Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Theoretical Insight into the Adsorption of Aromatic Compounds on Graphene Oxide

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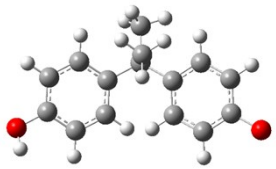
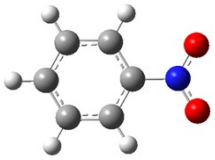
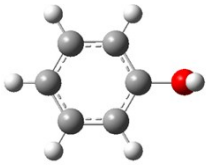
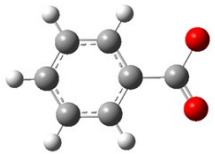
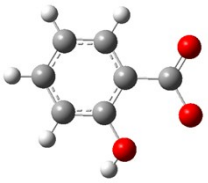
Preparing Methods for GO

Hummers method was used to produce GO.[1] 46 mL of concentrated sulfuric acid were cooled in a 500 mL beaker to 0 °C in an ice water bath. 2 g of natural graphite flakes and 1g anhydrous sodium nitrate were then added to the sulfuric acid. After stirring for 15 min, 6 g of $KMnO_4$ were slowly added to the mixture with stirring for 1h and further cooling to prevent the temperature from exceeding 20 °C. The mixture was then heated to 35±3°C, and held at that temperature for 30 min under constant stirring. 92mL of deionized (DI) water were then added to the mixture and stirred for 15 minutes. Then, the reaction was terminated through addition of 280 mL of 50 ℃ DI water. Finally, 10 mL of 30% H_2O_2 solution was slowly added to the mixture, and washed with 1.25 L of 1:10 HCl solution to remove metal ions and other contaminants. The mixture was then centrifuged at 300 r/min for 1 min to sediment the graphite flakes. Subsequently, the filtrate centrifuged for 10 min at 12000 rpm to sediment the GO, and the supernatant was decanted. This DI wash process was repeated many times until the GO was unable to be separated from water, and the final pH of the mixture was about ~6.5.

Table S1 Models of ACs used for DFT calculations and MD simulations.

Aromatic Compound	pKa[2-4]	Molecular Formula	Structure
BPA	9.0	$C_{15}H_{15}O_2$	
nitrobenzene	~	$C_6H_5NO_2$	
phenol	9.9	C_6H_5OH	
benzoic acid	4.2	$C_7H_5O_2$	
salicylic acid	2.98	$C_7H_5O_3$	

System Setup for DFT Calculations

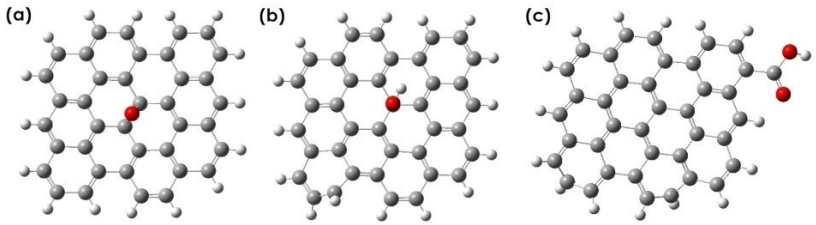


Fig. S1 Models of GO used for DFT calculations. Simplified GO models which contained only one kind of functional groups were used. (a) GO with only epoxy group. (b) GO with only hydroxyl group. (c) GO with only carboxyl group.

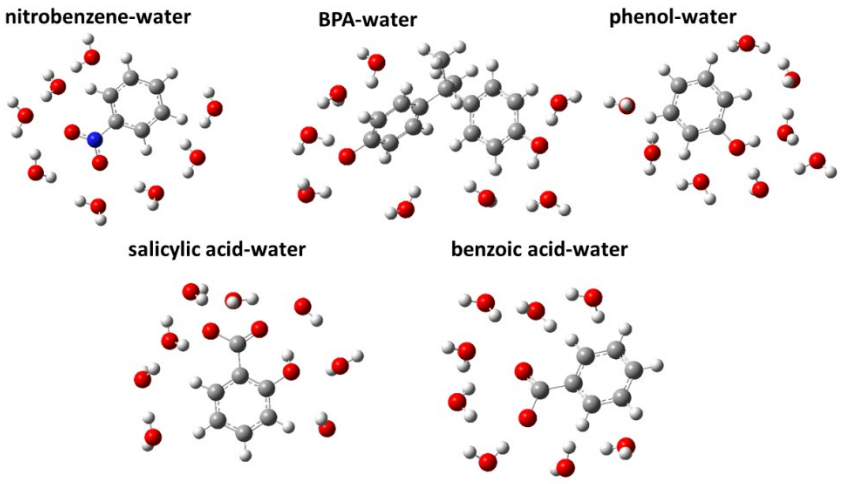


Fig. S2 Initial setup for the calculations of the H-bond between water and ACs.

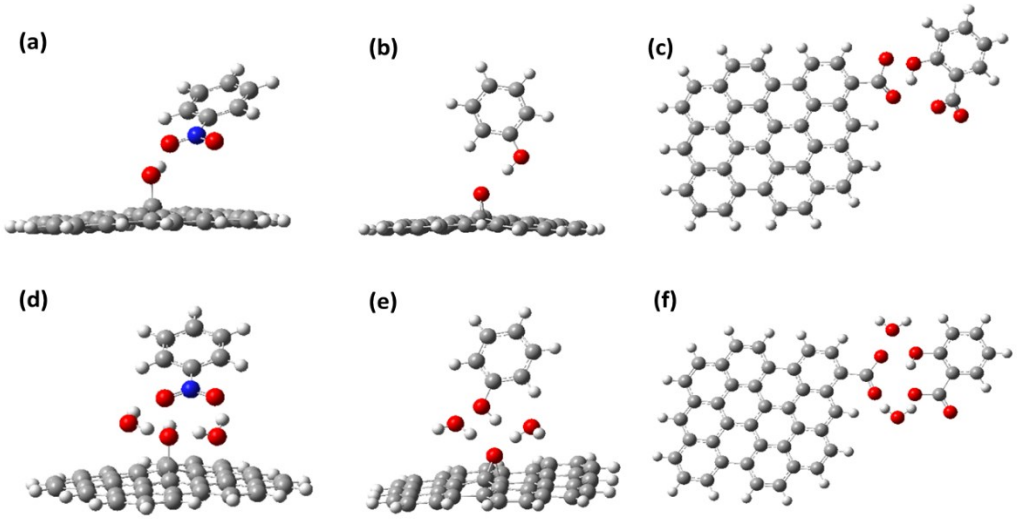


Fig. S3 Initial setup for the calculations of the H-bonds forming between ACs and different functional groups on GO. (a) H-bond interaction of hydroxyl in GO with nitrobenzene. (b) H-bond interaction of epoxy in GO with phenol. (c) H-bond interaction of carboxyl in GO with salicylic acid. (d) Water-bridged H-bond interaction of hydroxyl in GO with nitrobenzene. (e) Water-bridged H-bond interaction of epoxy in GO with phenol. (f) Water-bridged interaction of carboxyl in GO with salicylic acid.

The initial setup was similar for each AC-GO system, and we didn't list all the figures for the setups.

Table S2. Percentage of different functional groups in GO

Sample	% C-C	% C-O	% C=O	% O-C=O
GO	44.87	41.13	6.48	7.52

Table S3. Parameters for isotherms models for sorption of ACs on GO.

Aromatic Compound	Langmuir			Freundlich		
	q_m (mg/g)	K_L (L/mol)	R^2	K_F [(mg/g)/(mg/L)^n)]	n	R^2
nitrobenzene	263.24	0.002	0.9874	15.5510	0.4954	0.9083
BPA	224.32	0.029	0.9914	32.0975	0.3237	0.9135
phenol	56.56	0.172	0.9777	15.4508	0.1961	0.970
salicylic acid	33.64	0.001	0.9877	3.4775	0.4811	0.9332
benzoic acid	21.27	0.001	0.9874	0.8137	0.5283	0.9475

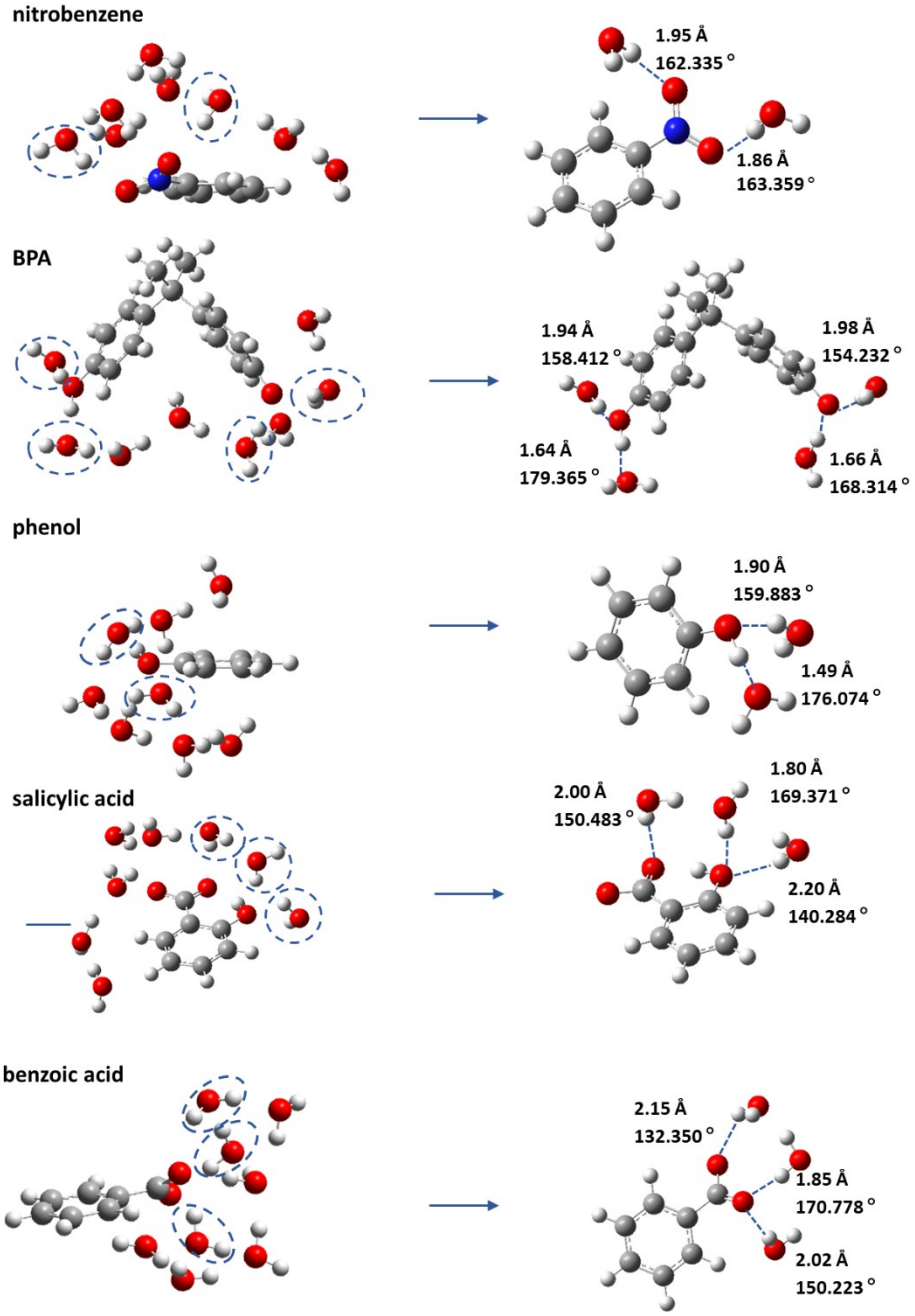


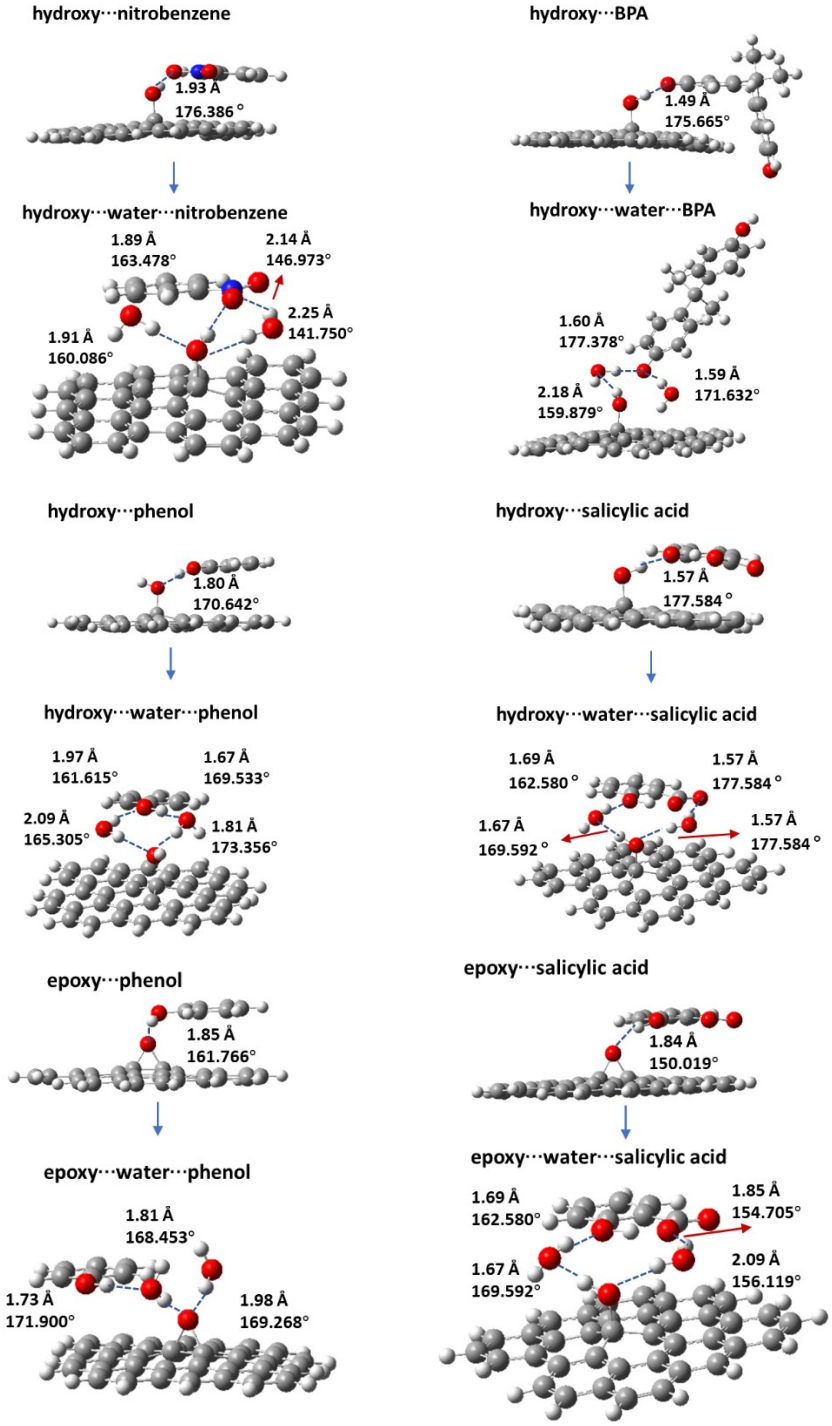
Fig. S4 H-bond configurations between ACs and water molecules. Left panels are the stable configurations for the water molecules around ACs and the water molecules that form H-bonds with ACs were circled, and the right panels are the H-bond details.

Table S4. Free energies of transfer between water and n-hexadecane of ACs

ACs	E_f (kJ/mol)
phenol	-1.25
benzoic acid	2.58
salicylic acid	11.60
BPA	-3.30
nitrobenzene	2.81

Table S5. Strong, moderate, and weak hydrogen bonds were following the classification of Jerrey[5].

	Strong	Moderate	Weak
bond lengths [Å]	1.2-1.5	1.5-2.2	> 2.2
bond angles [°]	170-180	> 130	> 90



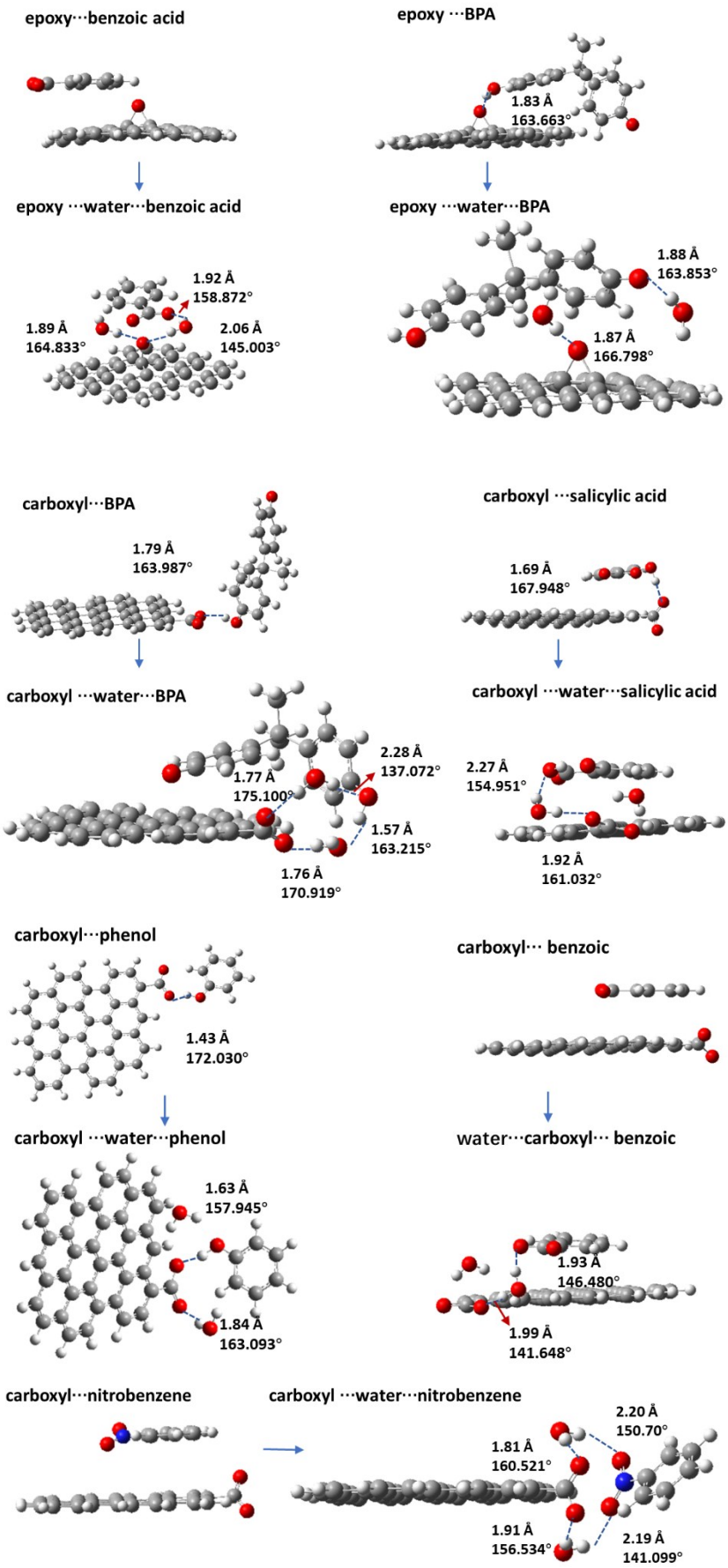


Fig. S5 Direct and water-bridged H-bond configurations between ACs and the functional groups on GO.

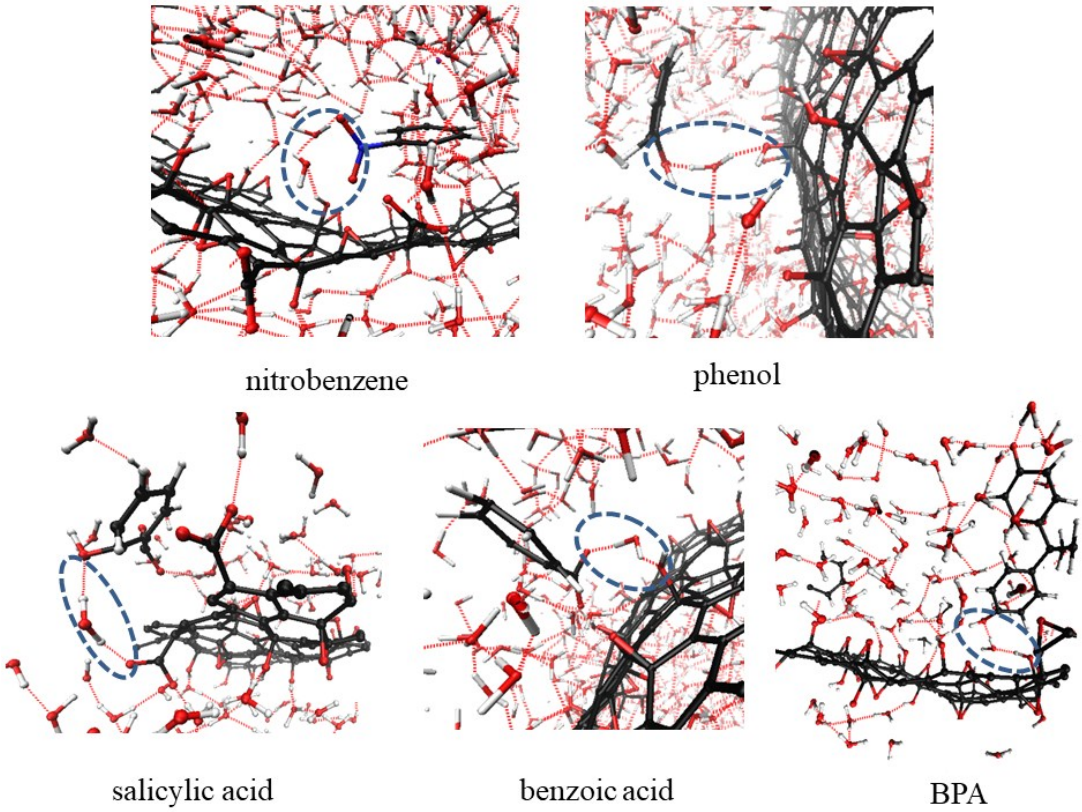


Fig. S6 Water-bridged H-bond interaction between ACs and GO during MD simulations. The red dashed lines are H-bonds. GO and ACs are surrounded by a H-bond network of water molecules, and the water-bridged H-bond is highlighted with blue dashed circle.

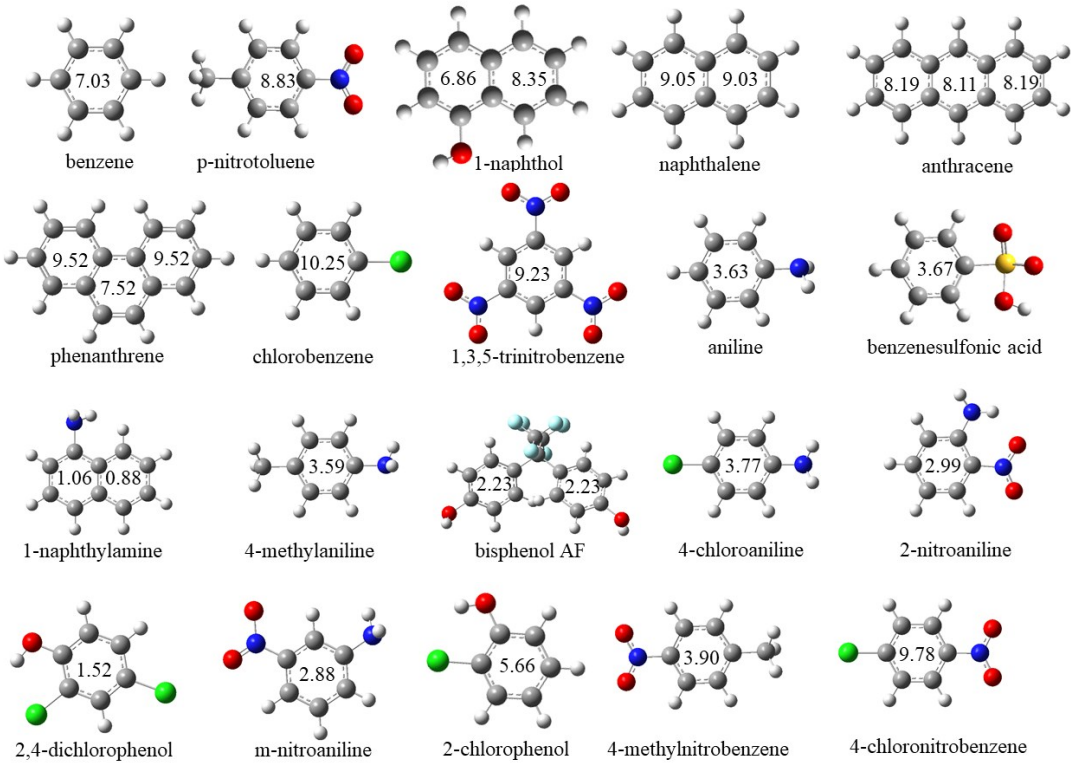


Fig. S7 LOLIPOP values of twenty common ACs.

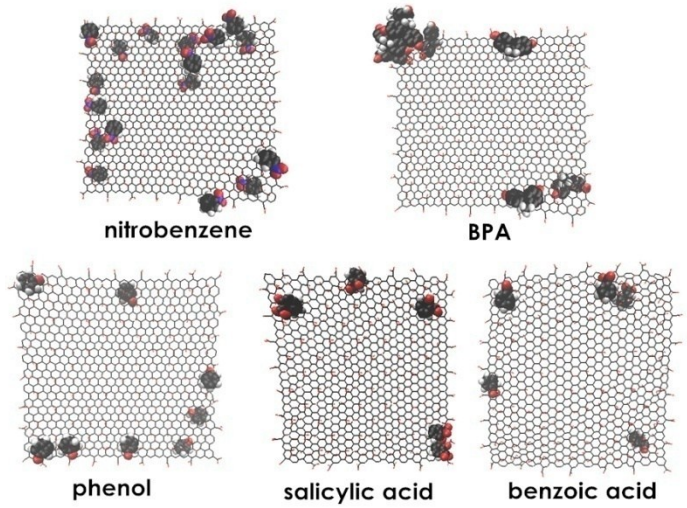


Fig. S8 Configurations of ACs adsorbed on GO in system i.

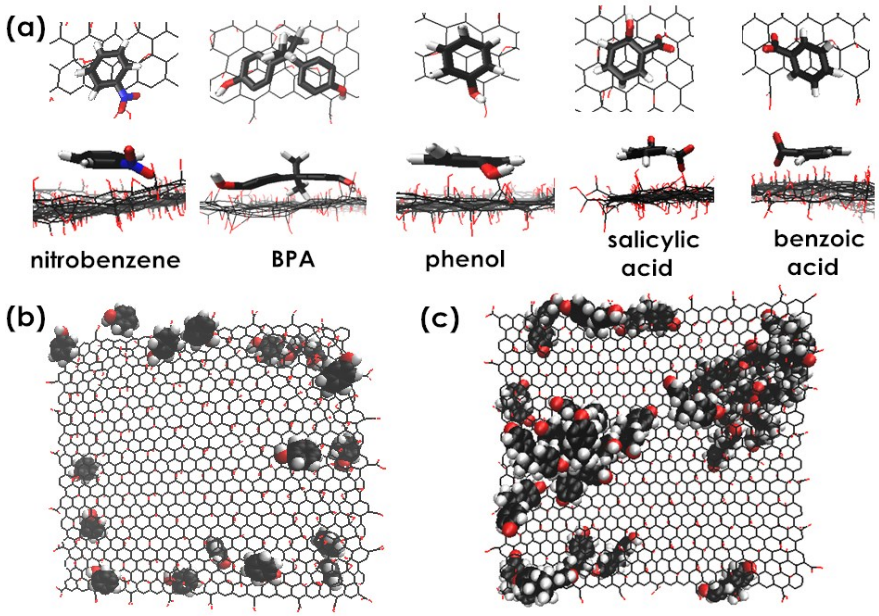


Fig. S9 (a) Configurations of ACs adsorbed on GO. (b) Monolayer adsorption of phenol on GO in system iii. (c) Multilayer adsorption of BPA on GO in system iii.

Table S6 MD parameters for kinetic models.

	pseudo-first-order kinetic model			pseudo-second-order model		
	q_e (mmol/g)	k_1 (1/ps)	R^2	q_e (mmol/g)	k_2(mmol /(g·ps)	R^2
nitrobenzene	0.84	0.03	0.979	1.03	0.01	0.746
BPA	0.41	0.08	0.939	0.91	0.05	0.439
phenol	0.45	0.02	0.927	0.42	0.01	0.544
salicylic acid	0.25	0.07	0.964	0.34	0.02	0.676
benzoic acid	0.15	0.05	0.954	0.18	0.01	0.725

Table S7 Experimental parameters for kinetic models.

	pseudo-first-order kinetic model			pseudo-second-order model		
	q_e (mmol/g)	k_1 (1/h)	R^2	q_e (mmol/g)	k_2(mmol /(g·h)	R^2
nitrobenzene	0.59	0.44	0.998	0.72	0.10	0.696
BPA	0.29	0.93	0.982	0.66	0.15	0.511
phenol	0.34	0.23	0.968	0.32	0.08	0.728
salicylic acid	0.15	0.69	0.984	0.19	0.18	0.576
benzoic acid	0.09	0.59	0.97	0.11	0.50	0.673

Forcefield Parameters

Forcefield Parameters for GO

```
[ defaults ]
1       3       yes       0.5       0.5
[ atomtypes ]
HW     1          1.00800        0.41            A       0.00000e+00    0.00000e+00 ;
OW     8         15.99940       -0.82            A       3.16557e-01    6.50194e-01 ;
CB     6         12.01100        0.000           A       3.55000e-01    2.92880e-01
CT     6         12.01100        0.140           A       3.50000e-01    2.76144e-01
OS     8         15.99940       -0.280           A       2.90000e-01    5.85760e-01
CF     6         12.01100        0.150           A       3.55000e-01    2.92880e-01
OH     8         15.99940       -0.585           A       3.07000e-01    7.11280e-01
HO     1          1.00800        0.435           A       0.00000e+00    0.00000e+00
C      6         12.01100        0.520           A       3.75000e-01    4.39320e-01
OH2    8         15.99940       -0.530           A       3.00000e-01    7.11280e-01
O_3    8         15.99940       -0.440           A       2.96000e-01    8.78640e-01
HO2    1          1.00800        0.450           A       0.00000e+00    0.00000e+00
NA     11        22.98977        1.000           A       3.33045e-01    1.15980e-02
CL     17        35.45300       -1.000           A       4.41724e-01    4.92833e-01
[ bondtypes ]
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HW        OW          1       0.09572     502080.0
CB        CT          1       0.15100     265265.6
CB        C           1       0.14000     392459.2
CT        OS          1       0.14100     267776.0
C         O_3         1       0.12290     476976.0
C         OH2         1       0.13640     376560.0
HO        OH          1       0.09450     462750.4
CF        OH          1       0.13640     376560.0
CT        CT          1       0.15290     224262.4
CB        OH          1       0.13640     376560.0
CT        CF          1       0.15100     265265.6
CF        CF          1       0.14000     392459.2
HO2       OH2         1       0.09450     462750.4
[ angletypes ]
CB        CB        CB          1     120.000       527.184
HW        OW        HW          1     109.500       627.600
CT        OS        CT          1     109.500       502.080
CB        CB        CT          1     120.000       585.760
CB        CT        CT          1     114.000       527.184
CB        CT        OS          1     109.500       418.400
CB        C         O_3         1     120.400       669.440
CB        CB        C           1     120.000       711.280
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CB      C       OH2     1    120.000    585.760
O_3     C       OH2     1    121.000    669.440
CF      OH      HO      1    113.000    292.880
CB      CF      OH      1    120.000    585.760
CB      CF      CB      1    120.000    527.184
CB      CB      CF      1    120.000    527.184
CB      C       OH      1    120.000    585.760
CT      OH      HO      1    113.000    292.880
CF      CB      CT      1    119.700    585.760
CB      CT      CB      1    109.500    334.720
CT      CT      OS      1    109.500    418.400
CB      OH      HO      1    113.000    292.880
CB      CB      OH      1    120.000    585.760
CF      CB      CF      1    120.000    527.184
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CB      CF      CT      1    120.000    585.760
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CF      CT      CT      1    114.000    527.184
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[ dihedraltypes ]
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Forcefield Parameters for BPA

[defaults]

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[atomtypes]

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CP1	6	12.01100	0.000	A	3.50000e-01	2.76144e-01
CP2	6	12.01100	-0.159	A	3.50000e-01	2.76144e-01
HP2	1	1.00800	0.053	A	2.50000e-01	1.25520e-01
CF	6	12.01100	0.042	A	3.55000e-01	2.92880e-01
OH	8	15.99940	-0.452	A	3.07000e-01	7.11280e-01
HO	1	1.00800	0.41	A	0.00000e+00	0.00000e+00
CB	6	12.01100	0	A	3.55000e-01	2.92880e-01

[bondtypes]

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HO	OH	1	0.09450	462750.4
CF	OH	1	0.13640	376560.0
CF	CA	1	0.14000	392459.2
CB	CP1	1	0.15100	265265.6
CP1	CP2	1	0.15100	265265.6
CP2	HP2	1	0.14000	392459.2
CA	CB	1	0.14000	392459.2
CA	HA	1	0.10800	307105.6

[angletypes]

CA	CA	CA	1	120.000	527.184
HW	OW	HW	1	109.500	627.600
CF	OH	HO	1	113.000	292.880
CA	CF	OH	1	120.000	585.760
CA	CF	CA	1	120.000	527.184
CA	CA	CF	1	120.000	527.184
CA	CF	OH	1	120.000	585.760
CA	CB	CP1	1	120.000	585.760
CB	CP1	CP2	1	120.000	585.760

```
CP1     CP2     HP2      1    130.700     292.880
CB      CP1     CB       1    120.000     585.760
CP2     CP1     CP2      1    120.000     585.760
HP2     CP2     HP2      1    107.800     276.144
CA      CA      CB       1    120.000     527.184
CA      CB      CA       1    120.000     527.184
CA      CA      HA       1    120.000     292.880
CF      CA      HA       1    120.000     292.880
CB      CA      HA       1    120.000     292.880
[ dihedraltypes ]
CA   CA   CA   CA   3    30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
CA   CF   OH   HO   3     7.03749   0.00000   -7.03749   0.00000   0.00000   0.00000
CA   CA   CA   CF   3    30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
CA   CA   CF   CA   3    30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
CA   CA   CA   HA   3    30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
HA   CA   CA   HA   3    30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
HA   CA   CF   OH   3    30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
CF   CA   CA   CP1  3    44.97800   0.00000 -44.97800   0.00000   0.00000   0.00000
CA   CA   CP1  CP2  3    44.97800   0.00000 -44.97800   0.00000   0.00000   0.00000
CB   CP1  CP2  HP2  3    44.97800   0.00000 -44.97800   0.00000   0.00000   0.00000
CA   CA   CA   CP1  3    44.97800   0.00000 -44.97800   0.00000   0.00000   0.00000
CB   CP1  CB   CA   3    44.97800   0.00000 -44.97800   0.00000   0.00000   0.00000
CA   CA   CB   CP1  3    44.97800   0.00000 -44.97800   0.00000   0.00000   0.00000
CF   CA   CA   CB   3    44.97800   0.00000 -44.97800   0.00000   0.00000   0.00000
CA   CA   CB   CA   3    44.97800   0.00000 -44.97800   0.00000   0.00000   0.00000
```

Forcefield Parameters for Nitrobenzene

```
[ defaults ]
1            3            yes            0.5         0.5
[ atomtypes ]
HW     1          1.00800        0.41            A       0.00000e+00    0.00000e+00 ;
OW     8         15.99940       -0.82            A       3.16557e-01    6.50194e-01 ;
CN     6 12.01100         0.010           A       3.55000e-01    2.92880e-01
ON     8         15.99940       -0.125           A       2.96000e-01    7.11280e-01
NO     7         14.00670        0.240           A       3.25000e-01    5.02080e-01
CA     6        12.01100       -0.1268           A       3.55000e-01    2.92880e-01
HA     1         1.00800        0.1268           A       2.42000e-01    1.25520e-01

[ bondtypes ]
HW      OW          1      0.09572     502080.0
NO      ON          1      0.12250     460240.0
CN      NO          1      0.14600     334720.0
CN      CA          1      0.14000     392459.2
CA      HA          1      0.10800     307105.6
```

```
CA      CA          1       0.14000     392459.2

[ angletypes ]
CA      CA      CA          1     120.000      527.184
HW      OW      HW          1     109.500      627.600
CA      CN      CA          1     120.000      527.184
CA      CA      CN          1     120.000      527.184
CA      CA      HA          1     120.000      292.880
CN      CA      HA          1     120.000      292.880
ON      NO      ON          1     125.000      669.440
CN      NO      ON          1     117.500      669.440
CA      CN      NO          1     120.000      711.280

[ dihedraltypes ]
CA    CA    CA    CA     3    30.33400    0.00000 -30.33400    0.00000    0.00000    0.00000
CA    CA    CA    CN     3    30.33400    0.00000 -30.33400    0.00000    0.00000    0.00000
CA    CA    CN    CA     3    30.33400    0.00000 -30.33400    0.00000    0.00000    0.00000
CA    CA    CA    HA     3    30.33400    0.00000 -30.33400    0.00000    0.00000    0.00000
HA    CA    CA    HA     3    30.33400    0.00000 -30.33400    0.00000    0.00000    0.00000
HA    CA    CN    NO     3    30.33400    0.00000 -30.33400    0.00000    0.00000    0.00000
CA    CN    NO    ON     3    4.81160     0.00000   -4.81160    0.00000    0.00000    0.00000
CA    CA    CN    NO     3    30.33400    0.00000 -30.33400    0.00000    0.00000    0.00000
```

Forcefield Parameters for Phenol

```
 [ defaults ]
1           3           yes        0.5        0.5
[ atomtypes ]
HW     1          1.00800        0.41             A       0.00000e+00    0.00000e+00 ;
OW     8         15.99940       -0.82             A       3.16557e-01    6.50194e-01 ;
CF     6         12.01100        0.042            A       3.55000e-01    2.92880e-01 ; 166    CA
OH     8         15.99940       -0.452            A       3.07000e-01    7.11280e-01 ;opls_167 -oh
HO     1          1.00800        0.41             A       0.00000e+00    0.00000e+00 ; opls_168 -oh
CA     6        12.01100       -0.1268           A       3.55000e-01    2.92880e-01;CA
HA     1         1.00800        0.1268              A       2.42000e-01    1.25520e-01;HA

[ bondtypes ]
HW      OW          1       0.09572     502080.0
HO      OH          1       0.09450     462750.4
CF      OH          1       0.13640     376560.0
CF      CA          1       0.14000     392459.2
CA      HA          1       0.10800     307105.6
CA      CA          1       0.14000     392459.2

[ angletypes ]
```

```
CA      CA      CA      1    120.000    527.184
HW      OW      HW      1    109.500    627.600
CF      OH      HO      1    113.000    292.880
CA      CF      OH      1    120.000    585.760
CA      CF      CA      1    120.000    527.184
CA      CA      CF      1    120.000    527.184
CA      CA      HA      1    120.000    292.880
CF      CA      HA      1    120.000    292.880

[ dihedraltypes ]
CA   CA   CA   CA   3   30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
CA   CF   OH   HO   3   7.03749    0.00000   -7.03749   0.00000   0.00000   0.00000
CA   CA   CA   CF   3   30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
CA   CA   CF   CA   3   30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
CA   CA   CA   HA   3   30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
HA   CA   CA   HA   3   30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
HA   CA   CF   OH   3   30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
```

Forcefield Parameters for Benzoic Acid

```
[ defaults ]
1           3           yes         0.5         0.5
[ atomtypes ]
HW    1     1.00800     0.41        A    0.00000e+00   0.00000e+00 ;
OW    8     15.99940    -0.82       A    3.16557e-01   6.50194e-01 ;
C     6     12.01100    0.530       A    3.75000e-01   4.39320e-01
OH2   8     15.99940    -0.455      A    3.00000e-01   7.11280e-01
O_3   8     15.99940    -0.45       A    2.96000e-01   8.78640e-01
HO2   1     1.00800     0.41        A    0.00000e+00   0.00000e+00
CA    6     12.01100    -0.1268     A    3.55000e-01   2.92880e-01
HA    1     1.00800     0.1268      A    2.42000e-01   1.25520e-01
CB    6     12.01100    -0.035      A    3.55000e-01   2.92880e-01

[ bondtypes ]
CA    CA    1    0.14000    392459.2
HW    OW    1    0.09572    502080.0
C     O_3   1    0.12290    476976.0
C     OH2   1    0.13640    376560.0
HO2   OH2   1    0.09450    462750.4
CB    CA    1    0.14000    392459.2
CB    C     1    0.14000    392459.2
CA    HA    1    0.10800    307105.6

[ angletypes ]
CA      CA      CA      1    120.000    527.184
```

```
CA      CA      CB      1    120.000    527.184
CA      CB      CA      1    120.000    527.184
HW      OW      HW      1    109.500    627.600
CB      C       O_3     1    120.400    669.440
CA      CB      C       1    120.000    711.280
CB      C       OH2     1    120.000    585.760
O_3     C       OH2     1    121.000    669.440
C       OH2     HO2     1    113.000    292.880
CA      CA      HA      1    120.000    292.880
CB      CA      HA      1    120.000    292.880

[ dihedraltypes ]
CA   CA   CA   CA   3   30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
CA   CA   CA   CB   3   30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
CA   CA   CB   CA   3   30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
CA   CA   CA   HA   3   30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
HA   CA   CA   HA   3   30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
CA   CB   C    O_3  3   8.78640    0.00000  -8.78640   0.00000   0.00000   0.00000
CB   C    OH2  HO2  3   29.28800  -8.36800 -20.92000   0.00000   0.00000   0.00000
C    CB   CA   HA   3   30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000
CA   CB   C    OH2  3   8.78640    0.00000  -8.78640   0.00000   0.00000   0.00000
```

Forcefield Parameters for Salicylic Acid

```
[ defaults ]
1               3           yes         0.5         0.5
[ atomtypes ]
HW    1        1.00800      0.41          A      0.00000e+00   0.00000e+00 ;
OW    8       15.99940     -0.82          A      3.16557e-01   6.50194e-01 ;
C     6       12.01100      0.530         A      3.75000e-01   4.39320e-01
OH2   8       15.99940     -0.455         A      3.00000e-01   7.11280e-01
O_3   8       15.99940     -0.45          A      2.96000e-01   8.78640e-01
HO2   1        1.00800      0.41          A      0.00000e+00   0.00000e+00
CA    6       12.01100     -0.1268        A      3.55000e-01   2.92880e-01
HA    1        1.00800      0.1268        A      2.42000e-01   1.25520e-01
CB    6       12.01100     -0.035         A      3.55000e-01   2.92880e-01
CF    6       12.01100      0.150         A      3.55000e-01   2.92880e-01
OH    8       15.99940     -0.585         A      3.07000e-01   7.11280e-01
HO    1        1.00800      0.435         A      0.00000e+00   0.00000e+00

[ bondtypes ]
CA      CA        1      0.14000     392459.2
HW      OW        1      0.09572     502080.0
C       O_3       1      0.12290     476976.0
```

```
C       OH2      1      0.13640     376560.0
HO2     OH2      1      0.09450     462750.4
CB      CA       1      0.14000     392459.2
CB      C        1      0.14000     392459.2
CA      HA       1      0.10800     307105.6
HO      OH       1      0.09450     462750.4 ;-oh
CF      OH       1      0.13640     376560.0 ;-oh
CA      CF       1      0.15100     265265.6

[ angletypes ]
CA      CA      CA       1     120.000      527.184
CA      CA      CB       1     120.000      527.184
CA      CB      CA       1     120.000      527.184
HW      OW      HW       1     109.500      627.600
CB      C       O_3      1     120.400      669.440
CA      CB      C        1     120.000      711.280
CB      C       OH2      1     120.000      585.760
O_3     C       OH2      1     121.000      669.440
C       OH2     HO2      1     113.000      292.880
CA      CA      HA       1     120.000      292.880
CB      CA      HA       1     120.000      292.880
CF      OH      HO       1     113.000      292.880
CA      CF      OH       1     120.000      585.760

[ dihedraltypes ]
CA    CA    CA    CA     3   30.33400    0.00000 -30.33400    0.00000    0.00000    0.00000
CA    CA    CA    CB     3   30.33400    0.00000 -30.33400    0.00000    0.00000    0.00000
CA    CA    CB    CA     3   30.33400    0.00000 -30.33400    0.00000    0.00000    0.00000
CA    CA    CA    HA     3   30.33400    0.00000 -30.33400    0.00000    0.00000    0.00000
HA    CA    CA    HA     3   30.33400    0.00000 -30.33400    0.00000    0.00000    0.00000
CA    CB    C     O_3    3   8.78640     0.00000   -8.78640    0.00000    0.00000    0.00000
CB    C     OH2   HO2    3   29.28800   -8.36800 -20.92000    0.00000    0.00000    0.00000
C     CB    CA    HA     3   30.33400    0.00000 -30.33400    0.00000    0.00000    0.00000
CA    CB    C     OH2    3   8.78640     0.00000   -8.78640    0.00000    0.00000    0.00000
CA    C     OH    HO     3   29.28800   -8.36800 -20.92000    0.00000    0.00000    0.00000
```

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