

```
* STREAM FILE PREPARED VIA PYTHON
* GAAMP 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 GAAMP 2CLE
*
36 1
```

```
MASS -1 CG320 12.01100 C
MASS -1 CG321 12.01100 C
MASS -1 OG301 15.99940 O
MASS -1 CLGA0 35.45000 CL
MASS -1 HGA2 1.00800 H
```

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

```
RESI 2CLE 0.000
GROUP
```

```
ATOM C1 CG320 0.080000
ATOM C2 CG321 0.080000
ATOM C3 CG321 -0.269000
ATOM C4 CG321 -0.269000
ATOM O1 OG301 -0.316000
ATOM CL1 CLGA0 -0.171000
ATOM CL2 CLGA0 -0.171000
ATOM H1 HGA2 0.081000
ATOM H2 HGA2 0.081000
ATOM H3 HGA2 0.081000
ATOM H4 HGA2 0.081000
ATOM H5 HGA2 0.178000
ATOM H6 HGA2 0.178000
ATOM H7 HGA2 0.178000
ATOM H8 HGA2 0.178000
```

```
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 GAAMP 2CLE
*
```

```
ATOMS
MASS -1 CG320 12.01100
MASS -1 CG321 12.01100
MASS -1 OG301 15.99940
MASS -1 CLGA0 35.45000
MASS -1 HGA2 1.00800
```

```
BONDS
CG320 CG321 222.50000 1.53000
OG301 CG320 360.00000 1.41500
CG321 CG321 222.50000 1.53000
CG321 OG301 360.00000 1.41500
CG321 CLGA0 220.00000 1.77680
CG320 HGA2 309.00000 1.11100
CG321 HGA2 309.00000 1.11100
```

ANGLES

OG301	CG320	CG321	45.00000	111.50000
CG321	CG320	HGA2	26.50000	110.10000
OG301	CG320	HGA2	45.90000	108.89000
HGA2	CG320	HGA2	35.50000	109.00000
CG321	CG321	OG301	45.00000	111.50000
HGA2	CG321	CG321	26.50000	110.10000
HGA2	CG321	OG301	45.90000	108.89000
HGA2	CG321	HGA2	35.50000	109.00000
CG320	CG321	CLGA0	32.00000	112.20000
CG320	CG321	HGA2	26.50000	110.10000
HGA2	CG321	CLGA0	35.00000	108.99000
CG321	CG321	CLGA0	32.00000	112.20000
CG320	OG301	CG321	95.00000	109.70000

DIHEDRALS

CG320	OG301	CG321	CG321	0.14987	1	0.00
CG320	OG301	CG321	CG321	0.33668	2	0.00
CG320	OG301	CG321	CG321	0.19590	3	0.00
CG320	OG301	CG321	CG321	0.15787	4	0.00
CG320	OG301	CG321	CG321	0.06586	6	0.00
CG320	OG301	CG321	HGA2	0.28400	3	0.00
CG321	OG301	CG320	CG321	0.13614	1	0.00
CG321	OG301	CG320	CG321	0.35440	2	0.00
CG321	OG301	CG320	CG321	0.20069	3	0.00
CG321	OG301	CG320	CG321	0.15293	4	0.00
CG321	OG301	CG320	CG321	0.05655	6	0.00
CG321	OG301	CG320	HGA2	0.28400	3	0.00
OG301	CG320	CG321	CLGA0	0.53642	1	180.00
OG301	CG320	CG321	CLGA0	0.82941	2	0.00
OG301	CG320	CG321	CLGA0	0.57937	3	0.00
OG301	CG320	CG321	CLGA0	0.03442	4	180.00
OG301	CG320	CG321	CLGA0	0.13589	6	180.00
OG301	CG320	CG321	HGA2	0.19000	3	0.00
OG301	CG321	CG321	CLGA0	0.52946	1	180.00
OG301	CG321	CG321	CLGA0	0.81918	2	0.00
OG301	CG321	CG321	CLGA0	0.58081	3	0.00
OG301	CG321	CG321	CLGA0	0.03721	4	180.00
OG301	CG321	CG321	CLGA0	0.14137	6	180.00
HGA2	CG321	CG321	OG301	0.19000	3	0.00
CLGA0	CG321	CG320	HGA2	0.19500	3	0.00
HGA2	CG321	CG321	CLGA0	0.19500	3	0.00
HGA2	CG320	CG321	HGA2	0.22000	3	0.00
HGA2	CG321	CG321	HGA2	0.22000	3	0.00

IMPROPERS

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

CG320	0.0	-0.05600	2.01000	0.0	-0.01000	1.90000
CLGA0	0.0	-0.03000	1.90820			
CG321	0.0	-0.05600	2.01000	0.0	-0.01000	1.90000
OG301	0.0	-0.10000	1.65000			
HGA2	0.0	-0.03500	1.34000			

HBOND CUTHB 0.5

END

RETURN