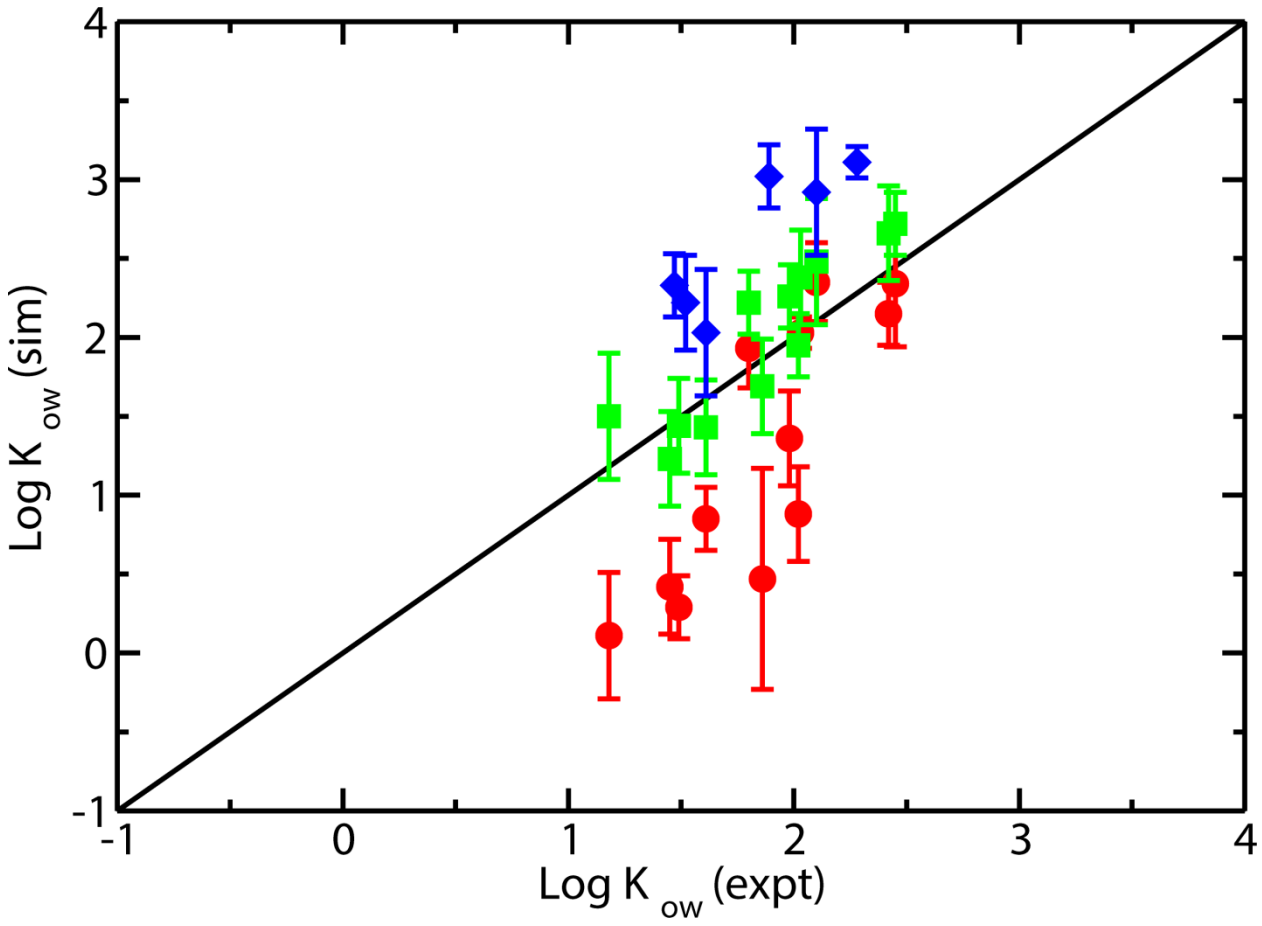

Figure S1: Comparison of Log K_{ow} values predicted by various charge distributions. Charges determined from a CHELPG analysis of MP2/6-31+G(d,p) *ab initio* calculations (blue diamonds), HF/6-31+G(d,p) (red circles), HF/6-31+G(d,p) scaled by 0.9 (green squares).

Table S1: Predicted free energies of transfer for models using HF/6-31+G(d,p) charges

Species	ΔG_{water} (kcal/mol)	ΔG_{oct} (kcal/mol)	ΔG_{net} (kcal/mol)	log Kow	Log K_H
14DNB	-9.90	-10.47	0.57	0.42	-7.26
13DNB	-10.22	-10.61	0.39	0.29	-7.50
DNAN	-10.59	-11.75	1.16	0.85	-7.77
MNA	-4.51	-7.72	3.21	2.35	-3.31
2NAN	-4.72	-7.35	2.63	1.93	-3.46
4NAN	-4.59	-7.35	2.76	2.03	-3.37
PNT	-3.55	-6.88	3.33	2.15	-2.60
MNT	-3.5	-6.53	3.03	2.22	-2.57
24DNT	-9.63	-11.48	1.85	1.36	-7.06
26DNT	-9.78	-10.98	1.2	0.88	-7.17
TNB	-17.03	-17.18	0.15	0.11	-12.49
TNT	-16.62	-17.26	0.64	0.47	-12.19

Table S2: Predicted free energies of transfer for models using HF/6-31+G(d,p) charges scaled by 0.9.

Species	ΔG_{water} (kcal/mol)	ΔG_{oct} (kcal/mol)	ΔG_{net} (kcal/mol)	log K_{ow}	Log K_H
14DNB	-7.84	-9.19	1.35	1.23	-5.75
13DNB	-7.65	-9.61	1.96	1.44	-5.61
DNAN	-8.21	-10.4	2.19	1.6	-6.02
MNA	-3.33	-7.14	3.81	2.48	-2.44
2NAN	-3.68	-6.72	3.04	2.29	-2.70
4NAN	-3.6	-6.85	3.25	2.38	-2.64
PNT	-2.48	-6.11	3.63	2.66	-1.82
MNT	-2.33	-6.05	3.72	2.72	-1.71
24DNT	-7.46	-10.54	3.08	2.26	-5.47
26DNT	-7.41	-10.08	2.67	1.95	-5.44
NTO	-15.36	-15.65	0.29	0.21	-11.26
DNP	-12.34	-13.2	0.86	0.63	-8.78
TNB	-13.27	-15.32	2.05	1.5	-9.73
TNT	-12.63	-14.95	2.31	1.69	-9.26

Table S3: Predicted free energies of transfer for models using MP2/6-31+G(d,p) charges.

Species	ΔG_{water} (kcal/mol)	ΔG_{oct} (kcal/mol)	ΔG_{net} (kcal/mol)	log Kow	Log K_H
14DNB	-5.19	-8.37	3.18	2.33	-3.81
13DNB	-5.52	-8.54	3.02	2.22	-4.05
DNAN	-7.09	-9.83	2.74	2.03	-5.2
MNA	-3.86	-7.81	3.95	2.91	-2.83
2NAN	-1.21	-5.54	4.33	3.11	-0.9
4NAN	-3.11	-7.22	4.11	3.02	-2.28

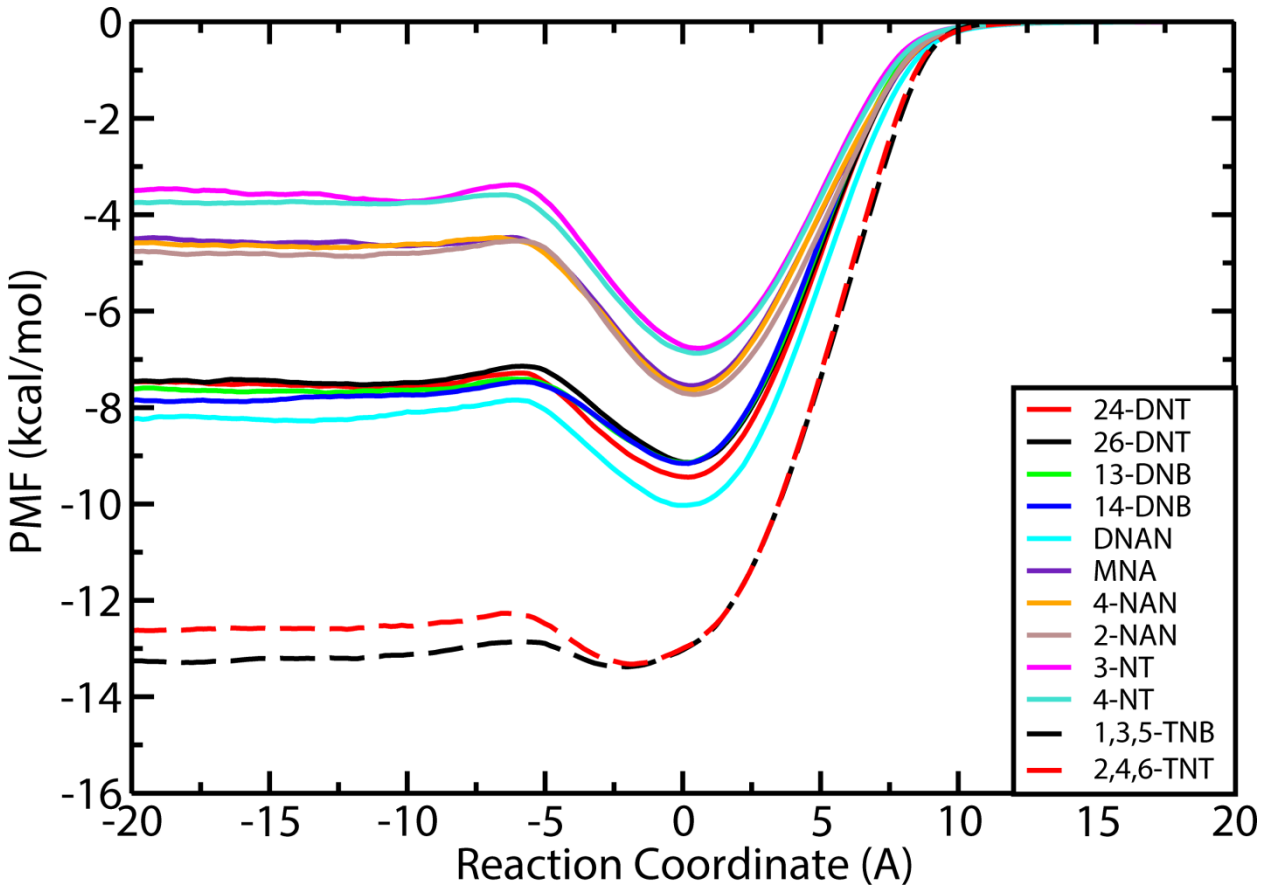

Figure S2: Potential of mean force as function of reaction coordinate for the transfer of solute from vacuum to water.

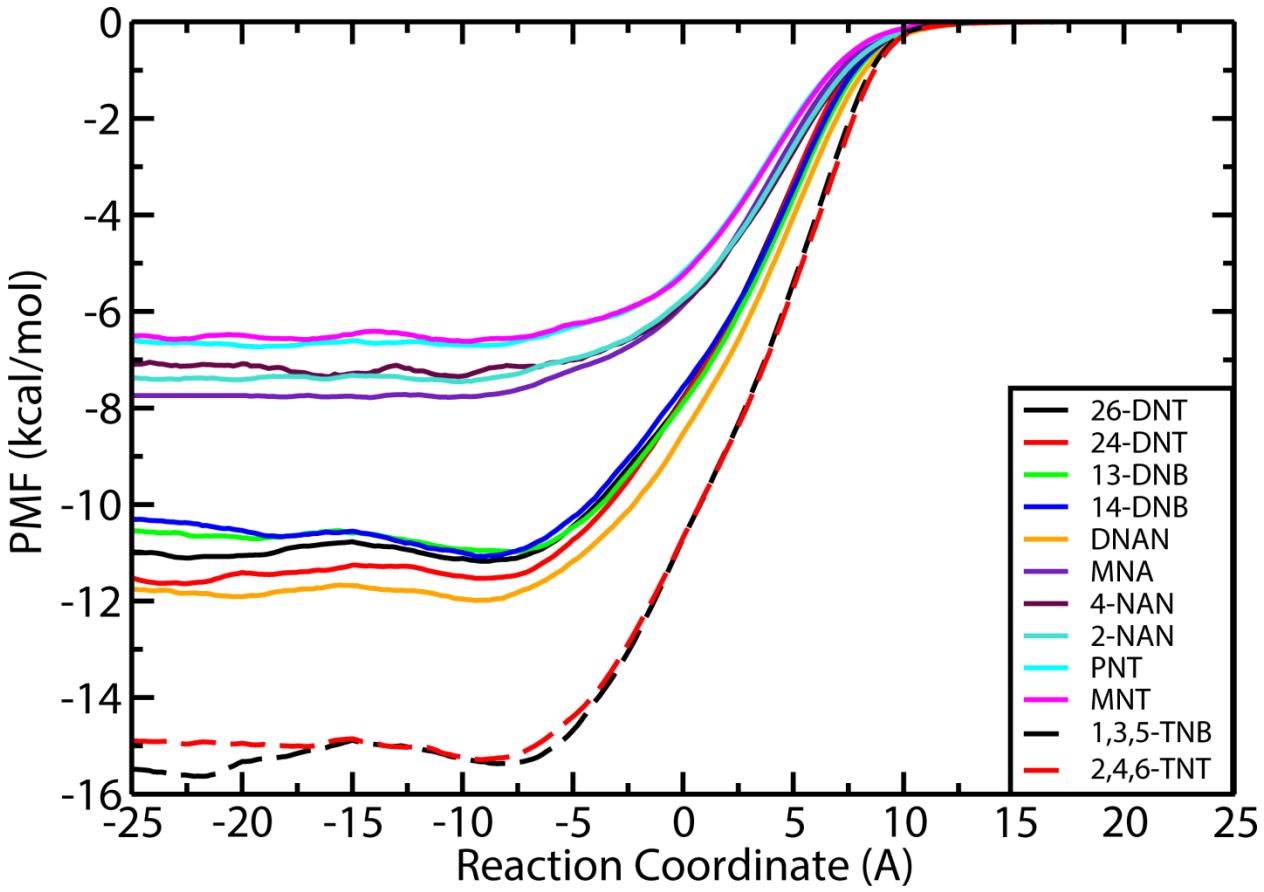

Figure S3: Potential of mean force as a function of reaction coordinate for the transfer of solute from vacuum to 1-octanol.

```
* Topology file for DNAN, 13DNB, 14DNB, MNA, 2NAN, 4NAN, 1-OCTANOL, SPCE
WATER
* 3-NT, 4-NT, 24-DNT, 26-DNT, NTO, DNP, 135-TNB, 2,4,6-TNT
* Parameters from TraPPE-UA
27  1

! Partial charges of CHELPG analysis of HF/6-31+g(d,p) calculations.
! 0.9*HF charges for dinitro compounds
! 0.5*HF charges for trinitro compounds

MASS     1 OE     15.9994 O ! Ether O
MASS     2 CA     13.0187 C ! Aromatic carbon (Benzene)
MASS     3 CA2    12.0107 C ! Alpha carbon (aromatics)
MASS     4 CN     12.0107 C ! Alpha cabon (nitro)
MASS     5 NO     14.0070 N ! Nitro (nitrogen)
MASS     6 ON     15.9990 O ! Nitro (oxygen)
MASS     7 OC     15.9990 O ! sp2 oxygen (carbonyl)
MASS   8 CT3       15.0347 C ! aliphatic sp3 C for CH3  - MASS CHANGED
MASS   9 OH1       15.9994 O ! O in alcohol
MASS  10 NP   14.0070 N ! Nitro (nitrogen)
MASS    11 OT     15.9994 O ! Oxygen in water
MASS    12 HT     1.00800 H ! H in water
MASS  13 CT2       14.0267 C ! aliphatic sp3 C for CH2
MASS  14 H      1.00800 H ! H in alcohol
MASS    15 NH     14.0267 N ! N in amine
MASS    16 HN     1.00800 N ! H in amine
MASS    17 NA     14.0267 N ! N in ring
MASS    18 NH1    14.0267 N ! N bonded to H in ring
MASS    19 HN1    1.00800 H ! H bonded to ring nitrogen
MASS    20 CR     12.0107 C ! C in 5 membered ring
MASS    21 CR2     12.0107 C ! C in 5 membered ring
MASS    22 CR3     12.0107 C ! C in 5 membered ring
MASS    23 HC      1.00800 H ! H in alcohol


AUTOGENERATE ANGLES DIHEDRALS

! 1,3 Dinitrobenzene     OK         PARTIAL CHARGES FROM HF/6-31+G(d, p)
! OPTIMIZED 0.9*HF Charges
RESI DNB        0.00   !
ATOM C1  CA     0.00   !        C1     O3
ATOM C2  CN     0.126  !       /  \     /
ATOM C3  CA     0.00   !     C6   C2-N1
ATOM C4  CN     0.126  !     |    |    \
ATOM C5  CA     0.00   !     C5   C3    O4
ATOM C6  CA     0.00   !      \  /
ATOM N   NP     0.738  !        C4
ATOM O1  ON    -0.432  !         N
ATOM O2  ON    -0.432  !        / \
ATOM N1  NP     0.738  !       O1  O2
ATOM O3  ON    -0.432  !
ATOM O4  ON    -0.432  !
```

```
BOND C1 C2  C2 C3  C3 C4  C4 C5  C5 C6  C6 C1  C4 N  N O1  N O2

BOND C2 N1  N1 O3 N1 O4

AUTOGENERATE ANGLES DIHEDRALS
PATCHING FIRS NONE LAST NONE


! 1,4 dinitrobenzene     OK          PARTIAL CHARGES FROM HF/6-31+G(d, p)
! OPTIMIZED 0.9*HF Charges
RESI DNB2   0.0
ATOM C1  CN     0.126  !     O1   O2
ATOM C2  CA     0.000  !       \  /
ATOM C3  CA     0.000  !        N1
ATOM C4  CN     0.126  !        C1
ATOM C5  CA     0.000  !       /  \
ATOM C6  CA     0.000  !      C6   C2
ATOM N1  NP     0.738  !      |    |
ATOM O1  ON    -0.432  !      C5   C3
ATOM O2  ON    -0.432  !       \  /
ATOM N2  NP     0.738  !        C4
ATOM O3  ON    -0.432  !        N2
ATOM O4  ON    -0.432  !       / \
                     !         O4  O3

BOND C1 C2  C2 C3  C3 C4  C4 C5  C5 C6  C6 C1  C4 N2  N2 O3  N2 O4

BOND C1 N1  N1 O1 N1 O2

AUTOGENERATE ANGLES DIHEDRALS
PATCHING FIRS NONE LAST NONE


! n-methyl-p-nitro-aniline (MNA)  OK  PARTIAL CHARGES FROM HF/6-31+G(d,
p)
RESI MNA        0.00   !
ATOM C1  CN    0.140  !          C7  H1
ATOM C2  CA     0.000  !           \ /
ATOM C3  CA     0.000  !           N2
ATOM C4  CA2    0.140  !           C4
ATOM C5  CA     0.000  !          /  \
ATOM C6  CA     0.000  !         C5   C3
ATOM N1  NP     0.820  !         |    |
ATOM O1  ON    -0.480  !         C6   C2
ATOM O2  ON    -0.480  !          \  /
ATOM C7  CT3    0.25   !           C1
ATOM N2  NH    -0.78   !           N1
ATOM H1  HN     0.39   !          / \
                       !        O2   O1

BOND C1 C2  C2 C3  C3 C4  C4 C5  C5 C6  C6 C1  C1 N1  N1 O1  N1 O2
BOND C4 N2  N2 H1 C7 N2
AUTOGENERATE ANGLES DIHEDRALS
```

```
! 2-nitroanisole          OK      PARTIAL CHARGES FROM HF/6-31+G(d, p)
! OPTIMIZED HF Charges
RESI NA2        0.00   !
ATOM C1  CA2    0.09   !               C7
ATOM C2  CN     0.140  !               /
ATOM C3  CA     0.000  !             O
ATOM C4  CA     0.000  !             C1      O3
ATOM C5  CA     0.000  !           /  \    /
ATOM C6  CA     0.000  !          C6   C2-N1
ATOM N1  NO     0.820  !          |    |   \
ATOM O2  ON    -0.480  !          C5   C3   O4
ATOM O3  ON    -0.480  !           \  /
ATOM O1  OE    -0.35   !            C4
ATOM C7  CT3    0.260  !

BOND C1 C2  C2 C3  C3 C4  C4 C5  C5 C6  C6 C1
BOND C7 O1  O1 C1  C2 N1
BOND N1 O2  N1 O3

AUTOGENERATE ANGLES DIHEDRALS
PATCHING FIRS NONE LAST NONE


! 4-Nitroanisole (NAN)       OK       True PARTIAL CHARGES FROM HF/6-
31+G(d, p)
! OPTIMIZED HF Charges
RESI NAN        0.00   !         C7
ATOM C1  CA2    0.09   !          \
ATOM C2  CA     0.00   !          O1
ATOM C3  CA     0.000  !          C1
ATOM C4  CN     0.14   !         /  \
ATOM C5  CA     0.000  !        C6  C2
ATOM C6  CA     0.000  !        |   |
ATOM C7  CT3    0.260  !        C5  C3
ATOM O1  OE    -0.35   !         \  /
ATOM N2  NP     0.82   !          C4
ATOM O4  ON    -0.480  !          |
ATOM O5  ON    -0.480  !          N2
                   !             / \
                   !            O5  O4

BOND C1 C2  C2 C3  C3 C4  C4 C5  C5 C6  C6 C1
BOND C7 O1  O1 C1  C4 N2
BOND N2 O4  N2 O5
AUTOGENERATE ANGLES DIHEDRALS
PATCHING FIRS NONE LAST NONE
```

```
! Dinitroanisole (DNAN)   OK  True   PARTIAL CHARGES FROM HF/6-31+G(d, p)
! OPTIMIZED: 0.9*HF/6-31+g(d,p) charges
RESI DNAN   0.00    !                  C7
ATOM C1  CA2    0.081   !               \
ATOM C2  CN     0.126   !                O1
ATOM C3  CA     0.00    !                 C1      O2
ATOM C4  CN     0.126   !                /  \    /
ATOM C5  CA     0.00    !              C6   C2-N1
ATOM C6  CA     0.00    !              |    |   \
ATOM C7  CT3    0.234   !              C5   C3   O3
ATOM O1  OE    -0.315   !                \  /
ATOM N1  NO     0.738   !                 C4
ATOM O2  ON    -0.432   !                  |
ATOM O3  ON    -0.432   !                 N2
ATOM N2  NP     0.738   !                /  \
ATOM O4  ON    -0.432   !             O5    O4
ATOM O5  ON    -0.432   !

BOND C1 C2  C2 C3  C3 C4  C4 C5  C5 C6  C6 C1
BOND C7 O1  O1 C1  C2 N1  C4 N2
BOND N1 O2  N1 O3  N2 O4  N2 O5

AUTOGENERATE ANGLES DIHEDRALS
PATCHING FIRS NONE LAST NONE

! para-nitrotoluene
! OPTIMIZED HF Charges
RESI PNT        0.0    !
ATOM C1  CA2    0.00    !               C7
ATOM C2  CA     0.00    !               |
ATOM C3  CA     0.000   !               C1
ATOM C4  CN     0.14    !              /  \
ATOM C5  CA     0.000   !            C6   C2
ATOM C6  CA     0.000   !            |    |
ATOM C7  CT3    0.000   !            C5   C3
ATOM N1  NP     0.82    !             \  /
ATOM O1  ON    -0.480   !               C4
ATOM O2  ON    -0.480   !                |
                        !               N1
                        !              /  \
                        !           O1    O2

BOND C1 C2  C2 C3  C3 C4  C4 C5  C5 C6  C6 C1  C1 C7
BOND C4 N1  N1 O1  N1 O2
AUTOGENERATE ANGLES DIHEDRALS
PATCHING FIRS NONE LAST NONE
```

```
! meta-nitrotoluene
! OPTIMIZED HF Charges
RESI MNT        0.0    !
ATOM C1  CA2    0.00   !             C7
ATOM C2  CA     0.00   !             |
ATOM C3  CN     0.14   !             C1
ATOM C4  CA     0.00   !            /  \
ATOM C5  CA     0.000  !           C6   C2
ATOM C6  CA     0.000  !           |    |
ATOM C7  CT3    0.000  !           C5   C3    O2
ATOM N1  NP     0.82   !            \  /  \  /
ATOM O1  ON    -0.480  !              C4    N1
ATOM O2  ON    -0.480  !                     \
                       !                      O1
                       !
BOND C1 C2  C2 C3  C3 C4  C4 C5  C5 C6  C6 C1  C1 C7
BOND C3 N1  N1 O1  N1 O2
AUTOGENERATE ANGLES DIHEDRALS
PATCHING FIRS NONE LAST NONE

! 2,4-dinitrotoluene
! OPTIMIZED 0.9*HF Charges
RESI DNT        0.0    !
ATOM C1  CA2    0.00   !             C7
ATOM C2  CN     0.126  !             |
ATOM C3  CA     0.00   !             C1       O2
ATOM C4  CN     0.126  !            /  \     /
ATOM C5  CA     0.000  !           C6   C2-N1
ATOM C6  CA     0.000  !           |    |    \
ATOM C7  CT3    0.000  !           C5   C3    O1
ATOM N1  NO     0.738  !            \  /
ATOM O1  ON    -0.432  !              C4
ATOM O2  ON    -0.432  !              |
ATOM N2  NP     0.738  !              N2
ATOM O3  ON    -0.432  !             /  \
ATOM O4  ON    -0.432  !           O3    O4
BOND C1 C2  C2 C3  C3 C4  C4 C5  C5 C6  C6 C1  C1 C7
BOND C2 N1  N1 O1  N1 O2
BOND C4 N2  N2 O3  N2 O4

AUTOGENERATE ANGLES DIHEDRALS
PATCHING FIRST NONE LAST NONE
```

```
! 2,6-dinitrotoluene
! OPTIMIZED 0.9*HF Charges
RESI DNT2       0.0    !
ATOM C1  CA2    0.00   !             C7
ATOM C2  CN     0.126  !             |
ATOM C3  CA     0.00   !     O3      C1       O2
ATOM C4  CA     0.00   !       \    /  \     /
ATOM C5  CA     0.000  !        N2-C6   C2-N1
ATOM C6  CN     0.126  !       /   |    |    \
ATOM C7  CT3    0.000  !     O4    C5   C3    O1
ATOM N1  NO     0.738  !            \  /
ATOM O1  ON    -0.432  !             C4
ATOM O2  ON    -0.432  !
ATOM N2  NO     0.738  !
ATOM O3  ON    -0.432  !
ATOM O4  ON    -0.432  !

BOND C1 C2  C2 C3  C3 C4  C4 C5  C5 C6  C6 C1  C1 C7
BOND C2 N1  N1 O1  N1 O2
BOND C6 N2  N2 O3  N2 O4
AUTOGENERATE ANGLES DIHEDRALS
PATCHING FIRS NONE LAST NONE

! NTO: OPTIMIZED
RESI NTO 0.0  ! Nitro charges tuned to be consistent with 0.9*HF charges
ATOM    C1 CR   0.446   !                      /H2
ATOM    C2 CR   0.72    !       O2        N2-N3
ATOM    N1 NH1 -0.50    !         \      /     \
ATOM    H1 HN1  0.37    !          N4-C1       C2=O3
ATOM    H2 HN1  0.34    !         /      \    /
ATOM    N2 NA  -0.41    !       O1         N1
ATOM    N3 NH1 -0.20    !                 /
ATOM    N4 NP   0.738   !               H1
ATOM    O1 ON  -0.432   !
ATOM    O2 ON  -0.432   !
ATOM    O3 OC  -0.64    !

BOND O2 N4  O1 N4  N4 C1  C1 N2  C1 N1  N2 N3  N3 H2  N3 C2  C2 O3  C2 N1
BOND N1 H1
```

```
AUTOGENERATE ANGLES DIHEDRALS
PATCHING FIRS NONE LAST NONE
! DNP: OPTIMIZED
RESI DNP        0.00                        H2
ATOM C1  CR    -0.33   !                     |
ATOM C2  CR2    0.342  !     O3            C1          O1
ATOM C3  CR3    0.10   !       \      //       \      /
ATOM N1  NA    -0.42   !         N4---C3         C2--N3
ATOM N2  NH1    0.00   !        /      \        //     \
ATOM N3  NP     0.738  !     O4         N2 -- N1       O2
ATOM N4  NP     0.738  !                 /
ATOM H1  HN1    0.34   !              H1
ATOM H2  HC     0.22   !
ATOM O1  ON    -0.432  !
ATOM O2  ON    -0.432  !
ATOM O3  ON    -0.432  !
ATOM O4  ON    -0.432  !

BOND C1 C2  C2 N1  N1 N2  N2 C3  C3 C1 N2 H1  H2 C1
BOND C2 N3  N3 O1  N3 O2
BOND C3 N4  N4 O3  N4 O4

! 1,3,5 Trinitrobenzene
!OPTIMIZED 0.5*HF Charges
RESI TNB        0.00   !         O1    O2
ATOM C1  CN     0.07   !           \  /
ATOM C2  CA     0.00   !            N1
ATOM C3  CN     0.07   !            C1
ATOM C4  CA     0.00   !           /  \
ATOM C5  CN     0.07   !    O6   C6   C2    O3
ATOM C6  CA     0.00   !     \   |    |    /
ATOM N1  NP     0.41   !       N3-C5   C3-N2
ATOM O1  ON    -0.24   !     /    \  /     \
ATOM O2  ON    -0.24   !   O5      C4       O4
ATOM N2  NP     0.41   !
ATOM O3  ON    -0.24   !
ATOM O4  ON    -0.24   !
ATOM N3  NP     0.41   !
ATOM O5  ON    -0.24   !
ATOM O6  ON    -0.24   !

BOND C1 C2  C2 C3  C3 C4  C4 C5  C5 C6  C6 C1  C1 N1  N1 O1  N1 O2
BOND C3 N2  N2 O3  N2 O4  C5 N3  N3 O5  N3 O6

AUTOGENERATE ANGLES DIHEDRALS
```

```
! 1,3,5 Trinitrotoulene          PARTIAL CHARGES FROM HF/6-31+G(d, p)
RESI TNT        0.00   !            O1   O2
ATOM C1  CN     0.126  !              \  /
ATOM C2  CA     0.00   !               N1
ATOM C3  CN     0.126  !               C1
ATOM C4  CA2    0.00   !              /  \
ATOM C5  CN     0.126  !       O6    C6   C2    O3
ATOM C6  CA     0.00   !        \    |    |    /
ATOM N1  NP     0.738  !          N3-C5   C3-N2
ATOM O1  ON    -0.432  !         /    \  /     \
ATOM O2  ON    -0.432  !       O5     C4       O4
ATOM N2  NO     0.738  !                |
ATOM O3  ON    -0.432  !                C7
ATOM O4  ON    -0.432  !
ATOM N3  NO     0.738  !
ATOM O5  ON    -0.432  !
ATOM O6  ON    -0.432  !
ATOM C7      CT3    0.00   !

BOND C1 C2  C2 C3  C3 C4  C4 C5  C5 C6  C6 C1  C7 C4
BOND C1 N1  N1 O1  N1 O2
BOND C3 N2  N2 O3  N2 O4  C5 N3  N3 O5  N3 O6

AUTOGENERATE ANGLES DIHEDRALS
PATCHING FIRS NONE LAST NONE


!SPC/E Water
RESI SPCE   0.00
ATOM OH2  OT  -0.8476
ATOM H1   HT   0.4238
ATOM H2   HT   0.4238
BOND OH2 H1 OH2 H2
ANGLE H1 OH2 H2
PATCHING FIRS NONE LAST NONE

!1-octanol
RESI OCL      0.00
GROUP
ATOM H         H     0.435
ATOM OH       OH1  -0.70
ATOM C1       CT2  0.265
ATOM C2       CT2 0.00
ATOM C3       CT2 0.00
ATOM C4       CT2 0.00
ATOM C5       CT2 0.00
ATOM C6       CT2 0.00
ATOM C7       CT2 0.00
ATOM C8       CT3 0.00

BOND H OH  OH C1  C1 C2  C2 C3  C3 C4  C4 C5  C5 C6  C6 C7 C7 C8
AUTOGENERATE ANGLES DIHEDRALS
PATCHING FIRS NONE LAST NONE
```

```
*Parameter file for TraPPE-UA nitro aromatics
BONDS
!
!V(bond) = Kb(b - b0)**2
!
!Kb: kcal/mole/A**2
!b0: A
!
!atom type Kb          b0  All constants from Charmm
CA   CA    528.275     1.4000 ! Aromatic
CA   CA2   528.275     1.4000 ! Aromatic
CA2  OE    480.357     1.4100 ! Ether
CT3  OE    289.566     1.4100 ! Ether to CH3
CT3  NH    413.414     1.4480 ! methyl-amine
CA   CN    528.275     1.4000 ! Aromatic
CA2  CN    528.275     1.4000 ! Aromatic
CA2  NH    528.947     1.3500 ! Aromatic
CN   NO    363.083     1.4900 ! nitro
CN   NP    363.083     1.4900 ! nitro
NP   ON    866.459     1.2250 ! nitro
NO   ON    866.459     1.2250 ! nitro
NH   HN    614.358     0.9900 ! Amine
CT2  CT2   222.500     1.5400 ! Alkane
CT2  CT3   222.500     1.5400 ! Alkane
OH1  CT2   428.000     1.4300 ! Alcohol
OH1  H     545.000     0.9450 ! Alcohol
OT   HT    450.000     1.0000 ! SPC bond length
HT   HT      0.000     1.6333 ! H-H pseudo bond in SPC water.
CT3  CA2   480.000     1.54   ! CH3-C(aro) in nitrotoluene
! NTO parameters
NP   CR    377.165     1.44  ! N(nitro)-C(ring NTO)
CR   NH1   428.831     1.36
CR   NA     932.049    1.26
NA   NH1   435.909     1.35
NH1  HN1   611.646     0.993
CR   OC    1061.0      1.20
! DNP parameters
CR3 CR  377.165  1.36
CR2 CR  377.165  1.36
CR2 NA  932.049  1.30
CR3 NH1 428.831  1.26
CR2 NP  377.165  1.44
CR3 NP  377.165  1.44
CR  HC  611.65   1.07
```

```
ANGLES
!
!V(angle) = Ktheta(Theta - Theta0)**2
!
!Kub: kcal/mole/A**2 (Urey-Bradley)
!S0: A
!
!atom types     Ktheta    Theta0   Kub     S0
!
CA   CA   CA    189.7    120.0    0.0      0.0 ! Aromatic
CA   CA   CA2   189.7    120.0    0.0      0.0 ! Aromatic
CA   CA2  CA    189.7    120.0    0.0      0.0 ! Aromatic
CA   CN   CA2   189.7    120.0    0.0      0.0 ! Aromatic
CN   CA   CN    189.7    120.0    0.0      0.0 ! Aromatic
CN   CA2   CN   189.7    120.0    0.0      0.0 ! Aromatic
CA   CN   CA    189.7    120.0    0.0      0.0 ! Aromatic
CA2   CA   CN   189.7    120.0    0.0      0.0 ! Aromatic
CT3  CA2  CA    189.7    120.0    0.0      0.0 ! nitrotoluene
CT3  OE   CA2   97.94    112.0    0.0      0.0 ! Anisole
OE   CA2  CA    138.72   120.0    0.0      0.0 ! Anisole
OE   CA2  CN    138.72   120.0    0.0      0.0 ! Anisole
CT3   CA2  CN   138.72   120.0    0.0      0.0 ! Anisole
ON   NO   ON    181.13   124.1    0.0      0.0 ! Nitro
CA2  CN   NO    154.793  120.0    0.0      0.0 ! Nitro
CA   CN   NO    154.793  120.0    0.0      0.0 ! Nitro
CA   CN   NP    154.793  120.0    0.0      0.0 ! Nitro
CN   NO   ON    167.892  117.95   0.0      0.0 ! Nitro
CN   NP   ON    167.892  117.95   0.0      0.0 ! Nitro
NH   CA2  CA    145.4    120.0    0.0      0.0 ! Amine
CA2  NH   CT3    89.2    124.0    0.0      0.0 !
HN   NH   CT3    72.9    119.7    0.0      0.0 !
CA2  NH   HN     73.9    116.3    0.0      0.0 !
ON   NP   ON    181.13   124.1    0.0      0.0 ! Nitro
CA   CA   CN    189.7    120.0    0.0      0.0 ! Nitro
CA   CA2  CN    189.7    120.0    0.0      0.0 ! Nitro
CT2  CT2  CT2    62.1    114.0    0.0      0.0 ! Octanol
CT2  CT2  CT3    62.1    114.0    0.0      0.0 ! Octanol
H    OH1  CT2    55.0    108.5    0.0      0.0 ! octanol
OH1  CT2  CT2    50.1    109.5    0.0      0.0 ! octanol
HT   OT   HT     55.0    109.5    0.0      0.0 ! water

! NTO ANGLES
CR   NP   ON     167.9       117.95      0.0      0.0 ! Nitro
NP   CR   NA     149.9       124.5       0.0      0.0 !
NP   CR   NH1    149.9       121.5       0.0      0.0 !
NA   CR   NH1    273.8       114.0       0.0      0.0
CR   NA   NH1    2401.5      103.5       0.0      0.0
CR   NH1  CR     2514.5      106.7       0.0      0.0
NH1  CR   NH1    1347.1      102.0       0.0      0.0
CR   NH1  NA     314.4       113.8       0.0      0.0
NH1  CR   OC     231.3       129.0       0.0      0.0
CR   NH1  HN1    84.0        126.65      0.0      0.0
```

```
!NA   NH1  HN1   84.0       119.55        0.0      0.0  !uncomment for
NTO

! DNP ANGLES
CR3  CR   CR2    165.0 101.2   0.0     0.0
CR2  NA   NH1   2400.0 105.0   0.0     0.0
CR3  NH1  NA     314.5 111.6   0.0     0.0
HC   CR   CR2     84.0 129.4   0.0     0.0
HC   CR   CR3     84.0 129.4   0.0     0.0
CR   CR2  NA     314.5 113.43  0.0     0.0
CR   CR3   NH1   314.5 108.8   0.0     0.0
NP   CR3   CR    150.0 130.7   0.0     0.0
NP   CR2   CR    150.0 125.74  0.0     0.0
NP   CR2   NA    150.0 120.83  0.0     0.0
NP   CR3   NH1   150.0 120.5   0.0     0.0
HN1  NH1   CR3    84.0 127.26  0.0     0.0
ON   NP    CR2   167.8 117.95  0.0     0.0
ON   NP    CR3   167.8 117.95  0.0     0.0
HN1  NH1   NA     84.0 121.14  0.0     0.0 !uncomment for DNP

DIHEDRALS
!
!V(dihedral) = Kchi(1 + cos(n(chi) - delta))
!
!Kchi: kcal/mole
!n: multiplicity
!delta: degrees
!
!atom types             Kchi    n   delta
!
X    CA   CA   X        3.230  2   180.00 ! Benzene
X    CA2  CA   X        3.230  2   180.00 ! Benzene
X    CA   CN   X        3.230  2   180.00 ! Benzene
X    CA2  CN   X        3.230  2   180.00 ! Benzene
CT3  NH   CA2  CA       1.3  2   180.00 ! MNA Amine group; refit
11/21/2012
HN   NH   CA2  CA       1.3   2  180.00 ! MNA Amine group; refit
11/21/2012
CA2  CN   CA   CA       3.230  2   180.00 ! Benzene
CA   CA   CA2  CN       3.230  2   180.00 ! Benzene
CT3  OE   CA2  CA       0.5  1   180.00 ! Refit 11/19/2012
CT3  OE   CA2  CA       0.5  2   180.00 ! Refit 11/19/2012
CT3  OE   CA2  CA       0.7  3   180.00 ! Refit 11/19/2012
CT3  OE   CA2  CN       0.5  1     0.00 ! Refit 11/19/2012
CT3  OE   CA2  CN       0.5  2     0.00 ! Refit 11/19/2012
CT3  OE   CA2  CN       0.7  3     0.00 ! Refit 11/19/2012
ON   NO   CN   CA2     -1.35 2     0.0 ! Ortho Nitro for 24/26 DNT
ON   NO   CN   CA2     -0.5  3     0.0 ! Ortho Nitro for 24/26 DNT
ON   NO   CN   CA      -1.35 2     0.0 ! Ortho Nitro for 24/26 DNT
!ON   NO   CN   CA2     0.24 1   180.00 ! Ortho nitro for DNAN, 2NAN rf
11/20/2012
!ON   NO   CN   CA2    -0.35 2     0.00 ! Ortho nitro for DNAN, 2NAN rf
11/20/2012
```

```
!ON   NO   CN   CA2      0.25   3     0.00 ! Ortho nitro for DNAN, 2NAN
rf 11/20/2012
!ON   NO   CN   CA       0.24   1    180.00 ! Ortho nitro for DNAN, 2NAN
rf 11/20/2012
!ON   NO   CN   CA      -0.35   2     0.00 ! Ortho nitro for DNAN, 2NAN
rf 11/20/2012
ON   NP   CN   CA       1.1460    2   180.00 ! para nitro, refit
11/19/2012
CT2  CT2  CT2  CT2      -2.200  1     0.00 ! octanol
CT2  CT2  CT2  CT2       0.600  2   180.00 ! octanol
CT2  CT2  CT2  CT2       1.300  3     0.00 ! octanol
CT3  CT2  CT2  CT2      -2.1    1     0.00 ! octanol
CT3  CT2  CT2  CT2       0.60   2   180.00 ! octanol
CT3  CT2  CT2  CT2       1.5    3     0.00 ! octanol
OH1  CT2  CT2  CT2       0.6964 1     0.00 ! octanol
OH1  CT2  CT2  CT2      -0.6166  2    180.00 ! octanol
OH1  CT2  CT2  CT2       2.018   3     0.00 ! octanol
H    OH1  CT2  CT2       0.4566  1     0.00 ! octanol
H    OH1  CT2  CT2      -0.1645  2   180.00 ! octanol
H    OH1  CT2  CT2       0.5731  3     0.00 ! octanol

!NTO DIHEDRALS
CR NA NH1 HN1    3.0   1     0.0  !
CR NA NH1 CR     3.0   1   180.0  !
CR NH1 CR NH1    3.0   1   180.0  !
CR NH1 CR OC     3.0   1     0.0  !
CR NH1 CR NP     3.0   1     0.0  !
CR NH1 CR NA     3.0   1   180.0  !
NH1 CR NH1 NA    3.0   1   180.0  !
NH1 CR NH1 HN1   3.0   1     0.0  ! repeated for DNP
NH1 CR NA NH1    3.0   1   180.0  !
HN1 NH1 CR NP    3.0   1   180.0  !
HN1 NH1 CR NA    3.0   1     0.0  !
HN1 NH1 CR OC    3.0   1   180.0  !
NA NH1 CR OC     3.0   1     0.0  !
NA CR NP ON       0.9   2   180.0  !
NH1 CR NP ON     0.9   2   180.0  !
NH1 NA CR NP     3.0   1     0.0  !

! DNP DIHEDRALS
CR CR3 NH1 NA  3.0   1   180.0
CR CR3 NH1 HN1 3.0   1     0.0
CR CR3 NP  ON  1.5   2   180.0
NH1 CR3 NP ON  1.5   2   180.0
CR CR2 NP  ON  1.5   2   180.0
NA CR2 NP  ON  1.5   2   180.0
CR CR2 NA  NH1 3.0   1   180.0
CR2 NA NH1 CR3 3.0   1   180.0
CR2 NA NH1 HN1 3.0   1     0.0
CR2 CR CR3 NH1 3.0   1   180.0
CR2 CR CR3 NP  3.0   1     0.0
CR3 CR CR2 NA  3.0   1   180.0
CR3 CR CR2 NP  3.0   1     0.0
NA NH1 CR3 NP  3.0   1     0.0
```

```
NA CR2 CR  HC  3.0   1     0.0
NH1 NA CR2 NP  3.0   1     0.0
NH1 CR3 CR HC  3.0   1     0.0
NP CR2 CR HC   3.0   1     0.0
NP CR3 NH1 HN1 3.0   1     0.0
NP CR3 CR HC   3.0   1     0.0

NONBONDED nbxmod  5 atom cdiel shift vatom vdistance vswitch -
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 1.0 wmin 1.5
                !adm jr., 5/08/91, suggested cutoff scheme
!
!V(Lennard-Jones) = Eps,i,j[(Rmin,i,j/ri,j)**12 - 2(Rmin,i,j/ri,j)**6]
!
!epsilon: kcal/mole, Eps,i,j = sqrt(eps,i * eps,j)
!Rmin/2: A, Rmin,i,j = Rmin/2,i + Rmin/2,j
!
!atom  ignored    epsilon      Rmin/2   ignored   eps,1-4       Rmin/2,1-
4
!
!Anisole /: Parameters from TraPPE 4
CA      0.000000    -0.095400  2.099000   0.0   0.0   0.0
CA2     0.000000    -0.029800  2.525500   0.0   0.0   0.0
OE      0.000000    -0.109300  1.571400   0.0   0.0   0.0
CN      0.000000    -0.029800  2.525500   0.0   0.0   0.0
NO      0.000000    -0.079500  1.857700   0.0   0.0   0.0
ON      0.000000    -0.159000  1.627600   0.0   0.0   0.0
NP      0.000000    -0.079500  1.857700   0.0   0.0   0.0
CT3     0.000000    -0.194735  2.104616   0.0   0.0   0.0
NH      0.000000    -0.11524   1.975533   0.0   0.0   0.0
HN      0.000000    -0.00000   0.000000   0.0   0.0   0.0
! NTO
HN1    0.000000    -0.023843  0.280615    0.0   0.0   0.0
NH1    0.000000    -0.280166  1.908185    0.0   0.0   0.0
NA     0.000000    -0.113258  1.795939    0.0   0.0   0.0
CR     0.000000    -0.061000  2.02043     0.0   0.0   0.0
OC     0.000000    -0.156972  1.711754    0.0   0.0   0.0
!Additional params for DNP
HC      0.000000    -0.050569  1.324505    0.0   0.0   0.0
CR2     0.000000    -0.061000  2.02043     0.0   0.0   0.0
CR3     0.000000    -0.061000  2.02043     0.0   0.0   0.0
!SPC/E Water
HT    0.000000     0.00000   0.00000      0.0   0.0   0.0
OT    0.000000    -0.15541   1.7774185  0.0   0.0   0.0
! Octanol
H     0.000000     0.000000   0.000000   0.0   0.0   0.0
OH1   0.000000    -0.184799   1.694918   0.0   0.0   0.0
CT2   0.000000    -0.091406   2.216863   0.0   0.0   0.0
```