This appendix details the Parameter-Topology file format used extensively by the AMBER software suite for biomolecular simulation and analysis, referred to as the *prmtop* file for short. The format specification of the AMBER topology file was written initially over a decade ago and posted on http://ambermd.org/formats.html. I have recently expanded that document to account for the drastic change to the file format that occurred with the 2004 release of Amber 7. The pre-Amber 7 format (*old format*) is described more briefly afterwards, although each section provided in the original format contains exactly the same information as the newer version.

This appendix also details the format changes and additions introduced by *chamber*—the program that translates a CHARMM parameter file (PSF) into a topology file that can be used with the *sander* and *pmemd* programs in AMBER.

This appendix draws from the information on http://ambermd.org/formats.html that was added by both me and others, as well as the experience I gleaned while writing the ParmEd program and working with the various codes in AMBER.

As a warning, the prmtop file is a result of bookkeeping that becomes increasingly complex as the system size increases. Therefore, hand-editing the topology file for all but the smallest systems is discouraged—a program or script should be written to automate the procedure.

0.1 Layout

The first line of the Amber topology file is the version string. An example is shown below in which XX is replaced by the actual date and time.

```
%VERSION  VERSION_STAMP = V0001.000  DATE = XX/XX/XX  XX:XX:XX
```

The topology format is divided into several sections in a way that is designed to be parsed easily using simple Fortran code. A consequence of this is that it is difficult for parsers written in other languages (*e.g.,* C, C++, Python, etc.) to strictly adhere to the standard. These parsers should try, however, to support as much of the standard as possible.

```
%FLAG SECTION
%COMMENT an arbitrary number of optional comments may be put here
%FORMAT(<FORTRAN FORMAT>)
... data formatted according to <FORTRAN FORMAT>
```

All names (*e.g.,* atom names, atom type names, and residue names) are limited to 4 characters and are printed in fields of width *exactly* 4 characters wide, left-justified. This means that names may not be space-delimited if any of the names have 4 characters.

Requirements for prmtop parsers.

Parsers, regardless of the language they are written in, should conform to a list of attributes to maximize the likelihood that they are parsed correctly.

- Parsers should expect that some 4-character fields (*e.g.,* atom or residue names) may have some names that have 4 characters and therefore may not be whitespace-delimited.
- Parsers should not expect SECTIONs in the prmtop to be in any particular order.
- Parsers should not expect or require %COMMENT lines to exist, but should properly parse the file if any number of %COMMENT lines appear as indicated above

- The topology file may be assumed to have been generated 'correctly' by *tleap* or some other credible source. No graceful error checking is required.

  Requirements for modifying SECTION**s.**

  To minimize the impact of prmtop changes to existing, third-party parsers, the following conventions should be followed.

- Any new SECTION should be added to the end of the topology file to avoid conflicts with order-dependent parsers.
- The <FORTRAN FORMAT> should be as simple as possible (and avoid adding new formats) to maintain simplicity for non-Fortran parsers.
- Avoid modifying if possible. Consider if this section truly belongs in the prmtop.

0.2 List of SECTIONs

TITLE

This section contains the title of the topology file on one line (up to 80 characters). While the title serves a primarily cosmetic purpose, this section must be present.

%FORMAT(20a4)

POINTERS

This section contains the information about how many parameters are present in all of the sections. There are 31 or 32 integer pointers (NCOPY may not be present). The format and names of all of the pointers are listed below, followed by a description of each pointer.

```
%FLAG POINTERS
%FORMAT(10I8)
NATOM    NTYPES NBONH   MBONA   NTHETH MTHETA NPHIH   MPHIA   NHPARM NPARM
NNB      NRES   NBONA   NTHETA  NPHIA  NUMBND NUMANG NPTRA   NATYP   NPHB
IFPERT  NBPER  NGPER   NDPER   MBPER  MGPER  MDPER   IFBOX   NMXRS   IFCAP
NUMEXTRA NCOPY
```

NATOM Number of atoms
NTYPES Number of distinct Lennard-Jones atom types
NBONH Number of bonds containing Hydrogen
MBONA Number of bonds not containing Hydrogen
NTHETH Number of angles containing Hydrogen
MTHETA Number of angles not containing Hydrogen
NPHIH Number of torsions containing Hydrogen
MPHIA Number of torsions not containing Hydrogen
NHPARM Not currently used for anything
NPARM Used to determine if this is a LES-compatible prmtop
NNB Number of excluded atoms (length of total exclusion list)
NRES Number of residues
NBONA MBONA + number of constraint bonds [1]

---

[1] AMBER codes no longer support constraints in the topology file.

NTHETA MTHETA + number of constraint angles [1]
NPHIA MPHIA + number of constraint torsions [1]
NUMBND Number of unique bond types
NUMANG Number of unique angle types
NPTRA Number of unique torsion types
NATYP Number of SOLTY terms. Currently unused.
NPHB Number of distinct 10-12 hydrogen bond pair types [2]
IFPERT Set to 1 if topology contains residue perturbation information. [3]
NBPER Number of perturbed bonds [3]
NGPER Number of perturbed angles [3]
NDPER Number of perturbed torsions [3]
MBPER Number of bonds in which both atoms are being perturbed
MGPER Number of angles in which all 3 atoms are being perturbed
MDPER Number of torsions in which all 4 atoms are being perturbed [1]
IFBOX Flag indicating whether a periodic box is present. Values can be 0 (no box), 1 (orthorhombic box) or 2 (truncated octahedron)
NMXRS Number of atoms in the largest residue
IFCAP Set to 1 if a solvent CAP is being used
NUMEXTRA Number of extra points in the topology file
NCOPY Number of PIMD slices or number of beads
ATOM_NAME

This section contains the atom name for every atom in the prmtop.
`%FORMAT(20a4)` There are `NATOM` 4-character strings in this section.
CHARGE

This section contains the charge for every atom in the prmtop. Charges are multiplied by 18.2223 ($\sqrt{k_{ele}}$ where k_{ele} is the electrostatic constant in $kcal\,\mathring{A}\,mol^{-1}\,q^{-2}$, where q is the charge of an electron).
`%FORMAT(5E16.8)`
There are `NATOM` floating point numbers in this section.
ATOMIC_NUMBER

This section contains the atomic number of every atom in the prmtop. This section was first introduced in AmberTools 12. [**?**]
`%FORMAT(10I8)`
There are `NATOM` integers in this section.
MASS

This section contains the atomic mass of every atom in $g\,mol^{-1}$.
`%FORMAT(5E16.8)`
There are `NATOM` floating point numbers in this section.

---

[2] Modern AMBER force fields do not use a 10-12 potential

[3] No AMBER codes support perturbed topologies anymore

ATOM_TYPE_INDEX

This section contains the Lennard-Jones atom type index. The Lennard-Jones potential contains parameters for every pair of atoms in the system. To minimize the memory requirements of storing NATOM × NATOM [2] Lennard-Jones A-coefficients and B-coefficients, all atoms with the same σ and ε parameters are assigned to the same type (regardless of whether they have the same AMBER_ATOM_TYPE). This significantly reduces the number of LJ coefficients which must be stored, but introduced the requirement for bookkeeping sections of the topology file to keep track of what the LJ type index was for each atom.

This section is used to compute a pointer into the NONBONDED_PARM_INDEX section, which itself is a pointer into the LENNARD_JONES_ACOEF and LENNARD_JONES_BCOEF sections (see below).

%FORMAT(10I8)

There are NATOM integers in this section.

NUMBER_EXCLUDED_ATOMS

This section contains the number of atoms that need to be excluded from the non-bonded calculation loop for atom i because i is involved in a bond, angle, or torsion with those atoms. Each atom in the prmtop has a list of excluded atoms that is a subset of the list in EXCLUDED_ATOMS_LIST (see below). The ith value in this section indicates how many elements of EXCLUDED_ATOMS_LIST belong to atom i.

For instance, if the first two elements of this array is 5 and 3, then elements 1 to 5 in EXCLUDED_ATOMS_LIST are the exclusions for atom 1 and elements 6 to 8 in EXCLUDED_ATOMS_LIST are the exclusions for atom 2. Each exclusion is listed only once in the topology file, and is given to the atom with the smaller index. That is, if atoms 1 and 2 are bonded, then atom 2 is in the exclusion list for atom 1, but atom 1 is *not* in the exclusion list for atom 2. If an atom has no excluded atoms (either because it is a monoatomic ion or all atoms it forms a bonded interaction with has a smaller index), then it is given a value of 1 in this list which corresponds to an exclusion with (a non-existent) atom 0 in EXCLUDED_ATOMS_LIST.

The exclusion rules for extra points are more complicated. When determining exclusions, it is considered an 'extension' of the atom it is connected (bonded) to. Therefore, extra points are excluded not only from the atom they are connected to, but also from every atom that its parent atom is excluded from.

NOTE: The non-bonded interaction code in *sander* and *pmemd* currently (as of Amber 12) recalculates the exclusion lists for simulations of systems with periodic boundary conditions, so this section is effectively ignored. The GB code uses the exclusion list in the topology file.

%FORMAT(10I8)

There are NATOM integers in this section.

---

[2] Only half this number would be required, since $a_{i,j} \equiv a_{j,i}$

NONBONDED_PARM_INDEX

This section contains the pointers for each pair of LJ atom types into the LENNARD_JONES_ACOEF and LENNARD_JONES_BCOEF arrays (see below). The pointer for an atom pair in this array is calculated from the LJ atom type index of the two atoms (see ATOM_TYPE_INDEX above).

The index for two atoms i and j into the LENNARD_JONES_ACOEF and LENNARD_JONES_BCOEF arrays is calculated as

$$index = \text{NONBONDED\_PARM\_INDEX}\left[\text{NTYPES} \times (\text{ATOM\_TYPE\_INDEX}(i) - 1) + \text{ATOM\_TYPE\_INDEX}(j)\right]$$
(1)

Note, each atom pair can interact with either the standard 12-6 LJ potential *or* via a 12-10 hydrogen bond potential. If $index$ in Eq. 1 is negative, then it is an index into HBOND_ACOEF and HBOND_BCOEF instead (see below).
%FORMAT(10I8)
There are NTYPES $\times$ NTYPES integers in this section.

RESIDUE_LABEL

This section contains the residue name for every residue in the prmtop. Residue names are limited to 4 letters, and may not be whitespace-delimited if any residues have 4-letter names.
%FORMAT(20a4)
There are NRES 4-character strings in this section.

RESIDUE_POINTER

This section lists the first atom in each residue.
%FORMAT(10i8)
There are NRES integers in this section.

BOND_FORCE_CONSTANT

Bond energies are calculated according to the equation

$$E_{bond} = \frac{1}{2}k\left(\vec{r} - \vec{r}_{eq}\right)^2$$
(2)

This section lists all of the bond force constants (k in Eq. 2) in units $kcal\,mol^{-1}\,\mathring{A}^{-2}$ for each unique bond type. Each bond in BONDS_INC_HYDROGEN and BONDS_WITHOUT_HYDROGEN (see below) contains an index into this array.
%FORMAT(5E16.8)
There are NUMBND floating point numbers in this section.

BOND_EQUIL_VALUE

This section lists all of the bond equilibrium distances ($\vec{r}_{eq}$ in Eq. 2) in units of Åfor each unique bond type. This list is indexed the same way as BOND_FORCE_CONSTANT.
%FORMAT(5E16.8)
There are NUMBND floating point numbers in this section.

ANGLE_FORCE_CONSTANT

Angle energies are calculated according to the equation

$$E_{angle} = \frac{1}{2}k_\theta\left(\theta - \theta_{eq}\right)^2$$
(3)

This section lists all of the angle force constants (θ in Eq. 3) in units of $kcal\,mol^{-1}\,rad^2$ for each unique angle type. Each angle in `ANGLES_INC_HYDROGEN` and `ANGLES_WITHOUT_HYDROGEN` contains an index into this (and the next) array.

`%FORMAT(5E16.8)`

There are `NUMANG` floating point numbers in this section.

ANGLE_EQUIL_VALUE

This section contains all of the angle equilibrium angles (θ_{eq} in Eq. 3) in radians. *NOTE:* the AMBER parameter files list equilibrium angles in degrees and are converted to radians in *tleap*. This list is indexed the same way as `ANGLE_FORCE_CONSTANT`.

`%FORMAT(5E16.8)`

There are `NUMBND` floating point numbers in this section.

DIHEDRAL_FORCE_CONSTANT

Torsion energies are calculated for each term according to the equation

$$E_{torsion} = k_{tor} \cos\left(n\phi + \psi\right) \tag{4}$$

This section lists the torsion force constants (k_{tor} in Eq. 4) in units of $kcal\,mol^{-1}$ for each unique torsion type. Each torsion in `DIHEDRALS_INC_HYDROGEN` and `DIHEDRALS_WITHOUT_HYDRO` has an index into this array.

Amber parameter files contain a dividing factor and barrier height for each dihedral. The barrier height in the parameter files are divided by the provided factor inside *tleap* and then discarded. As a result, the torsion barriers in this section may not match those in the original parameter files.

`%FORMAT(5E16.8)`

There are `NPTRA` floating point numbers in this section.

DIHEDRAL_PERIODICITY

This section lists the periodicity (n in Eq. 4) for each unique torsion type. It is indexed the same way as `DIHEDRAL_FORCE_CONSTANT`. *NOTE:* only integers are read by *tleap*, although the AMBER codes support non-integer periodicities.

`%FORMAT(5E16.8)`

There are `NPTRA` floating point numbers in this section.

DIHEDRAL_PHASE

This section lists the phase shift (ψ in Eq. 4) for each unique torsion type in radians. It is indexed the same way as `DIHEDRAL_FORCE_CONSTANT`.

`%FORMAT(5E16.8)`

There are `NPTRA` floating point numbers in this section.

SCEE_SCALE_FACTOR

This section was introduced in Amber 11. In previous versions, this variable was part of the input file and set a single scaling factor for every torsion.

This section lists the factor by which 1-4 electrostatic interactions are divided (*i.e.,* the two atoms on either end of a torsion). For torsion types in which 1-4 non-bonded interactions are not calculated (*e.g.,* improper torsions, multi-term torsions, and those involved in ring systems of 6 or fewer atoms), a value of 0 is assigned by *tleap*. This section is indexed the same way as `DIHEDRAL_FORCE_CONSTANT`.

`%FORMAT(5E16.8)`

There are `NPTRA` floating point numbers in this section.

SCNB_SCALE_FACTOR

This section was introduced in Amber 11. In previous versions, this variable was part of the input file and set a single scaling factor for every torsion.

This section lists the factor by which 1-4 van der Waals interactions are divided (*i.e.,* the two atoms on either end of a torsion). This section is analogous to `SCEE_SCALE_FACTOR` described above.

`%FORMAT(5E16.8)`

There are `NPTRA` floating point numbers in this section.

SOLTY

This section is currently unused, and while 'future use' is planned, this assertion has laid dormant for some time.

`%FORMAT(5E16.8)`

There are `NATYP` floating point numbers in this section.

LENNARD_JONES_ACOEF

LJ non-bonded interactions are calculated according to the equation

$$E_{LJ} = \frac{a_{i,j}}{r^{12}} - \frac{b_{i,j}}{r^6} \tag{5}$$

This section contains the LJ A-coefficients ($a_{i,j}$ in Eq. 5) for all pairs of distinct LJ types (see sections `ATOM_TYPE_INDEX` and `NONBONDED_PARM_INDEX` above).

`%FORMAT(5E16.8)`

There are $[\text{NTYPES} \times (\text{NTYPES} + 1)]/2$ floating point numbers in this section.

LENNARD_JONES_BCOEF

This section contains the LJ B-coefficients ($b_{i,j}$ in Eq. 5) for all pairs of distinct LJ types (see sections `ATOM_TYPE_INDEX` and `NONBONDED_PARM_INDEX` above).

`%FORMAT(5E16.8)`

There are $[\text{NTYPES} \times (\text{NTYPES} + 1)]/2$ floating point numbers in this section.

BONDS_INC_HYDROGEN

This section contains a list of every bond in the system in which at least one atom is Hydrogen. Each bond is identified by 3 integers—the two atoms involved in the bond and the index into the `BOND_FORCE_CONSTANT` and `BOND_EQUIL_VALUE`. For run-time efficiency, the atom indexes are actually indexes into a coordinate array, so the actual atom index A is calculated from the coordinate array index N by $A = N/3 + 1$.

`%FORMAT(10I8)`

There are $3 \times \text{NBONH}$ integers in this section.

BONDS_WITHOUT_HYDROGEN

This section contains a list of every bond in the system in which neither atom is Hydrogen. It has the same structure as `BONDS_INC_HYDROGEN` described above.

`%FORMAT(10I8)`

There are $3 \times \text{NBONA}$ integers in this section.

ANGLES_INC_HYDROGEN

This section contains a list of every angle in the system in which at least one atom is Hydrogen. Each angle is identified by 4 integers—the three atoms involved in the

angle and the index into the `ANGLE_FORCE_CONSTANT` and `ANGLE_EQUIL_VALUE`. For run-time efficiency, the atom indexes are actually indexes into a coordinate array, so the actual atom index A is calculated from the coordinate array index N by $A = N/3 + 1$.
`%FORMAT(10I8)`
There are $4 \times$ `NTHETH` integers in this section.

ANGLES_WITHOUT_HYDROGEN

This section contains a list of every angle in the system in which no atom is Hydrogen. It has the same structure as `ANGLES_INC_HYDROGEN` described above.
`%FORMAT(10I8)`
There are $4 \times$ `NTHETA` integers in this section.

DIHEDRALS_INC_HYDROGEN

This section contains a list of every torsion in the system in which at least one atom is Hydrogen. Each torsion is identified by 5 integers—the four atoms involved in the torsion and the index into the `DIHEDRAL_FORCE_CONSTANT`, `DIHEDRAL_PERIODICITY`, `DIHEDRAL_PHASE`, `SCEE_SCALE_FACTOR` and `SCNB_SCALE_FACTOR` arrays. For run-time efficiency, the atom indexes are actually indexes into a coordinate array, so the actual atom index A is calculated from the coordinate array index N by $A = N/3 + 1$.

If the third atom is negative, then the 1-4 non-bonded interactions for this torsion is not calculated. This is required to avoid double-counting these non-bonded interactions in some ring systems and in multi-term torsions.

If the fourth atom is negative, then the torsion is improper.

NOTE: The first atom has an index of zero. Since 0 cannot be negative and the 3rd and 4th atom indexes are tested for their sign to determine if 1-4 terms are calculated, the first atom in the topology file must be listed as either the first or second atom in whatever torsions it is defined in. The atom ordering in a torsion can be reversed to accommodate this requirement if necessary.
`%FORMAT(10I8)`
There are $5 \times$ `NPHIH` integers in this section.

DIHEDRALS_WITHOUT_HYDROGEN

This section contains a list of every torsion in the system in which no atom is Hydrogen. It has the same structure as `DIHEDRALS_INC_HYDROGEN` described above.
`%FORMAT(10I8)`
There are $5 \times$ `NPHIA` integers in this section.

EXCLUDED_ATOMS_LIST

This section contains a list for each atom of excluded partners in the non-bonded calculation routines. The subset of this list that belongs to each atom is determined from the pointers in `NUMBER_EXCLUDED_ATOMS`—see that section for more information.

NOTE: The periodic boundary code in *sander* and *pmemd* currently recalculates this section of the topology file. The GB code, however, uses the exclusion list defined in the topology file.
`%FORMAT(10I8)`
There are `NNB` integers in this section.

HBOND_ACOEF

This section is analogous to the `LENNARD_JONES_ACOEF` array described above, but refers to the A-coefficient in a 12-10 potential instead of the familiar 12-6 potential. This term has been dropped from most modern force fields.

`%FORMAT(5E16.8)`

There are `NPHB` floating point numbers in this section.

HBOND_BCOEF

This section is analogous to the `LENNARD_JONES_BCOEF` array described above, but refers to the B-coefficient in a 12-10 potential instead of the familiar 12-6 potential. This term has been dropped from most modern force fields.

`%FORMAT(5E16.8)`

There are `NPHB` floating point numbers in this section.

HBCUT

This section used to be used for a cutoff parameter in the 12-10 potential, but is no longer used for anything.

`%FORMAT(5E16.8)`

There are `NPHB` floating point numbers in this section.

AMBER_ATOM_TYPE

This section contains the atom type name for every atom in the prmtop.

`%FORMAT(20a4)`

There are `NATOM` 4-character strings in this section.

TREE_CHAIN_CLASSIFICATION

This section contains information about the tree structure (borrowing concepts from *graph theory*) of each atom. Each atom can have one of the following character indicators:

M This atom is part of the "main chain"

S This atom is part of the "sidechain"

E This atom is a chain-terminating atom (*i.e.,* an "end" atom)

3 The structure branches into 3 chains at this point

BLA If none of the above are true

`%FORMAT(20a4)`

There are `NATOM` 4-character strings in this section.

JOIN_ARRAY

This section is no longer used and is currently just filled with zeros.

`%FORMAT(10a8)`

There are `NATOM` integers in this section.

IROTAT

This section is not used and is currently just filled with zeros.

`%FORMAT(10a8)`

There are `NATOM` integers in this section.

SOLVENT_POINTERS

This section is only present if `IFBOX` is greater than 0 (*i.e.,* if the system was set up for use with periodic boundary conditions). There are 3 integers present in

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this section—the final residue that is part of the solute (IPTRES), the total number of 'molecules' (NSPM), and the first solvent 'molecule' (NSPSOL).

A 'molecule' is defined as a closed graph—that is, there is a pathway from every atom in a molecule to every other atom in the molecule by traversing bonds, and there are no pathways to 'other' molecules.

```
%FLAG SOLVENT_POINTERS
%FORMAT(3I8)
IPTRES    NSPM     NSPSOL
```

ATOMS_PER_MOLECULE

This section is only present if IFBOX is greater than 0 (*i.e.,* if the system was set up for use with periodic boundary conditions). This section lists how many atoms are present in each 'molecule' as defined in the SOLVENT_POINTERS section above.

```
%FORMAT(10I8)
```

There are NSPM integers in this section (see the SOLVENT_POINTERS section above).

BOX_DIMENSIONS

This section is only present if IFBOX is greater than 0 (*i.e.,* if the system was set up for use with periodic boundary conditions). This section lists the box angle (OLDBETA) and dimensions (BOX(1) × BOX(2) × BOX(3)). The values in this section are deprecated now since newer and more accurate information about the box size and shape is stored in the coordinate file. Since constant pressure simulations can change the box dimensions, the values in the coordinate file should be trusted over those in the topology file.

```
%FLAG BOX_DIMENSIONS
%FORMAT(5E16.8)
OLDBETA          BOX(1)           BOX(2)           BOX(3)
```

CAP_INFO

This section is present only if IFCAP is not 0. If present, it contains a single integer which is the last atom before the water cap begins (NATCAP)

```
%FORMAT(10I8)
```

CAP_INFO2

This section is present only if IFCAP is not 0. If present, it contains four numbers—the distance from the center of the cap to outside the cap (CUTCAP), and the Cartesian coordinates of the cap center.

```
%FLAG CAP_INFO2
%FORMAT(5E16.8)
CUTCAP           XCAP             YCAP             ZCAP
```

RADIUS_SET

This section contains a one-line string (up to 80 characters) describing the intrinsic implicit solvent radii set that are defined in the topology file. The available radii sets with their 1-line descriptions are:

bondi `Bondi radii (bondi)`
amber6 `amber6 modified Bondi radii (amber6)`
mbondi `modified Bondi radii (mbondi)`
mbondi2 `H(N)-modified Bondie radii (mbondi2)`

Table 1: List of all of the perturbed topology file sections.

FLAG name	%FORMAT	of values	Description
PERT_BOND_ATOMS	10I8	$2 \times$ NBPER	perturbed bond list
PERT_BOND_PARAMS	10I8	$2 \times$ NBPER	perturbed bond pointers
PERT_ANGLE_ATOMS	10I8	$3 \times$ NGPER	perturbed angle list
PERT_ANGLE_PARAMS	10I8	$2 \times$ NGPER	perturbed angle pointers
PERT_DIHEDRAL_ATOMS	10I8	$4 \times$ NDPER	perturbed torsion list
PERT_DIHEDRAL_PARAMS	10I8	$2 \times$ NDPER	perturbed torsion pointers
PERT_RESIDUE_NAME	20a4	NRES	end state residue names
PERT_ATOM_NAME	20a4	NATOM	end state atom names
PERT_ATOM_SYMBOL	20a4	NATOM	end state atom types
ALMPER	5E16.8	NATOM	Unused
IAPER	10I8	NATOM	Is Atom PERturbed?
PERT_ATOM_TYPE_INDEX	10I8	NATOM	Perturbed LJ Type
PERT_CHARGE	5E16.8	NATOM	Perturbed charge

mbondi3 `ArgH and AspGlu0 modified Bondi2 radii (mbondi3)`
`%FORMAT(1a80)`
There is a single line description in this section.
RADII
    This section contains the intrinsic radii of every atom used for implicit solvent calculations (typically Generalized Born).
`%FORMAT(5E16.8)`
There are `NATOM` floating point numbers in this section.
IPOL
    This section was introduced in Amber 12. In previous versions of Amber, this was a variable in the input file.
    This section contains a single integer that is 0 for fixed-charge force fields and 1 for force fields that contain polarization.
POLARIZABILITY
    This section is only present if `IPOL` is not 0. It contains the atomic polarizabilities for every atom in the prmtop.
`%FORMAT(5E16.8)`
There are `NATOM` floating point numbers in this section.
`%FORMAT(1I8)`
0.3   Deprecated Sections
    All of the sections of the topology file listed here are only present if `IFPERT` is 1. However, no modern programs support such prmtops so these sections are rarely (if ever) used. They are included here for completeness, only.
    More info can be found online at http://ambermd.org/formats.html
0.4   CHAMBER Topologies
    Here we will describe the general format of topology files generated by the *chamber* program. The *chamber* program was developed to translate CHARMM topology (PSF) files into Amber topology files for use with the AMBER program suite.

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Due to differences in the CHARMM force field (*e.g.,* the extra CMAP and Urey-Bradley terms and the different way that improper dihedrals are treated), chamber topologies contain more sections than Amber topologies. Furthermore, to ensure rigorous reproduction of CHARMM energies inside the AMBER program suites, some of the sections that are common between AMBER and CHARMM topology files have a different format for their data to support a different level of input data precision.

Due to the differences in the *chamber* topology files, a mechanism to differentiate between *chamber* topologies and AMBER topologies was introduced. If the topology file has a `%FLAG TITLE` then it is an AMBER topology. If it has a `%FLAG CTITLE` instead, then it is a *chamber* topology.

The following sections of the *chamber* topology are exacly the same as those from the AMBER topology files:

- POINTERS
- ATOM_NAME
- MASS
- ATOM_TYPE_INDEX
- NUMBER_EXCLUDED_ATOMS
- EXCLUDED_ATOMS_LIST
- NONBONDED_PARM_INDEX
- RESIDUE_LABEL
- BOND_FORCE_CONSTANT
- BOND_EQUIL_VALUE
- ANGLE_FORCE_CONSTANT
- DIHEDRAL_FORCE_CONSTANT
- DIHEDRAL_PERIODICITY
- DIHEDRAL_PHASE
- SCEE_SCALE_FACTOR
- SCNB_SCALE_FACTOR
- SOLTY
- BONDS_INC_HYDROGEN
- BONDS_WITHOUT_HYDROGEN
- ANGLES_INC_HYDROGEN
- ANGLES_WITHOUT_HYDROGEN
- DIHEDRALS_INC_HYDROGEN
- DIHEDRALS_WITHOUT_HYDROGEN
- HBOND_ACOEF
- HBOND_BCOEF
- HBCUT
- AMBER_ATOM_TYPE
- TREE_CHAIN_CLASSIFICATION [3]

---

[3] Not really supported. Every entry is BLA

Table 2: List of flags that are common between Amber and chamber topology files, but have different `FORMAT` identifiers.

FLAG name	AMBER Format	chamber Format
CHARGE	5E16.8	3E24.16
ANGLE_EQUIL_VALUE	5E16.8	3E25.17
LENNARD_JONES_ACOEF	5E16.8	3E24.16
LENNARD_JONES_BCOEF	5E16.8	3E24.16

- JOIN_ARRAY
- IROTAT
- RADIUS_SET
- RADII
- SCREEN
- SOLVENT_POINTERS
- ATOMS_PER_MOLECULE

FORCE_FIELD_TYPE

This section is a description of the CHARMM force field that is parametrized in the topology file. It is a single line (it can be read as a single string of length 80 characters). It does not affect any numerical results.

`%FORMAT(i2,a78)`

CHARMM_UREY_BRADLEY_COUNT

This section contains the number of Urey-Bradley parameters printed in the topology file. It contains two integers, the total number of Urey-Bradley terms (`NUB`) and the number of unique Urey-Bradley types (`NUBTYPES`).

`%FLAG CHARMM_UREY_BRADLEY_COUNT`
`%FORMAT(2i8)`
`NUB     NUBTYPES`

CHARMM_UREY_BRADLEY

This section contains all of the Urey-Bradley terms. It is formatted exactly like `BONDS_INC_HYDROGEN` and `BONDS_WITHOUT_HYDROGEN`.

`%FORMAT(10i8)`

There are $3 \times$ `NUB` integers in this section.

CHARMM_UREY_BRADLEY_FORCE_CONSTANT

This section contains all of the force constants for each unique Urey-Bradley term in $kcal\,mol^{-1}\,\mathring{A}^2$. It is formatted exactly the same as `BOND_FORCE_CONSTANT`.

`%FORMAT(5E16.8)`

There are `NUBTYPES` floating point numbers in this section.

CHARMM_UREY_BRADLEY_EQUIL_VALUE

This section contains all of the equilibrium distances for each unique Urey-Bradley term in Å. It is formatted exactly the same as `BOND_EQUIL_VALUE`.

`%FORMAT(5E16.8)`

There are `NUBTYPES` floating point numbers in this section.

CHARMM_NUM_IMPROPERS

This section contains the number of improper torsions in the topology file. It contains one integer, the total number of improper torsions.

`%FLAG CHARMM_NUM_IMPROPERS`
`%FORMAT(i8)`
`NIMPHI`

CHARMM_IMPROPERS

This section contains all of the improper torsion terms. It is formatted exactly like `DIHEDRALS_INC_HYDROGEN` and `DIHEDRALS_WITHOUT_HYDROGEN`.

`%FORMAT(10i8)`

There are $5 \times$ `NIMPHI` integers in this section.

CHARMM_NUM_IMPROPER_TYPES

This section contains the number of unique improper torsion types in the topology file. It contains one integer, the total number of improper torsions types.

`%FLAG CHARMM_NUM_IMPROPERS`
`%FORMAT(i8)`
`NIMPRTYPES`

CHARMM_IMPROPER_FORCE_CONSTANT

This section contains the force constant for each unique improper torsion type. It is formatted exactly like `DIHEDRAL_FORCE_CONSTANT`.

`%FORMAT(5E16.8)`

There are `NIMPRTYPES` integers in this section.

CHARMM_IMPROPER_PHASE

This section contains the phase shift for each unique improper torsion type. It is formatted exactly like `DIHEDRAL_PHASE`

`%FORMAT(5E16.8)`

There are `NIMPRTYPES` integers in this section.

LENNARD_JONES_14_ACOEF

Instead of scaling the 1-4 van der Waals interactions, the CHARMM force field actually assigns entirely different LJ parameters to each atom type. Therefore, *chamber* topologies have two extra sections that correspond to the set of LJ parameters for 1-4 interactions. The way these tables are set up is identical to the way `LENNARD_JONES_ACOEF` and `LENNARD_JONES_BCOEF` are set up in chamber topologies.

`%FORMAT(5E16.8)`

There are $[\text{NTYPES} \times (\text{NTYPES} + 1)] / 2$ floating point numbers in this section.

LENNARD_JONES_BCOEF

This section contains the LJ B-coefficients for 1-4 interactions. See LENNARD_JONES_14_AC above.

`%FORMAT(5E16.8)`

There are $[\text{NTYPES} \times (\text{NTYPES} + 1)] / 2$ floating point numbers in this section.

CHARMM_CMAP_COUNT

This section contains two integers—the number of total correction map (CMAP terms and the number of unique CMAP 'types.'

`%FLAG CHARMM_CMAP_COUNT`

```
%FORMAT(2i8)
CMAP_TERM_COUNT  CMAP_TYPE_COUNT
```
CHARM_CMAP_RESOLUTION

This section stores the resolution (*i.e.,* number of steps along each phi/psi CMAP axis) for each CMAP grid.

```
%FORMAT(20I4)
```

There are `CMAP_TERM_COUNT` integers in this section.

CHARMM_CMAP_PARAMETER_

There are `CMAP_TYPE_COUNT` of these sections, where is replaced by a 2-digit integer beginning from 01. It is a 2-dimensional Fortran array whose 1-D sequence is stored in column-major order.

```
%FORMAT(8(F9.5))
```

There are `CHARMM_CMAP_RESOLUTION(i)`^{2} floating point numbers in this section, where i is the in the FLAG title.