/Users/jessica/EEX_scratch/examples/amber/alkanes/trappe_tetradecane_single_molecule.prmtop, Top line: 1

```
%VERSION··VERSION STAMP·=·V0001.000··DATE·=·
%FLAG·TITLE·····
%FORMAT(20a4)·····
Molecule·····
%FLAG·POINTERS·····
%FORMAT(10I8)·····
·····14·····2·····0·····13·····0····
·····37·····1·····13·····12·····44····
·····0·····0·····0·····0·····0····
·····0
%FLAG·ATOM NAME·····
%FORMAT(20a4)·····
C1··C2··C3··C4··C5··C6··C7··C8··C9··C10·C11·
%FLAG·CHARGE·····
%FORMAT(5E16.8)·····
··0.00000000E+00··0.00000000E+00··0.00000000
··0.00000000E+00··0.00000000E+00··0.00000000
··0.00000000E+00··0.00000000E+00··0.00000000
%FLAG·ATOMIC NUMBER·····
%FORMAT(10I8)·····
·····6·····6·····6·····6·····6····
·····6·····6·····6
%FLAG·MASS·····
%FORMAT(5E16.8)·····
··1.50452000E+01··1.40265800E+01··1.40265800
··1.40265800E+01··1.40265800E+01··1.40265800
··1.40265800E+01··1.40265800E+01··1.40265800
%FLAG·ATOM TYPE INDEX·····
%FORMAT(10I8)·····
·····1·····2·····2·····2·····2····
·····2·····2·····2·····1
%FLAG·NUMBER EXCLUDED ATOMS·····
%FORMAT(10I8)·····
·····3·····3·····3·····3·····3····
·····3·····2·····1·····1
%FLAG·NONBONDED PARM INDEX·····
%FORMAT(10I8)·····
·····1·····2·····2·····3
%FLAG·RESIDUE LABEL·····
%FORMAT(20a4)·····
ule·
%FLAG·RESIDUE POINTER·····
%FORMAT(10I8)·····
·····1
%FLAG·BOND FORCE CONSTANT·····
%FORMAT(5E16.8)·····
··3.00900000E+02··3.00900000E+02
%FLAG·BOND EQUIL VALUE·····
%FORMAT(5E16.8)·····
··1.54000000E+00··1.54000000E+00
%FLAG·ANGLE FORCE CONSTANT·····
%FORMAT(5E16.8)·····
··6.21001125E+01··6.21001125E+01
%FLAG·ANGLE EQUIL VALUE·····
%FORMAT(5E16.8)·····
··1.98967620E+00··1.98967620E+00
%FLAG·DIHEDRAL FORCE CONSTANT·····
%FORMAT(5E16.8)·····
··0.00000000E+00··7.05516894E-01·-1.35507413
%FLAG·DIHEDRAL PERIODICITY·····
%FORMAT(5E16.8)·····
··0.00000000E+00··1.00000000E+00··2.00000000
%FLAG·DIHEDRAL PHASE·····
%FORMAT(5E16.8)·····
··0.00000000E+00··0.00000000E+00·-3.14159400
%FLAG·SCEE SCALE FACTOR·····
%FORMAT(5E16.8)·····
··0.00000000E+00··0.00000000E+00··0.00000000
%FLAG·SCNB SCALE FACTOR·····
%FORMAT(5E16.8)·····
··0.00000000E+00··0.00000000E+00··0.00000000
%FLAG·SOLTY·····
%FORMAT(5E16.8)·····
··0.00000000E+00··0.00000000E+00
%FLAG·LENNARD JONES ACOEF·····
%FORMAT(5E16.8)·····
··6.02425914E+06··5.66008645E+06··5.27503488
%FLAG·LENNARD JONES BCOEF·····
%FORMAT(5E16.8)·····
··2.16628722E+03··1.73803568E+03··1.38880977
```

/Users/jessica/EEX_scratch/examples/amber/alkanes/trappe_tetradecane_exclusions_single_molecule.prmtop, Top line: 1

```
%VERSION··VERSION_STAMP·=·V0001.000··DATE·=·
%FLAG·TITLE
%FORMAT(20a4)
Molecule
%FLAG·POINTERS
%FORMAT(10I8)
·····14·····2·····0·····13·····0····
·····38·····1·····13·····12·····44····
·····0·····0·····0·····0·····0····
·····0
%FLAG·ATOM NAME
%FORMAT(20a4)
C1··C2··C3··C4··C5··C6··C7··C8··C9··C10·C11·
%FLAG·CHARGE
%FORMAT(5E16.8)
··0.00000000E+00··0.00000000E+00··0.00000000
··0.00000000E+00··0.00000000E+00··0.00000000
··0.00000000E+00··0.00000000E+00··0.00000000
%FLAG·ATOMIC NUMBER
%FORMAT(10I8)
·····6·····6·····6·····6·····6····
·····6·····6·····6
%FLAG·MASS
%FORMAT(5E16.8)
··1.50452000E+01··1.40265800E+01··1.40265800
··1.40265800E+01··1.40265800E+01··1.40265800
··1.40265800E+01··1.40265800E+01··1.40265800
%FLAG·ATOM TYPE_INDEX
%FORMAT(10I8)
·····1·····2·····2·····2·····2····
·····2·····2·····2·····1
%FLAG·NUMBER EXCLUDED_ATOMS
%FORMAT(10I8)
·····4·····3·····3·····3·····3····
·····3·····2·····1·····1
%FLAG·NONBONDED_PARM_INDEX
%FORMAT(10I8)
·····1·····2·····2·····3
%FLAG·RESIDUE_LABEL
%FORMAT(20a4)
ule·
%FLAG·RESIDUE_POINTER
%FORMAT(10I8)
·····1
%FLAG·BOND FORCE_CONSTANT
%FORMAT(5E16.8)
··3.00900000E+02··3.00900000E+02
%FLAG·BOND EQUIL_VALUE
%FORMAT(5E16.8)
··1.54000000E+00··1.54000000E+00
%FLAG·ANGLE FORCE_CONSTANT
%FORMAT(5E16.8)
··6.21001125E+01··6.21001125E+01
%FLAG·ANGLE EQUIL_VALUE
%FORMAT(5E16.8)
··1.98967620E+00··1.98967620E+00
%FLAG·DIHEDRAL FORCE_CONSTANT
%FORMAT(5E16.8)
··0.00000000E+00··7.05516894E-01·-1.35507413
%FLAG·DIHEDRAL PERIODICITY
%FORMAT(5E16.8)
··0.00000000E+00··1.00000000E+00··2.00000000
%FLAG·DIHEDRAL PHASE
%FORMAT(5E16.8)
··0.00000000E+00··0.00000000E+00·-3.14159400
%FLAG·SCEE SCALE_FACTOR
%FORMAT(5E16.8)
··0.00000000E+00··0.00000000E+00··0.00000000
%FLAG·SCNB SCALE_FACTOR
%FORMAT(5E16.8)
··0.00000000E+00··0.00000000E+00··0.00000000
%FLAG·SOLTY
%FORMAT(5E16.8)
··0.00000000E+00··0.00000000E+00
%FLAG·LENNARD JONES_ACOEF
%FORMAT(5E16.8)
··6.02425914E+06··5.66008645E+06··5.27503488
%FLAG·LENNARD JONES_BCOEF
%FORMAT(5E16.8)
··2.16628722E+03··1.73803568E+03··1.38880977
```

/Users/jessica/EEX_scratch/examples/amber/alkanes/trappe_tetradecane_single_molecule.prmtop, Top line: 81

```
%FLAG BONDS INC HYDROGEN
%FORMAT(10I8)

%FLAG BONDS WITHOUT HYDROGEN
%FORMAT(10I8)
       0       3       1       3       6
      12       2      12      15       2
       2      21      24       2      24
      30      33       2      33      36
%FLAG ANGLES INC HYDROGEN
%FORMAT(10I8)

%FLAG ANGLES WITHOUT HYDROGEN
%FORMAT(10I8)
       0       3       6       1       3
      12       2       9      12      15
      15      18      21       2      18
      27       2      24      27      30
      30      33      36       2      33
%FLAG DIHEDRALS INC HYDROGEN
%FORMAT(10I8)

%FLAG DIHEDRALS WITHOUT HYDROGEN
%FORMAT(10I8)
       0       3       6       9       1
       0       3      -6       9       3
       3       6       9      12       1
       3       6      -9      12       3
       6       9      12      15       1
       6       9     -12      15       3
       9      12      15      18       1
       9      12     -15      18       3
      12      15      18      21       1
      12      15     -18      21       3
      15      18      21      24       1
      15      18     -21      24       3
      18      21      24      27       1
      18      21     -24      27       3
      21      24      27      30       1
      21      24     -27      30       3
      24      27      30      33       1
      24      27     -30      33       3
      27      30      33      36       1
      27      30     -33      36       3
      30      33      36      39       1
      30      33     -36      39       3
%FLAG EXCLUDED ATOMS LIST
%FORMAT(10I8)
       2       3       4       3       4
       6       7       6       7       8
      10       9      10      11      10
      12      13      14      13      14
%FLAG HBOND ACOEF
%FORMAT(5E16.8)

%FLAG HBOND BCOEF
%FORMAT(5E16.8)

%FLAG HBCUT
%FORMAT(5E16.8)

%FLAG AMBER ATOM TYPE
%FORMAT(20a4)
C3  C2  C2  C2  C2  C2  C2  C2  C2  C2  C2  C2
%FLAG TREE CHAIN CLASSIFICATION
%FORMAT(20a4)
BLA BLA BLA BLA BLA BLA BLA BLA BLA BLA BLA BLA
%FLAG JOIN ARRAY
%FORMAT(10I8)
       0       0       0       0       0
       0       0       0       0
%FLAG IROTAT
%FORMAT(10I8)
       0       0       0       0       0
       0       0       0       0
%FLAG RADIUS SET
%FORMAT(1a80)
modified Bondi radii (mbondi)
%FLAG RADII
%FORMAT(5E16.8)
```

/Users/jessica/EEX_scratch/examples/amber/alkanes/trappe_tetradecane_exclusions_single_molecule.prmtop, Top line: 81

```
%FLAG BONDS INC_HYDROGEN
%FORMAT(10I8)

%FLAG BONDS WITHOUT_HYDROGEN
%FORMAT(10I8)
       0       3       1       3       6
      12       2      12      15       2
       2      21      24       2      24
      30      33       2      33      36
%FLAG ANGLES INC_HYDROGEN
%FORMAT(10I8)

%FLAG ANGLES WITHOUT_HYDROGEN
%FORMAT(10I8)
       0       3       6       1       3
      12       2       9      12      15
      15      18      21       2      18
      27       2      24      27      30
      30      33      36       2      33
%FLAG DIHEDRALS_INC_HYDROGEN
%FORMAT(10I8)

%FLAG DIHEDRALS_WITHOUT_HYDROGEN
%FORMAT(10I8)
       0       3       6       9       1
       0       3      -6       9       3
       3       6       9      12       1
       3       6      -9      12       3
       6       9      12      15       1
       6       9     -12      15       3
       9      12      15      18       1
       9      12     -15      18       3
      12      15      18      21       1
      12      15     -18      21       3
      15      18      21      24       1
      15      18     -21      24       3
      18      21      24      27       1
      18      21     -24      27       3
      21      24      27      30       1
      21      24     -27      30       3
      24      27      30      33       1
      24      27     -30      33       3
      27      30      33      36       1
      27      30     -33      36       3
      30      33      36      39       1
      30      33     -36      39       3
%FLAG EXCLUDED_ATOMS_LIST
%FORMAT(10I8)
       2       3       4       5       3
       5       6       7       6       7
       9      10       9      10      11
      13      12      13      14      13
%FLAG HBOND ACOEF
%FORMAT(5E16.8)

%FLAG HBOND BCOEF
%FORMAT(5E16.8)

%FLAG HBCUT
%FORMAT(5E16.8)

%FLAG AMBER_ATOM_TYPE
%FORMAT(20a4)
C3  C2  C2  C2  C2  C2  C2  C2  C2  C2  C2  C2
%FLAG TREE_CHAIN_CLASSIFICATION
%FORMAT(20a4)
BLA BLA BLA BLA BLA BLA BLA BLA BLA BLA BLA BLA
%FLAG JOIN ARRAY
%FORMAT(10I8)
       0       0       0       0       0
       0       0       0       0
%FLAG IROTAT
%FORMAT(10I8)
       0       0       0       0       0
       0       0       0       0
%FLAG RADIUS SET
%FORMAT(1a80)
modified Bondi radii (mbondi)
%FLAG RADII
%FORMAT(5E16.8)
```

/Users/jessica/EEX_scratch/examples/amber/alkanes/trappe_tetradecane_single_molecule.prmtop, Top line: 161

```
  ··1.50000000E+00··1.50000000E+00··1.50000000
  ··1.50000000E+00··1.50000000E+00··1.50000000
  ··1.50000000E+00··1.50000000E+00··1.50000000
  %FLAG·SCREEN·····································
  %FORMAT(5E16.8)··································
  ··8.00000000E-01··8.00000000E-01··8.00000000
  ··8.00000000E-01··8.00000000E-01··8.00000000
  ··8.00000000E-01··8.00000000E-01··8.00000000
  %FLAG·IPOL·····································
  %FORMAT(1I8)·····································
  ·······0
```

/Users/jessica/EEX_scratch/examples/amber/alkanes/trappe_tetradecane_exclusions_single_molecule.prmtop, Top line: 161

```
  ··1.50000000E+00··1.50000000E+00··1.50000000
  ··1.50000000E+00··1.50000000E+00··1.50000000
  ··1.50000000E+00··1.50000000E+00··1.50000000
  %FLAG·SCREEN
  %FORMAT(5E16.8)
  ··8.00000000E-01··8.00000000E-01··8.00000000
  ··8.00000000E-01··8.00000000E-01··8.00000000
  ··8.00000000E-01··8.00000000E-01··8.00000000
  %FLAG·IPOL
  %FORMAT(1I8)
  ·······0
```