Electronic Supplementary Information for

Structure and Dynamics of CO_2 and N_2 in a Tetracyanoborate Based Ionic Liquid

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Table S1. Simulated density and diffusivity of the CO_2/N_2 emimB$(CN)_4$ mixtures. The uncertainty in density is within 1% and in self-diffusivity within 10%, based on averaging over multiple independent runs.

Temperature (K)	Mole fraction (%)	Density (g/cm^3)	D_+ (10^{-8} m^2/s)	D_- (10^{-8} m^2/s)	D_{solute} (10^{-8} m^2/s)
Neat IL					
400		0.899	0.093	0.073	
360		0.927	0.047	0.037	
340		0.945	0.028	0.023	
320		0.963	0.017	0.013	
300		0.983	0.009	0.006	
CO_2 mixture					
400	2.5	0.891	0.092	0.074	0.438
360	2.5	0.926	0.047	0.038	0.254
320	2.5	0.964	0.016	0.014	0.117
300	2.5	0.983	0.010	0.007	0.075
400	5.0	0.890	0.095	0.074	0.405
400	10.0	0.890	0.102	0.081	0.397
N_2 mixture					
400	2.5	0.888	0.091	0.074	0.558
360	2.5	0.924	0.048	0.039	0.286
320	2.5	0.962	0.018	0.014	0.150
300	2.5	0.980	0.009	0.008	0.089
400	5.0	0.886	0.093	0.079	0.565
400	10.0	0.880	0.094	0.081	0.577

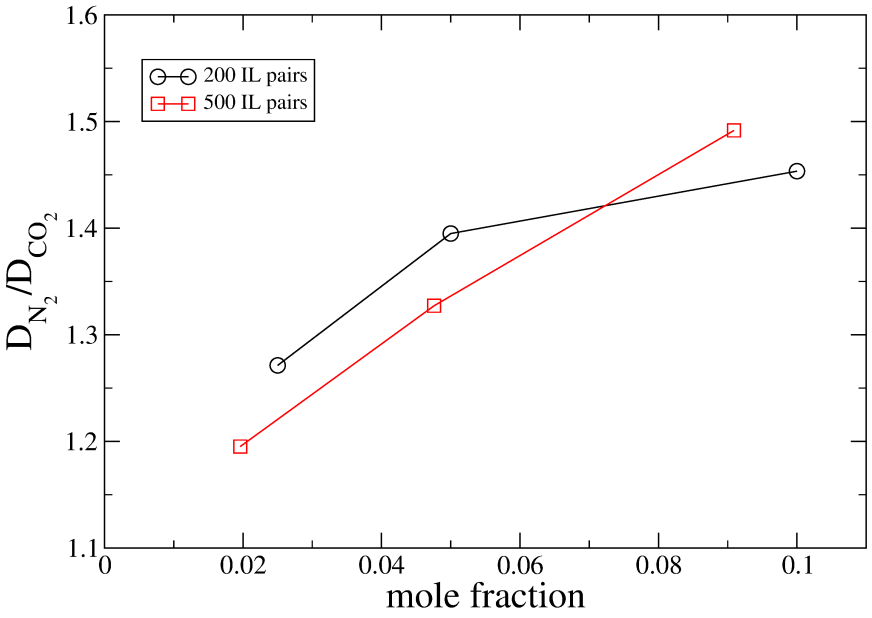

Figure S1. System size effect on the diffusivity ratio of D_{N2}/D_{CO2}.

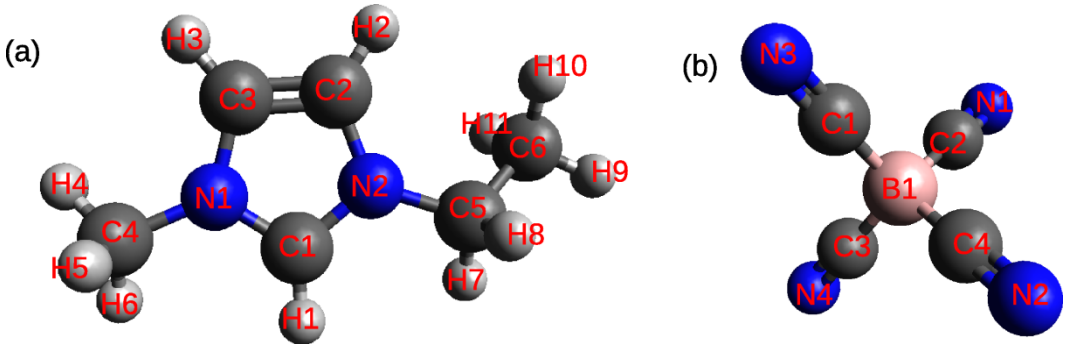

Figure S2. Atom names (in red) in the force fields of (a) emim cation and (b) $B(CN)_4$ anion. Each atom is given an atom name from which one can readily retrieve the atom type information for the specific atom. Lennard-Jones and bonded parameters are categorized in atom types.

```
##############################################################
# Force field originally built via Antechamber using GAFF
# For AMBER-style impropers, atom #3 is the central atom.
##############################################################
FORCEFIELD 2MI

! ATOM:
!! index (int): atom index
!! name (str): atom name (required)
!! mass (float, amu): atomic mass
!! element (str): element symbol
!! epsilon (float, Ken): LJ well depth
!! sigma (float, angstrom): LJ zero-energy distance
ATOM name mass element epsilon sigma ! 8
  cc   12.010  C  43.277 3.400  ! 1
  cd   12.010  C  43.277 3.400  ! 2
  na   14.010  N  85.547 3.250  ! 3
  h5    1.008  H   7.548 2.421  ! 4
  h4    1.008  H   7.548 2.511  ! 5
  c3   12.010  C  55.052 3.400  ! 6
  h1    1.008  H   7.901 2.471  ! 7
  hc    1.008  H   7.901 2.650  ! 8

! BOND:
!! harmonic: K * (R - R0)**2
!!! K (float, Ken/angstrom^2): force constant
!!! R0 (float, angstrom): equilibrium bond length
!! fixed: R = R0
!!! R0 (float, angstrom): equilibrium bond length
BOND  ! 10
  cc   na harmonic  220812.0  1.371  ! 1    1.353
  cc   h5 harmonic  179146.0  1.079  ! 2    1.080
  cc   cd harmonic  253622.0  1.371  ! 3    1.363
  cc   h4 harmonic  176177.0  1.083  ! 4    1.079
  cd   na harmonic  220812.0  1.371  ! 5    1.383
  cd   h4 harmonic  176177.0  1.083  ! 6    1.079
  c3   na harmonic  168427.0  1.456  ! 7    1.477
  c3   h1 harmonic  169031.0  1.093  ! 8    1.092
  c3   c3 harmonic  152526.0  1.535  ! 9    1.527
  c3   hc harmonic  169736.0  1.092  ! 10    1.094

! ANGLE:
!! harmonic: K * (A - A0)**2
!!! K (float, Ken/radian^2): force constant
!!! A0 (float, degrees): equilibrium angle
!! fixed: A = A0
!!! A0 (float, degrees): equilibrium angle
ANGLE  ! 18
  cc   na   cd harmonic   32146.0  128.01  ! 1  108.328
  c3   na   cc harmonic   31481.0  125.09  ! 2  125.847
  cc   na   cc harmonic   34692.0  109.90  ! 3  108.324
  cc   cd   na harmonic   36690.0  109.42  ! 4  107.113
  cc   cd   h4 harmonic   23747.0  129.11  ! 5  130.932
  cd   cc   h4 harmonic   23747.0  129.11  ! 6  130.728
  cd   cc   na harmonic   36690.0  109.42  ! 7  107.214
  c3   na   cd harmonic   31481.0  125.09  ! 8  125.776
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```
  h5   cc   na harmonic   25040.0  122.10  ! 9  125.489
  na   cc   na harmonic   37062.0  109.33  ! 10  109.020
  h4   cd   na harmonic   25272.0  119.66  ! 11  121.954
  h1   c3   na harmonic   25111.0  109.45  ! 12  108.213
  h4   cc   na harmonic   25272.0  119.66  ! 13  122.057
  c3   c3   na harmonic   33077.0  112.81  ! 14  112.336
  h1   c3   h1 harmonic   19716.0  109.55  ! 15  109.162
  c3   c3   hc harmonic   23334.0  110.05  ! 16  110.640
  c3   c3   h1 harmonic   23329.0  110.07  ! 17  111.646
  hc   c3   hc harmonic   19842.0  108.35  ! 18  108.266

! DIHEDRAL:
!! charmm: Kn * (1 + cos(N * A - A0))
!!! Kn (float, Ken): interaction energy
!!! N (int): periodicity
!!! A0 (float, degrees): equilibrium angle
!! opls: K1*(1+cos(A)) + K2*(1-cos(2*A)) + K3*(1+cos(3*A)) + K4*(1-cos(4*A))
!!! K1 (float, Ken): interaction energy
!!! K2 (float, Ken): interaction energy
!!! K3 (float, Ken): interaction energy
!!! K4 (float, Ken): interaction energy
DIHEDRAL  ! 23
  cc   cd   na   cc charmm   855.470  2  180.0  ! 1   -0.022
  h4   cd   na   cc charmm   855.470  2  180.0  ! 2 -179.606
  h1   c3   na   cc charmm     0.000  2    0.0  ! 3    8.438
  cd   cc   na   cc charmm   855.470  2  180.0  ! 4    0.146
  h4   cc   na   cc charmm   855.470  2  180.0  ! 5  179.866
  c3   c3   na   cc charmm   4822.97  1    0.0  # min: -199 max: 304 rms: 180
  c3   c3   na   cc charmm    -59.10  2  180.0  # min: -97 max: 137 rms: 86
  c3   c3   na   cc charmm    219.01  3    0.0  # min: -32 max: 19 rms: 17
  c3   c3   na   cc charmm    102.66  4  180.0  # min: -177 max: 222 rms: 139
  cc   cd   na   c3 charmm   855.470  2  180.0  ! 7  179.568
  na   cc   na   cc charmm   855.470  2  180.0  ! 8   -0.161
  h5   cc   na   cc charmm   855.470  2  180.0  ! 9 -179.857
  cd   cc   na   c3 charmm   855.470  2  180.0  ! 10  178.271
  h5   cc   na   cd charmm   855.470  2  180.0  ! 11  179.811
  na   cc   na   cd charmm   855.470  2  180.0  ! 12    0.114
  h1   c3   na   cd charmm     0.000  2    0.0  ! 13   59.507
  na   cc   na   c3 charmm    855.470  2  180.0  ! 14 -178.882
  h4   cc   cd   na charmm   2012.880  2  180.0  ! 15 -179.763
  na   cc   cd   na charmm   2012.880  2  180.0  ! 16   -0.075
  h5   cc   na   c3 charmm    855.470  2  180.0  ! 17    1.118
  h4   cc   cd   h4 charmm   2012.880  2  180.0  ! 18   -0.230
  h4   cc   na   c3 charmm    855.470  2  180.0  ! 19   -2.009
  na   cc   cd   h4 charmm   2012.880  2  180.0  ! 20  179.458
  h4   cd   na   c3 charmm    855.470  2  180.0  ! 21   -0.016
  hc   c3   c3   na charmm     78.500  3    0.0  ! 22   60.022
  h1   c3   c3   hc charmm     78.500  3    0.0  ! 23   -0.131

! IMPROPER:
!! cosine: Kn * (1 + cos(N * A - A0))
!!! Kn (float, Ken): interaction energy
!!! N (int): periodicity
!!! A0 (float, degrees): equilibrium angle
!! harmonic: K * (A - A0)**2
!!! K (float, Ken/radian^2): force constant
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!!! A0 (float, degrees): equilibrium angle
IMPROPER  ! 5
  h5   na   cc   na cosine   553.540  2  180.0  ! 1 -179.697
  cd   h4   cc   na cosine   553.540  2  180.0  ! 2 -179.648
  cc   h4   cd   na cosine   553.540  2  180.0  ! 3  179.474
  c3   cc   na   cd cosine   553.540  2  180.0  ! 4  179.589
  c3   cc   na   cc cosine   553.540  2  180.0  ! 5 -178.125
```

MOLECULE 2MI

```
! ATOM:
!! index (int): atom index
!! name (str): atom name (required)
!! type (str): atomtype name
!! charge (float, e): partial atomic charge
!! x (float, angstrom): atom coordinate
!! y (float, angstrom): atom coordinate
!! z (float, angstrom): atom coordinate
ATOM name type charge x y z ! 19
  C1   cc -0.090000   -1.89400   -0.67700    0.15500  ! 1
  C2   cc -0.121000   -0.17900    0.67000   -0.17500  ! 2
  C3   cd -0.145000   -1.31200    1.42800   -0.16400  ! 3
  N1   na  0.191000   -2.37500    0.56800    0.04400  ! 4
  H1   h5  0.186000   -2.48600   -1.56400    0.32500  ! 5
  H2   h4  0.189000    0.85500    0.95100   -0.30400  ! 6
  H3   h4  0.185000   -1.45200    2.49200   -0.27800  ! 7
  N2   na  0.044000   -0.56300   -0.64300    0.02800  ! 8
  C4   c3 -0.286000   -3.79000    0.95700    0.13700  ! 9
  H4   h1  0.139000   -4.09400    1.44300   -0.79200  ! 10
  H5   h1  0.139000   -4.39300    0.06300    0.29500  ! 11
  H6   h1  0.139000   -3.92400    1.64000    0.97800  ! 12
  C5   c3  0.015000    0.34100   -1.81900    0.05500  ! 13
  C6   c3 -0.141000    0.84200   -2.19800   -1.33700  ! 14
  H7   h1  0.076000   -0.22200   -2.63500    0.51500  ! 15
  H8   h1  0.076000    1.16500   -1.56700    0.72700  ! 16
  H9   hc  0.068000    0.01400   -2.46200   -2.00100  ! 17
 H10   hc  0.068000    1.41500   -1.38600   -1.79500  ! 18
 H11   hc  0.068000    1.50200   -3.06700   -1.25100  ! 19

! BOND:
BOND  ! 19
  C1   N1   ! 1    1.339
  C1   H1   ! 2    1.080
  C1   N2   ! 3    1.337
  C2   C3   ! 4    1.363
  C2   H2   ! 5    1.079
  C2   N2   ! 6    1.383
  C3   N1   ! 7    1.383
  C3   H3   ! 8    1.079
  C4   N1   ! 9    1.470
  C5   N2   ! 10    1.484
  C4   H4   ! 11    1.092
  C4   H5   ! 12    1.090
  C4   H6   ! 13    1.092
  C5   C6   ! 14    1.527
  C5   H7   ! 15    1.093
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  C5   H8   ! 16    1.093
  C6   H9   ! 17    1.094
  C6  H10   ! 18    1.094
  C6  H11   ! 19    1.095

! ANGLE:
ANGLE  ! 33
  C1   N1   C3   ! 1  108.328
  C1   N1   C4   ! 2  125.894
  C1   N2   C2   ! 3  108.324
  C1   N2   C5   ! 4  125.769
  C2   C3   N1   ! 5  107.113
  C2   C3   H3   ! 6  130.932
  C2   N2   C5   ! 7  125.878
  C3   C2   H2   ! 8  130.728
  C3   C2   N2   ! 9  107.214
  C3   N1   C4   ! 10  125.776
  H1   C1   N1   ! 11  125.431
  N1   C1   N2   ! 12  109.020
  H3   C3   N1   ! 13  121.954
  H4   C4   N1   ! 14  109.386
  H5   C4   N1   ! 15  108.940
  H6   C4   N1   ! 16  109.412
  H1   C1   N2   ! 17  125.548
  H2   C2   N2   ! 18  122.057
  C6   C5   N2   ! 19  112.336
  H7   C5   N2   ! 20  106.595
  H8   C5   N2   ! 21  106.731
  H4   C4   H5   ! 22  109.542
  H4   C4   H6   ! 23  110.053
  H5   C4   H6   ! 24  109.488
  C5   C6   H9   ! 25  111.403
  C5   C6  H10   ! 26  111.661
  C5   C6  H11   ! 27  108.857
  C6   C5   H7   ! 28  111.552
  C6   C5   H8   ! 29  111.740
  H7   C5   H8   ! 30  107.566
 H10   C6   H9   ! 31  108.750
 H11   C6   H9   ! 32  108.213
 H10   C6  H11   ! 33  107.834

! DIHEDRAL:
DIHEDRAL  ! 41
  H1   C1   N1   C3   ! 1  179.811
  N2   C1   N1   C3   ! 2    0.114
  H1   C1   N1   C4   ! 3    0.221
  N2   C1   N1   C4   ! 4 -179.475
  N1   C1   N2   C2   ! 5   -0.161
  H1   C1   N2   C2   ! 6 -179.857
  N1   C1   N2   C5   ! 7 -178.289
  H1   C1   N2   C5   ! 8    2.015
  H2   C2   C3   N1   ! 9 -179.763
  N2   C2   C3   N1   ! 10   -0.075
  H2   C2   C3   H3   ! 11   -0.230
  N2   C2   C3   H3   ! 12  179.458
  C3   C2   N2   C1   ! 13    0.146
```

```
  H2   C2   N2   C1   ! 14  179.866
  C3   C2   N2   C5   ! 15  178.271
  H2   C2   N2   C5   ! 16   -2.009
  C2   C3   N1   C1   ! 17   -0.022
  H3   C3   N1   C1   ! 18 -179.606
  C2   C3   N1   C4   ! 19  179.568
  H3   C3   N1   C4   ! 20   -0.016
  H4   C4   N1   C1   ! 21 -120.670
  H4   C4   N1   C3   ! 22   59.811
  H5   C4   N1   C1   ! 23   -0.957
  H5   C4   N1   C3   ! 24  179.523
  H6   C4   N1   C1   ! 25  118.706
  H6   C4   N1   C3   ! 26  -60.814
  C6   C5   N2   C1   ! 27  104.237
  C6   C5   N2   C2   ! 28  -73.570
  H7   C5   N2   C1   ! 29  -18.233
  H7   C5   N2   C2   ! 30  163.961
  H8   C5   N2   C1   ! 31 -132.968
  H8   C5   N2   C2   ! 32   49.226
  N2   C5   C6   H9   ! 33  -60.833
  H7   C5   C6   H9   ! 34   58.788
  H8   C5   C6   H9   ! 35  179.240
  N2   C5   C6  H10   ! 36   60.980
  H7   C5   C6  H10   ! 37 -179.399
  H8   C5   C6  H10   ! 38  -58.947
  N2   C5   C6  H11   ! 39  179.918
  H7   C5   C6  H11   ! 40  -60.461
  H8   C5   C6  H11   ! 41   59.992

! IMPROPER:
IMPROPER  ! 5
  H1   N1   C1   N2   ! 1 -179.697
  C3   H2   C2   N2   ! 2 -179.648
  C2   H3   C3   N1   ! 3  179.474
  C4   C1   N1   C3   ! 4  179.589
  C5   C2   N2   C1   ! 5 -178.125
```

FORCEFIELD BCN

```
! ATOM:
!! index (int): atom index
!! name (str): atom name (required)
!! mass (float, amu): atomic mass
!! element (str): element symbol
!! epsilon (float, Ken): LJ well depth
!! sigma (float, angstrom): LJ zero-energy distance
ATOM name mass element epsilon sigma ! 3
   c1  12.010  C  30.696 3.118  ! 1
   b   10.810  B  47.811 3.581  ! 2
   n1  14.010  N  85.554 3.401  ! 3

! BOND:
!! harmonic: K * (R - R0)**2
!!! K (float, Ken/angstrom^2): force constant
!!! R0 (float, angstrom): equilibrium bond length
```

```
!! fixed: R = R0
!!! R0 (float, angstrom): equilibrium bond length
BOND  ! 2
   b    c1 harmonic  35228.3  1.572  ! 1    1.423
   c1   n1 harmonic  60389.7  1.150  ! 2    1.423

! ANGLE:
!! harmonic: K * (A - A0)**2
!!! K (float, Ken/radian^2): force constant
!!! A0 (float, degrees): equilibrium angle
!! fixed: A = A0
!!! A0 (float, degrees): equilibrium angle
ANGLE  ! 2
   c1    b    c1 harmonic   50276.6  109.50  ! 1  109.471
   b     c1   n1 harmonic   50276.6  180.00  ! 2  180.00
```

MOLECULE BCN

```
! ATOM:
!! index (int): atom index
!! name (str): atom name (required)
!! type (str): atomtype name
!! charge (float, e): partial atomic charge
!! x (float, angstrom): atom coordinate
!! y (float, angstrom): atom coordinate
!! z (float, angstrom): atom coordinate
ATOM name type charge x y z ! 5
  B1    b  0.200000    0.33500    0.55900   -0.84400  ! 1
  C1    c1 0.160000    1.75700    0.67700   -1.56700  ! 2
  C2    c1 0.160000   -0.62100   -0.39400   -1.70100  ! 3
  C3    c1 0.160000   -0.32500    2.01000   -0.72600  ! 4
  C4    c1 0.160000    0.53100   -0.05900    0.61800  ! 5
  N1    n1 -0.41000   -1.31700   -1.08700   -2.32500  ! 6
  N2    n1 -0.41000    0.67300   -0.50700    1.68200  ! 7
  N3    n1 -0.41000    2.79000    0.76300   -2.09300  ! 8
  N4    n1 -0.41000   -0.80600    3.06600   -0.64000  ! 9

! BOND:
BOND  !8
  B1   C1   ! 1    1.423
  B1   C2   ! 2    1.423
  B1   C3   ! 3    1.423
  B1   C4   ! 4    1.423
  C1   N3   ! 5    1.423
  C2   N1   ! 6    1.423
  C3   N4   ! 7    1.423
  C4   N2   ! 8    1.423

! ANGLE:
ANGLE  ! 6
  C1   B1   C2   ! 1  109.533
  C1   B1   C3   ! 2  109.463
  C1   B1   C4   ! 3  109.458
  C2   B1   C3   ! 4  109.463
  C2   B1   C4   ! 5  109.458
  C3   B1   C4   ! 6  109.453
```

```
B1    C1    N3    ! 7  180.00
B1    C2    N1    ! 8  180.00
B1    C3    N4    ! 9  180.00
B1    C4    N2    ! 10 180.00
```