ADVANCED ENERGY MATERIALS

# Supporting Information

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## Characterization of the Solid Electrolyte Interphase at the Li Metal–Ionic Liquid Interface

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**This PDF file includes:**

## COMPUTATIONAL DETAILS

### ReaxFF Reactive Force Field

ReaxFF is a general bond order (BO) based force field method that allows bond breaking and formation processes during simulations. The ReaxFF parameters are based on fitting to quantum mechanics (QM) calculations. The general form of the ReaxFF energy terms are following:

$$E_{\text{system}} = E_{\text{bond}} + E_{\text{over}} + E_{\text{under}} + E_{\text{lp}} + E_{\text{val}} + E_{\text{tor}} + E_{\text{Coul}} + E_{\text{vdW}} \quad (1)$$

where the partial contributions to the total energy are valence terms: bond, over-coordination penalty, and under-coordination stability, lone-pair, valence angle and torsion, and non-bonding terms: Coulombic and van der Waals (vdW) energies.

ReaxFF uses the concept of BOs to determine the bonded interactions among all the atoms in a system. BOs are a continuous function of the distance between bonded atoms, and contributions from σ, π, and ππ bonds are calculated from the following equation.

$$BO'_{ij} = BO^{\sigma}_{ij} + BO^{\pi}_{ij} + BO^{\pi\pi}_{ij}$$

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

where $BO^{\sigma}_{ij}$, $BO^{\pi}_{ij}$, and $BO^{\pi\pi}_{ij}$ are the partial contributions of σ-, π- and, ππ-bonds between atoms $i$ and $j$, $r_{ij}$ is the distance between $i$ and $j$, $r_o^{\sigma}$, $r_o^{\pi}$, and $r_o^{\pi\pi}$ are the bond radii of σ-, π- and, ππ-bonds, respectively, and $p_{\text{bo}}$ terms are empirical parameters fit quantum mechanics (QM) data.

Non-bonded interactions (vdW and Coulomb) are calculated between every pair of atoms, regardless of their connectivity. A more detailed description of the ReaxFF method is provided in previous studies.[1,2]

### ReaxFF Development

The ReaxFF parameters for the Li anode/IL electrolyte system were developed based on the previous study for Li-S systems.[3] In the fitting procedure, the parameters were trained extensively against QM data describing bond dissociation (Fig. S1 to S3) and equation of state (Fig. S4). Here the QM calculations were performed using the Gaussian09 program[4] at the B3LYP/6-31G(d,p) level. Moreover, heats of formation of crystalline phases (Table. S1) and density of the [TFSI][BMIM] IL electrolyte (Fig. S5) data were included to fit the ReaxFF parameters. The optimization of the parameters was performed to minimize the sum of the following error

$$Error = \sum_i^n \left[\frac{x_{i,\text{QM}} - x_{i,\text{ReaxFF}}}{\sigma_i}\right]^2 \quad (3)$$

where $x_{\text{QM}}$ is the QM value, $x_{\text{ReaxFF}}$ is the ReaxFF value, and $\sigma_i$ is the weight assigned to a data point, $i$. The optimized ReaxFF parameters show overall good fitting to the QM data and reproduce well experimental data. Although the ReaxFF bond dissociation curves do not exactly fit the whole DFT plots, they are in reasonable agreement with the QM data and, more importantly, reproduce well the equilibrium bond length and bond dissociation energy that are critical for proper modeling of the bond breaking and formation processes.

The developed ReaxFF parameters are at the end of the Supporting Information.

**ReaxFF MD Simulations**

We started with ReaxFF MD on a small system containing 4 TFSI to validate the optimized ReaxFF parameters against QM. The system was constructed based on our previous QM-MD simulations,[5] where five Li layers (84 Li) were increased to sixteen layers (196 Li), leading to the system size of 13.4 × 13.4 × 27.5 $Å^3$. After the minimization, a short NVT (constant particles, volume, and temperature) MD was carried out at 10 K for 1 ps to generate initial velocities for the atoms. The system temperature was increased from 10 K to 400 K over 5 ps using NVT, which was followed by NPT (constant particles, volume, and pressure) at 400 K for 100 ps.

For the production runs, a larger system was prepared to describe the SEI layer formation at realistic distance and time scales. The system consisted of a ~10 nm thick Li anode and a ~19 nm thick [TFSI][BMIM] IL electrolyte with periodic lateral dimensions of 4.5 nm × 4.5 nm, where ~10 % of the BMIM was replaced with Li-ion. The electrolyte was constructed based on our previous study.[6] Two layers of Li and IL molecules at each end were fixed to force the reactions to occur at only one interface. After the minimization, a short NVT MD was carried out at 10 K for 10 ps to generate initial velocities for the atoms. The system temperature was gradually increased from 10 K to 300 K or 400 K over 50 ps using NVT MD. The production runs were performed at the target temperature for 1 ns. The model for 400 K had a slightly longer electrolyte, ~20 nm, than that of 300 K to take into account the lower density at the higher temperature (Fig. S5B).

All MD simulations were performed under ambient conditions using LAMMPS program.[7] The time step was set to 0.5 fs. The Nose-Hoover thermostat and barostat were employed for NVT and NPT simulations. The charge equilibration (QEq) method was used for Coulomb interactions.[8] VMD was used for bond and radial distribution function (RDF) analyses and visualization.[9] The IL molecules were regarded as decomposed if the structure contains one or more bond lengths longer than its original distance by 50 %.

The chemical reactions and SEI formation occurred in our simulations under ambient conditions. The reactions at the interface between the Li-metal and IL are basically driven by highly reactive Li-metal.

**FIGURES**

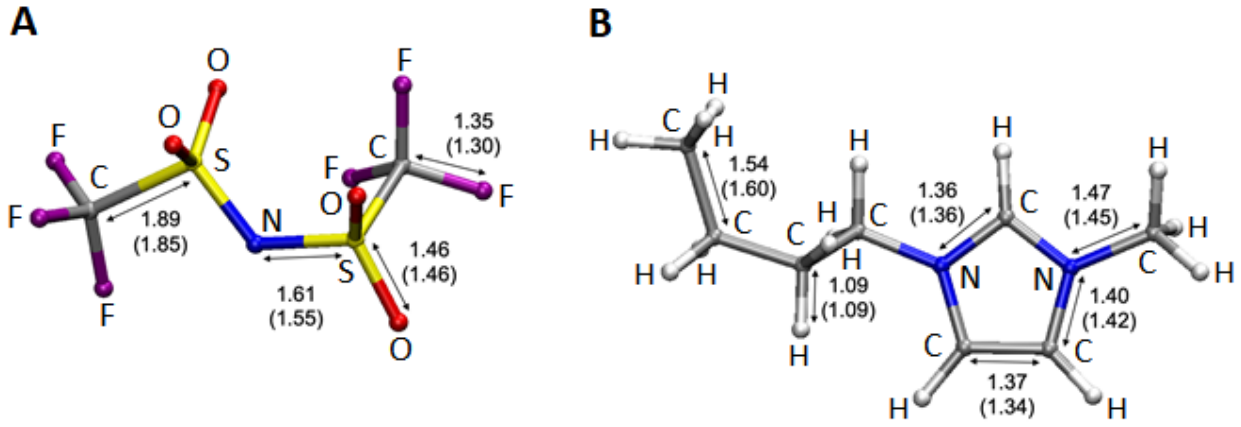


**Figure S1.** Molecular structures of the electrolyte. The structures and bond lengths between two atoms within (A) TFSI and (B) BMIM molecules, respectively, optimized by DFT and ReaxFF (provided in parentheses).

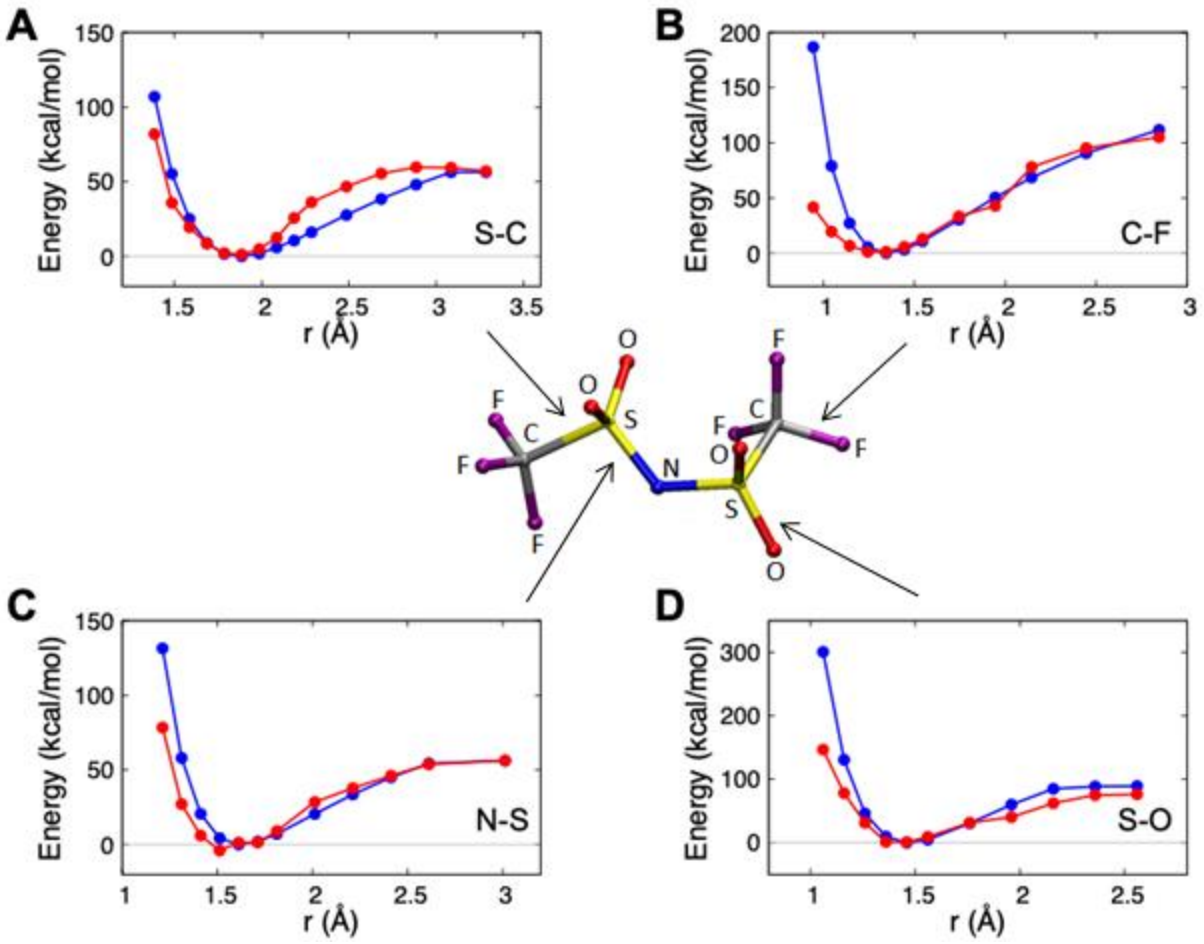


**Figure S2.** ReaxFF parameter optimization for TFSI. Bond dissociation energies of TFSI, where blue and red represent DFT and ReaxFF.

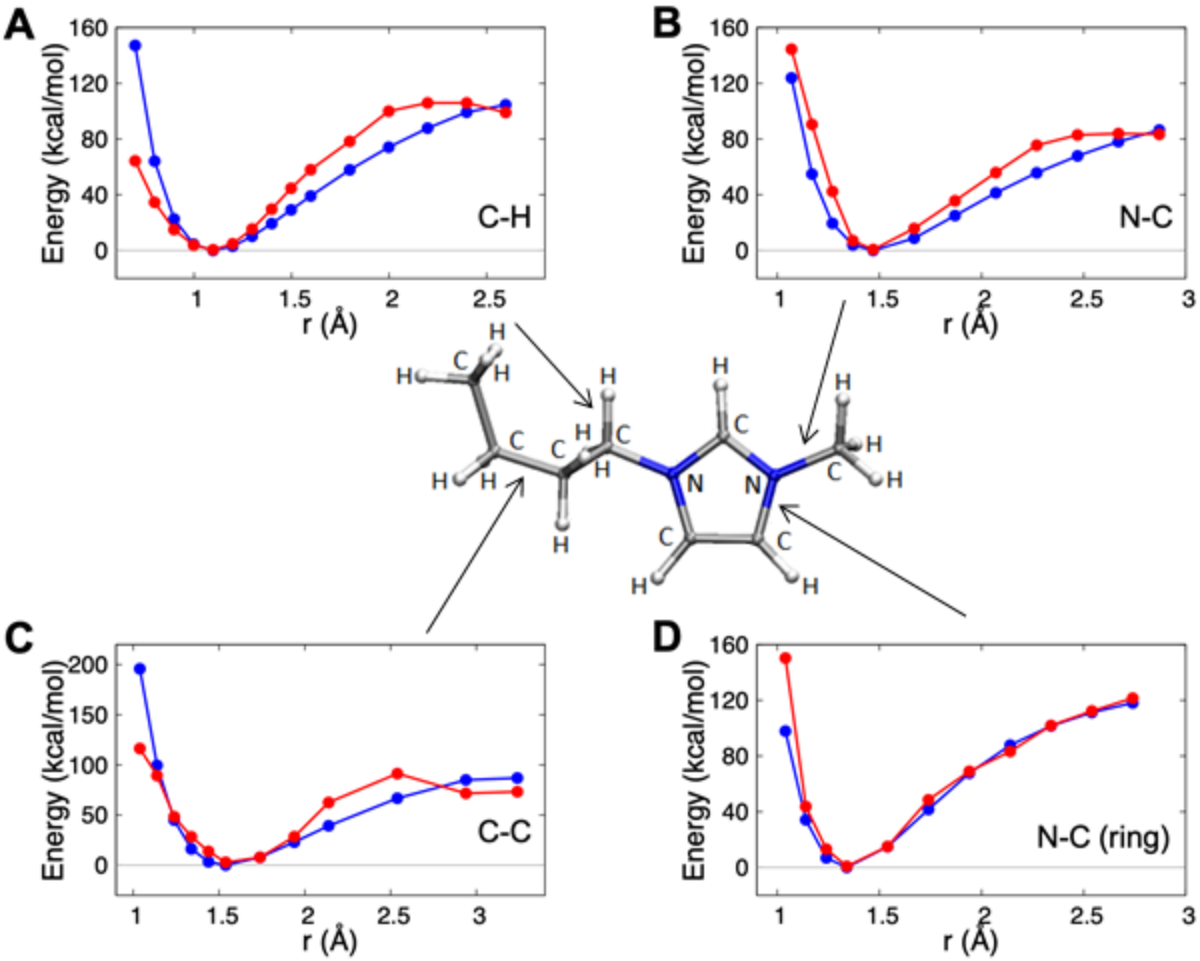


**Figure S3.** ReaxFF parameter optimization for BMIM. Bond dissociation energies of BMIM, where blue and red represent DFT and ReaxFF.

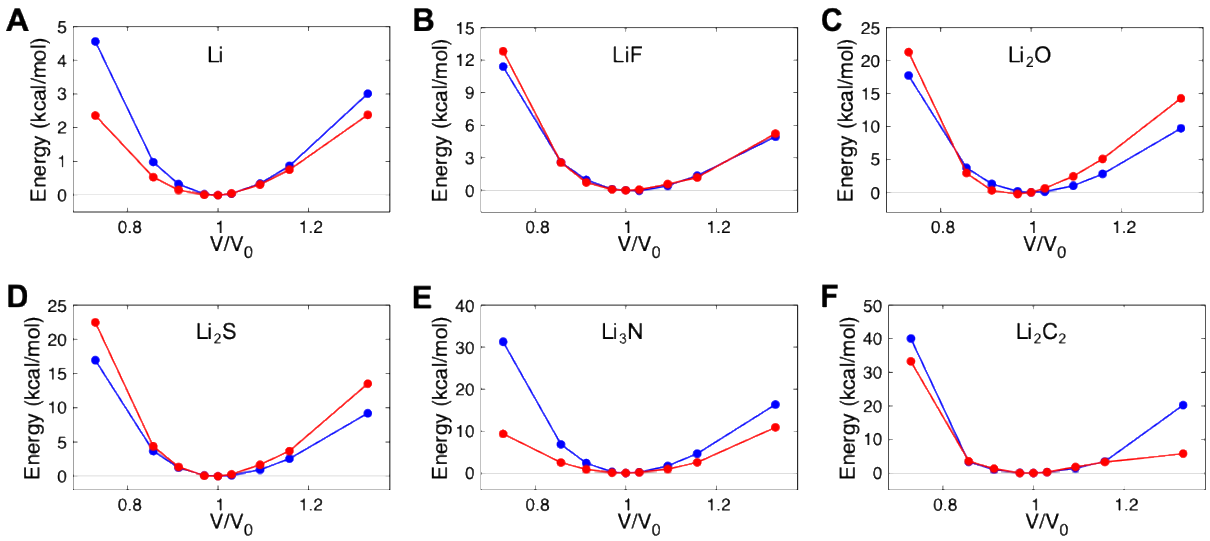


**Figure S4.** ReaxFF parameter optimization for crystalline phases. Equation of states of (A) Li (bcc), (B) LiF, (C) $Li_2O$, (D) $Li_2S$, (E) $Li_3N$, and (F) $Li_2C_2$, where blue and red represent DFT and ReaxFF results, respectively.

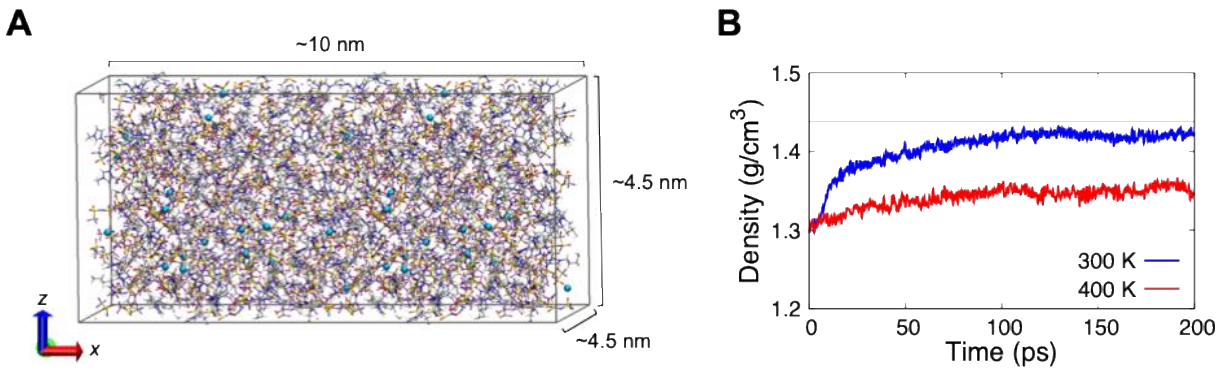


**Figure S5.** The densities of the IL electrolyte from ReaxFF MD simulations. (A) The structure of the [TFSI][BMIM] electrolyte, where about 10% of BMIM was replaced by Li (Li: cyan, F: purple, C: gray, N: blue, O: red, S: yellow, and H: white). (B) The estimated densities at 300 K (blue) and 400 K (red) from the 200 ps NPT MD simulations. The experimental density at room temperature is shown with a gray line.[10]

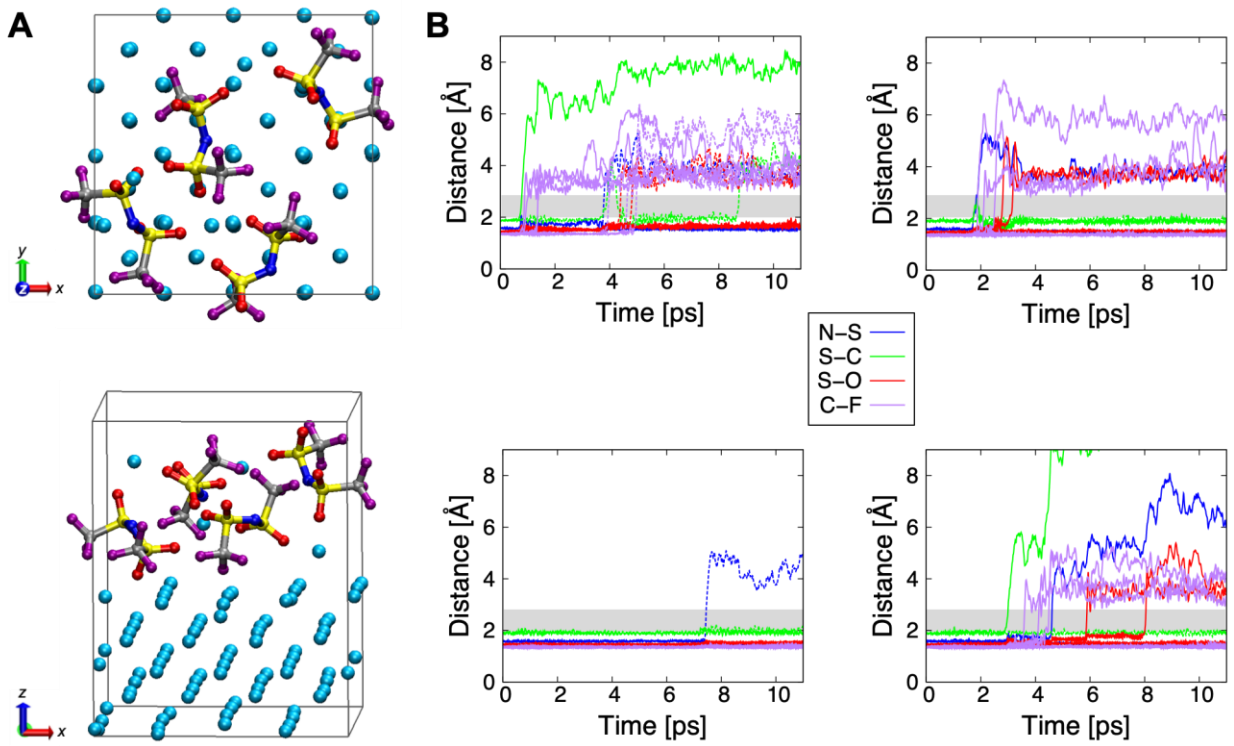


**Figure S6.** The DFT-MD simulation for a small system at 400 K.[5] (A) Top view (upper) and side view (bottom) of the initial structure containing 4 TFSI molecules on the Li slab layer (84 Li). (B) Bond distances within each TFSI molecule at the beginning of the simulation.
The following colors represent the species: Li – cyan, F – purple, C – gray, N – blue, O – red, S – yellow, and H – white. The gray box indicates a bond breaking range from 2.0 Å to 2.8 Å, which is ~50 % longer than the original bond length for the shortest C–F bond, 1.35 Å, and the longest C–S bond, 1.89 Å.

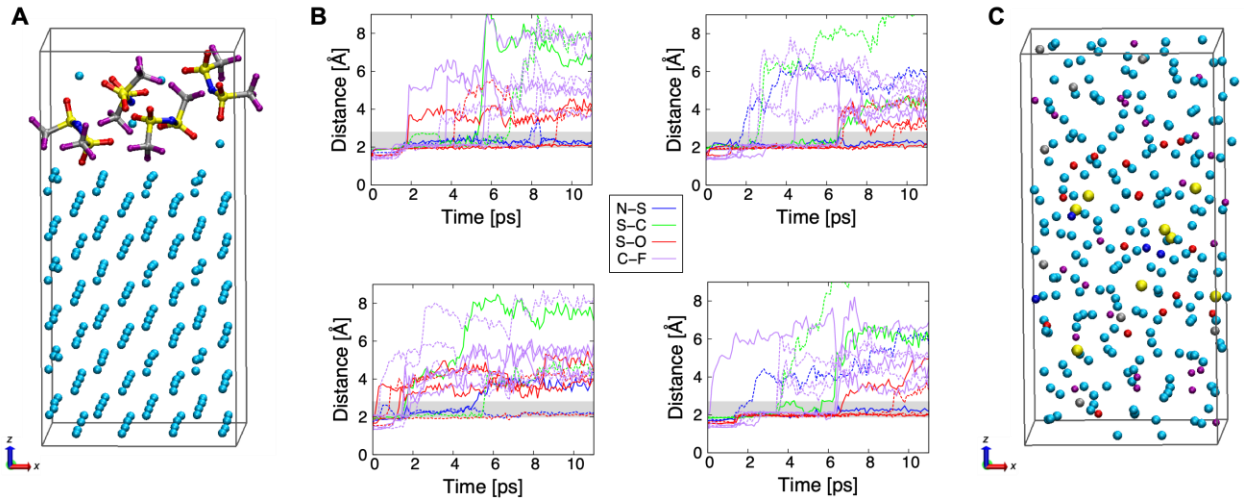


**Figure S7.** The ReaxFF MD simulation for a small system at 400 K. (A) The initial structure of the system containing 4 TFSI molecules on the thicker Li slab layers (196 Li) compared to that of DFT-MD. (B) Bond distances within each TFSI molecule at the beginning of the simulation. (C) A snapshot structure after 100 ps MD simulation showing fully decomposed anions by Li, where the bond distance cutoff for visualization was set to 2.0 Å.

The following colors represent the species: Li – cyan, F – purple, C – gray, N – blue, O – red, S – yellow, and H – white. The gray box indicates a bond breaking range from 2.0 Å to 2.8 Å, which is ~50 % longer than the original bond length for the shortest C–F bond, 1.35 Å, and the longest C–S bond, 1.89 Å.

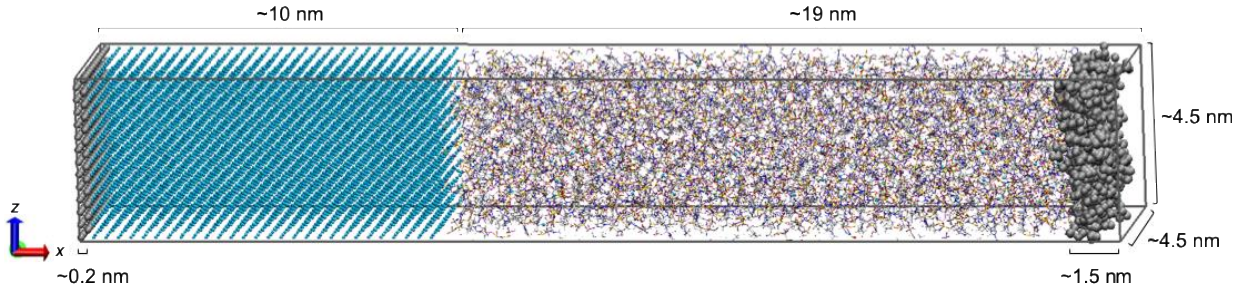


**Figure S8.** The initial Li-metal – [TFSI][BMIM] model system (Li: cyan, F: purple, C: gray, N: blue, O: red, S: yellow, and H: white). Li and IL molecules at both ends (dark gray) were fixed to allow the reactions only at one interface.

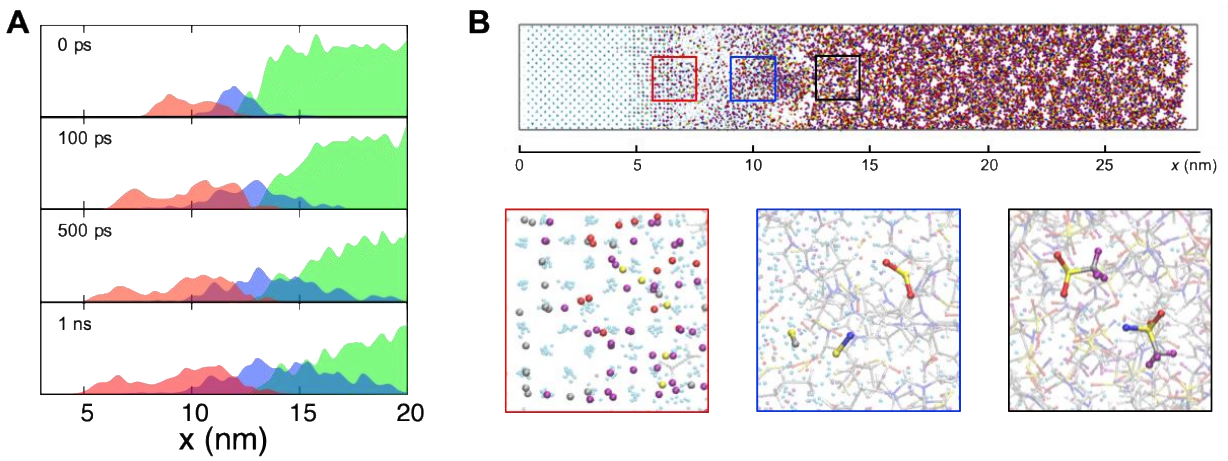


**Figure S9.** (A) The distribution of the atomic densities of the fully decomposed (red), partially decomposed (blue), and not decomposed (green) TFSI, at different time steps. (B) The snapshots of representative decomposition products of the TFSI anions from the final frame (Li: cyan, F: purple, C: gray, N: blue, O: red, S: yellow, and H: white). The anode side of the SEI consists of the fully decomposed components (red box), while small fragments (blue box) and large fragments (black box) mainly contribute to the middle and electrolyte parts of the SEI, respectively.

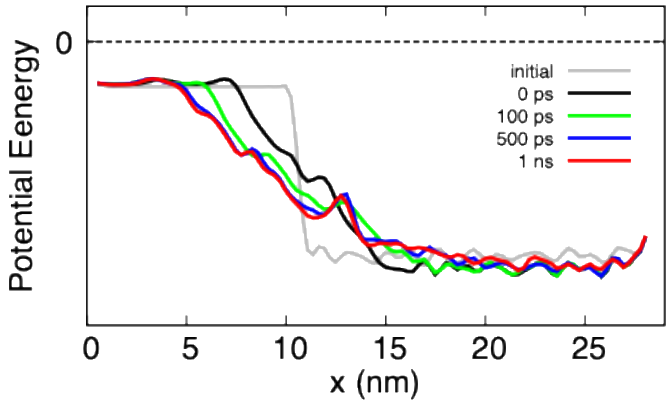


**Figure S10.** The estimated potential energy of the Li-metal – [TFSI][BMIM] system along the *x*-direction after different time intervals of the simulation.

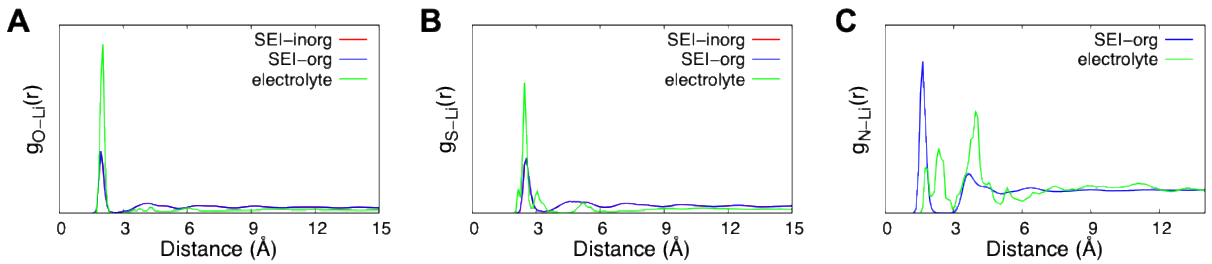


**Figure S11.** The RDF plots for (A) O-Li, (B) S-Li, and (C) N-Li pairs, respectively. The ranges of each region are indicated in Figure 3A. The SEI-inorg is not shown in C, because no N species are in the inorganic layer.

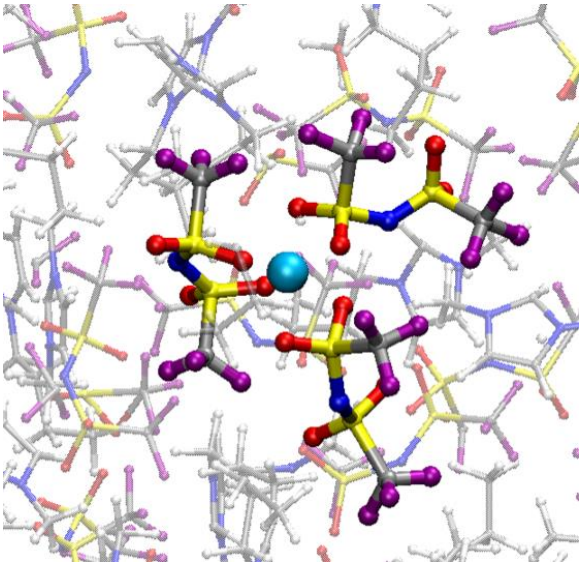

**Figure S12.** Representative interactions between a Li-ion and TFSI anions in the [TFSI][BMIM] IL. Oxygens of the TFSI anions interact strongly with the Li-ion (Li: cyan, F: purple, C: gray, N: blue, O: red, S: yellow, and H: white).

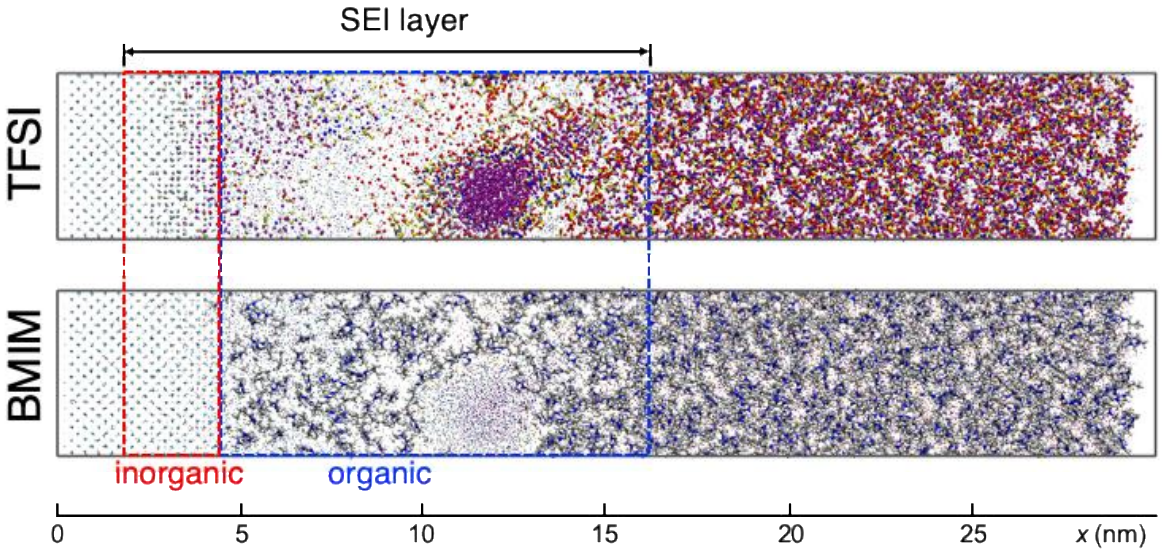


**Figure S13.** The SEI layer showing two distinct phases: inorganic (~2.5 nm thick) and organic (~12.5 nm thick). The inorganic phase is composed only of products of fully decomposed TFSI. The following colors represent the species: Li – cyan, F – purple, C – gray, N – blue, O – red, S – yellow, and H – white.

## TABLES

**Table S1.** ReaxFF parameter optimization: experimental and ReaxFF heat of formation (kcal/mol) for various crystalline phases.

| Crystalline phases | Experiment[Refs] | ReaxFF |
|---|---|---|
| LiF | -147.23[11] | -146.09 |
| $Li_2O$ | -142.90[11] | -142.83 |
| $Li_2S$ | -105.50[11] | -106.92 |
| $Li_3N$ | -40.94[12] | -47.13 |
| $Li_2C_2$ | -15.60[13] | -16.77 |

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**ReaxFF reactive force field parameters for the Li-metal and [TFSI][BMIM] ionic liquid system:**

```
Reactive MD-force field: C/O/H/F/Li/S/N force field;
 39       ! Number of general parameters
   50.0000 !p(boc1)        Overcoordination parameter
    9.5469 !p(boc2)        Overcoordination parameter
   26.5405 !p(coa2)        Valency angle conjugation parameter
    1.5105 !p(trip4)       Triple bond stabilization parameter
    6.6630 !p(trip3)       Triple bond stabilization parameter
   70.0000 !kc2            C2-correction
    1.0588 !p(ovun6)       Undercoordination parameter
    4.6000 !p(trip2)       Triple bond stabilization parameter
   12.1176 !p(ovun7)       Undercoordination parameter
   13.3056 !p(ovun8)       Undercoordination parameter
  -10.1292 !p(trip1)       Triple bond stabilization parameter
    0.0000 !(swa)          Lower Taper-radius
   10.0000 !(swb)          Upper Taper-radius
    0.0000 !p(fe1)         Fe dimer correction
   33.8667 !p(val6)        Valency undercoordination
    6.0891 !p(lp1)         Valency angle/lone pair parameter
    1.0563 !p(val9)        Valency angle parameter
    2.0384 !p(val10)       Valency angle parameter
    6.1431 !p(fe2)         Fe dimer correction
    6.9290 !p(pen2)        Double bond/angle parameter
    0.3989 !p(pen3)        Double bond/angle parameter: overcoord
    3.9954 !p(pen4)        Double bond/angle parameter: overcoord
    0.0000 !p(fe3)         Fe dimer correction
    5.7796 !p(tor2)        Torsion/BO parameter
   10.0000 !p(tor3)        Torsion overcoordination
    1.9487 !p(tor4)        Torsion overcoordination
    0.0000 !p(elho)        eReaxFF
    2.1645 !p(cot2)        Conjugation
    1.5591 !p(vdW1)        vdW shielding
    0.1000 !               Cutoff for bond order (*100)
    2.1365 !p(coa4)        Valency angle conjugation parameter
    0.6991 !p(ovun4)       Overcoordination parameter
   50.0000 !p(ovun3)       Overcoordination parameter
    1.8512 !p(val8)        Valency/lone pair parameter
    0.0000 !not used
    0.0000 !not used
    0.0000 !not used
    0.0000 !not used
    2.6962 !p(coa3)        Valency angle conjugation parameter
 11    ! Nr of atoms; atomID;ro(sigma); Val;atom mass;Rvdw;Dij;gamma
            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     1.3825   4.0000  12.0000   1.9133   0.1853   0.9000   1.1359   4.0000
       9.7602   2.1346   4.0000  33.2433  79.5548   5.8678   7.0000   0.0000
       1.2306   0.0000 199.0303   8.6991  34.7289  13.3894   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   5.3200   7.4366   1.0000
      -0.1000   0.0000  54.5000   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   1.9236   0.0904   1.0503   1.0863   6.0000
      10.2127   7.7719   4.0000  36.9573 116.0768   8.5000   8.9989   2.0000
       0.9088   1.0003  60.8726  20.4140   3.3754   0.2702   0.9745   0.0000
      -3.6141   2.7025   1.0493   4.0000   2.9225   0.0000   0.0000   0.0000
 S     1.9186   2.0000  32.0600   1.6516   0.4937   0.7530   1.6593   6.0000
       9.0227   4.9055   4.0000  30.0000 112.1416   6.5745   9.0000   2.0000
       1.0000   3.4994  65.0000  12.0000  22.1978  15.3230   0.9745   0.0000
     -15.7363   2.8802   1.0338   6.2998   2.8793   0.0000   0.0000   0.0000
 Mo    2.4695   5.6375  95.9400   1.8471   0.3413   1.0000   0.1000   6.0000
      13.1958  44.8826   4.0000   0.0000   0.0000   0.7695   6.0677   0.0000
       0.1000   0.0000 152.6300   3.4529   0.0722   3.1767   0.8563   0.0000
     -17.9815   3.1072   1.0338   8.0000   3.4590   0.0000   0.0000   0.0000
```

```
Ni   1.8201   2.0000  58.6900   1.9449   0.1880   0.8218   0.1000   2.0000
    12.1594   3.8387   2.0000   0.0000   0.0000   4.8038   7.3852   0.0000
    -1.0000   0.0000  95.6300  50.6786   0.6762   0.0981   0.8563   0.0000
    -3.7733   3.6035   1.0338   8.0000   2.5791   0.0000   0.0000   0.0000
Li   1.9814   1.0000   6.9410   1.8000   0.2939   0.9387  -0.1000   1.0000
     9.0616   1.3258   1.0000   0.0000   0.0000  -3.0000  10.0241   0.0000
    -1.0000   0.0000  37.5000   5.4409   6.9107   0.1973   0.8563   0.0000
    -2.5068   2.2989   1.0338   1.0000   2.8103   1.3000   0.2000  13.0000
B    1.5530   3.0000  10.8110   1.6512   0.1000   0.9480   1.0000   3.0000
    10.3025   2.3647   3.0000   0.7036  80.0000   4.0000   7.0000   0.0000
    -1.3000   0.0000 151.3700   7.6069   1.9324   1.0943   0.0000   0.0000
    -3.1611   4.0000   1.0564   3.0000   2.8413   0.0000   0.0000   0.0000
F    1.1620   1.0000  18.9984   1.5562   0.1213   0.5000  -0.1000   7.0000
    10.2712   7.5000   1.0000   9.2533   0.2000   9.0000   8.0000   0.0000
    -1.0000   3.4296  18.0000   6.9821   4.1799   1.0561   0.0000   0.0000
    -7.3000   2.6656   1.0493   4.0000   2.9225   0.0000   0.0000   0.0000
P    1.5994   3.0000  30.9738   1.7000   0.1743   1.0000   1.3000   5.0000
     9.1909  14.9482   5.0000   0.0000   0.0000   1.8000   7.0946   0.0000
    -1.0000  25.0000   1.5000   0.2187  21.4305  15.1425   0.0000   0.0000
    -3.9294   3.4831   1.0338   5.0000   2.8793   0.0000   0.0000   0.0000
N    1.6157   3.0000  14.0000   1.9376   0.1203   1.0000   1.2558   5.0000
     9.4267  26.8500   4.0000   8.6294 100.0000   7.6099   7.7500   2.0000
     1.0439   0.1000 119.9837   1.7640   2.7409   2.3814   0.9745   0.0000
    -6.5798   4.4843   1.0183   4.0000   2.8793   0.0000   0.0000   0.0000
51      ! Nr of bonds; at1;at2;De(sigma);De(pi);De(pipi);p(be1);p(b
                    p(be2);p(bo3);p(bo4);n.u.;p(bo1);p(bo2)
 1  1 156.6463  99.9144  80.0715  -0.8028  -0.4648   1.0000  37.6741   0.4292
       0.4291  -0.1024   9.2608   1.0000  -0.0500   6.8233   1.0000   0.0000
 1  2 170.2316   0.0000   0.0000  -0.5931   0.0000   1.0000   6.0000   0.7140
       5.2267   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  3 146.4038 154.9131  61.1630  -0.9704  -0.0842   1.0000  11.0135   0.1548
       2.3427  -0.2649   6.5137   1.0000  -0.1868   6.1410   0.0000   0.0000
 3  3  60.1463 176.6202  51.1430  -0.2802  -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  4 210.9101  78.3627  55.2528  -0.2963  -0.5211   1.0000  18.9617   0.5938
       2.1958  -0.1912  14.0034   1.0000  -0.1261   4.8222   1.0000   0.0000
 2  4 183.1582   0.0000   0.0000  -0.7544   0.0000   1.0000   6.0000   0.3725
      11.7366   1.0000   0.0000   1.0000  -0.0595   4.6177   0.0000   0.0000
 4  4  84.3765  31.1563   0.0000  -0.8610  -0.4781   1.0000  17.8574   0.3198
       0.4942  -0.1773   8.4125   1.0000  -0.0889   6.8515   1.0000   0.0000
 1  5   0.5356   0.9614   0.0000   0.3817  -0.3000   1.0000  36.0000   0.2142
       0.6116  -0.2579   6.1366   1.0000  -0.0913   6.6008   1.0000   0.0000
 2  5 101.0000   0.0000   0.0000  -0.5019  -0.3000   0.0000  36.0000   0.3712
       0.0705  -0.3027  15.0243   1.0000  -0.0950   6.5090   0.0000   0.0000
 3  5 108.9868  10.5806 137.5564   0.8861  -0.2172   1.0000  19.1047   1.2087
       0.9510  -0.1831   7.2198   1.0000  -0.1266   6.0906   1.0000   0.0000
 4  5  82.5107  27.2572 137.6546   1.0000  -0.2304   1.0000  19.1688   0.4660
       1.0151  -0.1596   7.8950   1.0000  -0.0909   5.5509   1.0000   0.0000
 5  5  51.8235   0.0000   0.0000   0.8271  -0.3000   0.0000  16.0000   0.2670
       0.2248  -0.3000  16.0000   1.0000  -0.1908   7.3978   0.0000   0.0000
 3  4 184.8866 217.1354   0.0000   0.1769  -0.2406   1.0000  22.1005   0.1418
       0.9091  -0.2751   8.4347   1.0000  -0.1424   6.7434   1.0000   0.0000
 1  6  83.5810   9.0383   0.0000   0.2531  -0.2000   1.0000  16.0000   0.0529
       1.4085  -0.1113  13.3900   1.0000  -0.1436   4.5683   1.0000   0.0000
 2  6 114.7566   0.0000   0.0000  -0.8939   0.0000   1.0000   6.0000   0.1256
       0.1054   1.0000   0.0000   1.0000  -0.1196   5.0815   0.0000   0.0000
 3  6 105.3618   0.0000   0.0000  -0.0456  -0.2000   1.0000  16.0000   0.1870
       0.7193  -0.2500  15.0000   1.0000  -0.0880   5.7169   1.0000   0.0000
 6  6  91.2220   0.0000   0.0000  -0.2538  -0.2000   0.0000  16.0000   0.2688
       1.4651  -0.2000  15.0000   1.0000  -0.1435   4.3908   0.0000   0.0000
 5  6  56.5379   0.0000   0.0000  -0.3241  -0.2000   0.0000  16.0000   0.1607
```

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        2.6232  -0.2000  15.0000   1.0000  -0.1790   4.4051   0.0000   0.0000
 4  6  79.7256   0.0000   0.0000   0.3100  -0.2000   0.0000  16.0000   0.1466
        0.7435  -0.2500  25.0000   1.0000  -0.0929   5.3027   0.0000   0.0000
 1  7  45.7211  -0.0200   0.0000   0.6313  -0.5000   0.0000  35.0000   0.1810
        0.8439  -0.2500  11.9965   1.0000  -0.0522   4.3603   0.0000   0.0000
 2  7  36.3483   0.0000   0.0000  -0.9999   0.0000   0.0000   6.0000   0.4500
        2.0000   0.0000  12.0000   1.0000  -0.0697   5.0219   0.0000   0.0000
 3  7  97.9383   0.0000   0.0000  -0.3751   0.3000   0.0000   6.0000   0.4328
        1.3021  -0.2500  11.9965   1.0000  -0.0592   5.4275   0.0000   0.0000
 4  7  88.5127   0.0000   0.0000  -0.4648  -0.5000   0.0000  25.0000   0.2776
        0.4455  -0.2500  20.0000   1.0000  -0.1826   5.4446   0.0000   0.0000
 7  7  34.3154   0.0000   0.0000   0.5995   0.3000   0.0000  26.0000   0.5445
        0.5752   0.0000  12.0000   1.0000  -0.1382   4.5000   0.0000   0.0000
 1  8 180.3526  50.0000   0.0000  -0.1860  -0.4591   1.0000  37.7369   0.2590
        0.2807  -0.2047  10.2887   1.0000  -0.0641   5.9561   1.0000   0.0000
 2  8 165.3660   0.0000   0.0000  -0.2658  -0.3000   1.0000  25.0000   0.3019
        6.1522   0.0000   0.0000   1.0000  -0.0933   5.4815   1.0000   0.0000
 3  8 236.5417  65.2243   0.0000  -0.4987  -0.2500   1.0000  25.0000   1.0000
        0.9994  -0.2342  17.4842   1.0000  -0.1262   5.8863   1.0000   0.0000
 4  8   0.0000   0.0000   0.0000   0.9000  -0.2500   1.0000  25.0000   0.5201
        1.0000  -0.1488  10.0786   1.0000  -0.1647   6.3839   1.0000   0.0000
 8  8  85.8601   0.0000   0.0000   1.0000  -0.2500   1.0000  25.0000   0.7894
        0.8860  -0.2000  25.0000   1.0000  -0.0820   8.6292   1.0000   0.0000
 1  9 185.5699   0.0000   0.0000  -0.6826  -0.5000   1.0000  35.0000   0.8994
        4.7452  -0.2500  15.0000   1.0000  -0.1214   4.1366   1.0000   0.0000
 2  9 265.0555   0.0000   0.0000  -0.6839  -0.2000   0.0000  16.0000   0.4242
       49.7545  -0.2000  15.0000   1.0000  -0.0758   6.0344   0.0000   0.0000
 3  9 112.9341   0.0000   0.0000  -0.4700  -0.5000   1.0000  45.0000   0.5656
        1.4209  -0.2500  15.0000   1.0000  -0.0406   5.5704   1.0000   0.0000
 4  9 208.5797   0.0000   0.0000  -0.9477  -0.5000   1.0000  45.0000   1.1437
        1.4579  -0.2500  15.0000   1.0000  -0.1925   4.8604   1.0000   0.0000
 7  9 100.5404   0.0000   0.0000  -0.5542  -0.5000   0.0000  45.0000   0.2773
        3.4090  -0.2500  15.0000   1.0000  -0.0786   4.3125   0.0000   0.0000
 8  9 150.6978   0.0000   0.0000   0.1373  -0.1418   1.0000  13.1260   0.3916
        0.2867  -0.1310  10.7257   1.0000  -0.1182   6.8737   1.0000   0.0000
 9  9  75.6988 100.5231   0.0000   0.8760  -0.3500   1.0000  25.0000   1.5575
        0.0200  -0.2500  15.0000   1.0000  -0.1183   5.1151   1.0000   0.0000
 1 10   0.0000   0.0000   0.0000   0.2500  -0.5000   1.0000  45.0000   0.6000
        0.4000  -0.2500  15.0000   1.0000  -0.1000  10.0000   1.0000   0.0000
 2 10   0.0000   0.0000   0.0000   0.2500  -0.5000   1.0000  45.0000   0.6000
        0.4000  -0.2500  15.0000   1.0000  -0.1000  10.0000   1.0000   0.0000
 3 10   0.0000   0.0000   0.0000   0.2500  -0.5000   1.0000  45.0000   0.6000
        0.4000  -0.2500  15.0000   1.0000  -0.1000  10.0000   1.0000   0.0000
 7 10   0.0000   0.0000   0.0000   0.2500  -0.5000   1.0000  45.0000   0.6000
        0.4000  -0.2500  15.0000   1.0000  -0.1000  10.0000   1.0000   0.0000
 9 10 153.5200   0.0000   0.0000   0.3010  -0.5000   1.0000  50.0000   0.1025
        0.4150  -0.5000  15.0000   1.0000  -0.0723   5.3872   1.0000   0.0000
10 10   0.0000   0.0000   0.0000   0.2500  -0.5000   1.0000  45.0000   0.6000
        0.4000  -0.2500  15.0000   1.0000  -0.1000  10.0000   1.0000   0.0000
 1 11 230.6480  83.4300 132.3859  -0.7257  -0.2709   1.0000  29.9009   0.8275
        3.9750  -0.3406   7.9815   1.0000  -0.1620   6.6589   1.0000   0.0000
 2 11 161.1063   0.0000   0.0000  -0.1387   0.0000   1.0000   6.0000   0.7276
        0.6127   1.0000   0.0000   1.0000  -0.0395   7.2218   0.0000   0.0000
 3 11  85.9770  90.1220   0.0000  -0.1794  -0.4462   1.0000  34.9336   0.2655
        2.1655  -0.2173   7.0137   1.0000  -0.2489   4.7873   1.0000   0.0000
 4 11  83.8728 158.4962  10.6453   0.5906  -0.2136   1.0000  42.7701   0.3124
        1.2522  -0.3679   5.1968   1.0000  -0.1670   4.3060   1.0000   0.0000
 7 11  59.9489   0.0000   0.0000  -0.8676  -0.5000   0.0000  25.0000   0.3001
        0.5172  -0.2500  20.0000   1.0000  -0.1067   4.4438   0.0000   0.0000
 9 11 219.0435   0.0000   0.0000  -0.7851  -0.5000   1.0000  45.0000   0.4632
        4.7945  -0.2500  15.0000   1.0000  -0.1655   4.9080   1.0000   0.0000
11 11 134.6492  66.2329 149.2707  -0.7228  -0.1000   1.0000  19.0850   1.0000
        0.6060  -0.2050   9.7308   1.0000  -0.1791   5.8008   1.0000   0.0000
36    ! Nr of off-diagonal terms. at1;at2;Dij;RvdW;alfa;ro(sigma);r
 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    0.1745    1.6542  10.4231   1.3184   1.1401   1.1191
  1  4    0.3656    1.6119  10.7207   1.6790   1.3635  -1.0000
  2  4    0.1017    1.7755   9.6088   1.3696  -1.0000  -1.0000
  1  5    0.1495    2.0794  12.2376   0.0100   1.4060  -1.0000
  2  5    0.1361    1.5875  11.9875   1.4900  -1.0000  -1.0000
  3  5    0.2011    2.0377  10.4646   1.6025   1.4785   1.6595
  4  5    0.2161    1.8729   9.9069   2.0896   1.6848  -1.0000
  3  4    0.1822    1.8309  11.4304   1.4943   1.2907  -1.0000
  1  6    0.0800    1.7085  10.0895   1.5504   1.4005  -1.0000
  2  6    0.0366    1.7306  11.1019   1.2270  -1.0000  -1.0000
  3  6    0.0500    1.8000  11.6139   1.4652  -1.0000  -1.0000
  4  6    0.1664    1.7078  11.8610   1.7692  -1.0000  -1.0000
  5  6    0.3188    2.0391  11.1208   2.3703  -1.0000  -1.0000
  1  7    0.1117    1.6762  12.4579   1.6944   1.0000   1.0000
  2  7    0.1165    1.5761  10.6684   1.4759  -1.0000  -1.0000
  3  7    0.3585    1.4416  10.8424   1.5535   1.0000   1.0000
  4  7    0.2252    2.1533  10.3744   2.1038  -1.0000  -1.0000
  1  8    0.0956    1.7010  11.7436   1.3003   1.1889  -1.0000
  2  8    0.0472    1.4236  11.8887   1.1333  -1.0000  -1.0000
  3  8    0.0907    2.3192   9.8579   1.3103   1.2629  -1.0000
  4  8    0.1000    2.0000  10.0000  -1.0000  -1.0000  -1.0000
  1  9    0.0556    1.6739  11.0578   1.2427  -1.0000  -1.0000
  2  9    0.0752    1.9606   9.9948   1.0331  -1.0000  -1.0000
  3  9    0.1055    1.7390  10.2770   1.2126  -1.0000  -1.0000
  4  9    0.3409    1.6930  10.6301   1.4936  -1.0000  -1.0000
  7  9    0.1664    1.9808   9.7107   1.6587  -1.0000  -1.0000
  8  9    0.0830    1.7419  10.8641   1.3592  -1.0000  -1.0000
  9 10    0.1211    1.7575   9.6653   1.3555  -1.0000  -1.0000
  1 11    0.1147    1.6475  10.4840   1.5441   1.0839   1.0216
  2 11    0.0480    2.3000   9.0050   1.0156  -1.0000  -1.0000
  3 11    0.0557    1.9804  10.1404   1.2503   1.1170   1.0125
  4 11    0.2413    1.7461   9.9357   1.5934   1.4658   1.0220
  7 11    0.1726    1.5073   9.4702   1.5174  -1.0000  -1.0000
  9 11    0.1658    1.7458  10.5176   1.4246  -1.0000  -1.0000
132   ! Nr of angles. at1;at2;at3;Thetao,o;p(val1);p(val2);p(coa1);
  3  4  3  62.5000   9.9619   3.2919  -1.0365   0.4516   0.0000   1.3077
  1  4  3  75.1000  16.4780   5.0545   0.0000   0.7250   0.0000   1.0384
  4  1  9  70.1233  23.4636   4.9273   0.0000   3.3034   0.0000   3.3671
  9  1  9  75.1477  27.4433   4.9794   0.0000   3.4269   0.0000   3.2642
  3  4 11  65.9219  42.8194   4.5719   0.0000   2.2424   0.0000   1.6980
  4 11  4  58.7095  26.3208   1.0000   0.0000   1.0764   0.0000   3.3900
  7  1  7  71.1401   7.4370   3.8886   0.0000   2.5612   0.0000   1.1416
  7  3  7  95.7136   2.2375   4.0707   0.0000   2.7428   0.0000   2.1527
  7  4  7 110.0000   2.8100   4.1060   0.0000   1.5751   0.0000   1.7554
  7  9  7  92.0257   1.3076   2.5528   0.0000   2.3697   0.0000   1.0624
  7 11  7  60.9696   2.0706   3.5501   0.0000   2.3388   0.0000   1.1372
  1  1  1  67.2326  22.0695   1.6286   0.0000   1.7959  15.4141   1.8089
  1  1  3  49.5561   7.3771   4.9568   0.0000   0.7533  15.9906   1.0010
  3  1  3 124.0171  37.6945   2.5635 -24.3902   1.8646 -42.9758   2.0610
  1  3  1  74.3994  44.7500   0.7982   0.0000   3.0000   0.0000   1.0528
  1  3  3 119.0854  37.6478   2.0268   0.0000   0.8037  67.0264   2.9826
  3  3  3  80.7324  30.4554   0.9953   0.0000   1.6310  50.0000   1.0783
  3  3  4 150.2283  45.0000   5.9341   0.0000   2.7893   0.0000   1.0782
  3  4  4  65.0000  45.8401   2.9557   0.0000   2.0952   0.0000   1.0323
  1  1  4  68.9986  31.4057   4.8471   0.1463   0.1076   0.0000   2.5166
  1  4  1  30.7500   4.5000   7.0000   0.1463   1.4452   0.0000   2.8788
  1  4  4  84.4685   5.2103   6.6033   0.1463   0.0905   0.0000   2.9037
  4  4  4  70.3671   5.7180   7.0000   0.0000   0.3683   0.0000   2.4869
  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
  2  1  3  65.0000  14.2057   4.8649   0.0000   0.3504   0.0000   1.7185
```

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 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 |
| 1 | 2 | 4 | 0.0000 | 0.0019 | 6.0000 | 0.0000 | 0.0000 | 0.0000 | 1.0400 |
| 2 | 1 | 4 | 30.9196 | 11.3010 | 0.5535 | 0.0000 | 0.0050 | 0.0000 | 1.9267 |
| 1 | 4 | 2 | 100.0000 | 14.2598 | 4.2424 | 0.0000 | 0.0050 | 0.0000 | 3.0000 |
| 2 | 4 | 2 | 92.1229 | 42.8350 | 0.6163 | 0.0000 | 1.0235 | 0.0000 | 1.0010 |
| 2 | 4 | 4 | 70.9476 | 9.9024 | 0.6923 | 0.0000 | 0.2031 | 0.0000 | 2.9811 |
| 2 | 3 | 5 | 88.3222 | 7.1767 | 2.4747 | 0.0000 | 0.6219 | 0.0000 | 3.1507 |
| 2 | 4 | 5 | 90.0000 | 20.3126 | 0.7222 | 0.0000 | 0.6873 | 0.0000 | 2.2146 |
| 2 | 5 | 5 | 57.6230 | 6.3083 | 5.0722 | 0.0000 | 0.6873 | 0.0000 | 1.5510 |
| 2 | 5 | 4 | 54.6337 | 8.6317 | 6.9912 | 0.0000 | 1.6873 | 0.0000 | 2.8674 |
| 2 | 5 | 2 | 76.2482 | 11.2841 | 7.6230 | 0.0000 | 0.9375 | 0.0000 | 1.0586 |
| 2 | 3 | 4 | 45.6742 | 13.4413 | 1.5725 | 0.0000 | 0.7737 | 0.0000 | 2.6616 |
| 4 | 2 | 4 | 0.0000 | 7.5000 | 2.0000 | 0.0000 | 0.0000 | 0.0000 | 1.0400 |
| 4 | 2 | 5 | 0.0000 | 7.5000 | 2.0000 | 0.0000 | 0.0000 | 0.0000 | 1.0400 |
| 5 | 2 | 5 | 0.0000 | 7.5000 | 2.0000 | 0.0000 | 0.0000 | 0.0000 | 1.0400 |
| 2 | 5 | 3 | 70.0000 | 12.0000 | 4.0000 | 0.0000 | 1.0000 | 0.0000 | 1.2500 |
| 3 | 2 | 5 | 0.0000 | 15.0000 | 2.0000 | 0.0000 | 0.0000 | 0.0000 | 1.0500 |
| 2 | 1 | 9 | 85.4658 | 0.0100 | 1.9807 | 0.0000 | 1.4400 | 0.0000 | 2.9068 |
| 2 | 1 | 11 | 62.2465 | 35.4859 | 2.1648 | 0.0000 | 0.0110 | 0.0000 | 2.4442 |
| 2 | 3 | 11 | 81.0695 | 20.0000 | 2.0285 | 0.0000 | 0.1218 | 0.0000 | 1.4477 |
| 1 | 11 | 2 | 76.9847 | 49.2262 | 0.9407 | 0.0000 | 0.0300 | 0.0000 | 2.6196 |
| 2 | 11 | 3 | 85.4080 | 40.0000 | 1.7549 | 0.0000 | 0.0222 | 0.0000 | 1.0774 |
| 2 | 11 | 11 | 83.5658 | 40.0000 | 1.3540 | 0.0000 | 0.0222 | 0.0000 | 2.6397 |
| 2 | 11 | 2 | 58.0387 | 1.1862 | 3.9770 | 0.0000 | 0.0222 | 0.0000 | 1.0000 |
| 3 | 5 | 3 | 80.0647 | 49.0226 | 1.1861 | 0.7271 | 0.1000 | 0.0000 | 1.5321 |
| 5 | 3 | 5 | 16.5418 | 38.3796 | 0.5347 | 0.0000 | 0.1000 | 0.0000 | 2.3535 |
| 3 | 3 | 5 | 34.0844 | 11.5602 | 1.5428 | 0.0000 | 0.4319 | 0.0000 | 1.0500 |
| 3 | 5 | 5 | 6.0985 | 0.0302 | 0.1000 | 0.0000 | 0.6142 | 0.0000 | 1.7575 |
| 1 | 3 | 5 | 76.5850 | 8.7797 | 0.8099 | 0.0000 | 2.5889 | 0.0000 | 1.0500 |
| 4 | 5 | 4 | 66.1778 | 17.0744 | 4.2862 | 0.0984 | 1.4056 | 0.0000 | 1.7545 |
| 5 | 4 | 5 | 35.4696 | 10.5159 | 5.6990 | 0.0000 | 3.9985 | 0.0000 | 1.3642 |
| 4 | 4 | 5 | 90.0000 | 32.0246 | 1.1683 | 0.0000 | 3.9500 | 0.0000 | 1.3617 |
| 4 | 5 | 5 | 41.9144 | 0.5409 | 7.1700 | 0.0000 | 3.4295 | 0.0000 | 3.2326 |
| 3 | 5 | 4 | 75.0000 | 25.0000 | 2.0000 | 0.0984 | 1.0000 | 0.0000 | 1.5000 |
| 4 | 3 | 5 | 35.0000 | 12.5000 | 1.5000 | 0.0000 | 0.5000 | 0.0000 | 1.0500 |
| 3 | 4 | 5 | 90.0000 | 30.0000 | 1.2500 | 0.0000 | 3.0000 | 0.0000 | 1.3000 |
| 1 | 6 | 1 | 62.5000 | 16.6806 | 0.7981 | 0.0000 | 0.9630 | 0.0000 | 1.0711 |
| 1 | 1 | 6 | 87.6241 | 12.6504 | 1.8145 | 0.0000 | 0.6154 | 0.0000 | 1.5298 |
| 6 | 1 | 6 | 100.0000 | 40.4895 | 1.6455 | 0.0000 | 0.0100 | 0.0000 | 1.7667 |
| 1 | 6 | 6 | 5.0994 | 3.1824 | 0.7016 | 0.0000 | 0.7465 | 0.0000 | 2.2665 |
| 3 | 6 | 3 | 28.9047 | 27.3847 | 2.5790 | 0.0000 | 0.1078 | 0.0000 | 2.4145 |
| 3 | 3 | 6 | 90.0000 | 39.1857 | 4.8200 | 0.0000 | 0.9067 | 0.0000 | 1.9533 |
| 6 | 3 | 6 | 51.5671 | 2.9451 | 0.6657 | 0.0000 | 1.6341 | 0.0000 | 1.9057 |
| 3 | 6 | 6 | 56.7026 | 3.2665 | 4.3063 | 0.0000 | 0.6729 | 0.0000 | 2.7490 |
| 2 | 6 | 2 | 106.3969 | 30.0000 | 0.9614 | 0.0000 | 1.9664 | 0.0000 | 2.2693 |
| 2 | 2 | 6 | 0.0000 | 26.3327 | 4.6867 | 0.0000 | 0.8177 | 0.0000 | 1.0404 |
| 6 | 2 | 6 | 0.0000 | 60.0000 | 1.8471 | 0.0000 | 0.6331 | 0.0000 | 1.8931 |
| 2 | 6 | 6 | 30.3748 | 1.0000 | 4.8528 | 0.0000 | 0.1019 | 0.0000 | 3.1660 |
| 2 | 6 | 6 | 180.0000 | -27.2489 | 8.3752 | 0.0000 | 0.8112 | 0.0000 | 1.0004 |
| 1 | 6 | 2 | 97.5742 | 10.9373 | 2.5200 | 0.0000 | 1.8558 | 0.0000 | 1.0000 |
| 1 | 2 | 6 | 0.0000 | 0.2811 | 1.1741 | 0.0000 | 0.9136 | 0.0000 | 3.8138 |
| 2 | 1 | 6 | 84.0006 | 45.0000 | 0.6271 | 0.0000 | 3.0000 | 0.0000 | 1.0000 |
| 2 | 3 | 6 | 28.4774 | 12.0885 | 3.2396 | 0.5000 | 0.0778 | 0.0000 | 1.6733 |
| 1 | 6 | 3 | 70.0000 | 25.0000 | 1.0000 | 0.0000 | 1.0000 | 0.0000 | 1.2500 |
| 1 | 3 | 6 | 70.0000 | 25.0000 | 1.0000 | 0.0000 | 1.0000 | 0.0000 | 1.2500 |
| 3 | 1 | 6 | 70.0000 | 25.0000 | 1.0000 | 0.0000 | 1.0000 | 0.0000 | 1.2500 |
| 3 | 2 | 6 | 0.0000 | 1.0000 | 1.3402 | 0.5000 | 0.0500 | 0.0000 | 1.5379 |
| 4 | 6 | 4 | 2.7962 | 7.1073 | 0.5589 | 0.0000 | 0.0554 | 0.0000 | 1.1473 |
| 6 | 4 | 6 | 92.9945 | 26.8345 | 0.9189 | 0.0000 | 0.0100 | 0.0000 | 1.4683 |
| 4 | 6 | 6 | 48.7356 | 9.9227 | 0.1206 | 0.0000 | 0.0893 | 0.0000 | 1.1108 |

```
 4   4   6   64.5223    7.2562    5.2298    0.0000    0.5459    0.0000    1.0400
 2   4   6   83.4937   16.7605    0.8242    0.5000    0.5409    0.0000    1.1378
 4   2   6    0.0000   10.0000    1.0000    0.5000    0.2500    0.0000    1.5000
 5   4   6   61.8263   20.8696    0.2450    0.0000    0.7429    0.0000    1.0400
 4   5   6   60.0000    1.0000    1.0000    0.0000    1.0000    0.0000    1.2500
 4   6   5   60.0000    1.0000    1.0000    0.0000    1.0000    0.0000    1.2500
 5   3   6   44.9106    2.7940    0.5834    0.0000    0.9597    0.0000    1.3151
 3   5   6   60.0000    1.0000    1.0000    0.0000    1.0000    0.0000    1.2500
 3   6   5   60.0000    1.0000    1.0000    0.0000    1.0000    0.0000    1.2500
 2   8   2   50.0000   26.9005    1.7315    0.0000    0.1848    0.0000    1.0400
 2   8   8   55.2500   36.5272    6.0000    0.0000    0.4281    0.0000    2.1149
 2   2   8    0.0000   10.4651    0.1000    0.0000    0.0000    0.0000    3.0000
 2   3   8   75.9746   10.9523    0.8687    0.0000    1.8256    0.0000    2.9875
 2   8   3   65.0000   40.0000    6.0000    0.0000    0.1000    0.0000    3.0000
 3   8   3   50.4947   12.1095    3.5926    0.0000    3.0000   35.0000    1.0400
 8   3   8   90.0000   40.0000    4.7885    0.0000    2.7146    0.0000    1.0400
 3   2   8   52.0162    2.5267    0.3146    0.0000    2.2070    0.0000    2.9111
 3   3   8   90.0000   27.7492    6.0000    0.0000    0.1870    0.0000    1.0400
 8   2   8    0.5000    3.4405    0.9580    0.0000    0.8031    0.0000    1.0000
 8   8   8   60.9386   12.9033    7.8607    0.0000    1.7515    0.0000    2.2405
 3   8   8   70.7224    5.3644    3.4424    0.0000    0.8219    0.0000    2.8000
 1   1   8   30.0491   23.9749    3.2341    0.0000    1.0000    0.0000    1.0000
 1   8   1   80.6555   40.0000    5.6273    0.0000    1.0000    0.0000    3.7089
 1   8   8   70.5217   39.3118    7.9958    0.0000    1.0000    0.0000    1.0000
 8   1   8   47.0626    4.5590    5.6859    0.0000    1.0000    0.0000    1.4685
 1   8   3   75.0000   30.0000    2.0000    0.0000    1.0000    0.0000    2.0000
 1   8   2   65.0000   35.0000    4.0000    0.0000    0.5000    0.0000    2.0000
 9   8   9   65.0386   28.8263    2.2480    0.0000    1.1021    0.0000    1.0400
 8   9   9   70.0000   28.7353    1.2918    0.0000    1.0913    0.0000    1.0400
 8   8   9   70.0000   25.0000    2.5000    0.0000    1.0000    0.0000    1.0400
 9  10   9   92.7358   25.0000    2.5000    0.0000    1.1355    0.0000    1.1514
 1   1  11   77.4923   42.7218    4.3622    0.0000    3.2077   50.0000    2.7926
11   1  11   74.8600   52.6870    2.0030    0.0000    3.3760    0.0000    3.0686
 1  11   1   58.2601   47.8710    1.8642    0.0000    0.9406    0.0000    1.4461
 1   4  11   74.8583   48.5512    6.9669    0.0000    3.4134   50.0000    1.1985
11  11  11    0.0000   27.9213    5.8635    0.0000    0.0000    0.0000    1.0400
 1   4   7  130.8936    8.6656    6.9828    0.0000    3.4977   50.0000    1.5070
 4   1   7  130.8936    8.6656    6.9828    0.0000    3.4977   50.0000    1.5070
71     ! Nr of torsions. at1;at2;at3;at4;;V1;V2;V3;p(tor1);p(cot1);n
 1   1   1   1  -0.2775   10.1210    0.2025   -4.6886   -2.1309    0.0000    0.0000
 1   1   1   3  -0.7098   22.2951    0.0060   -2.5000   -2.1688    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   3  -0.0179    5.0603   -0.1894   -2.5000   -2.0399    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   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   3   0.0531  -17.3983    1.0000   -2.5000   -2.1584    0.0000    0.0000
 3   3   3   3  -2.5000  -25.0000    1.0000   -2.5000   -1.0000    0.0000    0.0000
 0   1   1   0  -0.0098   51.9046    0.2435   -4.5500   -1.9721    0.0000    0.0000
 0   3   3   0   0.5611   25.0350    1.0000   -5.3564   -0.9918    0.0000    0.0000
 4   4   4   4   1.8397  -10.0688   -0.4387   -2.4875   -0.0258    0.0000    0.0000
 3   4   4   4   0.2500   90.0000    0.5000   -6.0000    0.0000    0.0000    0.0000
 3   4   4   3   0.2247   90.0000    0.6100   -6.0339    0.0320    0.0000    0.0000
 1   4   4   1   0.0490   49.6276    0.0785   -7.5561    0.0128    0.0000    0.0000
 4   4   4   7   0.0000    2.0000    0.0100   -9.0000    0.0000    0.0000    0.0000
 7   4   4   7   0.0263   22.1907    0.0085   -5.3761   -0.0153    0.0000    0.0000
 1   1   1   9   0.0016   19.4325   -0.2470   -4.3189   -1.8976    0.0000    0.0000
 9   1   1   9   0.0100   37.2385    0.5751   -5.1000   -1.9746    0.0000    0.0000
 1   1   3   7   0.0100   49.0000    0.2500   -3.8312   -0.0971    0.0000    0.0000
 3   1   3   7  -0.0049   48.3830    0.2500   -3.9625   -0.0201    0.0000    0.0000
 0   1  11   0  -0.7705   47.5626    0.7704   -4.3365   -3.0000    0.0000    0.0000
 3   1  11   1   0.0000   90.0000   -0.2000   -2.5000   -2.0000    0.0000    0.0000
 3   4  11   4   1.9416   39.7453   -1.0000   -6.4779   -2.2386    0.0000    0.0000
 1   4  11   4   1.8981   39.5179   -0.9868   -6.6438   -2.2836    0.0000    0.0000
```

```
 1   4 11   7    1.8670   39.7586  -0.9292   -6.5627   -2.4025    0.0000    0.0000
 9   1   4 11   -0.3544   85.7240   0.3880   -3.1316   -0.1007    0.0000    0.0000
 9   1   4   3   -0.2837   86.3003   0.4231   -2.6099   -0.1107    0.0000    0.0000
 0   4 11   0    2.0000   90.0000  -0.7545   -9.1181   -2.0510    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
 2   1   1   3   -0.3568   22.6472   0.6045   -4.0088   -1.0000    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
 2   1   3   3   -0.5583   80.0000   1.0000   -4.4000   -3.0000    0.0000    0.0000
 3   1   3   2    0.0345   78.9586  -0.6810   -4.1777   -3.0000    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
 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   2   4   0    0.0000    0.0000   0.0000    0.0000    0.0000    0.0000    0.0000
 2   1   3   5    2.1344   29.9850   0.3398   -3.1459   -2.1000    0.0000    0.0000
 1   1   3   5    0.4573   10.0000   1.0000   -7.3632   -2.1000    0.0000    0.0000
 2   3   5   3    0.3709   10.0000   0.9625   -9.0000   -1.0000    0.0000    0.0000
 2   3   4   3    2.5000    2.5000   0.2237  -10.0000    0.0000    0.0000    0.0000
 1   4   4   2    0.0000   50.0000   0.0000   -8.0000    0.0000    0.0000    0.0000
 2   4   4   2    0.0000   50.0000   0.0000   -8.0000    0.0000    0.0000    0.0000
 1   1   1   6    0.0000    5.0000   0.4000   -6.0000    0.0000    0.0000    0.0000
 6   1   1   6    0.0000   44.3024   0.4000   -4.0000    0.0000    0.0000    0.0000
 2   1   1   6    0.0000   21.7038   0.0100   -4.0000    0.0000    0.0000    0.0000
 2   1   6   1    0.0000    5.2500   0.0100   -6.0000    0.0000    0.0000    0.0000
 1   1   6   1    0.0000    5.1676   0.0100   -5.9539    0.0000    0.0000    0.0000
 1   1   6   2    0.0000    5.1676   0.0100   -5.9539    0.0000    0.0000    0.0000
 6   3   3   6    0.0509   30.0000   0.5000   -4.0000    0.0000    0.0000    0.0000
 0   8   8   0    0.0000   42.3911  -0.3192   -4.3105    0.0000    0.0000    0.0000
 0   3   8   0   -2.0000   48.7726  -0.5000   -2.5000    0.0000    0.0000    0.0000
 8   3   3   8    2.0000   75.0000   0.3000   -5.0000    0.0000    0.0000    0.0000
 0   1   8   0    0.0000   30.0000  -0.1000   -5.0000    0.0000    0.0000    0.0000
 1   1   1   8    0.0000    2.0000   0.0000   -6.0000    0.0000    0.0000    0.0000
 8   1   1   8    0.0000    2.0000   0.0000   -6.0000    0.0000    0.0000    0.0000
 2   1   3   7    0.0000   50.0000   0.2000   -4.0000    0.0000    0.0000    0.0000
 1 11   1   2   -0.4607   73.2745   0.8057   -6.5581   -2.7334    0.0000    0.0000
11   1   1   2   -0.2828   45.1749   0.1156   -6.2783   -2.5478    0.0000    0.0000
 1   1   1 11   -0.5541   76.7989   0.7541   -8.0269   -1.9959    0.0000    0.0000
 1   1 11   1   -0.4431   75.1291  -0.7926   -1.6886   -2.8003    0.0000    0.0000
11   1 11   1   -2.2533   83.2815  -0.4856   -7.9986   -1.0007    0.0000    0.0000
 7     ! 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   4    2.5000   -1.0000    1.7976    3.0000
 4   2   3    2.5000   -1.0000    1.7976    3.0000
 4   2   4    1.5000   -2.0000    1.7976    3.0000
 3   2 11    2.0000   -2.5000    1.7976    3.0000
11   2   3    2.0000   -2.5000    1.7976    3.0000
11   2 11    2.0000   -2.5000    1.7976    3.0000
```

**Atom section (by order)**

```
r0(sigma);          Sigma bond covalent radius
Val;                Valency
atom mass;          Atomic mass
Rvdw;               van der Waals radius
Dij;                van der Waals dissociation energy
gamma;              EEM shielding
r0(pi);             Pi bond covalent radius
Val(e);             Number of valence electrons
alfa;               van der Waals parameter
gamma(w);           van der Waals shielding
Val(angle);         Valency for 1,3-BO correction
p(ovun5);           Undercoordination energy
n.u.;
chiEEM;             EEM electronegativity
etaEEM;             EEM hardness
n.u.
r0(pipi);           Double pi bond covalent radius
p(lp2);             Lone pair energy
Heat increment;     Atomic heat of formation
p(boc4);            Bond order correction
p(boc3);            Bond order correction
p(boc5),            Bond order correction
n.u.;
n.u.;
p(ovun2);           Valence angle parameter
p(val3);            Valence angle parameter
n.u.;
Val(boc);           Number of lone pairs
p(val5);            Valence angle parameter
n.u.;
n.u.;
n.u.;
```

**Bond section (by order)**

```
De(sigma);          Sigma bond dissociation energy
De(pi);             Pi bond dissociation energy
De(pipi);           Double pi bond dissociation energy
p(be1);             Bond energy parameter
p(bo5);             Double pi bond order parameter
13corr;             1,3-BO correction
p(bo6);             Double pi bond order parameter
p(ovun1);           Overcoordination penalty
p(be2);             Bond energy parameter
p(bo3);             Pi bond order parameter
p(bo4);             Pi bond order parameter
n.u.;
p(bo1);             Sigma bond order parameter
p(bo2);             Sigma bond order parameter
n.u.;
n.u.;
```

**Off-diagonal section (by order)**

```
Dij;                vdW energy
RvdW;               vdW radius
alfa;               vdW parameter
r0(sigma);          Sigma bond length
r0(pi);             Pi bond length
r0(pipi);           Double pi bond length
```

**Angle section (by order)**

```
Dij;                vdW energy
Thetao,o;           180 – (equilibrium angle)
p(val1);            Valence angle parameter
p(val2);            Valence angle parameter
```

```
p(coa1);            Valence conjugation
p(val7);            Undercoordination
p(pen1);            Penalty energy
p(val4);            Valence angle parameter

Torsion section (by order)
V1;                 V1 torsion barrier
V2;                 V2 torsion barrier
V3;                 V3 torsion barrier
p(tor1);            Torsion angle parameter
p(cot1);            Conjugation energy
n.u.;
n.u.;

Hydrogen bond section (by order)
r(hb);              Hydrogen bond equilibrium distance
p(hb1);             Hydrogen bond energy
p(hb2);             Hydrogen bond/bond order
p(hb3);             Hydrogen bond parameter
```