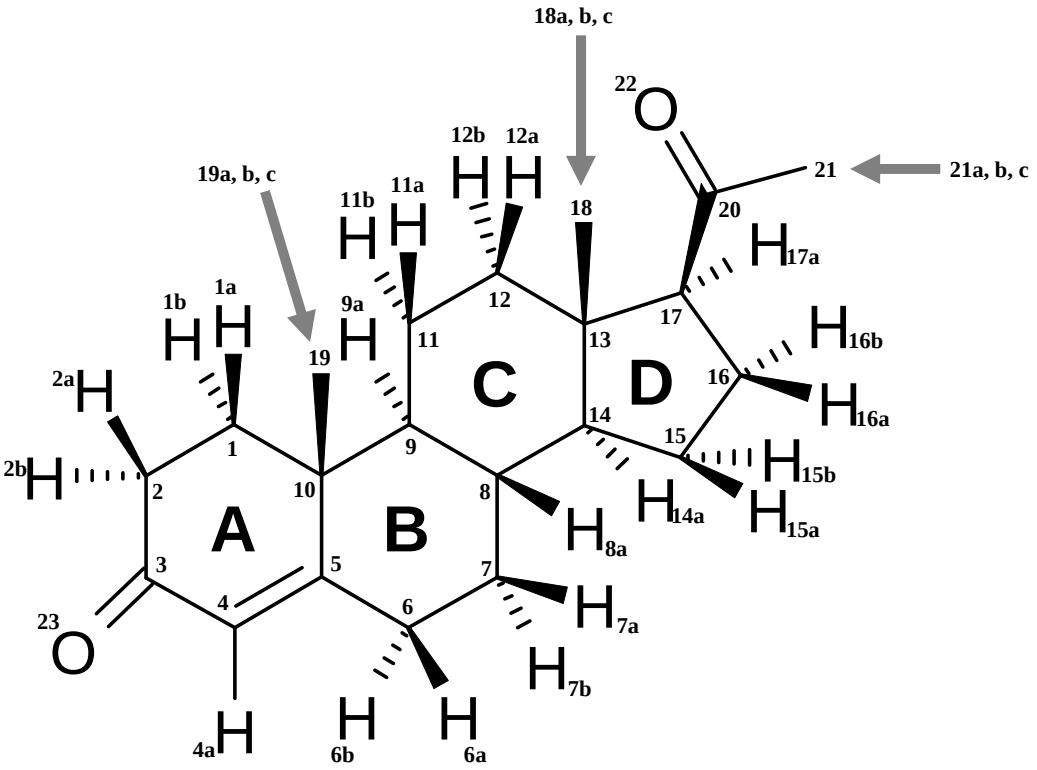
Charges and Charmm parameters for progesterone



Atom	Charge	Kind of atom
1	-0.180000	CTL2
2	-0.180000	CTL2
3	0.510000	CL
4	-0.150000	CEL1
5	0.000000	CEL1
6	-0.180000	CTL2
7	-0.180000	CTL2
8	-0.090000	CTL1
9	-0.090000	CTL1
10	0.000000	CTL1
11	-0.180000	CTL2
12	-0.180000	CTL2
13	0.000000	CTL1
14	-0.090000	CTL1
15	-0.180000	CTL2
16	-0.180000	CTL2
17	-0.090000	CTL1
18	-0.270000	CTL3
19	-0.270000	CTL3
20	0.510000	CL
21	-0.270000	CTL3
22	-0.510000	OBL
23	-0.510000	OBL

1a	0.090000	HAL2
1b	0.090000	HAL2
2a	0.090000	HAL2
2b	0.090000	HAL2
4a	0.150000	HEL1
6a	0.090000	HAL2
6b	0.090000	HAL2
7a	0.090000	HAL2
7b	0.090000	HAL2
8a	0.090000	HAL1
9a	0.090000	HAL1
11a	0.090000	HAL2
11b	0.090000	HAL2
12a	0.090000	HAL2
12b	0.090000	HAL2
14a	0.090000	HAL1
15a	0.090000	HAL2
15b	0.090000	HAL2
16a	0.090000	HAL2
16b	0.090000	HAL2
17a	0.090000	HAL1
18a	0.090000	HAL3
18b	0.090000	HAL3
18c	0.090000	HAL3
19a	0.090000	HAL3
19b	0.090000	HAL3
19c	0.090000	HAL3
21a	0.090000	HAL3
21b	0.090000	HAL3
21c	0.090000	HAL3

Parameters

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* progesterone parameters
*

BONDS

!V(bond) = Kb(b - b0)**2

!Kb: kcal/mole/A**2
!b0: A

!atom type  Kb          b0
CTL2  CL    200.000     1.522
CTL3  CL    200.000     1.522
CTL1  CL    200.000     1.522
OBL   CL    750.000     1.220
CTL2  HAL2  309.000     1.111
CTL3  HAL3  322.000     1.111
CTL2  CTL2  222.500     1.530
CTL0  CTL3  222.500     1.538
CTL1  CTL2  222.500     1.538
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CTL0  CTL2  222.500     1.538
CTL1  CTL1  222.500     1.500
CTL0  CTL1  222.500     1.500
CEL0  CEL1  440.000     1.340
HEL1  CEL1  360.500     1.100
CEL0  CTL0  240.000     1.502
CL    CEL1  269.151     1.476
CEL0  CTL2  365.000     1.502
CTL1  HAL1  309.000     1.111


ANGLES

!V(angle) = Ktheta(Theta - Theta0)**2

!Ktheta: kcal/mole/rad**2
!Theta0: degrees

!atom types     Ktheta    Theta0
OBL  CL   CTL3    70.0     125.00
OBL  CL   CTL2    70.0     125.00
OBL  CL   CTL1    70.0     125.00
HAL2 CTL2 CL      33.00    109.50
HAL3 CTL3 CL      33.00    109.50
CTL2 CTL2 CL      52.0     108.00
HAL2 CTL2 HAL2    35.50    109.00
HAL3 CTL3 HAL3   35.500    108.40
HAL1 CTL1 CTL1   34.500    110.10
HAL1 CTL1 CTL2   34.500    110.10
HAL1 CTL1 CTL0   34.500    110.10
HAL2 CTL2 CTL1   26.500    110.10
HAL2 CTL2 CTL0   26.500    110.10
HAL2 CTL2 CTL2   26.500    110.10
HAL3 CTL3 CTL0   33.430    110.10
CTL1 CTL1 CTL2   58.350    113.50
CTL1 CTL0 CTL2   58.350    113.50
CTL1 CTL0 CTL3   53.350    108.50
CTL1 CTL2 CTL2   58.350    113.50
CTL0 CTL2 CTL2   58.350    113.50
CTL0 CTL1 CTL2   58.350    113.50
CEL1 CEL0 CTL2   48.00     123.50
HEL1 CEL1 CEL0   52.00     119.50
CEL0 CTL2 CTL2   32.00     112.20
HAL2 CTL2 CEL0   45.00     111.50
CTL2 CTL0 CEL0   32.00     112.20
CTL1 CTL0 CEL0   32.00     112.20
CTL3 CTL0 CEL0   32.00     112.20
CTL0 CEL0 CTL2   50.00     113.00
CEL1 CEL0 CTL0   48.00     123.50
OBL  CL   CEL1   39.348    121.73
CEL1 CL   CTL2   19.827    115.70
CL   CEL1 CEL0   21.034    124.11
CTL2 CTL1 CL     13.128    113.54
HAL1 CTL1 CL      5.992    107.36
CTL0 CTL1 CL     11.547    115.74
CTL1 CL   CTL3   40.941    117.12
CTL2 CTL0 CTL3   58.350    113.50
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DIHEDRALS

!V(dihedral) = Kchi(1 + cos(n(chi) - delta))

!Kchi: kcal/mole
!n: multiplicity
!delta: degrees

!atom types				Kchi	n	delta
OBL	CL	CTL2	HAL2	0.00	6	180.00
X	CTL2	CL	X	0.05	6	180.00
X	CTL3	CL	X	0.05	6	180.00
X	CTL1	CTL1	X	0.200	3	0.00
X	CTL0	CTL1	X	0.200	3	0.00
X	CTL1	CTL2	X	0.200	3	0.00
X	CTL0	CTL2	X	0.200	3	0.00
X	CTL0	CTL3	X	0.200	3	0.00
X	CTL2	CTL2	X	0.1900	3	0.00
X	CEL1	CEL0	X	0.1300	1	180.00
CEL1	CEL0	CTL2	HAL2	0.0300	3	0.00
CEL1	CEL0	CTL2	CTL2	0.4000	3	0.00
CTL2	CEL0	CTL0	CTL1	0.00	3	180.0
CTL2	CEL0	CTL0	CTL3	0.00	3	180.0
CTL2	CEL0	CTL0	CTL2	0.30	3	180.0
HAL2	CTL2	CEL0	CTL0	0.0300	3	0.0
CEL1	CEL0	CTL0	CTL1	1.3000	3	180.0
CEL1	CEL0	CTL0	CTL2	1.3000	3	180.0
CEL1	CEL0	CTL0	CTL3	1.3000	3	180.0
OBL	CL	CEL1	CEL0	0.7024	2	180.00
OBL	CL	CEL1	HEL1	0.7510	2	180.00
CTL2	CL	CEL1	CEL0	0.7190	2	180.00
CTL2	CL	CEL1	HEL1	0.6697	2	180.00
CTL2	CTL2	CEL0	CTL0	0.1021	6	128.37
CTL2	CTL1	CL	OBL	0.0757	6	0.00
HAL1	CTL1	CL	CTL3	0.0738	6	205.59
HAL1	CTL1	CL	OBL	0.0730	6	0.00
CTL0	CTL1	CL	CTL3	0.0867	6	0.00
CTL1	CTL1	CL	OBL	0.0807	6	0.00

IMPROPER

!V(improper) = Kpsi(psi - psi0)**2

!Kpsi: kcal/mole/rad**2
!psi0: degrees

!atom types				Kpsi	0	psi0
OBL	X	X	CL	100.0000	0	0.0000
CTL2	HAL1	CTL1	CTL1	3.9867	0	-43.8026
CTL1	CTL1	CTL2	CTL1	2.5233	0	-33.5596
CTL2	HAL2	CTL1	CTL2	4.2669	0	39.3636
CTL2	CTL1	CTL1	CTL1	2.6763	0	-35.1164
CTL2	HAL2	CTL1	CTL2	4.0981	0	34.8234
CTL1	CTL2	CTL1	CTL1	2.7562	0	28.9907
CEL1	CTL1	CTL2	CTL1	3.0750	0	-35.8315
CL	CTL2	HAL2	CTL2	3.7008	0	-29.7072
CTL2	CEL1	CTL0	CEL0	0.5213	0	-0.8903
CL	CEL0	HEL1	CEL1	0.8082	0	-1.4242
HAL2	CEL0	CTL2	CTL2	3.8267	0	35.1361

CTL1	CTL2	HAL2	CTL2	3.1498	0	28.0810
HAL3	HAL3	HAL3	CTL3	8.1219	0	-38.0521
CTL2	CTL1	CL	CTL1	2.7133	0	-29.3745
CTL2	HAL2	CTL1	CTL2	3.5963	0	35.9089
CTL1	CTL3	CTL2	CTL1	2.6043	0	35.0995
CEL0	CTL1	CTL3	CTL0	2.8937	0	34.3759