C_7H_7ClO_3$)	-103.90	-101.58	2.2
5-Chloro-2,2-hydroxyethyl furan-3-carbaldehyde ($C_7H_7ClO_3$)	-104.29	-101.57	2.6
4-Chloro-2-hydroxyphenyl methanendiol ($C_7H_7ClO_3$)	-104.74	-101.74	2.9
4-Chloro-3-hydroxymethyl benzene-1,2-diol ($C_7H_7ClO_3$)	-104.77	-103.82	0.9

3-Chloro-2-hydroxy-2,3,3a,6a-tetrahydrocyclopenta[b]turan-4-one ($C_7H_7ClO_3$)	-104.71	-101.94		2.6
Methyl 2-chlorobenzoate ($C_8H_7ClO_2$)	-107.57	-107.85		0.3
Phenoxyacetyl chloride ($C_8H_7ClO_2$)	-107.09	-109.14		1.9
3-chloro-4,1-methyl-2-propenyl 3-cyclobutene-1,2-dione ($C_8H_7ClO_2$)	-105.25	-104.81		0.4
5-chloromethyl-2-hydroxycyclohepta 2,4,6-trien-1-one ($C_8H_7ClO_2$)	-106.78	-107.85		1.0
E-3-chloro-1-2-methylfuran-3-yl, prop-2-en-1-one ($C_8H_7ClO_2$)	-106.39	-105.94		0.4
5-1-chlorovinyl 1,3-benzodioxole ($C_9H_7ClO_2$)	-115.22	-115.92		0.6
4-2-chlorophenyl oxetane-2-one ($C_9H_7ClO_2$)	-116.13	-115.97		0.1
1-(5-chlorofuran-2-yl) pent-4-yn-1-one ($C_9H_7ClO_2$)	-113.70	-114.45		0.7
2-chloro-3-hydroxy-2,3-dihydroinden-1-one ($C_9H_7ClO_2$)	-116.23	-117.02		0.7
2-2-furanyl-3-chloro-4-methylfuran ($C_9H_7ClO_2$)	-115.18	-116.06		0.8
(4S)-4-[(1E)-4,4-dichlorobuta-1,3-dienyl]-2,2-dimethyl-1,3-dioxolane ($C_9H_{12}Cl_2O_2$)	-130.63	-132.52		1.4
2-24-Dichlorophenoxy propan-1-ol ($C_9H_{10}Cl_2O_2$)	-125.80	-127.56		1.4
2-hydroxypentanoyl chloride ($C_5H_9ClO_2$)	-86.03	-87.54		1.7
5-chloropentanoic acid ($C_5H_9ClO_2$)	-86.69	-87.13		0.5
2-chloropentanoic acid ($C_5H_9ClO_2$)	-86.48	-86.51		0.0
R-3-Methoxybutanoic acid chloride ($C_5H_9ClO_2$)	-85.91	-85.94		0.0
2S-2-Chloro-2-methylbutanoic acid ($C_5H_9ClO_2$)	-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 seventy molecules.

● PES using the new ReaxFF for reactive bonding interactions

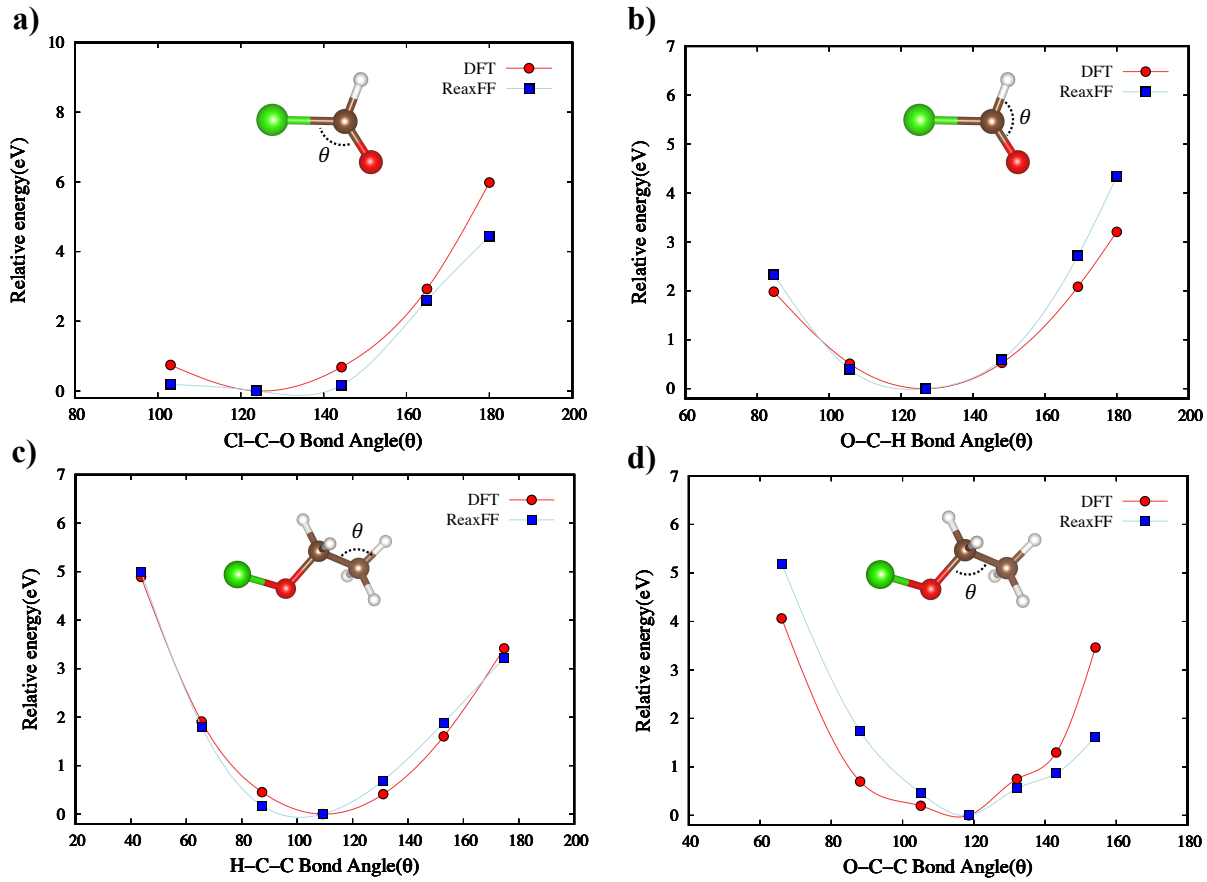


Fig. S1 Relative energies comparison of DFT and the new ReaxFF calculations for a) Cl-C-O and b) O-C-H bond angles in CHClO as well as for c) H-C-C and O-C-C bond angles in C_2H_5ClO.

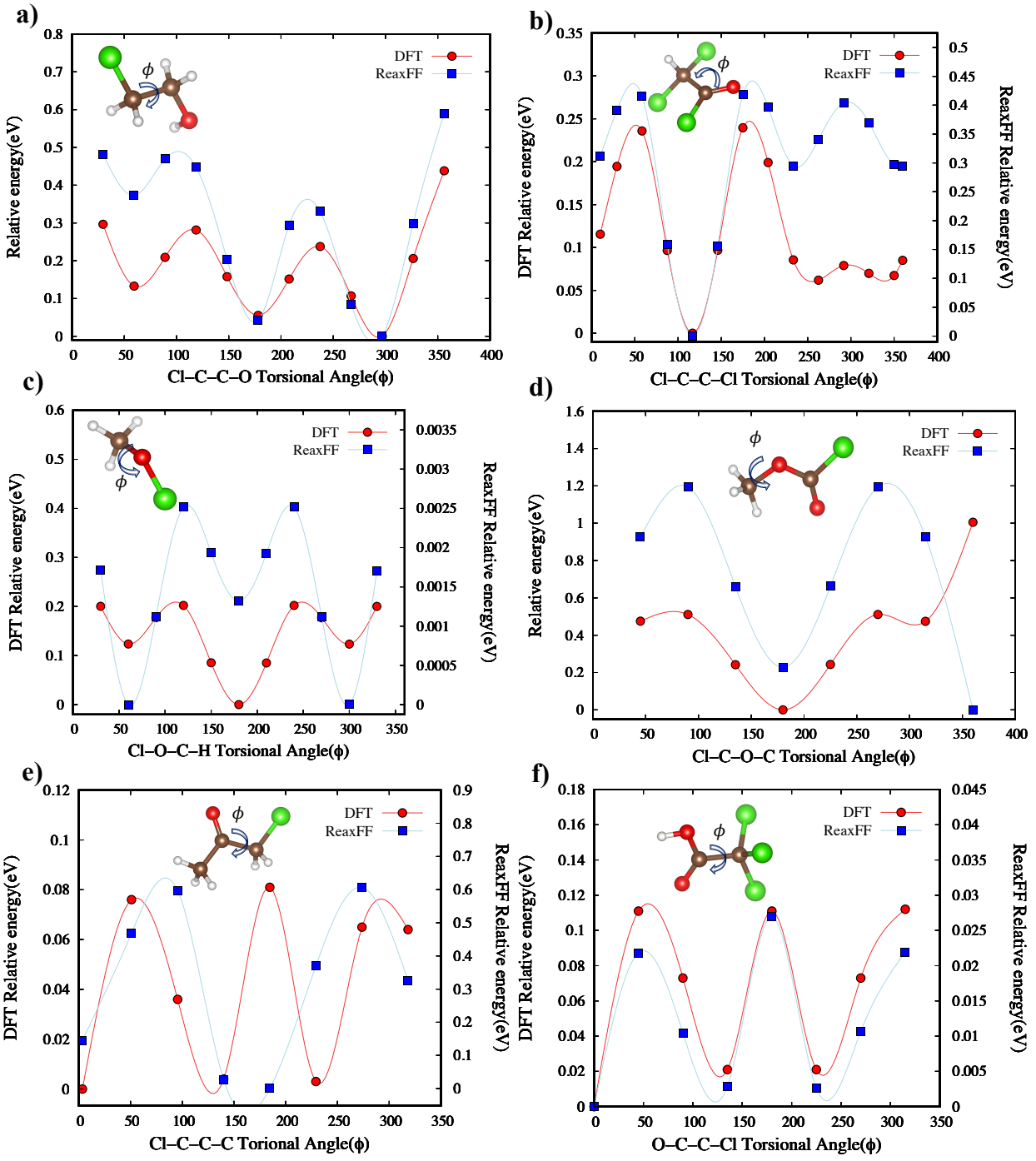


Fig. S2 Relative energies comparison of DFT and the new ReaxFF calculations for a) Cl-C-C-O, b) Cl-C-C-Cl, c) Cl-O-C-H, and d) Cl-C-O-C, e) Cl-C-C-C, and f) O-C-C-Cl torsional angles in C_2H_5ClO, C_2HCl_3O, CH_3ClO, $C_2H_3ClO_2$, C_3H_5ClO, and $C_2HCl_3O_2$, respectively. These different conformational 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 charge[1] values calculated by Bader analysis with PBE functional[2].

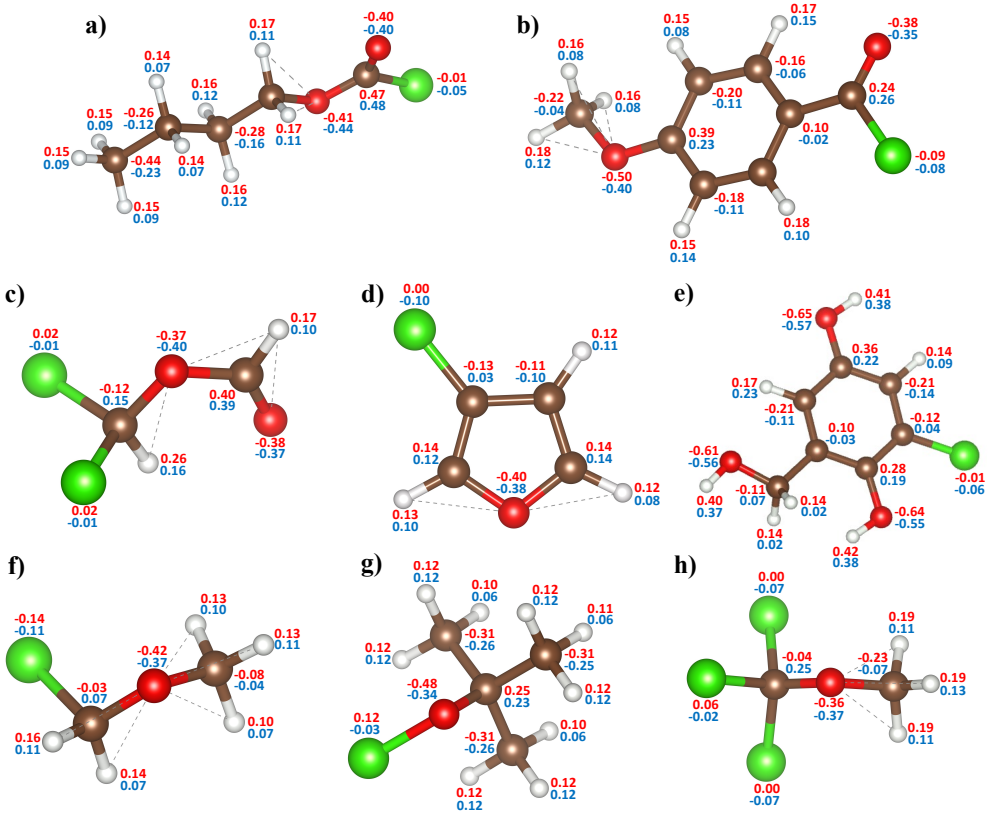


Fig. S3 Charge distributions comparison of DFT and the new ReaxFF calculations in a) $C_5H_9ClO_2$, b) $C_8H_7ClO_2$, c) $C_2H_2Cl_2O_2$, d) C_4H_3ClO, e) $C_7H_7ClO_3$ f) C_2H_5ClO, g) C_4H_9ClO, and h) $C_2H_3Cl_3O$ molecules, respectively.

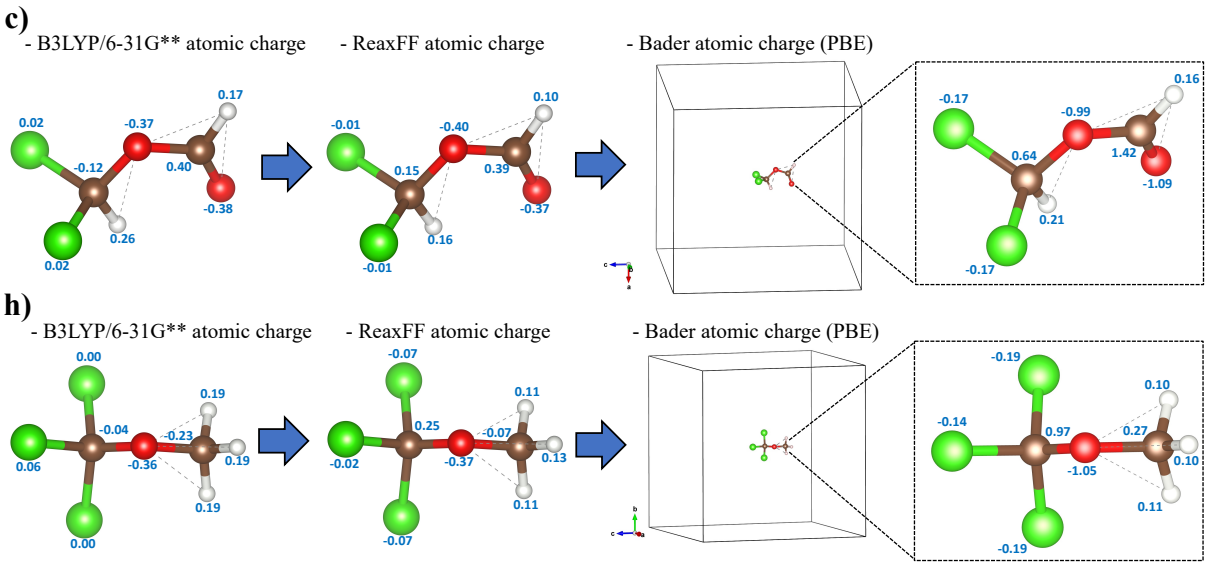


Fig. S4 Bader charge analysis of the atomic charge interpretations, shown Fig. S3, whose patterns are well consistent with the new ReaxFF atomic charges, whereas there is the discrepancy in atomic charges between B3LYP and the new ReaxFF.

- 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 ~ 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 such as 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 1.1 eV, displayed in 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 Goddard[3] that we based our C/H/O/Cl parameter set on.

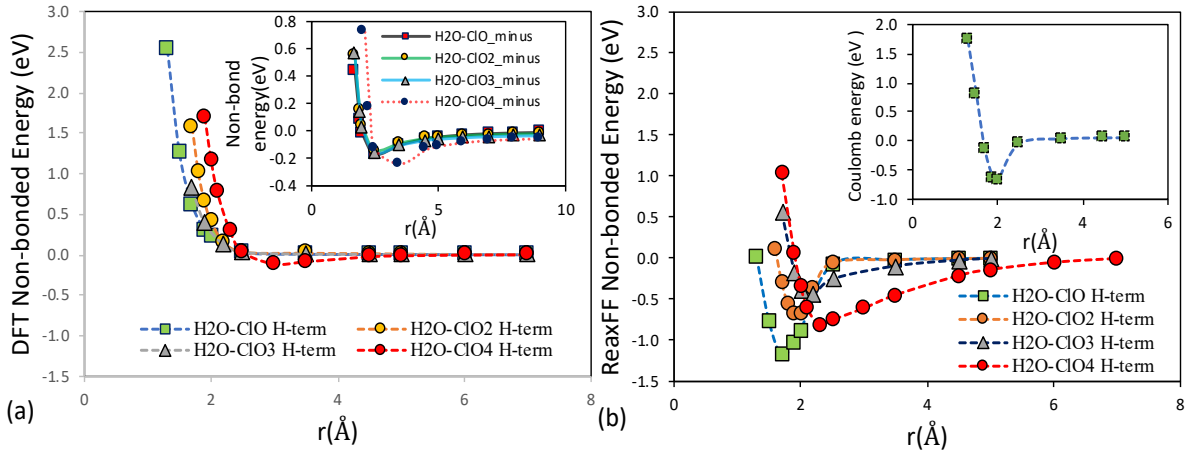
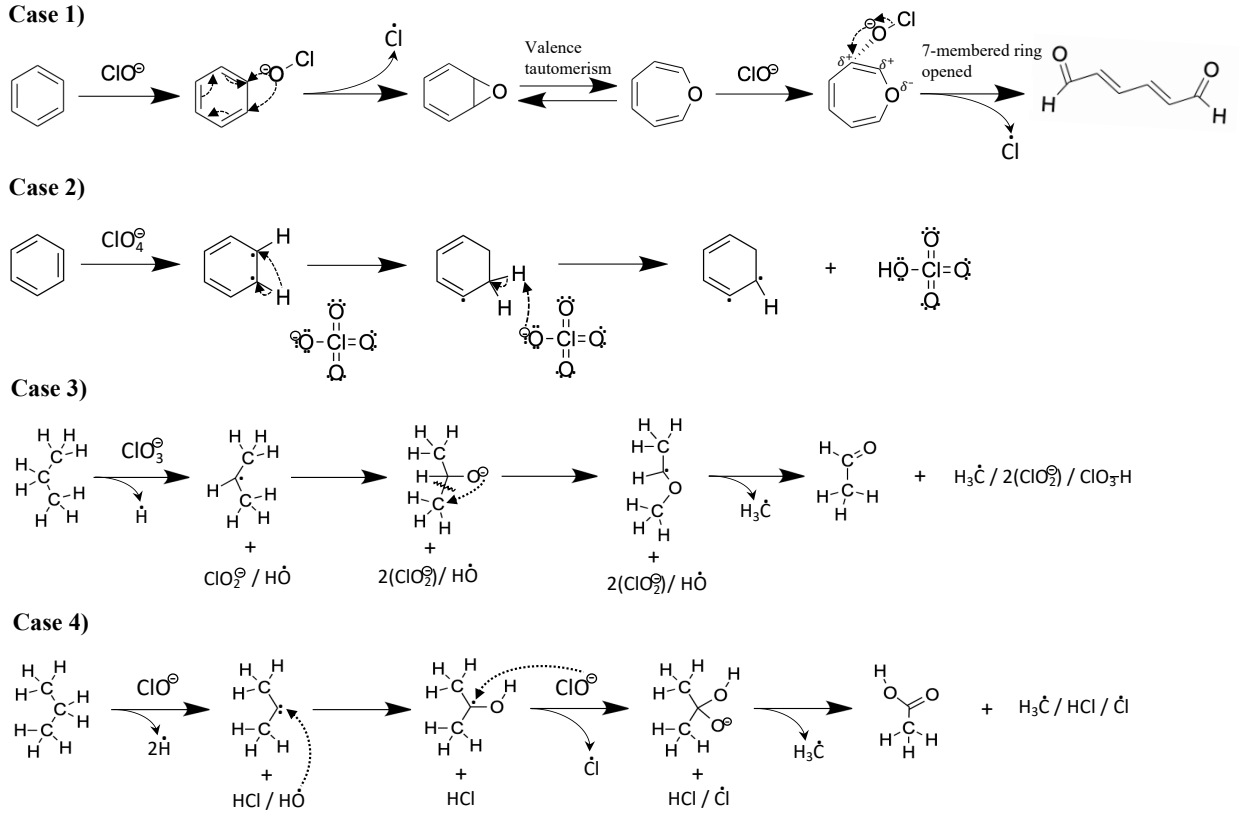


Fig. S5 The comparison between a) DFT and b) ReaxFF non-bonded energies for water and hydrogen-terminated ClO_n^- oxidizers. The inset in graph a) shows the non-bonded energy between water and ClO_n^- oxidizers at the DFT (B3LYP/6-31++G**(D3)). The inset in part b) shows the coulombic contributions to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

● Transition state (TS) simulations of hydrocarbon oxidation

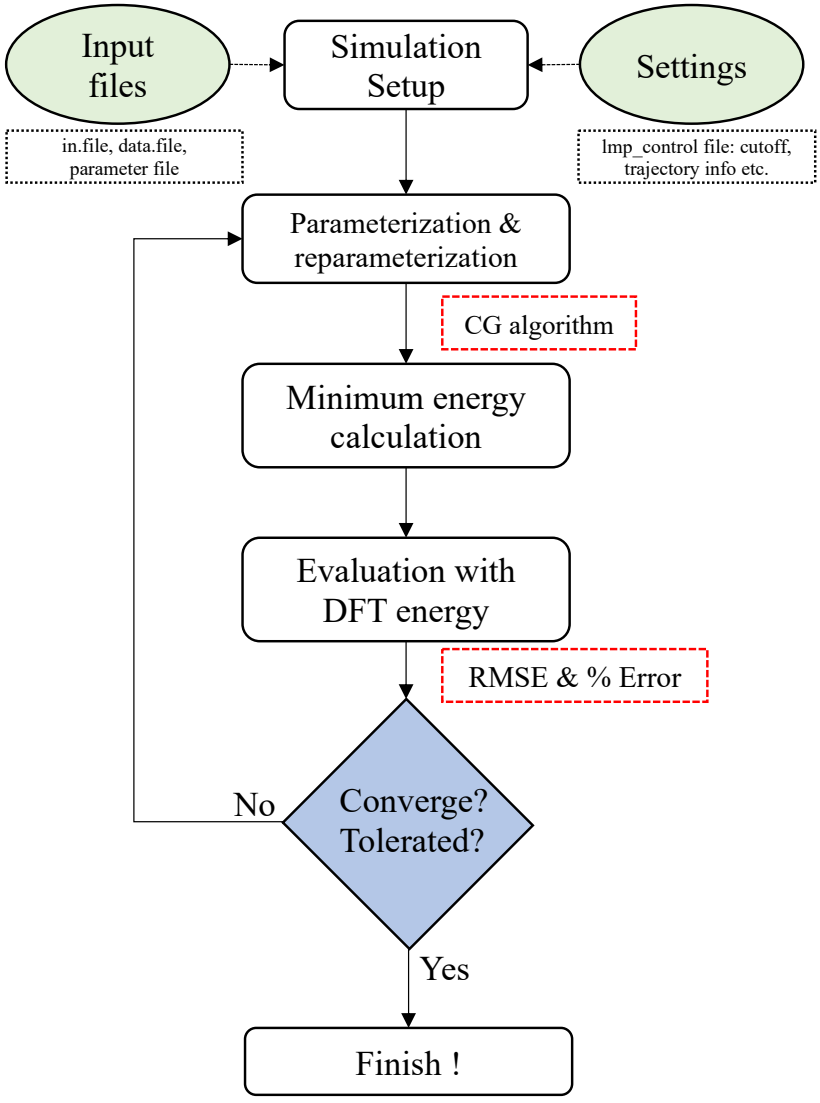
The reasonable reaction paths defined by *ab-initio* MD simulations for an oxidation of a small hydrocarbon using chlorate oxidizers ($ClO_n^-; 1 \leq n \leq 4$) were proposed and validated for the new ReaxFF force field. In Case 1) reaction path, benzene oxygenation begins with causing epoxidation on 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 iso-propyl backbone, and the generation of an acetaldehyde containing a CHO hydrophilic polar end are observed. Case 4) shows radical-radical combination of $\cdot H$ and $\cdot Cl$ 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 H/C/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
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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;Thetao,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
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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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