

```
* STREAM FILE PREPARED VIA PYTHON
* CGenFF 2CLE
* PSH
*
```

```
!Something something bug in parser
set nat ?NATC
set app
if "@NAT" ne "?NATC" if @nat ne 0 set app append
```

```
read rtf card @app
* Custom Made RTF file from PSH for CGenFF 2CLE
*
36 1
```

```
MASS -1 CG321 12.01100 C
MASS -1 OG301 15.99940 O
MASS -1 CLGA1 35.45300 CL
MASS -1 HGA2 1.00800 H
```

```
DEFA FIRS NONE LAST NONE
AUTO ANGLES DIHE PATCH DRUDE
```

```
RESI 2CLE 0.000
```

```
GROUP
```

```
ATOM C1 CG321 -0.212000
ATOM C2 CG321 -0.212000
ATOM C3 CG321 0.121000
ATOM C4 CG321 0.121000
ATOM O1 OG301 -0.338000
ATOM CL1 CLGA1 -0.100000
ATOM CL2 CLGA1 -0.100000
ATOM H1 HGA2 0.090000
ATOM H2 HGA2 0.090000
ATOM H3 HGA2 0.090000
ATOM H4 HGA2 0.090000
ATOM H5 HGA2 0.090000
ATOM H6 HGA2 0.090000
ATOM H7 HGA2 0.090000
ATOM H8 HGA2 0.090000
```

```
BOND C1 C3 C1 O1 C2 C4 C2 O1
BOND C3 CL1 C4 CL2 C1 H1 C1 H2
BOND C2 H3 C2 H4 C3 H5 C3 H6
BOND C4 H7 C4 H8
```

```
END
```

```
READ PARAM CARD FLEX @APP
```

```
* Custom Made PRM file from PSH for CGenFF 2CLE
*
```

```
ATOMS
```

```
MASS -1 CG321 12.01100
MASS -1 OG301 15.99940
MASS -1 CLGA1 35.45300
MASS -1 HGA2 1.00800
```

```
BONDS
```

```
CG321 CG321 222.50000 1.53000
CG321 OG301 360.00000 1.41500
CG321 CLGA1 220.00000 1.78800
CG321 HGA2 309.00000 1.11100
```

```
ANGLES
```

```
CG321 CG321 OG301 45.00000 111.50000
CG321 CG321 HGA2 26.50000 110.10000 22.53000 2.17900
OG301 CG321 HGA2 45.90000 108.89000
HGA2 CG321 HGA2 35.50000 109.00000 5.40000 1.80200
CLGA1 CG321 HGA2 42.00000 107.00000
```

CG321	OG301	CG321	95.00000	109.70000
CG321	CG321	CLGA1	71.00000	112.20000

## DIHEDRALS

CG321	CG321	OG301	CG321	0.57000	1	0.00
CG321	CG321	OG301	CG321	0.29000	2	0.00
CG321	CG321	OG301	CG321	0.43000	3	0.00
HGA2	CG321	OG301	CG321	0.28400	3	0.00
OG301	CG321	CG321	HGA2	0.19000	3	0.00
HGA2	CG321	CG321	HGA2	0.22000	3	0.00
OG301	CG321	CG321	CLGA1	0.80000	3	0.00
CLGA1	CG321	CG321	HGA2	0.30000	3	0.00

## IMPROPERS

NONBONDED nbxmod 5 atom cdiel fshift vatom vdistance vswitch -  
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 1.0 wmin 1.5

CG321	0.0	-0.05600	2.01000	0.0	-0.01000	1.90000
OG301	0.0	-0.10000	1.65000			
CLGA1	0.0	-0.34300	1.91000			
HGA2	0.0	-0.03500	1.34000			

HBOND CUTHB 0.5

END

RETURN