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]	ϵ [Kcal/mol]	σ [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)]	θ_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]	δ_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
```