# Supplementary Material I

Below are listed all the GAFF-IC force-field parameters. Partial charges are not provided, since they should be obtained from ab-initio calculations by using RESP method. A MOL2 file containing the specifications for an HDI molecule is provided at the end of this document, where RESP partial charges are reported.

## Atom types and non-bonded parameters

LJ parameters for the atom types appearing in isocyanates. The source of the parameters is also reported: GAFF-IC is this work, GAFFlipid is from Dickson et al. (Ref. 33 in main text), default means the GAFF standard values.

| Atom type | Mass [amu] | $\epsilon$ [Kcal/mol] | $\sigma$ [Å] | comment (source) |
|---|---|---|---|---|
| n2 | 14.010 | 1.795 | 0.155 | N in isocyanate (GAFF-IC) |
| c1 | 12.010 | 1.874 | 0.155 | C in isocyanate (GAFF-IC) |
| o | 16.000 | 1.632 | 0.175 | O in isocyanurate/isocyanate (GAFF-IC) |
| c3 | 12.010 | 2.010 | 0.055 | sp3 carbon (GAFFlipid) |
| hc | 1.008 | 1.340 | 0.024 | hydrogen in -CH3- (GAFFlipid) |
| h1 | 1.008 | 1.340 | 0.024 | hydrogen in -CH2- (GAFFlipid) |
| c | 12.010 | 1.908 | 0.086 | sp2 C in isocyanurate (default) |
| n | 14.010 | 1.824 | 0.175 | sp2 N in isocyanurate (default) |

## Bond parameters

All bond equilibrium lengths were adjusted to match the B3LYP-6311++G(d,p) calculations. The bond energy term in the force field is:

$$E_{bond} = \frac{k_b}{2} \left(r_{ij} - b_0\right)^2$$

| Bond | $k_b$ [Kcal/(mol·Å$^2$)] | $b_0$ [Å] |
|---|---|---|
| c - n | 478.20 | 1.379 |
| c - o | 648.00 | 1.200 |
| n - c3 | 330.60 | 1.478 |
| c3 - h1 | 335.90 | 1.095 |
| c3 - c3 | 303.10 | 1.525 |
| c3 - hc | 337.30 | 1.096 |
| c3 - n2 | 313.80 | 1.450 |
| n2 - c1 | 769.80 | 1.199 |
| c1 - o | 777.00 | 1.171 |

## Angle parameters

All equilibrium angle values were adjusted to match the B3LYP-6311++G(d,p) calculations. The angle energy term in the force field is:

$$E_{angle} = \frac{k_a}{2} \left(\theta_{ijk} - \theta_0\right)^2$$

| angle | $k_a$ [Kcal/(mol·deg$^2$)] | $\theta_0$ [deg]] |
|---|---|---|
| c - n - c | 65.33 | 124.13 |
| c - n - c3 | 63.92 | 118.02 |
| n - c - o | 75.83 | 122.03 |
| n - c - n | 74.80 | 115.80 |
| n - c3 - h1 | 49.82 | 112.32 |
| n - c3 - c3 | 65.85 | 112.13 |
| n - cc - n2 | 74.78 | 122.59 |
| c3 - c3 - hc | 46.37 | 109.50 |
| c3 - c3 - c3 | 63.21 | 112.69 |
| h1 - c3 - h1 | 39.18 | 109.55 |
| h1 - c3 - c3 | 46.36 | 110.20 |
| hc - c3 - hc | 39.43 | 106.25 |
| c3 - c3 - n2 | 66.40 | 113.13 |
| c3 - n2 - c1 | 58.67 | 138.85 |
| h1 - c3 - n2 | 49.26 | 109.01 |
| n2 - c1 - o | 69.15 | 173.76 |

## Dihedral parameters

All dihedral values were refitted as described in the main text. The dihedral energy term of the force field is:

$$V_{dihe}(\phi) = \sum_{i=1}^{4} V_i \left[1 + cos\left(i\phi + \delta_i\right)\right]$$

| Dihedral | i | $V_i$ [Kcal/mol] | $\delta_i$ [degrees] |
|---|---|---|---|
| c -n -c -n | 2 | 25.0000 | 180 |
| c -n -c -o | 2 | 25.0000 | 180 |
| c -n -c3-c3 | 4 | -0.1439 | 0 |
| c -n -c3-c3 | 2 | 0.3789 | 0 |
| n -c -n -c3 | 2 | 25.0000 | 180 |
| n -c3-c3-hc | 3 | 0.1353 | 0 |
| n -c3-c3-c3 | 4 | 0.0106 | 180 |
| n -c3-c3-c3 | 3 | 0.1393 | 0 |
| n -c3-c3-c3 | 2 | -0.0779 | 180 |
| n -c3-c3-c3 | 1 | -0.4949 | 0 |
| o -c -n -c | 2 | 25.0000 | 180 |
| c3-c3-c3-hc | 3 | 0.1392 | 0 |
| h1-c3-c3-hc | 3 | 0.1827 | 0 |
| h1-c3-c3-c3 | 3 | 0.1827 | 0 |
| hc-c3-c3-hc | 3 | 0.1392 | 0 |
| c3-c3-c3-c3 | 4 | -0.0751 | 180 |
| c3-c3-c3-c3 | 3 | 0.1392 | 0 |
| c3-c3-c3-c3 | 2 | -0.1686 | 180 |
| c3-c3-c3-c3 | 1 | 0.3456 | 0 |
| c3-c3-c3-n2 | 4 | -0.0493 | 0 |
| c3-c3-c3-n2 | 3 | 0.1827 | 0 |
| c3-c3-c3-n2 | 2 | -0.1918 | 180 |
| c3-c3-c3-n2 | 1 | -0.0956 | 0 |
| c3-c3-n2-c1 | 3 | 0.0000 | 0 |
| hc-c3-c3-n2 | 3 | 0.1827 | 0 |
| c3-n2-c1-o | 2 | 0.0000 | 0 |
| h1-c3-n2-c1 | 3 | 0.0000 | 0 |

## MOL2 file for the HDI molecule

```
#This is the MOL2 file for the HDI molecule.
#Last column of the ATOM section contains the RESP partial charged,
#already scaled by the 1/sqrt(2) factor.


@<TRIPOS>MOLECULE
HDI
24    23     1     0     0
SMALL
resp


@<TRIPOS>ATOM
1 C1          -1.6810   -0.6270   -0.1450 c3        1 HDI      0.090994
2 H1          -1.4040   -1.6860   -0.0740 h1        1 HDI      0.0424462
3 H2          -1.1910   -0.2320   -1.0390 h1        1 HDI      0.0424462
4 C2          -1.2070    0.1280    1.0920 c3        1 HDI      0.0224422
5 H3          -1.5170    1.1770    1.0100 hc        1 HDI      0.0176105
6 H4          -1.7120   -0.2790    1.9770 hc        1 HDI      0.0176105
7 C3           0.3040    0.0410    1.2700 c3        1 HDI     -0.00190212
8 H5           0.8040    0.4430    0.3780 hc        1 HDI     -0.00738785
9 H6           0.6080   -1.0120    1.3400 hc        1 HDI     -0.00738785
10 C4          0.7960    0.7900    2.5050 c3        1 HDI     -0.00190212
11 H7          0.2960    0.3890    3.3970 hc        1 HDI     -0.00738785
12 H8          0.4920    1.8430    2.4350 hc        1 HDI     -0.00738785
13 C5          2.3070    0.7030    2.6830 c3        1 HDI      0.0224422
14 H9          2.8120    1.1100    1.7980 hc        1 HDI      0.0176105
15 H10         2.6170   -0.3460    2.7650 hc        1 HDI      0.0176105
16 C6          2.7810    1.4580    3.9200 c3        1 HDI      0.090994
17 H11         2.2910    1.0630    4.8140 h1        1 HDI      0.0424462
18 H12         2.5040    2.5170    3.8490 h1        1 HDI      0.0424462
19 N1          4.2020    1.3630    4.1300 n2        1 HDI     -0.40123678
20 N2         -3.1020   -0.5330   -0.3550 n2        1 HDI     -0.40123678
21 C7         -4.1150   -0.6080    0.2810 c1        1 HDI      0.513372
22 C8          5.2160    1.4440    3.4950 c1        1 HDI      0.513372
23 O1         -5.1680   -0.6570    0.7930 o         1 HDI     -0.329007
24 O2          6.2680    1.4980    2.9840 o         1 HDI     -0.329007
@<TRIPOS>BOND
1    1    2 1
2    1    3 1
3    1    4 1
4    1   20 1
5    4    5 1
6    4    6 1
```

```
7    4    7 1
8    7    8 1
9    7    9 1
10    7   10 1
11   10   11 1
12   10   12 1
13   10   13 1
14   13   14 1
15   13   15 1
16   13   16 1
17   16   17 1
18   16   18 1
19   16   19 1
20   19   22 2
21   20   21 2
22   21   23 2
23   22   24 2
@<TRIPOS>SUBSTRUCTURE
1 HDI        1 TEMP              0 ****  ****    0 ROOT
```