Supplementary Material for “Retinal Conformation Governs pKa of Protonated Schiff Base in Rhodopsin Activation” by S. Zhu, M.F. Brown, and S.E. Feller

CHARMM style stream files for protonated and deprotonated model retinal Schiff base compounds

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* Toppar stream file for protonated retinal parameters
*
read rtf card append
* retinal/retinol and related model compounds
*
32  1

RESI RTNH       1.00
GROUP
ATOM C1   CT    0.00
ATOM C2   CT2  -0.18
ATOM H21  HA    0.09
ATOM H22  HA    0.09
GROUP
ATOM C3   CT2  -0.18
ATOM H31  HA    0.09
ATOM H32  HA    0.09
GROUP
ATOM C4   CT2  -0.18
ATOM H41  HA    0.09
ATOM H42  HA    0.09
ATOM C5   CC1A  0.00
ATOM C6   CC1A  0.00
GROUP
ATOM C7   CC1B -0.15
ATOM H71  HE1   0.15
ATOM C8   CC1B -0.15
ATOM H81  HE1   0.15
GROUP
ATOM C9   CC1A  0.00
ATOM C10  CR10 -0.15
ATOM H101 HE1   0.15
GROUP
ATOM C11  CR11 -0.15
ATOM H111 HE1   0.15
GROUP
ATOM C12  CR12 -0.15
ATOM H121 HE1   0.15
GROUP
ATOM C13  CR13  0.00
ATOM C14  CR14 -0.15
ATOM H141 HE1   0.15 H162 H163  H171 H172
GROUP                     \  |    |  /
ATOM C15  CR15  0.37 H161-C16    C17-H173            H191 H192
ATOM H151 HR1   0.20         \  /                      \   /
Group                  H21    C1        H71    H81      C19
ATOM NZ   NS2  -0.40      \  /  \        |      |       /  \
ATOM HZ1  HC    0.38   H22-C2    C6------C7=====C8----C9    H193
GROUP                       |     ||                   ||
ATOM C16  CT3  -0.27   H31-C3    C5   H181            C10-H101
ATOM H161 HA    0.09      /  \  /  \  /               |
ATOM H162 HA    0.09   H32    C4    C18-H182          C11-H111
ATOM H163 HA    0.09         /  \     \               ||
GROUP                       H41  H42   H183            C12-H121 H201
ATOM C17  CT3  -0.27                                   |       /
ATOM H171 HA    0.09                                   C13---C20-H202
ATOM H172 HA    0.09                                   ||      \
ATOM H173 HA    0.09                                   C14-H141 H203
GROUP                                                  |
ATOM C18  CT3  -0.27                                   C15-H151
ATOM H181 HA    0.09                                   ||
ATOM H182 HA    0.09                                   NZ-HZ1
ATOM H183 HA    0.09                                   |
GROUP                                            H211-C21-H213
ATOM C19  CT3  -0.27                                   |
ATOM H191 HA    0.09                                   H212
ATOM H192 HA    0.09
ATOM H193 HA    0.09
GROUP
ATOM C20  CT3  -0.27
ATOM H201 HA    0.09
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ATOM H202 HA    0.09
ATOM H203 HA    0.09
GROUP
ATOM C21  CT3   0.18
ATOM H211 HA    0.09
ATOM H212 HA    0.09
ATOM H213 HA    0.09


BOND C1   C2   C2   C3   C3   C4   C4   C5   C5   C6   C6   C1
BOND C6   C7   C7   C8   C8   C9   C9   C10  C10  C11  C11  C12
BOND C12  C13  C13  C14  C14  C15  C15  NZ   NZ   HZ1
BOND C1   C16  C1   C17  C5   C18  C9   C19  C13  C20
BOND C2   H21  C2   H22  C3   H31  C3   H32  C4   H41  C4   H42
BOND C7   H71  C8   H81  C10  H101 C11  H111 C12  H121 C14  H141
BOND C15  H151 NZ   C21  C21  H211 C21  H212 C21  H213
BOND C16  H161 C16  H162 C16  H163 C17  H171 C17  H172 C17  H173
BOND C18  H181 C18  H182 C18  H183 C19  H191 C19  H192 C19  H193
BOND C20  H201 C20  H202 C20  H203

IMPR C6   C5  C7  C1
IMPR C5   C6  C4  C18
IMPR C9   C10 C8  C19
IMPR C13  C14 C12 C20
IMPR C7   C6  C8  H71
IMPR C8   C7  C9  H81
IMPR C10  C9  C11 H101
IMPR C11  C10 C12 H111
IMPR C12  C11 C13 H121
IMPR C14  C13 C15 H141
IMPR C15  C14 NZ  H151

IC C1    C2    C3    C4     0.0000    0.00    0.00    0.00   0.0000
IC C6    C1    C2    C3     0.0000    0.00    0.00    0.00   0.0000
IC C2    C3    C4    C5     0.0000    0.00    0.00    0.00   0.0000
IC C3    C4    C5    C6     0.0000    0.00    0.00    0.00   0.0000
IC C1    C6    C7    C8     0.0000    0.00  180.00    0.00   0.0000
IC C6    C7    C8    C9     0.0000    0.00  180.00    0.00   0.0000
IC C7    C8    C9    C10    0.0000    0.00  180.00    0.00   0.0000
IC C2    C6    *C1   C16    0.0000    0.00  120.00    0.00   0.0000
IC C2    C6    *C1   C17    0.0000    0.00 -120.00    0.00   0.0000
IC C3    C1    *C2   H21    0.0000    0.00  120.00    0.00   0.0000
IC C3    C1    *C2   H22    0.0000    0.00 -120.00    0.00   0.0000
IC C4    C2    *C3   H31    0.0000    0.00  120.00    0.00   0.0000
IC C4    C2    *C3   H32    0.0000    0.00 -120.00    0.00   0.0000
IC C5    C3    *C4   H41    0.0000    0.00  120.00    0.00   0.0000
IC C5    C3    *C4   H42    0.0000    0.00 -120.00    0.00   0.0000
IC C5    C1    *C6   C7     0.0000    0.00  180.00    0.00   0.0000
IC C8    C6    *C7   H71    0.0000    0.00  180.00    0.00   0.0000
IC C9    C7    *C8   H81    0.0000    0.00  180.00    0.00   0.0000
IC C10   C8    *C9   C19    0.0000    0.00  180.00    0.00   0.0000
IC C8    C9    C10   C11    0.0000    0.00  180.00    0.00   0.0000
IC C11   C9    *C10  H101   0.0000    0.00  180.00    0.00   0.0000
IC C9    C10   C11   C12    0.0000    0.00  180.00    0.00   0.0000
IC C12   C10   *C11  H111   0.0000    0.00  180.00    0.00   0.0000
IC C10   C11   C12   C13    0.0000    0.00  180.00    0.00   0.0000
IC C13   C11   *C12  H121   0.0000    0.00  180.00    0.00   0.0000
IC C11   C12   C13   C14    0.0000    0.00  180.00    0.00   0.0000
IC C14   C12   *C13  C20    0.0000    0.00  180.00    0.00   0.0000
IC C12   C13   C14   C15    0.0000    0.00  180.00    0.00   0.0000
IC C15   C13   *C14  H141   0.0000    0.00  180.00    0.00   0.0000
IC C13   C14   C15   NZ     0.0000    0.00  180.00    0.00   0.0000
IC NZ    C14   *C15  H151   0.0000    0.00  180.00    0.00   0.0000
IC C14   C15   NZ    C21    0.0000    0.00  180.00    0.00   0.0000
IC C15   NZ    C21   H211   0.0000    0.00    0.00    0.00   0.0000
IC NZ    H211  *C21  H212   0.0000    0.00  120.00    0.00   0.0000
IC NZ    H211  *C21  H213   0.0000    0.00 -120.00    0.00   0.0000
IC C6    C1    C16   H161   0.0000    0.00  180.00    0.00   0.0000
IC H161  C1    *C16  H162   0.0000    0.00  120.00    0.00   0.0000
IC H161  C1    *C16  H163   0.0000    0.00 -120.00    0.00   0.0000
IC C6    C1    C17   H171   0.0000    0.00  180.00    0.00   0.0000
IC H171  C1    *C17  H172   0.0000    0.00  120.00    0.00   0.0000
IC H171  C1    *C17  H173   0.0000    0.00 -120.00    0.00   0.0000
IC C6    C4    *C5   C18    0.0000    0.00  180.00    0.00   0.0000
IC C4    C5    C18   H181   0.0000    0.00    0.00    0.00   0.0000
IC H181  C5    *C18  H182   0.0000    0.00  120.00    0.00   0.0000
IC H181  C5    *C18  H183   0.0000    0.00 -120.00    0.00   0.0000
IC C8    C9    C19   H191   0.0000    0.00  180.00    0.00   0.0000
IC H191  C9    *C19  H192   0.0000    0.00  120.00    0.00   0.0000
IC H191  C9    *C19  H193   0.0000    0.00 -120.00    0.00   0.0000
IC C12   C13   C20   H201   0.0000    0.00    0.00    0.00   0.0000
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IC H201  C13   *C20  H202   0.0000    0.00  120.00    0.00   0.0000
IC H201  C13   *C20  H203   0.0000    0.00 -120.00    0.00   0.0000
IC C21   C15   *NZ   HZ1    0.0000    0.00  180.00    0.00   0.0000

PATCH FIRST NONE LAST NONE

PRES SCK1       1.00

DELETE ATOM 1HZ2
DELETE ATOM 1HZ3
DELETE ATOM 2O15
GROUP                   HE1 HE2
ATOM 1CE  CT2   0.27     \ /
ATOM 1HE1 HA    0.09   --1CE1       2H15
ATOM 1HE2 HA    0.09         \       /
ATOM 1NZ  NS2  -0.40         1NZ=2C15
ATOM HZ1  HC    0.38         /       \
ATOM 2C15 CC1B  0.37      2HZ1        2C14==
ATOM 2H15 HR1   0.20                 /
GROUP                          2HE14
ATOM 2C14 CC1A -0.15
ATOM 2H141 HE1  0.15

BOND 1NZ 2C15

IC 1CD    1CE    1NZ    2C15    0.0000    0.00  180.00    0.00   0.0000
IC 1CE    1NZ    2C15   2C14    0.0000    0.00  180.00    0.00   0.0000
IC 1NZ    2C15   2C14   2C13    0.0000    0.00  180.00    0.00   0.0000
IC 2C15   1CE    *1NZ   1HZ1    0.0000    0.00  180.00    0.00   0.0000
IC 2C14   1NZ    *2C15  2H15    0.0000    0.00  180.00    0.00   0.0000
IC 2C5    2C6    2C1    2C2     0.0000    0.00    0.00    0.00   0.0000

end

read parameter card append

BONDS
HE1   CC1A  360.500     1.100
HE1   CC1B  360.500     1.100
CC1A  CC1A  440.000     1.340
CC1B  CC1B  440.000     1.340
CC1A  CC1B  300.000     1.470
CC1A  CT2   365.000     1.502
CC1A  CT    365.000     1.502
CC1A  CT3   383.000     1.504
CT    CT2   222.500     1.538
CT    CT3   222.500     1.538
CT3   NS2   300.000     1.453
NS2   HC    455.000     1.000
CT2   NS2   300.000     1.453
CR10  HE1   370.000     1.070
CR11  HE1   370.000     1.070
CR12  HE1   370.000     1.070
CR14  HE1   370.000     1.070
CR15  HR1   370.000     1.070
CR10  CC1A  550.000     1.370
CR10  CR11  430.000     1.410
CR11  CR12  550.000     1.370
CR12  CR13  430.000     1.400
CR13  CT3   320.000     1.520
CR13  CR14  550.000     1.400
CR14  CR15  430.000     1.370
CR15  NS2   490.000     1.320

ANGLES
CC1A CC1A CT     48.00     123.50
CC1B CC1A CT     48.00     123.50
CC1A CC1A CT3    48.00     123.50
HA   CT2  CC1A   45.00     111.50
HA   CT3  CC1A   42.00     111.50
HE1  CC1A CC1A   42.00     119.00
HE1  CC1B CC1B   42.00     119.00
HE1  CC1A CT3    42.00     117.50
HE1  CC1B CC1A   42.00     118.00
HE1  CC1A CC1B   42.00     118.00
CC1A CC1B CC1B   48.00     123.50
CC1A CT   CT3    32.00     112.20
CC1A CT   CT2    32.00     112.20
CC1A CT2  CT2    32.00     112.20
CC1A CC1A CC1B   48.00     123.50
CC1A CC1A CT2    48.00     123.50
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CT2  CC1A CT3    48.00     123.50
CC1B CC1A CT3    48.00     113.00
CT2  CT   CT3    58.35     113.50   11.16   2.561
CT3  CT   CT3    58.35     113.50   11.16   2.561
CT   CT2  CT2    58.35     113.50   11.16   2.561
CT   CT2  HA     26.50     110.10   22.53   2.179
CT   CT3  HA     33.43     110.10   22.53   2.179
CT   CC1A CT3    48.00     123.50
CT3  CC1A CT3    47.00     125.20
HE1  CC1A CT2    40.00     116.00
CT3  NS2  HC     38.00     117.40
HA   CT3  NS2    42.00     110.10
CT2  NS2  HC     38.00     117.40
CT2  CT2  NS2    67.70     110.00
HA   CT2  NS2    42.00     110.10
CC1A CR10 HE1    35.00     119.70
CR10 CR11 HE1    35.00     119.70
CR11 CR12 HE1    35.00     119.70
CR13 CR14 HE1    35.00     119.70
CR14 CR15 HR1    35.00     119.70
HE1  CR10 CR11   35.00     119.00
HE1  CR11 CR12   35.00     119.70
HE1  CR12 CR13   35.00     119.70
HE1  CR14 CR15   35.00     119.70
HR1  CR15 NS2    35.00     119.70
CR15 NS2  HC     35.00     119.70
CR13 CT3  HA     50.00     109.50
CR10 CC1A CC1B   95.00     122.90
CC1A CR10 CR11   95.00     122.90
CR10 CR11 CR12   95.00     122.90
CR11 CR12 CR13   95.00     122.90
CR12 CR13 CR14   95.00     122.90
CR13 CR14 CR15   95.00     122.90
CR14 CR15 NS2    40.00     125.60
CR12 CR13 CT3    70.00     119.70
CR10 CC1A CT3    70.00     119.70
CR15 NS2  CT3    67.00     123.60
CR14 CR13 CT3    70.00     119.70

DIHEDRALS
CT2  CC1A CT3  HA       0.3920  3     0.00
HE1  CC1A CT3  HA       0.3000  3     0.00
CC1B CC1A CT3  HA       0.1230  3     0.00
CC1B CC1A CT3  HA       0.1290  2   180.00
CR10 CC1A CT3  HA       0.0640  3   180.00
CR12 CR13 CT3  HA       0.0640  3     0.00
HA   CT3  CR13 CR14     0.0880  3   180.00
HA   CT3  CR13 CR14     0.1500  6   180.00
CC1A CT   CT3  HA       0.1600  3     0.00
CT3  CT   CT3  HA       0.1600  3     0.00
CT2  CT   CT3  HA       0.1600  3     0.00
CC1A CC1A CT   CT2      0.5000  2     0.00
CC1A CC1A CT   CT2      0.3000  3     0.00
CC1A CC1A CT   CT3      0.5000  2     0.00
CC1A CC1A CT   CT3      0.4000  3     0.00
CC1B CC1A CT   CT2      0.3000  3     0.00
CC1B CC1A CT   CT3      0.3000  3     0.00
CC1A CC1A CT2  CT2      0.5000  2     0.00
CC1A CC1A CT2  CT2      0.3000  3     0.00
CT2  CT2  CC1A CT3      0.1900  3     0.00
CT3  CC1A CT2  HA       0.1900  3     0.00
CC1A CC1A CT2  HA       0.0300  3     0.00
CC1A CT2  CT2  CT2      0.1900  3     0.00
CC1A CT2  CT2  HA       0.1900  3     0.00
CT2  CT2  CT   CC1A     0.2000  3     0.00
CT2  CT2  CT   CT3      0.2000  3     0.00
CC1A CT   CT2  HA       0.1900  3     0.00
CT3  CT   CT2  HA       0.1900  3     0.00
CC1B CC1A CC1A CT2      0.5600  1   180.00
CC1B CC1A CC1A CT2      7.0000  2   180.00
CT   CC1A CC1A CT2     10.0000  2   180.00
CT   CC1A CC1A CT3     10.0000  2   180.00
CC1A CC1A CC1B CC1B     0.4850  1   180.00
CC1A CC1A CC1B CC1B     1.5790  2   180.00
CC1A CC1A CC1B CC1B     0.9060  3     0.00
CC1A CC1A CC1B CC1B     0.2030  4     0.00
CT   CC1A CC1B CC1B     0.5840  1      0.0
CT   CC1A CC1B CC1B     3.394   2   180.00
CT   CC1A CC1B CC1B     0.186   3      0.0
CT   CC1A CC1B CC1B     0.3330  4    180.0
CT   CC1A CC1B CC1B     0.1850  5    180.0
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CT	CC1A	CC1B	CC1B	0.0790	6	180.0
CT	CC1A	CC1B	HE1	0.1600	1	90.0
CT	CC1A	CC1B	HE1	0.4510	2	90.0
CT	CC1A	CC1B	HE1	0.0830	3	90.0
CT	CC1A	CC1B	HE1	0.1690	4	90.0
CT	CC1A	CC1B	HE1	0.119	5	90.00
CT	CC1A	CC1B	HE1	0.136	6	90.00
CC1A	CC1B	CC1B	CC1A	1.1000	1	180.00
CC1A	CC1B	CC1B	CC1A	14.460	2	180.00
CC1A	CC1B	CC1B	CC1A	0.0900	3	180.00
CC1A	CC1B	CC1B	CC1A	2.8000	4	0.00
CC1A	CC1B	CC1B	CC1A	0.0950	5	180.00
CC1A	CC1B	CC1B	CC1A	0.9790	6	180.00
HE1	CC1B	CC1B	HE1	0.6920	1	90.00
HE1	CC1B	CC1B	HE1	1.4020	2	90.00
HE1	CC1B	CC1B	HE1	0.6380	3	90.00
HE1	CC1B	CC1B	HE1	0.4520	4	-90.00
HE1	CC1B	CC1B	HE1	0.074	5	90.00
HE1	CC1B	CC1B	HE1	0.318	6	-90.00
CT3	CC1A	CC1B	HE1	1.0000	2	180.00
CT3	CC1A	CC1B	CC1B	0.9700	1	180.00
CT3	CC1A	CC1B	CC1B	0.5440	2	180.00
CT3	CC1A	CC1B	CC1B	0.5750	3	180.00
CT3	CC1A	CC1B	CC1B	0.3170	4	90.00
CC1B	CC1A	CC1A	CT3	7.0000	2	180.00
CR10	CC1A	CC1B	CC1B	0.7670	1	180.00
CR10	CC1A	CC1B	CC1B	3.5150	2	180.00
CR10	CC1A	CC1B	CC1B	0.5600	3	0.00
CR10	CC1A	CC1B	CC1B	0.535	4	0.00
CR11	CR10	CC1A	CC1B	0.2980	1	180.00
CR11	CR10	CC1A	CC1B	14.168	2	180.00
CR11	CR10	CC1A	CC1B	0.6010	3	0.00
CR11	CR10	CC1A	CC1B	3.4640	4	0.00
CR11	CR10	CC1A	CC1B	0.1590	5	180.00
CR11	CR10	CC1A	CC1B	1.5240	6	180.00
CR12	CR11	CR10	CC1A	1.1350	1	180.00
CR12	CR11	CR10	CC1A	8.0240	2	180.00
CR12	CR11	CR10	CC1A	0.4250	3	0.00
CR12	CR11	CR10	CC1A	0.6470	4	0.00
CR12	CR11	CR10	CC1A	0.3080	5	180.00
CR12	CR11	CR10	CC1A	0.3120	6	180.00
CR10	CR11	CR12	CR13	1.6900	1	180.00
CR10	CR11	CR12	CR13	13.093	2	180.00
CR10	CR11	CR12	CR13	0.4680	3	0.00
CR10	CR11	CR12	CR13	2.7660	4	0.00
CR10	CR11	CR12	CR13	0.4800	5	180.00
CR10	CR11	CR12	CR13	1.1900	6	180.00
CR10	CR11	CR12	HE1	0.2000	2	180.00
HE1	CR11	CR12	CR13	0.2000	2	180.00
CR11	CR12	CR13	CT3	1.4000	1	180.00
CR11	CR12	CR13	CT3	2.8000	2	180.00
CR11	CR12	CR13	CR14	1.3810	1	180.00
CR11	CR12	CR13	CR14	5.5040	2	180.00
CR11	CR12	CR13	CR14	0.8030	3	0.00
CR11	CR12	CR13	CR14	1.3460	4	0.00
CR11	CR12	CR13	CR14	0.2030	5	180.00
CR11	CR12	CR13	CR14	0.3130	6	180.00
CR12	CR13	CR14	CR15	1.4650	1	180.0
CR12	CR13	CR14	CR15	5.1460	2	180.0
CR12	CR13	CR14	CR15	0.7940	3	0.00
CR12	CR13	CR14	CR15	2.0720	4	0.00
CR12	CR13	CR14	CR15	0.2500	5	180.0
CR12	CR13	CR14	CR15	0.8100	6	180.0
CT3	CR13	CR14	CR15	0.5600	1	180.00
CT3	CR13	CR14	CR15	7.0000	2	180.00
CR13	CR14	CR15	NS2	1.0320	1	180.00
CR13	CR14	CR15	NS2	10.032	2	180.00
CR13	CR14	CR15	NS2	0.3460	3	0.00
CR13	CR14	CR15	NS2	1.4510	4	0.00
CR13	CR14	CR15	NS2	0.3860	5	180.00
CR13	CR14	CR15	NS2	0.6200	6	180.00
CR14	CR15	NS2	CT3	0.848	1	180.00
CR14	CR15	NS2	CT3	6.713	2	180.00

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CR14 CR15 NS2  CT3      0.114   3   180.00
CR14 CR15 NS2  CT3      0.8220  4     0.00
CR14 CR15 NS2  CT3      0.077   5   180.00
CR14 CR15 NS2  CT3      0.350   6   180.00
CR14 CR15 NS2  HC       5.0000  2   180.00
CT2  CT2  NS2  HC       0.1000  3     0.00
HA   CT2  NS2  HC       0.1000  3     0.00
CR15 NS2  CT3  HA       0.1500  3   180.00
HA   CT3  NS2  HC       0.1100  3     0.00

IMPROPER
CC1A X    X    CT3      100.0   0      0.0
CC1A X    X    CT       100.0   0      0.0
CC1B X    X    HE1      100.0   0      0.0
CC1A X    X    HE1      100.0   0      0.0
CR12 X    X    CT3      100.0   0      0.0
CR10 X    X    HE1      100.0   0      0.0
CR11 X    X    HE1      100.0   0      0.0
CR12 X    X    HE1      100.0   0      0.0
CR13 X    X    CT3      100.0   0      0.0
CR14 X    X    HE1      100.0   0      0.0
CR15 X    X    HE1      100.0   0      0.0
CR15 X    X    HR1      100.0   0      0.0

NONBONDED nbxmod  5 atom cdiel shift vatom vdistance vswitch -
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 1.0 wmin 1.5
                !adm jr., 5/08/91, suggested cutoff scheme

end
```

CHARMM style stream files for protonated and deprotonated model retinal Schiff base compounds

```
* Toppar stream file for deprotonated retinal parameters
*
read rtf card append
* retinal/retinol and related model compounds
*
32  1

RESI RTNE       0.00

GROUP
ATOM C1   CT    0.00
ATOM C2   CT2  -0.18
ATOM H21  HA    0.09
ATOM H22  HA    0.09
GROUP
ATOM C3   CT2  -0.18
ATOM H31  HA    0.09
ATOM H32  HA    0.09
GROUP
ATOM C4   CT2  -0.18
ATOM H41  HA    0.09
ATOM H42  HA    0.09
ATOM C5   CC1A  0.00
ATOM C6   CC1A  0.00
GROUP
ATOM C7   CC1B -0.15
ATOM H71  HE1   0.15
ATOM C8   CC1B -0.15
ATOM H81  HE1   0.15
GROUP
ATOM C9   CC1A  0.00
ATOM C10  CC1A -0.15
ATOM H101 HE1   0.15
GROUP
ATOM C11  CC1B -0.15
ATOM H111 HE1   0.15
GROUP
ATOM C12  CC1B -0.15
ATOM H121 HE1   0.15
GROUP
ATOM C13  CC1A  0.00
ATOM C14  CC1A -0.15
ATOM H141 HE1   0.15 H162 H163  H171 H172
GROUP                     \  |    |  /
```

```
ATOM C15  CC1B  0.23 H161-C16    C17-H173            H191 H192
ATOM H151 HE1   0.15         \  /                      \   /
Group                  H21    C1        H71    H81      C19
ATOM NZ   NS1  -0.60      \  /  \        |      |       /  \
                       H22-C2    C6------C7=====C8----C9    H193
GROUP                     |     ||                    ||
ATOM C16  CT3  -0.27   H31-C3    C5   H181            C10-H101
ATOM H161 HA    0.09      /  \  /  \  /               |
ATOM H162 HA    0.09   H32    C4    C18-H182          C11-H111
ATOM H163 HA    0.09         /  \     \               ||
GROUP                       H41  H42   H183            C12-H121 H201
ATOM C17  CT3  -0.27                                  |        /
ATOM H171 HA    0.09                                  C13---C20-H202
ATOM H172 HA    0.09                                  ||      \
ATOM H173 HA    0.09                                  C14-H141 H203
GROUP                                                 |
ATOM C18  CT3  -0.27                                  C15-H151
ATOM H181 HA    0.09                                  ||
ATOM H182 HA    0.09                                  NZ
ATOM H183 HA    0.09                                  |
GROUP                                            H211-C21-H213
ATOM C19  CT3  -0.27                                  |
ATOM H191 HA    0.09                                  H212
ATOM H192 HA    0.09
ATOM H193 HA    0.09
GROUP
ATOM C20  CT3  -0.27
ATOM H201 HA    0.09
ATOM H202 HA    0.09
ATOM H203 HA    0.09
GROUP
ATOM C21  CT3  -0.05
ATOM H211 HA    0.09
ATOM H212 HA    0.09
ATOM H213 HA    0.09

BOND C1   C2   C2   C3   C3   C4   C4   C5   C5   C6   C6   C1
BOND C6   C7   C7   C8   C8   C9   C9   C10  C10  C11  C11  C12
BOND C12  C13  C13  C14  C14  C15  C15  NZ
BOND C1   C16  C1   C17  C5   C18  C9   C19  C13  C20
BOND C2   H21  C2   H22  C3   H31  C3   H32  C4   H41  C4   H42
BOND C7   H71  C8   H81  C10  H101 C11  H111 C12  H121 C14  H141
BOND C15  H151 NZ   C21  C21  H211 C21  H212 C21  H213
BOND C16  H161 C16  H162 C16  H163 C17  H171 C17  H172 C17  H173
BOND C18  H181 C18  H182 C18  H183 C19  H191 C19  H192 C19  H193
BOND C20  H201 C20  H202 C20  H203

IMPR C6   C5  C7  C1
IMPR C5   C6  C4  C18
IMPR C9   C10 C8  C19
IMPR C13  C14 C12 C20
IMPR C7   C6  C8  H71
IMPR C8   C7  C9  H81
IMPR C10  C9  C11 H101
IMPR C11  C10 C12 H111
IMPR C12  C11 C13 H121
IMPR C14  C13 C15 H141
IMPR C15  C14 NZ  H151

IC C1    C2    C3    C4     0.0000    0.00  -62.00    0.00   0.0000
IC C6    C1    C2    C3     0.0000    0.00   46.00    0.00   0.0000
IC C2    C3    C4    C5     0.0000    0.00   46.00    0.00   0.0000
IC C3    C4    C5    C6     0.0000    0.00  -18.00    0.00   0.0000
IC C1    C6    C7    C8     0.0000    0.00 -120.00    0.00   0.0000
IC C6    C7    C8    C9     0.0000    0.00  180.00    0.00   0.0000
IC C7    C8    C9    C10    0.0000    0.00  180.00    0.00   0.0000
IC C2    C6    *C1   C16    0.0000    0.00  120.00    0.00   0.0000
IC C2    C6    *C1   C17    0.0000    0.00 -120.00    0.00   0.0000
IC C3    C1    *C2   H21    0.0000    0.00  120.00    0.00   0.0000
IC C3    C1    *C2   H22    0.0000    0.00 -120.00    0.00   0.0000
IC C4    C2    *C3   H31    0.0000    0.00  120.00    0.00   0.0000
IC C4    C2    *C3   H32    0.0000    0.00 -120.00    0.00   0.0000
IC C5    C3    *C4   H41    0.0000    0.00  120.00    0.00   0.0000
IC C5    C3    *C4   H42    0.0000    0.00 -120.00    0.00   0.0000
IC C5    C1    *C6   C7     0.0000    0.00  180.00    0.00   0.0000
IC C8    C6    *C7   H71    0.0000    0.00  180.00    0.00   0.0000
IC C9    C7    *C8   H81    0.0000    0.00  180.00    0.00   0.0000
IC C10   C8    *C9   C19    0.0000    0.00  180.00    0.00   0.0000
IC C8    C9    C10   C11    0.0000    0.00  180.00    0.00   0.0000
IC C11   C9    *C10  H101   0.0000    0.00  180.00    0.00   0.0000
IC C9    C10   C11   C12    0.0000    0.00  180.00    0.00   0.0000
```

```
IC C12   C10   *C11  H111   0.0000    0.00  180.00    0.00   0.0000
IC C10   C11   C12   C13    0.0000    0.00  180.00    0.00   0.0000
IC C13   C11   *C12  H121   0.0000    0.00  180.00    0.00   0.0000
IC C11   C12   C13   C14    0.0000    0.00  180.00    0.00   0.0000
IC C14   C12   *C13  C20    0.0000    0.00  180.00    0.00   0.0000
IC C12   C13   C14   C15    0.0000    0.00  180.00    0.00   0.0000
IC C15   C13   *C14  H141   0.0000    0.00  180.00    0.00   0.0000
IC C13   C14   C15   NZ     0.0000    0.00  180.00    0.00   0.0000
IC NZ    C14   *C15  H151   0.0000    0.00  180.00    0.00   0.0000
IC C14   C15   NZ    C21    0.0000    0.00  180.00    0.00   0.0000
IC C15   NZ    C21   H211   0.0000    0.00    0.00    0.00   0.0000
IC NZ    H211  *C21  H212   0.0000    0.00  120.00    0.00   0.0000
IC NZ    H211  *C21  H213   0.0000    0.00 -120.00    0.00   0.0000
IC C6    C1    C16   H161   0.0000    0.00  180.00    0.00   0.0000
IC H161  C1    *C16  H162   0.0000    0.00  120.00    0.00   0.0000
IC H161  C1    *C16  H163   0.0000    0.00 -120.00    0.00   0.0000
IC C6    C1    C17   H171   0.0000    0.00  180.00    0.00   0.0000
IC H171  C1    *C17  H172   0.0000    0.00  120.00    0.00   0.0000
IC H171  C1    *C17  H173   0.0000    0.00 -120.00    0.00   0.0000
IC C6    C4    *C5   C18    0.0000    0.00  180.00    0.00   0.0000
IC C4    C5    C18   H181   0.0000    0.00 -175.00    0.00   0.0000
IC H181  C5    *C18  H182   0.0000    0.00  120.00    0.00   0.0000
IC H181  C5    *C18  H183   0.0000    0.00 -120.00    0.00   0.0000
IC C8    C9    C19   H191   0.0000    0.00  180.00    0.00   0.0000
IC H191  C9    *C19  H192   0.0000    0.00  120.00    0.00   0.0000
IC H191  C9    *C19  H193   0.0000    0.00 -120.00    0.00   0.0000
IC C12   C13   C20   H201   0.0000    0.00  180.00    0.00   0.0000
IC H201  C13   *C20  H202   0.0000    0.00  120.00    0.00   0.0000
IC H201  C13   *C20  H203   0.0000    0.00 -120.00    0.00   0.0000

PATCH FIRST NONE LAST NONE

PRES SCK0       0.00


DELETE ATOM 1NZ
DELETE ATOM 1HZ1
DELETE ATOM 1HZ2
DELETE ATOM 1HZ3
DELETE ATOM 2C21
DELETE ATOM 2H211
DELETE ATOM 2H212
DELETE ATOM 2H213

GROUP                   HE1 HE2
ATOM 1CE  CT2   0.04      \ /
ATOM 1HE1 HA    0.09   --1CE       2H151
ATOM 1HE2 HA    0.09         \       /
                             2NZ=2C15
                                     \
BOND 1CE 2NZ

IC 1CG    1CD    1CE    2NZ     0.0000    0.00  180.00    0.00   0.0000
IC 1CD    1CE    2NZ    2C15    0.0000    0.00  180.00    0.00   0.0000
IC 1CE    2NZ    2C15   2C14    0.0000    0.00  180.00    0.00   0.0000
IC 2NZ    1CD   *1CE    1HE1   1.4604 110.4600  119.9100 110.5100  1.1128
IC 2NZ    1CD   *1CE    1HE2   1.4604 110.4600 -120.0200 110.5700  1.1123
IC 1HN    1N     1CA    1C      0.0000    0.00  180.00    0.00   0.0000
IC 1CB    1CA    1C     1O      0.0000    0.00 -110.00    0.00   0.0000
end

read parameter card append

BONDS
HE1   CC1A  360.500     1.100
HE1   CC1B  360.500     1.100
CC1A  CC1A  440.000     1.340
CC1B  CC1B  440.000     1.340
CC1A  CC1B  300.000     1.470
CC1A  CT3   383.000     1.504
CC1A  CT2   365.000     1.502
CC1A  CT    365.000     1.502
CT   CT2    222.500     1.538
CT   CT3    222.500     1.538
NS1   CC1B  500.000     1.276
CT3   NS1   310.000     1.440
CT2   NS1   310.000     1.440

ANGLES
CC1A CC1A CT3    48.00     123.50
HA   CT2  CC1A   45.00     111.50
```

HA	CT3	CC1A	42.00	111.50		
HE1	CC1A	CC1A	42.00	119.00		
HE1	CC1B	CC1B	42.00	119.00		
HE1	CC1A	CT3	42.00	117.50		
HE1	CC1B	CC1A	42.00	118.00		
HE1	CC1A	CC1B	42.00	118.00		
CC1A	CC1B	CC1B	48.00	123.50		
CC1A	CT	CT3	32.00	112.20		
CC1A	CT	CT2	32.00	112.20		
CC1A	CT2	CT2	32.00	112.20		
CC1A	CC1A	CC1B	48.00	123.50		
CC1A	CC1A	CT	48.00	123.50		
CC1A	CC1A	CT2	48.00	123.50		
CC1B	CC1A	CT	48.00	123.50		
CT2	CC1A	CT3	48.00	123.50		
CC1B	CC1A	CT3	48.00	113.00		
CT2	CT	CT3	58.35	113.50	11.16	2.561
CT3	CT	CT3	58.35	113.50	11.16	2.561
CT	CT2	CT2	58.35	113.50	11.16	2.561
CT	CT2	HA	26.50	110.10	22.53	2.179
CT	CT3	HA	33.43	110.10	22.53	2.179
CT	CC1A	CT3	48.00	123.50		
CT3	NS1	CC1B	67.00	111.00		
NS1	CC1B	HE1	38.00	119.50		
HA	CT3	NS1	42.00	113.50		
CT2	CT2	NS1	67.70	110.00		
HA	CT2	NS1	42.00	113.50		
CT2	NS1	CC1B	67.00	111.00		
NS1	CC1B	CC1A	40.00	123.00		

DIHEDRALS

CC1B	CC1A	CT3	HA	0.0116	6	180.00
CC1B	CC1A	CT3	HA	0.0870	3	0.00
CT2	CC1A	CT3	HA	0.475	3	0.00
CC1A	CC1A	CC1B	CC1B	2.9000	2	180.00
CC1A	CC1A	CC1B	CC1B	1.3440	3	0.00
CC1A	CC1A	CC1B	CC1B	0.2880	4	0.00
CT3	CC1A	CC1B	HE1	0.6620	1	180.00
CT3	CC1A	CC1B	HE1	1.0800	2	180.00
CT3	CC1A	CC1B	CC1B	0.8550	1	180.00
HE1	CC1A	CC1B	CC1B	1.0430	1	0.00
HE1	CC1A	CC1B	CC1B	1.312	2	180.00
HE1	CC1A	CC1B	CC1B	0.7050	3	0.00
CT	CC1A	CC1B	CC1B	1.5410	1	0.0
CT	CC1A	CC1B	CC1B	0.743	2	180.0
CT	CC1A	CC1B	CC1B	0.702	3	0.0
CT	CC1A	CC1B	CC1B	0.516	4	180.0
CT	CC1A	CC1B	CC1B	0.216	5	180.0
CT	CC1A	CC1B	CC1B	0.089	6	180.0
CT	CC1A	CC1B	HE1	0.5060	2	90.00
CT	CC1A	CC1B	HE1	0.1770	4	90.00
CT	CC1A	CC1B	HE1	0.0550	5	90.00
CT	CC1A	CC1B	HE1	0.094	6	90.00
CT3	NS1	CC1B	CC1A	0.2180	1	180.00
CT3	NS1	CC1B	CC1A	19.537	2	180.00
CT3	NS1	CC1B	CC1A	0.5970	3	0.00
CT3	NS1	CC1B	CC1A	4.4390	4	0.00
CT3	NS1	CC1B	CC1A	0.4640	5	180.00
CT3	NS1	CC1B	CC1A	1.8520	6	180.00
CC1A	CC1B	CC1B	CC1A	0.300	1	180.00
CC1A	CC1B	CC1B	CC1A	16.383	2	180.00
CC1A	CC1B	CC1B	CC1A	0.7460	3	0.00
CC1A	CC1B	CC1B	CC1A	3.6370	4	0.00
CC1A	CC1B	CC1B	CC1A	1.4132	6	180.00
HE1	CC1B	CC1B	HE1	1.376	1	180.00
HE1	CC1B	CC1B	HE1	0.867	2	0.00
CC1B	CC1A	CC1A	CC1B	0.7940	1	180.00
CC1B	CC1A	CC1A	CC1B	5.3480	2	180.00
CC1B	CC1A	CC1A	CC1B	0.6380	3	0.00
CC1B	CC1A	CC1A	CC1B	2.8060	4	0.00
CC1B	CC1A	CC1A	CC1	1.2890	6	180.00
CT3	CC1A	CC1A	CC1B	7.0000	2	180.00
CT3	CC1A	CC1A	HE1	5.2000	2	180.00
CT	CC1A	CC1A	CT2	10.0000	2	180.00
CT	CC1A	CC1A	CT3	10.0000	2	180.00
CC1A	CC1A	CT	CT2	0.5000	2	0.00
CC1A	CC1A	CT	CT2	0.3000	3	0.00
CC1A	CC1A	CT	CT3	0.5000	2	0.00
CC1A	CC1A	CT	CT3	0.4000	3	0.00
CC1B	CC1A	CT	CT2	0.3000	3	0.00

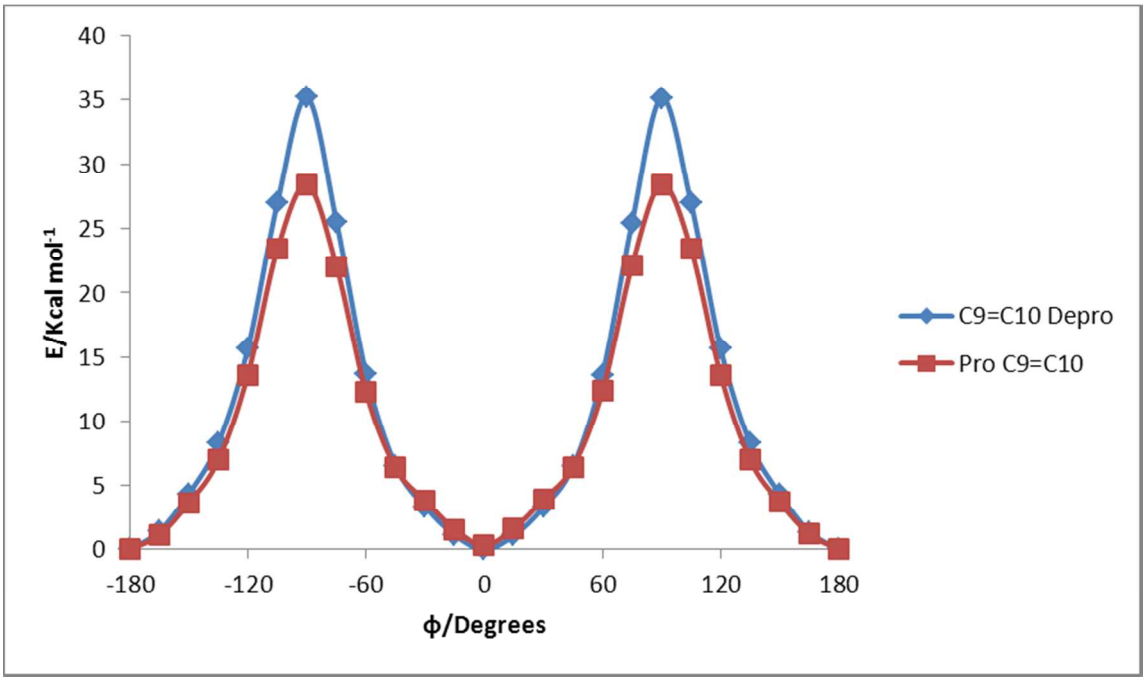
```
CC1B CC1A CT   CT3      0.3000  3     0.00
CC1A CC1A CT2  CT2      0.5000  2     0.00
CC1A CC1A CT2  CT2      0.3000  3     0.00
CT2  CT2  CC1A CT3      0.1900  3     0.00
CT3  CC1A CT2  HA       0.1900  3     0.00
CC1A CC1A CT2  HA       0.0300  3     0.00
CC1A CT2  CT2  CT2      0.1900  3     0.00
CC1A CT2  CT2  HA       0.1900  3     0.00
CT2  CT2  CT   CC1A     0.2000  3     0.00
CT2  CT2  CT   CT3      0.2000  3     0.00
CC1A CT   CT2  HA       0.1900  3     0.00
CT3  CT   CT2  HA       0.1900  3     0.00
CT2  CT   CT3  HA       0.1600  3     0.00
CC1A CT   CT3  HA       0.1600  3     0.00
CT3  CT   CT3  HA       0.1600  3     0.00
CC1B CC1A CC1A CT2      0.5600  1   180.00
CC1B CC1A CC1A CT2      7.0000  2   180.00
CC1B NS1  CT3  HA       0.3500  3   180.00
CT2  CT2  NS1  CC1B     0.1000  3     0.00
CT2  NS1  CC1B CC1A     12.0000 2   180.00
CT2  NS1  CC1B HE1      8.5000  2   180.00
HA   CT2  NS1  CC1B     0.1000  3     0.00
NS1  CC1B CC1A CC1A     2.9640  1    180.0
NS1  CC1B CC1A CC1A     2.9760  2    180.0
NS1  CC1B CC1A CC1A     0.3420  3     0.00
NS1  CC1B CC1A HE1      1.0000  2   180.00

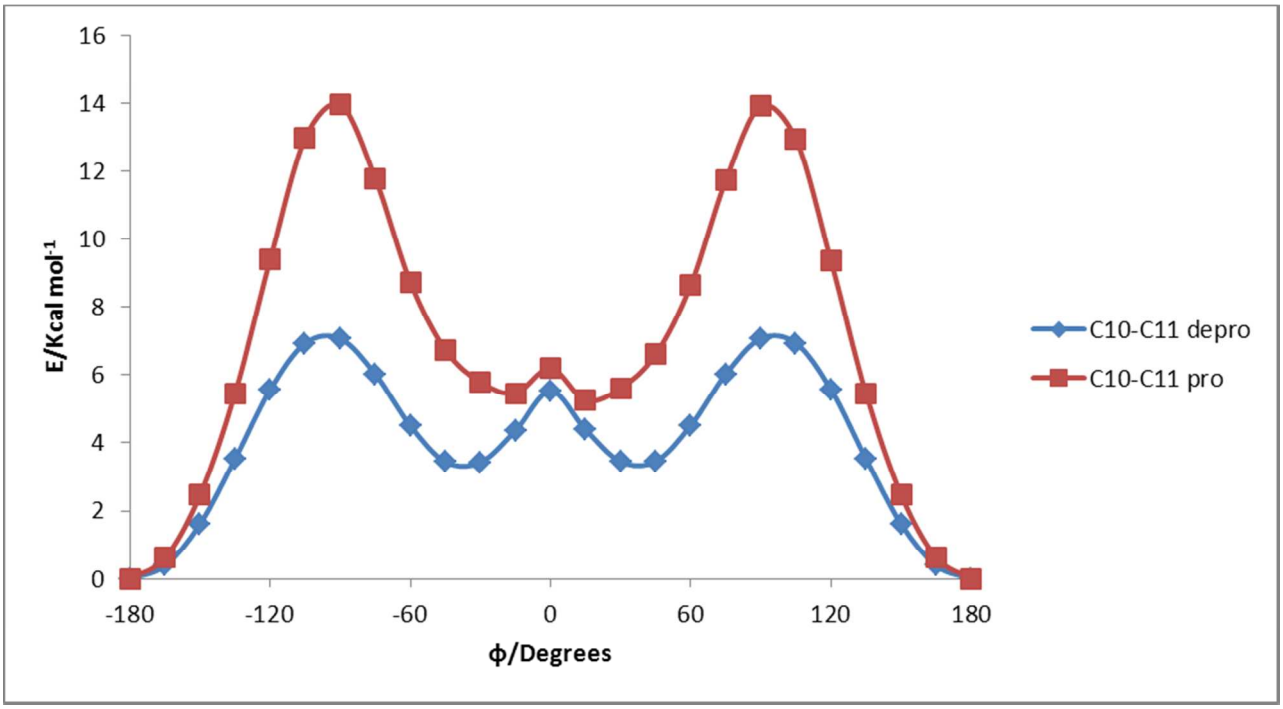
IMPROPER
CC1A X    X    CT       100.0   0      0.0
CC1A X    X    CT3      100.0   0      0.0
CC1B X    X    HE1      100.0   0      0.0
CC1A X    X    HE1      100.0   0      0.0

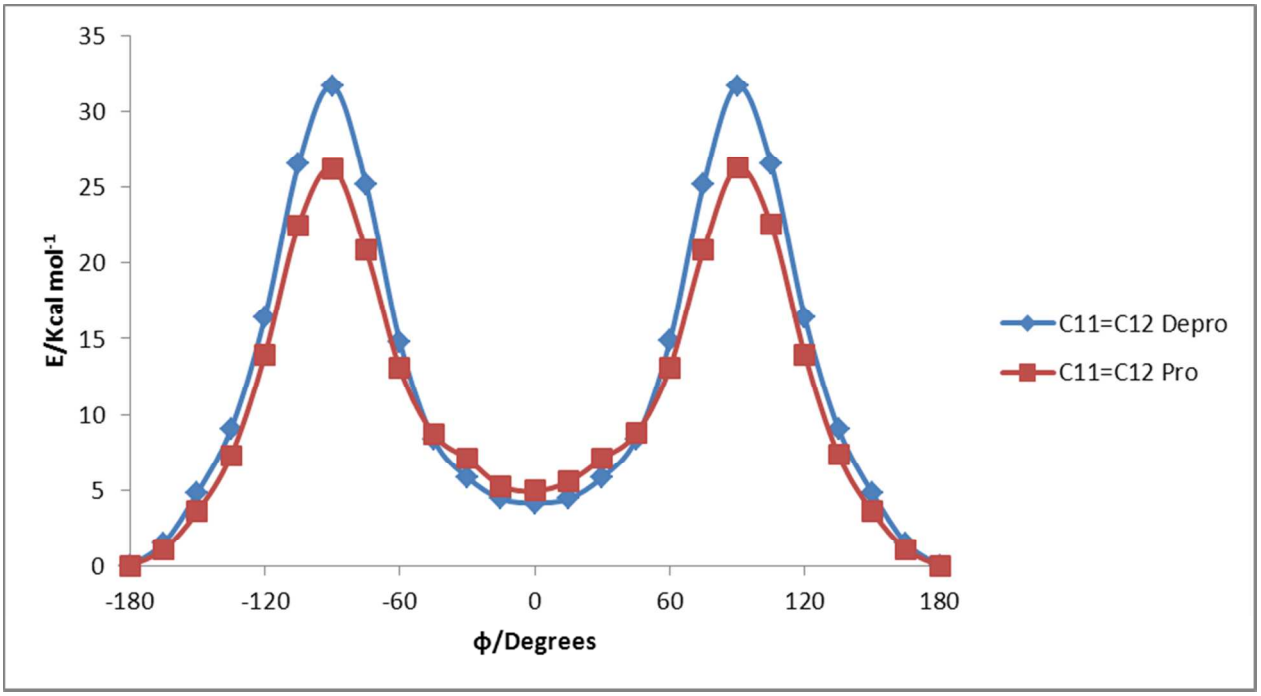
NONBONDED nbxmod  5 atom cdiel shift vatom vdistance vswitch -
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 1.0 wmin 1.5
                !adm jr., 5/08/91, suggested cutoff scheme

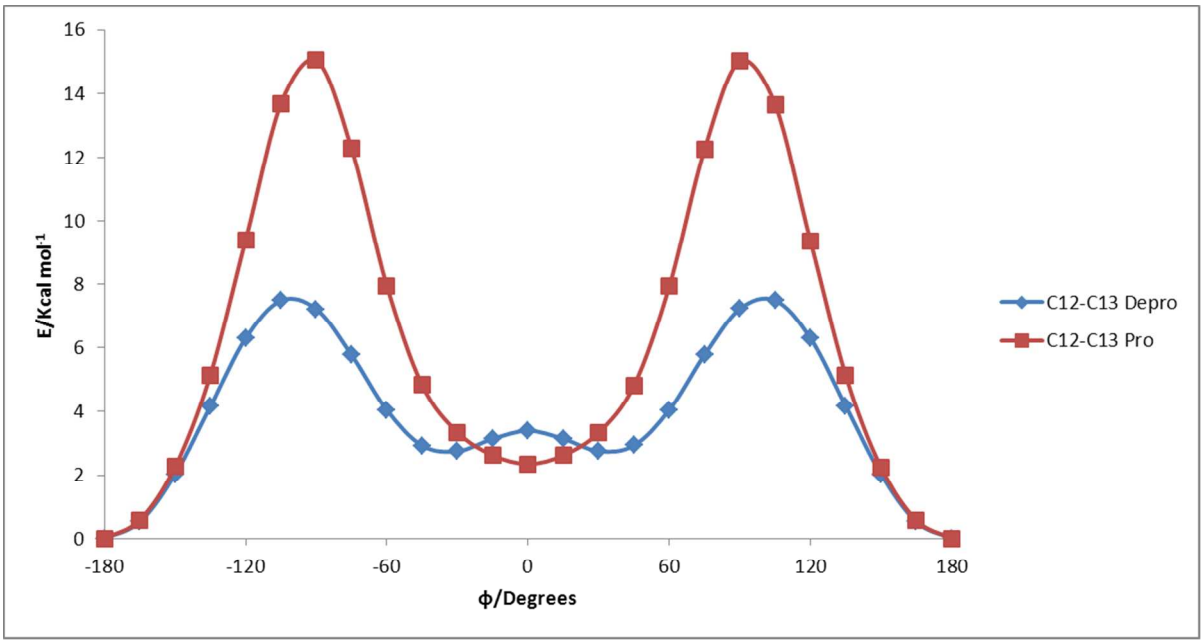
end
```

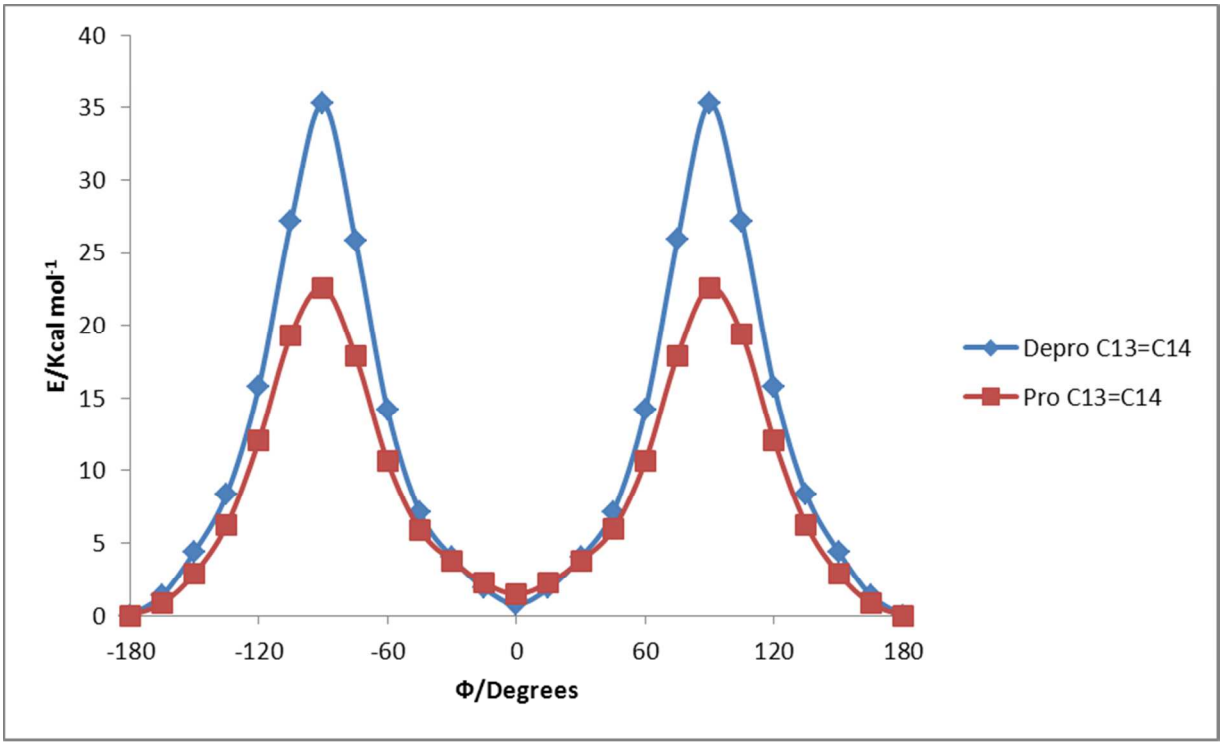
Torsional Energy Profiles for Polyene Torsions



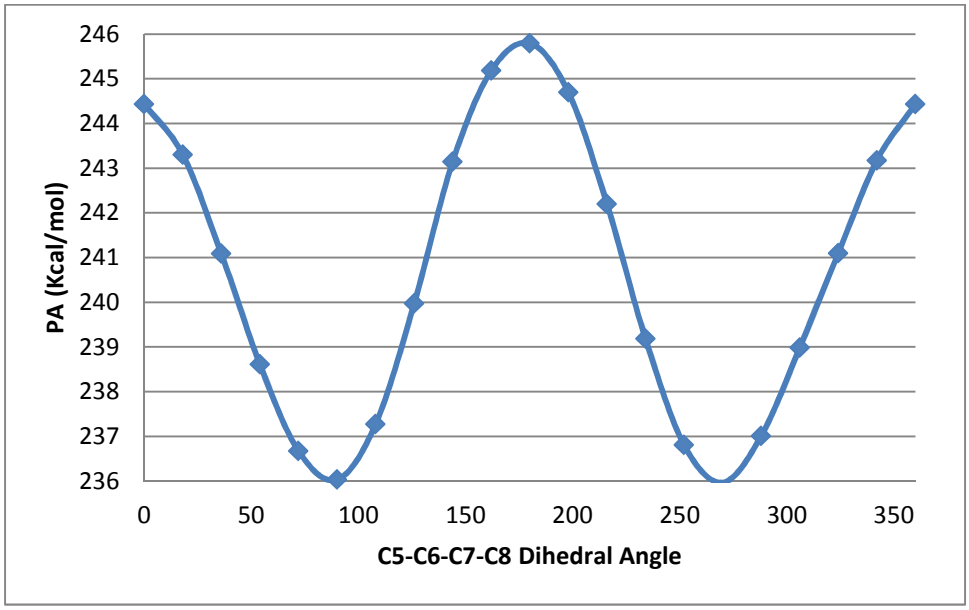



35
30
25
20
15
10
5
0
E/Kcal mol-1
-180
-120
-60
0
60
120
180
ϕ/Degrees
C11=C12 Depro
C11=C12 Pro


16
14
12
10
8
6
4
2
0
E/Kcal mol-1
-180
-120
-60
0
60
120
180
ϕ/Degrees
C12-C13 Depro
C12-C13 Pro


40
35
30
25
20
15
10
5
0
E/Kcal mol-1
-180
-120
-60
0
60
120
180
Φ/Degrees
Depro C13=C14
Pro C13=C14

Proton Affinity as a Function of the β-ionone Ring Orientation



Coordinates of energy minimized structures of retinal models

Protonated Retinal Model at global energy minimum (-870.93191061269 Hartrees) – PDB format

```
ATOM      1 C    UNK     1       4.983  -0.696   0.488                          C 0
ATOM      2 C    UNK     1       3.868   0.110  -0.188                          C 0
ATOM      3 C    UNK     1       4.024   1.408  -0.585                          C 0
ATOM      4 C    UNK     1       5.274   2.192  -0.281                          C 0
ATOM      5 C    UNK     1       6.137   1.548   0.792                          C 0
ATOM      6 C    UNK     1       6.310   0.075   0.458                          C 0
ATOM      7 H    UNK     1       6.745  -0.005  -0.548                          H 0
ATOM      8 H    UNK     1       7.014  -0.412   1.145                          H 0
ATOM      9 H    UNK     1       5.662   1.666   1.773                          H 0
ATOM     10 H    UNK     1       7.110   2.050   0.850                          H 0
ATOM     11 H    UNK     1       5.854   2.311  -1.210                          H 0
ATOM     12 H    UNK     1       4.979   3.210   0.011                          H 0
ATOM     13 C    UNK     1       3.027   2.180  -1.410                          C 0
ATOM     14 H    UNK     1       2.496   2.923  -0.802                          H 0
ATOM     15 H    UNK     1       2.289   1.542  -1.898                          H 0
ATOM     16 H    UNK     1       3.566   2.741  -2.183                          H 0
ATOM     17 C    UNK     1       2.614  -0.609  -0.381                          C 0
ATOM     18 H    UNK     1       2.684  -1.656  -0.671                          H 0
ATOM     19 C    UNK     1       1.372  -0.089  -0.153                          C 0
ATOM     20 H    UNK     1       1.299   0.933   0.216                          H 0
ATOM     21 C    UNK     1       0.137  -0.798  -0.349                          C 0
ATOM     22 C    UNK     1      -1.039  -0.111  -0.102                          C 0
ATOM     23 H    UNK     1      -0.947   0.926   0.226                          H 0
ATOM     24 C    UNK     1      -2.351  -0.617  -0.229                          C 0
ATOM     25 H    UNK     1      -2.485  -1.648  -0.547                          H 0
ATOM     26 C    UNK     1      -3.471   0.144   0.035                          C 0
ATOM     27 H    UNK     1      -3.323   1.177   0.350                          H 0
ATOM     28 C    UNK     1      -4.807  -0.318  -0.068                          C 0
ATOM     29 C    UNK     1      -5.827   0.580   0.240                          C 0
ATOM     30 H    UNK     1      -5.540   1.589   0.535                          H 0
ATOM     31 C    UNK     1      -7.193   0.290   0.206                          C 0
ATOM     32 H    UNK     1      -7.558  -0.695  -0.073                          H 0
ATOM     33 N    UNK     1      -8.140   1.165   0.504                          N 0
ATOM     34 C    UNK     1      -9.576   0.893   0.480                          C 0
ATOM     35 H    UNK     1      -9.998   1.044   1.476                          H 0
ATOM     36 H    UNK     1      -9.732  -0.142   0.175                          H 0
ATOM     37 H    UNK     1     -10.068   1.558  -0.231                          H 0
ATOM     38 H    UNK     1      -7.853   2.104   0.774                          H 0
ATOM     39 C    UNK     1      -5.068  -1.742  -0.489                          C 0
ATOM     40 H    UNK     1      -4.634  -2.436   0.236                          H 0
ATOM     41 H    UNK     1      -4.605  -1.939  -1.459                          H 0
ATOM     42 H    UNK     1      -6.128  -1.978  -0.580                          H 0
ATOM     43 C    UNK     1       0.179  -2.228  -0.814                          C 0
ATOM     44 H    UNK     1       0.767  -2.834  -0.118                          H 0
ATOM     45 H    UNK     1       0.660  -2.295  -1.795                          H 0
ATOM     46 H    UNK     1      -0.810  -2.678  -0.894                          H 0
ATOM     47 C    UNK     1       4.572  -0.995   1.938                          C 0
ATOM     48 H    UNK     1       5.337  -1.605   2.431                          H 0
ATOM     49 H    UNK     1       3.626  -1.547   1.968                          H 0
ATOM     50 H    UNK     1       4.440  -0.075   2.515                          H 0
ATOM     51 C    UNK     1       5.212  -2.029  -0.244                          C 0
ATOM     52 H    UNK     1       6.110  -2.509   0.159                          H 0
ATOM     53 H    UNK     1       5.366  -1.867  -1.316                          H 0
ATOM     54 H    UNK     1       4.386  -2.733  -0.109                          H 0
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Coordinates of energy minimized structures of retinal models

Deprotonated Retinal Model at global energy minimum (-870.53313097039 Hartrees) – PDB format

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ATOM      1 C    UNK     1      -4.854   0.619   0.679                        C 0
ATOM      2 C    UNK     1      -3.835  -0.073  -0.228                        C 0
ATOM      3 C    UNK     1      -4.039  -1.308  -0.761                        C 0
ATOM      4 C    UNK     1      -5.257  -2.139  -0.438                        C 0
ATOM      5 C    UNK     1      -6.014  -1.639   0.784                        C 0
ATOM      6 C    UNK     1      -6.193  -0.133   0.670                        C 0
ATOM      7 H    UNK     1      -6.716   0.086  -0.272                        H 0
ATOM      8 H    UNK     1      -6.824   0.257   1.480                        H 0
ATOM      9 H    UNK     1      -5.454  -1.887   1.693                        H 0
ATOM     10 H    UNK     1      -6.985  -2.141   0.864                        H 0
ATOM     11 H    UNK     1      -5.925  -2.151  -1.314                        H 0
ATOM     12 H    UNK     1      -4.942  -3.183  -0.297                        H 0
ATOM     13 C    UNK     1      -3.116  -1.964  -1.754                        C 0
ATOM     14 H    UNK     1      -2.568  -2.798  -1.298                        H 0
ATOM     15 H    UNK     1      -2.389  -1.268  -2.174                        H 0
ATOM     16 H    UNK     1      -3.710  -2.391  -2.573                        H 0
ATOM     17 C    UNK     1      -2.591   0.677  -0.468                        C 0
ATOM     18 H    UNK     1      -2.680   1.705  -0.815                        H 0
ATOM     19 C    UNK     1      -1.354   0.171  -0.232                        C 0
ATOM     20 H    UNK     1      -1.287  -0.846   0.160                        H 0
ATOM     21 C    UNK     1      -0.096   0.865  -0.443                        C 0
ATOM     22 C    UNK     1       1.063   0.196  -0.158                        C 0
ATOM     23 H    UNK     1       0.964  -0.825   0.217                        H 0
ATOM     24 C    UNK     1       2.412   0.678  -0.292                        C 0
ATOM     25 H    UNK     1       2.571   1.687  -0.664                        H 0
ATOM     26 C    UNK     1       3.492  -0.087   0.030                        C 0
ATOM     27 H    UNK     1       3.312  -1.098   0.402                        H 0
ATOM     28 C    UNK     1       4.881   0.317  -0.075                        C 0
ATOM     29 C    UNK     1       5.838  -0.582   0.296                        C 0
ATOM     30 H    UNK     1       5.524  -1.562   0.655                        H 0
ATOM     31 C    UNK     1       7.276  -0.397   0.273                        C 0
ATOM     32 H    UNK     1       7.688   0.560  -0.077                        H 0
ATOM     33 N    UNK     1       8.050  -1.355   0.663                        N 0
ATOM     34 C    UNK     1       9.479  -1.091   0.608                        C 0
ATOM     35 H    UNK     1       9.900  -1.212   1.611                        H 0
ATOM     36 H    UNK     1       9.729  -0.086   0.234                        H 0
ATOM     37 H    UNK     1       9.952  -1.838  -0.037                        H 0
ATOM     38 C    UNK     1       5.179   1.702  -0.587                        C 0
ATOM     39 H    UNK     1       4.713   2.455   0.058                        H 0
ATOM     40 H    UNK     1       4.768   1.834  -1.593                        H 0
ATOM     41 H    UNK     1       6.247   1.912  -0.630                        H 0
ATOM     42 C    UNK     1      -0.141   2.275  -0.965                        C 0
ATOM     43 H    UNK     1      -0.711   2.917  -0.284                        H 0
ATOM     44 H    UNK     1      -0.642   2.310  -1.938                        H 0
ATOM     45 H    UNK     1       0.852   2.709  -1.081                        H 0
ATOM     46 C    UNK     1      -4.290   0.690   2.105                        C 0
ATOM     47 H    UNK     1      -4.981   1.231   2.763                        H 0
ATOM     48 H    UNK     1      -3.328   1.213   2.110                        H 0
ATOM     49 H    UNK     1      -4.127  -0.308   2.522                        H 0
ATOM     50 C    UNK     1      -5.124   2.051   0.191                        C 0
ATOM     51 H    UNK     1      -5.948   2.484   0.770                        H 0
ATOM     52 H    UNK     1      -5.409   2.056  -0.866                        H 0
ATOM     53 H    UNK     1      -4.254   2.701   0.322                        H 0
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