```
C(sp3)==>
atom         81   13    CT    "Alkane >C<"  ("atom type" "atom class" "atom
name")
atom         82   36    HC    "Alkane H-C"
vdw          81               3.5000     0.0660 (sigma and epsilon)
vdw          82               2.5000     0.0300
bond         13   36          340.00     1.0900 (Kb and r0)
.
.
.

C(sp2)==>
atom         87   38    CA    "Aromatic C"
atom         88   39    HA    "Aromatic H-C"
vdw          87               3.5500     0.0700
vdw          88               2.4200     0.0300
bond         38   39          367.00     1.0800
.
.
.

C(sp3)-OH ==>
atom         93    5    OH    "Alcohol -OH"
atom         94    7    HO    "Alcohol -OH"
vdw          93               3.1200     0.1700
vdw          94               0.0000     0.0000
bond          5    7          553.00     0.9450
.
.
.

C(sp2)-OH ==>
atom        105   38    CA    "Phenol C-OH"
atom        106    5    OH    "Phenol -OH"
atom        107    7    HO    "Phenol -OH"
vdw         105               3.5500     0.0700
vdw         106               3.0700     0.1700
vdw         107               0.0000     0.0000
bond          5   38          450.00     1.3640
bond          5    7          553.00     0.9450
.
.
.

Epoxy ==>
atom        119   29    OS    "Dialkyl Ether -O-"
vdw         119               2.9000     0.1400
bond         13   29          320.00     1.4100
.
.
.

Carboxylic acid ==>
atom        206    3    C     "Carboxylic Acid -COOH"
atom        207    4    O     "Carboxylic Acid C=O"
atom        208    5    OH    "Carboxylic Acid -OH"
vdw         206               3.7500     0.1050
vdw         207               3.0000     0.1700
vdw         208               2.9600     0.2100
bond          3    4          570.00     1.2290
bond          3    5          450.00     1.3640
.
.
```