

Chlorophyll excitation energies and structural stability of the CP47 antenna of Photosystem II: a case study in the first-principles simulation of light-harvesting complexes

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Electronic Supplementary Information

Table S1. Computed site energies (in eV) of CP47 chromophores using the ω B97X-V functional with the Def2-TZVP basis set. Comparison of first excitation energies obtained *in vacuo*, in the electrostatic field of a PSII monomer, and in the electrostatic field of the PSII dimer. The pigment geometries in all cases are derived from QM/MM optimisations inside the complete PSII dimer. Parentheses indicate oscillator strengths.

| Site | Q_y (Vacuum) | Q_y (Monomer) | Q_y (Dimer) |
|------|-------------------|--------------------|------------------|
| B1 | 1.941(0.22) | 1.893 (0.24) | 1.899 (0.25) |
| B2 | 1.928 (0.22) | 1.948 (0.16) | 1.953 (0.17) |
| B3 | 1.888 (0.23) | 1.888 (0.19) | 1.884 (0.19) |
| B4 | 1.935 (0.23) | 1.928 (0.22) | 1.947 (0.21) |
| B5 | 1.909 (0.22) | 1.923 (0.17) | 1.921 (0.17) |
| B6 | 1.924 (0.21) | 1.923 (0.20) | 1.933 (0.19) |
| B7 | 1.925 (0.23) | 1.923 (0.19) | 1.915 (0.21) |
| B8 | 1.951 (0.21) | 1.998 (0.23) | 1.967 (0.23) |
| B9 | 1.981 (0.22) | 2.091 (0.20) | 2.102 (0.20) |
| B10 | 1.965 (0.21) | 1.974 (0.18) | 1.966 (0.20) |
| B11 | 1.967 (0.23) | 1.999 (0.24) | 1.996 (0.24) |
| B12 | 1.939 (0.21) | 1.944 (0.19) | 1.941 (0.20) |
| B13 | 1.917 (0.23) | 1.946 (0.25) | 1.921 (0.27) |
| B14 | 1.942 (0.22) | 1.957 (0.24) | 1.956 (0.24) |
| B15 | 1.933 (0.22) | 1.938 (0.20) | 1.930 (0.21) |
| B16 | 1.945 (0.22) | 2.009 (0.23) | 2.050 (0.22) |

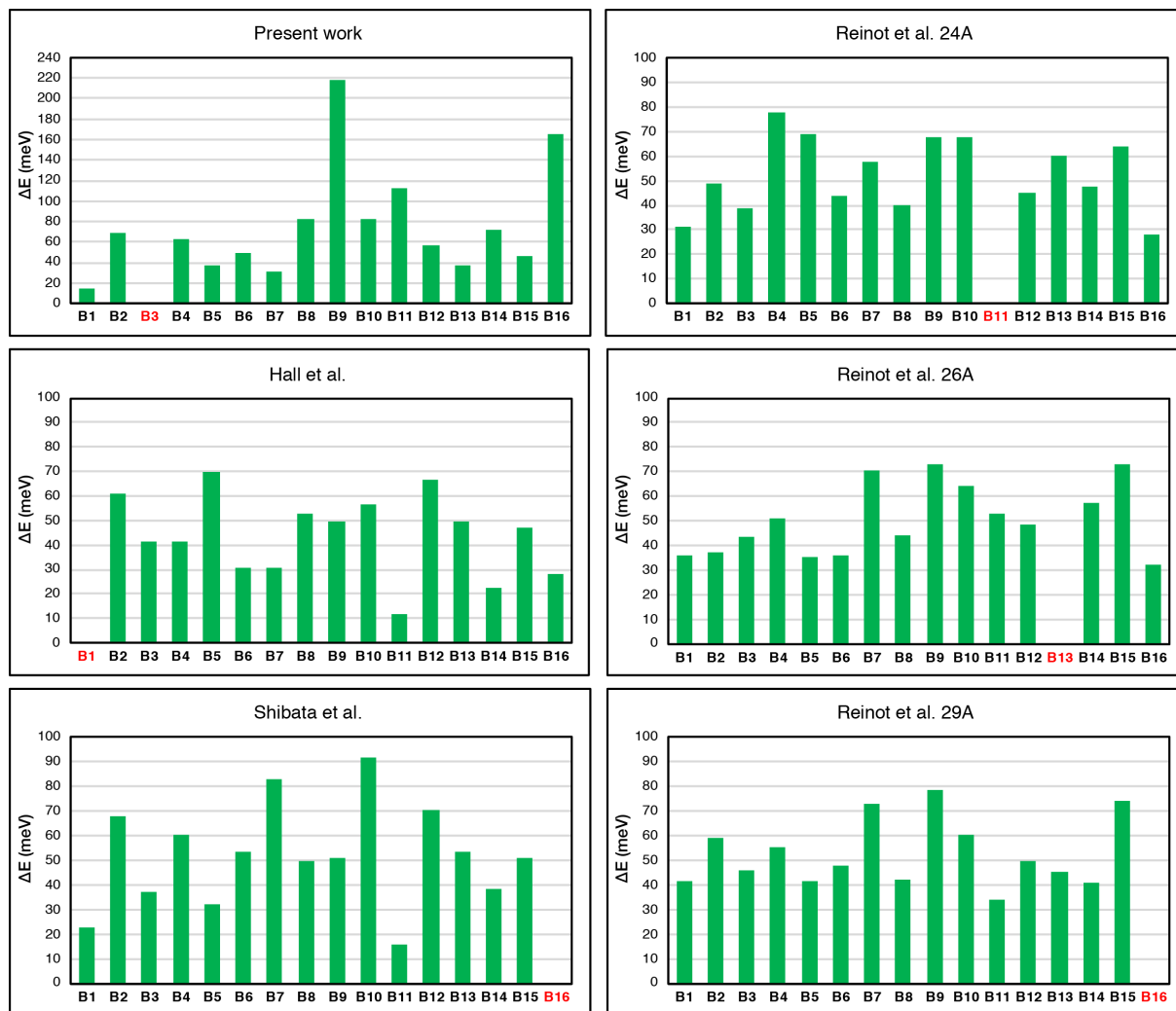


Figure S1. Comparison of vertical excitation energies for the CP47 chlorophylls computed in the present work with fitted site energies reported in selected past papers by Hall et al.,¹ Shibata et al.,² and Reinot et al.³

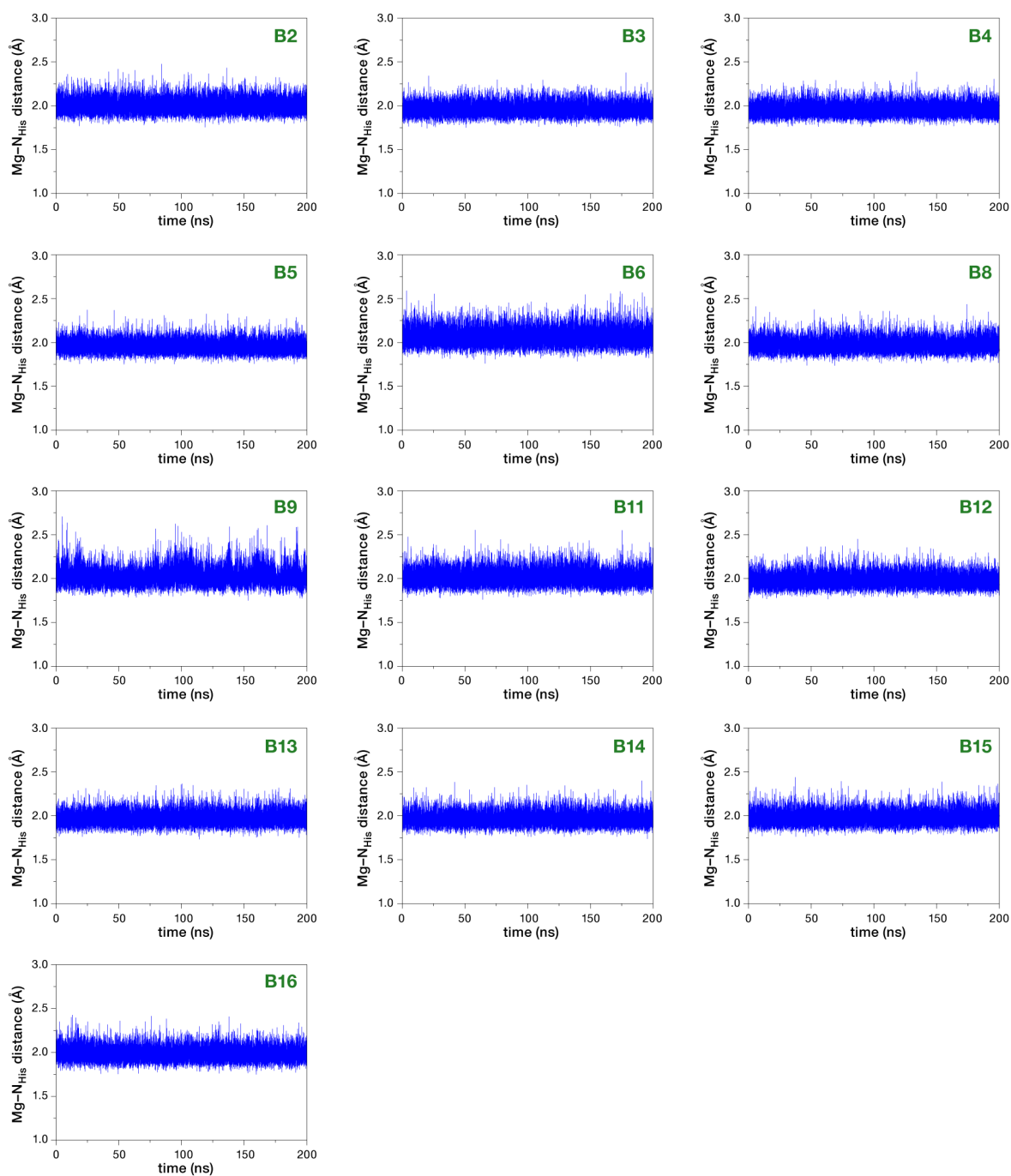


Figure S2. Distances between the Mg ion and the imidazole N atom for all CP47 chlorophylls that are formally coordinated by a histidine residue, from MD simulations carried out without specifying the presence of a Mg–N_{HIS} bond.

COFACTOR FORCE FIELD PARAMETERS

Definition of atoms types, bond connectivity and RESP charges for Chlorophyll a

@<TRIPOS>MOLECULE

CLA

137 145 1 0 0

SMALL

No Charge or Current Charge

@<TRIPOS>ATOM

| | | | | | | | | |
|----|------|----------|---------|---------|-----|------|-----|-----------|
| 1 | CAA | -7.0450 | 36.1740 | 7.9070 | ct2 | 2740 | CLA | -0.171036 |
| 2 | CAB | -3.7300 | 34.5260 | -0.6930 | cf | 2740 | CLA | 0.004602 |
| 3 | CAC | 2.5080 | 37.2040 | 3.4510 | ct2 | 2740 | CLA | 0.051556 |
| 4 | CAD | -2.4990 | 36.0040 | 9.9420 | c2k | 2740 | CLA | 0.700109 |
| 5 | NA | -4.6920 | 34.9520 | 5.9050 | ns | 2740 | CLA | -0.406343 |
| 6 | CBA | -6.8560 | 37.1890 | 6.7410 | ct2 | 2740 | CLA | -0.054130 |
| 7 | CBB | -4.6280 | 34.4210 | -1.6550 | c2 | 2740 | CLA | -0.352117 |
| 8 | CBC | 2.2640 | 38.7120 | 3.6060 | ct3 | 2740 | CLA | -0.161821 |
| 9 | CBD | -3.8660 | 35.5320 | 9.6270 | ct1 | 2740 | CLA | -0.684536 |
| 10 | NB | -3.7370 | 34.8980 | 3.0460 | nmh | 2740 | CLA | -0.460890 |
| 11 | OBD | -2.0730 | 36.1940 | 11.1240 | o2c | 2740 | CLA | -0.486229 |
| 12 | CGA | -7.7650 | 38.3670 | 6.9690 | c2a | 2740 | CLA | 0.661278 |
| 13 | CGD | -4.0530 | 34.1050 | 10.1490 | c2a | 2740 | CLA | 0.775843 |
| 14 | ND | -1.8910 | 35.7750 | 6.4000 | nmh | 2740 | CLA | -0.562974 |
| 15 | CED | -4.3760 | 32.7210 | 12.2440 | ct3 | 2740 | CLA | 0.023891 |
| 16 | CHA | -3.8660 | 35.4610 | 8.1530 | csb | 2740 | CLA | 0.215505 |
| 17 | CHB | -6.0140 | 34.3700 | 3.9770 | cab | 2740 | CLA | -0.412162 |
| 18 | CHC | -1.8280 | 35.2750 | 1.4160 | cab | 2740 | CLA | -0.294853 |
| 19 | CHD | 0.3970 | 36.3220 | 5.6940 | cab | 2740 | CLA | -0.409266 |
| 20 | CMA | -6.8010 | 32.6540 | 6.4090 | ct3 | 2740 | CLA | -0.284997 |
| 21 | CMB | -6.7410 | 33.8690 | 0.8460 | ct3 | 2740 | CLA | -0.414554 |
| 22 | CMC | 0.9540 | 36.4980 | 0.5370 | ct3 | 2740 | CLA | -0.376255 |
| 23 | CMD | 0.8770 | 36.7840 | 8.8420 | ct3 | 2740 | CLA | -0.347111 |
| 24 | C1 | -8.6360 | 40.5350 | 6.0970 | c3 | 2740 | CLA | 0.426615 |
| 25 | C1A | -4.8840 | 35.0930 | 7.1570 | ccs | 2740 | CLA | -0.015834 |
| 26 | C1B | -5.0500 | 34.5490 | 2.8370 | crb | 2740 | CLA | 0.074017 |
| 27 | C1C | -0.8290 | 35.7730 | 2.3840 | crb | 2740 | CLA | 0.080581 |
| 28 | C1D | -0.6310 | 36.1660 | 6.7240 | cpb | 2740 | CLA | 0.331507 |
| 29 | O1A | -8.4760 | 38.5020 | 7.9790 | o2c | 2740 | CLA | -0.524995 |
| 30 | O1D | -3.7340 | 33.1220 | 9.4970 | o2c | 2740 | CLA | -0.495118 |
| 31 | C2 | -8.5480 | 41.2380 | 4.7550 | c2 | 2740 | CLA | -0.554928 |
| 32 | C2A | -6.2910 | 34.8490 | 7.6040 | ct1 | 2740 | CLA | 0.114777 |
| 33 | C2B | -5.4130 | 34.3160 | 1.4200 | cbb | 2740 | CLA | 0.215950 |
| 34 | C2C | 0.4720 | 36.3340 | 1.9650 | cbb | 2740 | CLA | 0.152944 |
| 35 | C2D | -0.3890 | 36.3570 | 8.1300 | cbb | 2740 | CLA | 0.065292 |
| 36 | O2A | -7.7680 | 39.3980 | 5.9540 | o1c | 2740 | CLA | -0.451704 |
| 37 | O2D | -4.1950 | 33.9620 | 11.5440 | o1c | 2740 | CLA | -0.371917 |
| 38 | C3 | -9.2210 | 40.8860 | 3.6530 | c2 | 2740 | CLA | 0.294232 |
| 39 | C3A | -6.8630 | 34.2030 | 6.3470 | ct1 | 2740 | CLA | 0.032573 |
| 40 | C3B | -4.1480 | 34.5460 | 0.7400 | cbb | 2740 | CLA | -0.211021 |
| 41 | C3C | 1.1310 | 36.5860 | 3.2470 | cbb | 2740 | CLA | -0.231334 |
| 42 | C3D | -1.7150 | 36.0590 | 8.6940 | cbb | 2740 | CLA | -0.247617 |
| 43 | C4 | -10.1750 | 39.7320 | 3.6380 | c3 | 2740 | CLA | -0.407700 |
| 44 | C4A | -5.8190 | 34.5410 | 5.3130 | ccs | 2740 | CLA | 0.357959 |
| 45 | C4B | -3.1860 | 34.9180 | 1.8120 | cnb | 2740 | CLA | 0.260744 |
| 46 | C4C | 0.1090 | 36.1780 | 4.2590 | cnb | 2740 | CLA | 0.314971 |
| 47 | C4D | -2.5370 | 35.7760 | 7.6260 | cqb | 2740 | CLA | 0.083937 |
| 48 | C5 | -9.0260 | 41.6810 | 2.3920 | c3 | 2740 | CLA | -0.224157 |
| 49 | C6 | -10.3080 | 42.4310 | 2.0720 | c3 | 2740 | CLA | 0.110326 |
| 50 | C7 | -10.2390 | 42.9460 | 0.6500 | c3 | 2740 | CLA | -0.030187 |
| 51 | C8 | -11.5560 | 43.6590 | 0.3650 | c3 | 2740 | CLA | 0.251557 |
| 52 | C9 | -12.4020 | 42.7960 | -0.5730 | c3 | 2740 | CLA | -0.368354 |
| 53 | C10 | -11.2950 | 45.0990 | -0.1070 | c3 | 2740 | CLA | -0.274480 |
| 54 | C11 | -11.4660 | 46.1280 | 1.0390 | c3 | 2740 | CLA | 0.184319 |
| 55 | C12 | -10.1830 | 46.8020 | 1.5770 | c3 | 2740 | CLA | -0.230634 |
| 56 | C13 | -10.2850 | 48.3140 | 1.8780 | c3 | 2740 | CLA | 0.277050 |
| 57 | C14 | -9.9740 | 49.1400 | 0.6290 | c3 | 2740 | CLA | -0.296828 |
| 58 | C15 | -9.3560 | 48.7420 | 3.0260 | c3 | 2740 | CLA | -0.137174 |
| 59 | C16 | -9.9310 | 49.9130 | 3.8350 | c3 | 2740 | CLA | 0.075364 |
| 60 | C17 | -9.5600 | 49.8850 | 5.3270 | c3 | 2740 | CLA | -0.187234 |
| 61 | C18 | -9.7740 | 51.2180 | 6.0710 | c3 | 2740 | CLA | 0.411365 |
| 62 | C19 | -8.6700 | 51.5090 | 7.0880 | c3 | 2740 | CLA | -0.311376 |
| 63 | C20 | -11.1490 | 51.3190 | 6.7470 | c3 | 2740 | CLA | -0.419125 |
| 64 | NC | -1.0080 | 35.7330 | 3.6970 | ns | 2740 | CLA | -0.456670 |
| 65 | MG | -2.7780 | 34.9590 | 4.7430 | mgc | 2740 | CLA | 1.052289 |
| 66 | HAA1 | -6.6740 | 36.6050 | 8.8370 | hc | 2740 | CLA | 0.070073 |

| | | | | | | | | |
|-----|------|----------|---------|---------|----|------|-----|-----------|
| 67 | HAA2 | -8.1060 | 35.9710 | 8.0520 | hc | 2740 | CLA | 0.070073 |
| 68 | HAB | -2.6730 | 34.6010 | -0.9480 | ha | 2740 | CLA | 0.090045 |
| 69 | HAC1 | 3.1610 | 36.9980 | 2.6020 | hc | 2740 | CLA | 0.027001 |
| 70 | HAC2 | 2.9950 | 36.7930 | 4.3350 | hc | 2740 | CLA | 0.027001 |
| 71 | HBA1 | -7.0840 | 36.7140 | 5.7870 | hc | 2740 | CLA | 0.027329 |
| 72 | HBA2 | -5.8180 | 37.5180 | 6.6920 | hc | 2740 | CLA | 0.027329 |
| 73 | HBB1 | -5.6870 | 34.3460 | -1.4060 | ha | 2740 | CLA | 0.146195 |
| 74 | HBB2 | -4.3120 | 34.4070 | -2.6970 | ha | 2740 | CLA | 0.146195 |
| 75 | HBC1 | 3.2160 | 39.2210 | 3.7560 | hc | 2740 | CLA | 0.050268 |
| 76 | HBC2 | 1.6170 | 38.8890 | 4.4650 | hc | 2740 | CLA | 0.050268 |
| 77 | HBC3 | 1.7850 | 39.0960 | 2.7050 | hc | 2740 | CLA | 0.050268 |
| 78 | HBD | -4.6400 | 36.1680 | 10.0570 | hc | 2740 | CLA | 0.191948 |
| 79 | HED1 | -4.4560 | 32.9130 | 13.3140 | h1 | 2740 | CLA | 0.067353 |
| 80 | HED2 | -3.5210 | 32.0690 | 12.0570 | h1 | 2740 | CLA | 0.067353 |
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| 82 | HHB | -7.0180 | 34.0550 | 3.6920 | ha | 2740 | CLA | 0.149746 |
| 83 | HHC | -1.5410 | 35.1690 | 0.3700 | ha | 2740 | CLA | 0.171031 |
| 84 | HHD | 1.4160 | 36.5550 | 6.0010 | ha | 2740 | CLA | 0.186781 |
| 85 | HMA1 | -7.2180 | 32.2380 | 5.4930 | hc | 2740 | CLA | 0.076415 |
| 86 | HMA2 | -7.3770 | 32.3020 | 7.2640 | hc | 2740 | CLA | 0.076415 |
| 87 | HMA3 | -5.7640 | 32.3360 | 6.5130 | hc | 2740 | CLA | 0.076415 |
| 88 | HMB1 | -6.6620 | 33.7960 | -0.2390 | hc | 2740 | CLA | 0.125522 |
| 89 | HMB2 | -7.5130 | 34.5930 | 1.1060 | hc | 2740 | CLA | 0.125522 |
| 90 | HMB3 | -7.0040 | 32.8930 | 1.2560 | hc | 2740 | CLA | 0.125522 |
| 91 | HMC1 | 1.9520 | 36.9380 | 0.5390 | hc | 2740 | CLA | 0.117064 |
| 92 | HMC2 | 0.2710 | 37.1530 | -0.0040 | hc | 2740 | CLA | 0.117064 |
| 93 | HMC3 | 0.9880 | 35.5260 | 0.0490 | hc | 2740 | CLA | 0.117064 |
| 94 | HMD1 | 0.6940 | 36.8250 | 9.9160 | hc | 2740 | CLA | 0.115985 |
| 95 | HMD2 | 1.1780 | 37.7700 | 8.4880 | hc | 2740 | CLA | 0.115985 |
| 96 | HMD3 | 1.6710 | 36.0660 | 8.6350 | hc | 2740 | CLA | 0.115985 |
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| 99 | H11 | -8.3130 | 41.1840 | 6.9100 | h1 | 2740 | CLA | -0.003770 |
| 100 | H12 | -9.6590 | 40.2300 | 6.3210 | h1 | 2740 | CLA | -0.003770 |
| 101 | H13 | -11.3130 | 48.5030 | 2.1900 | hc | 2740 | CLA | -0.037920 |
| 102 | H18 | -9.7310 | 51.9800 | 5.2920 | hc | 2740 | CLA | -0.061702 |
| 103 | H2A | -6.3720 | 34.2630 | 8.5200 | hc | 2740 | CLA | 0.008180 |
| 104 | H41 | -10.6060 | 39.6290 | 2.6420 | hc | 2740 | CLA | 0.118056 |
| 105 | H42 | -10.9710 | 39.9070 | 4.3620 | hc | 2740 | CLA | 0.118056 |
| 106 | H43 | -9.6430 | 38.8170 | 3.8990 | hc | 2740 | CLA | 0.118056 |
| 107 | H3A | -7.8900 | 34.5280 | 6.1800 | hc | 2740 | CLA | 0.028468 |
| 108 | H51 | -8.7610 | 41.0200 | 1.5670 | hc | 2740 | CLA | 0.065906 |
| 109 | H52 | -8.2000 | 42.3840 | 2.5140 | hc | 2740 | CLA | 0.065906 |
| 110 | H61 | -10.4410 | 43.2610 | 2.7670 | hc | 2740 | CLA | -0.012985 |
| 111 | H62 | -11.1680 | 41.7730 | 2.1930 | hc | 2740 | CLA | -0.012985 |
| 112 | H71 | -10.0860 | 42.1250 | -0.0500 | hc | 2740 | CLA | 0.001818 |
| 113 | H72 | -9.3980 | 43.6290 | 0.5270 | hc | 2740 | CLA | 0.001818 |
| 114 | H91 | -13.3450 | 43.3000 | -0.7790 | hc | 2740 | CLA | 0.081706 |
| 115 | H92 | -12.6010 | 41.8340 | -0.1000 | hc | 2740 | CLA | 0.081706 |
| 116 | H93 | -11.8620 | 42.6370 | -1.5060 | hc | 2740 | CLA | 0.081706 |
| 117 | H101 | -11.9810 | 45.3450 | -0.9190 | hc | 2740 | CLA | 0.063428 |
| 118 | H102 | -10.2850 | 45.1720 | -0.5100 | hc | 2740 | CLA | 0.063428 |
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| 121 | H121 | -9.3850 | 46.6500 | 0.8500 | hc | 2740 | CLA | 0.042399 |
| 122 | H122 | -9.8840 | 46.2880 | 2.4910 | hc | 2740 | CLA | 0.042399 |
| 123 | H141 | -10.0520 | 50.2010 | 0.8660 | hc | 2740 | CLA | 0.066213 |
| 124 | H142 | -10.6860 | 48.8910 | -0.1580 | hc | 2740 | CLA | 0.066213 |
| 125 | H143 | -8.9630 | 48.9180 | 0.2880 | hc | 2740 | CLA | 0.066213 |
| 126 | H151 | -8.3850 | 49.0260 | 2.6190 | hc | 2740 | CLA | 0.030146 |
| 127 | H152 | -9.1870 | 47.8930 | 3.6900 | hc | 2740 | CLA | 0.030146 |
| 128 | H161 | -11.0180 | 49.9090 | 3.7410 | hc | 2740 | CLA | -0.011209 |
| 129 | H162 | -9.5780 | 50.8490 | 3.4010 | hc | 2740 | CLA | -0.011209 |
| 130 | H171 | -8.5140 | 49.5960 | 5.4210 | hc | 2740 | CLA | 0.032589 |
| 131 | H172 | -10.1500 | 49.1110 | 5.8190 | hc | 2740 | CLA | 0.032589 |
| 132 | H191 | -8.8710 | 52.4590 | 7.5830 | hc | 2740 | CLA | 0.063258 |
| 133 | H192 | -7.7080 | 51.5620 | 6.5770 | hc | 2740 | CLA | 0.063258 |
| 134 | H193 | -8.6420 | 50.7120 | 7.8320 | hc | 2740 | CLA | 0.063258 |
| 135 | H201 | -11.2360 | 52.2810 | 7.2530 | hc | 2740 | CLA | 0.092857 |
| 136 | H202 | -11.2560 | 50.5160 | 7.4750 | hc | 2740 | CLA | 0.092857 |
| 137 | H203 | -11.9310 | 51.2330 | 5.9940 | hc | 2740 | CLA | 0.092857 |

@<TRIPOS>BOND

| | | | |
|---|---|----|---|
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| 2 | 1 | 32 | 1 |
| 3 | 1 | 66 | 1 |
| 4 | 1 | 67 | 1 |
| 5 | 2 | 7 | 1 |
| 6 | 2 | 40 | 1 |
| 7 | 2 | 68 | 1 |
| 8 | 3 | 8 | 1 |

| | | | |
|----|----|-----|---|
| 9 | 3 | 41 | 1 |
| 10 | 3 | 69 | 1 |
| 11 | 3 | 70 | 1 |
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| 13 | 4 | 11 | 1 |
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| 15 | 5 | 25 | 1 |
| 16 | 5 | 44 | 1 |
| 17 | 5 | 65 | 1 |
| 18 | 6 | 12 | 1 |
| 19 | 6 | 71 | 1 |
| 20 | 6 | 72 | 1 |
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| 22 | 7 | 74 | 1 |
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| 26 | 9 | 13 | 1 |
| 27 | 9 | 16 | 1 |
| 28 | 9 | 78 | 1 |
| 29 | 10 | 26 | 1 |
| 30 | 10 | 45 | 1 |
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| 33 | 12 | 36 | 1 |
| 34 | 13 | 30 | 1 |
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| 68 | 23 | 95 | 1 |
| 69 | 23 | 96 | 1 |
| 70 | 24 | 31 | 1 |
| 71 | 24 | 36 | 1 |
| 72 | 24 | 99 | 1 |
| 73 | 24 | 100 | 1 |
| 74 | 25 | 32 | 1 |
| 75 | 26 | 33 | 1 |
| 76 | 27 | 34 | 1 |
| 77 | 27 | 64 | 1 |
| 78 | 28 | 35 | 1 |
| 79 | 31 | 38 | 1 |
| 80 | 31 | 97 | 1 |
| 81 | 32 | 39 | 1 |
| 82 | 32 | 103 | 1 |
| 83 | 33 | 40 | 1 |
| 84 | 34 | 41 | 1 |
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| 87 | 38 | 48 | 1 |
| 88 | 39 | 44 | 1 |

| | | | |
|-----|----|-----|---|
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| 90 | 40 | 45 | 1 |
| 91 | 41 | 46 | 1 |
| 92 | 42 | 47 | 1 |
| 93 | 43 | 104 | 1 |
| 94 | 43 | 105 | 1 |
| 95 | 43 | 106 | 1 |
| 96 | 46 | 64 | 1 |
| 97 | 48 | 49 | 1 |
| 98 | 48 | 108 | 1 |
| 99 | 48 | 109 | 1 |
| 100 | 49 | 50 | 1 |
| 101 | 49 | 110 | 1 |
| 102 | 49 | 111 | 1 |
| 103 | 50 | 51 | 1 |
| 104 | 50 | 112 | 1 |
| 105 | 50 | 113 | 1 |
| 106 | 51 | 52 | 1 |
| 107 | 51 | 53 | 1 |
| 108 | 51 | 98 | 1 |
| 109 | 52 | 114 | 1 |
| 110 | 52 | 115 | 1 |
| 111 | 52 | 116 | 1 |
| 112 | 53 | 54 | 1 |
| 113 | 53 | 117 | 1 |
| 114 | 53 | 118 | 1 |
| 115 | 54 | 55 | 1 |
| 116 | 54 | 119 | 1 |
| 117 | 54 | 120 | 1 |
| 118 | 55 | 56 | 1 |
| 119 | 55 | 121 | 1 |
| 120 | 55 | 122 | 1 |
| 121 | 56 | 57 | 1 |
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| 123 | 56 | 101 | 1 |
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| 125 | 57 | 124 | 1 |
| 126 | 57 | 125 | 1 |
| 127 | 58 | 59 | 1 |
| 128 | 58 | 126 | 1 |
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| 134 | 60 | 130 | 1 |
| 135 | 60 | 131 | 1 |
| 136 | 61 | 62 | 1 |
| 137 | 61 | 63 | 1 |
| 138 | 61 | 102 | 1 |
| 139 | 62 | 132 | 1 |
| 140 | 62 | 133 | 1 |
| 141 | 62 | 134 | 1 |
| 142 | 63 | 135 | 1 |
| 143 | 63 | 136 | 1 |
| 144 | 63 | 137 | 1 |
| 145 | 64 | 65 | 1 |

@<TRIPOS>SUBSTRUCTURE
1 CLA 1 TEMP 0 **** 0 ROOT

Bonded and LJ parameters for Chlorophyll a

Force Field modification file for CLA

MASS

| | | | |
|-----|--------|-------|--|
| mgc | 24.305 | 0.120 | magnesium |
| csb | 12.01 | 0.360 | Inner Sp2 carbons in conjugated systems |
| cab | 12.01 | 0.360 | Inner Sp2 carbons in conjugated systems |
| ccs | 12.01 | 0.360 | Inner Sp2 carbons in conjugated systems |
| ct1 | 12.01 | 0.878 | Sp3 C |
| ct2 | 12.01 | 0.878 | Sp3 C |
| ct3 | 12.01 | 0.878 | Sp3 C |
| crb | 12.01 | 0.360 | Sp2 carbons in non-pure aromatic systems |
| cbb | 12.01 | 0.360 | Sp2 carbons in non-pure aromatic systems |
| cnb | 12.01 | 0.360 | Sp2 carbons in non-pure aromatic systems |
| cpb | 12.01 | 0.360 | Sp2 carbons in non-pure aromatic systems |
| cqb | 12.01 | 0.360 | Sp2 carbons in non-pure aromatic systems |
| c2k | 12.01 | 0.616 | Sp2 C carbonyl group |

| | | | |
|-----|-------|-------|-----------------------------------|
| c2a | 12.01 | 0.616 | Sp2 C carbonyl group |
| nmh | 14.01 | 0.530 | Inner Sp2 N in conjugated systems |
| ns | 14.01 | 0.530 | Inner Sp2 N in conjugated systems |
| o2c | 16.00 | 0.434 | Oxygen with one connected atom |
| o1c | 16.00 | 0.465 | Ether and ester oxygen |

BOND

| | | | | |
|-----|-----|--------|-------|--------------------|
| nmh | mgc | 50.00 | 2.05 | |
| ns | mgc | 50.00 | 2.150 | |
| nmh | cnb | 316.00 | 1.375 | |
| nmh | crb | 316.00 | 1.380 | |
| ns | cnb | 316.00 | 1.375 | |
| ns | crb | 316.00 | 1.380 | |
| nmh | cpb | 316.00 | 1.393 | |
| nmh | cqb | 316.00 | 1.348 | |
| cnb | cbb | 263.00 | 1.456 | |
| crb | cbb | 263.00 | 1.439 | |
| cpb | cbb | 263.00 | 1.441 | |
| cqb | cbb | 283.00 | 1.421 | |
| cbb | cbb | 340.00 | 1.402 | |
| cbb | ct2 | 323.50 | 1.513 | # Same with c3-ca |
| cbb | ct3 | 200.00 | 1.497 | |
| cbb | c2e | 190.00 | 1.479 | |
| ct3 | c2e | 170.00 | 1.522 | |
| ns | ccs | 296.00 | 1.362 | |
| ccs | ct1 | 250.00 | 1.527 | |
| ct1 | ct1 | 250.00 | 1.552 | |
| ct1 | ct2 | 250.00 | 1.541 | |
| ct1 | ct3 | 250.00 | 1.541 | |
| ct1 | hc | 358.00 | 1.090 | |
| c2k | o2c | 700.00 | 1.226 | |
| c2k | cbb | 263.00 | 1.455 | |
| c2k | ct1 | 170.00 | 1.604 | |
| csb | ct1 | 250.00 | 1.525 | |
| cqb | csb | 305.00 | 1.404 | |
| cnb | cab | 350.00 | 1.404 | |
| crb | cab | 350.00 | 1.406 | |
| cpb | cab | 350.00 | 1.407 | |
| ccs | cab | 370.00 | 1.380 | |
| ccs | csb | 370.00 | 1.370 | |
| cab | ha | 376.00 | 1.092 | |
| ct3 | hc | 358.00 | 1.090 | |
| c2a | o2c | 700.00 | 1.222 | |
| c2a | o1c | 380.00 | 1.363 | |
| o1c | ct2 | 358.00 | 1.457 | |
| o1c | ct3 | 358.00 | 1.457 | |
| o1c | c3 | 358.00 | 1.457 | |
| c2a | ct1 | 250.00 | 1.522 | |
| c2a | ct2 | 250.00 | 1.522 | |
| ct2 | ct2 | 260.00 | 1.526 | |
| ct2 | ct3 | 260.00 | 1.526 | |
| ct2 | hc | 358.00 | 1.090 | |
| ct3 | hc | 358.00 | 1.090 | |
| ct3 | h1 | 358.00 | 1.090 | |
| c2e | o2c | 650.00 | 1.229 | |
| cbb | cf | 562.40 | 1.338 | # same as ce - cf. |

ANGLE

| | | | | | |
|-----|-----|-----|-------|--------|-------------------------|
| nmh | mgc | ns | 50.0 | 87.0 | |
| nmh | mgc | nmh | 50.0 | 158.39 | |
| ns | mgc | ns | 50.0 | 158.06 | |
| mgc | nmh | cnb | 70.0 | 125.45 | |
| mgc | nmh | cpb | 70.0 | 130.82 | |
| mgc | nmh | cqb | 70.0 | 122.4 | |
| mgc | nmh | crb | 70.0 | 126.83 | |
| mgc | ns | cnb | 70.0 | 128.15 | # Same with mgc-nmh-cnb |
| mgc | ns | crb | 70.0 | 126.4 | # Same with mgc-nmh-crb |
| mgc | ns | ccs | 70.0 | 125.8 | |
| cnb | nmh | crb | 100.0 | 107.18 | |
| cnb | ns | crb | 100.0 | 106.62 | # Same with cnb-nmh-crb |
| cpb | nmh | cqb | 100.0 | 106.17 | |
| nmh | cnb | cbb | 70.0 | 109.5 | |
| nmh | crb | cbb | 70.0 | 110.28 | |
| ns | cnb | cbb | 70.0 | 109.72 | # Same with nmh-cnb-cbb |
| ns | crb | cbb | 70.0 | 110.28 | # Same with nmh-crb-cbb |
| nmh | cpb | cbb | 70.0 | 109.75 | |
| nmh | cqb | cbb | 70.0 | 112.23 | |
| cnb | cbb | cbb | 63.0 | 106.19 | |
| crb | cbb | cbb | 63.0 | 106.41 | |
| cpb | cbb | cbb | 63.0 | 104.92 | |

| | | | | | |
|-----|-----|-----|--------|---------|-------------------------|
| cqb | cbb | cbb | 63.0 | 106.92 | |
| nmh | cnb | cab | 70.0 | 124.65 | |
| nmh | crb | cab | 70.0 | 124.5 | |
| ns | cnb | cab | 70.0 | 123.87 | # Same with nmh-cnb-cab |
| ns | crb | cab | 70.0 | 124.78 | # Same with nmh-crb-cab |
| nmh | cpb | cab | 70.0 | 122.04 | |
| nmh | cqb | csb | 70.0 | 133.38 | |
| cbb | cbb | c2k | 63.0 | 142.98 | |
| cbb | cbb | ct2 | 63.0 | 129.0 | |
| cbb | cbb | ct3 | 63.0 | 129.0 | |
| crb | cbb | ct3 | 63.0 | 123.5 | |
| cpb | cbb | ct3 | 63.0 | 127.11 | |
| cnb | cbb | c2e | 63.0 | 124.4 | |
| cnb | cbb | ct2 | 63.0 | 124.4 | # Same with cnb-cbb-c2e |
| cbb | cbb | c2e | 63.0 | 128.5 | |
| cbb | cnb | cab | 63.0 | 126.26 | |
| cbb | crb | cab | 63.0 | 126.5 | |
| cbb | cpb | cab | 63.0 | 128.14 | |
| ccs | ns | ccs | 120.0 | 109.95 | |
| ns | ccs | ct1 | 70.0 | 110.59 | |
| ccs | ct1 | ct1 | 63.0 | 101.61 | |
| ns | ccs | cab | 70.0 | 125.5 | |
| ns | ccs | csb | 70.0 | 123.21 | |
| ccs | ct1 | ct2 | 63.0 | 112.1 | |
| ccs | ct1 | ct3 | 63.0 | 112.1 | |
| ct1 | ct1 | ct2 | 63.0 | 114.0 | |
| ct1 | ct1 | ct3 | 63.0 | 114.0 | |
| ct1 | ct2 | ct2 | 63.0 | 114.0 | |
| ct1 | ct2 | ct3 | 63.0 | 114.0 | |
| cbb | ct2 | ct3 | 63.250 | 112.090 | # Same with c3-c3-ca |
| ccs | ct1 | hc | 35.0 | 109.5 | |
| ct1 | ct1 | hc | 35.0 | 109.5 | |
| ct1 | ct2 | hc | 35.0 | 109.5 | |
| cbb | ct2 | hc | 46.960 | 110.15 | # Same with ca-c3-hc |
| ct2 | ct1 | hc | 35.0 | 109.5 | |
| cbb | c2k | ct1 | 63.0 | 105.16 | |
| cbb | c2k | o2c | 80.0 | 130.7 | |
| ct1 | c2k | o2c | 80.0 | 124.0 | |
| c2k | ct1 | csb | 63.0 | 104.67 | |
| cqb | csb | ct1 | 63.0 | 106.69 | |
| cqb | cbb | c2k | 63.0 | 109.41 | |
| ct1 | csb | ccs | 63.0 | 128.26 | |
| c2k | ct1 | c2a | 63.0 | 111.0 | |
| csb | ct1 | c2a | 63.0 | 112.5 | |
| csb | ct1 | hc | 35.0 | 109.5 | |
| c2k | ct1 | hc | 35.0 | 109.5 | |
| csb | cqb | cbb | 63.0 | 114.03 | |
| cnb | cab | cpb | 63.0 | 126.9 | # Same with csb-cqb-ccs |
| cnb | cab | ccs | 63.0 | 129.9 | |
| crb | cab | ccs | 63.0 | 127.92 | |
| crb | cab | cnb | 63.0 | 128.48 | |
| cqb | csb | ccs | 63.0 | 123.92 | |
| cnb | cab | ha | 25.0 | 116.33 | |
| crb | cab | ha | 25.0 | 115.48 | |
| cpb | cab | ha | 25.0 | 116.72 | |
| ccs | cab | ha | 25.0 | 115.98 | |
| cab | ccs | ct1 | 63.0 | 122.0 | |
| csb | ccs | ct1 | 63.0 | 125.8 | |
| c2a | o1c | ct2 | 45.0 | 106.0 | |
| c2a | o1c | ct3 | 45.0 | 106.0 | |
| c2a | o1c | c3 | 45.0 | 106.0 | |
| o1c | c2a | ct1 | 70.0 | 111.5 | |
| o1c | c2a | ct2 | 70.0 | 111.5 | |
| o2c | c2a | ct1 | 90.0 | 126.5 | |
| o2c | c2a | ct2 | 90.0 | 126.5 | |
| o2c | c2a | o1c | 100.0 | 122.0 | |
| c2a | ct1 | hc | 35.0 | 109.5 | |
| c2a | ct2 | hc | 35.0 | 109.5 | |
| o1c | ct2 | hc | 35.0 | 109.5 | |
| o1c | ct2 | h1 | 35.0 | 109.5 | |
| o1c | ct3 | hc | 35.0 | 109.5 | |
| o1c | ct3 | h1 | 35.0 | 109.5 | |
| o1c | c3 | h1 | 35.0 | 109.5 | |
| c2a | ct2 | ct2 | 63.0 | 116.6 | |
| cbb | ct3 | hc | 35.0 | 109.5 | |
| cbb | c2e | o2c | 80.0 | 121.9 | |
| cbb | c2e | ct3 | 63.0 | 118.0 | |
| ct1 | ct3 | ct3 | 40.0 | 114.2 | |
| ct1 | ct3 | hc | 35.0 | 109.5 | |
| ct3 | ct1 | hc | 35.0 | 109.5 | |

| | | | | |
|-----|-----|-----|--------|---------------------------------|
| ct3 | c2e | o2c | 80.0 | 122.4 |
| c2e | ct3 | hc | 35.0 | 109.5 |
| ct2 | ct2 | hc | 35.0 | 109.5 |
| ct2 | ct3 | hc | 35.0 | 109.5 |
| ct3 | ct2 | hc | 35.0 | 109.5 |
| ct3 | ct3 | hc | 35.0 | 109.5 |
| hc | ct2 | hc | 35.0 | 109.5 |
| hc | ct3 | hc | 35.0 | 109.5 |
| h1 | ct3 | h1 | 35.0 | 109.5 |
| o2c | cqo | cq2 | 60.0 | 120.0 |
| olc | cq2 | cqo | 60.0 | 120.0 |
| olc | cq2 | cq2 | 60.0 | 120.0 |
| cq2 | olc | ct3 | 60.0 | 112.0 |
| cqo | cq2 | cq2 | 30.0 | 120.0 |
| cq2 | cqo | cq2 | 30.0 | 120.0 |
| cqo | cq2 | ct2 | 50.0 | 115.7 |
| cq2 | cq2 | ct2 | 50.0 | 124.1 |
| cqo | cq2 | ct3 | 50.0 | 115.2 |
| cq2 | cq2 | ct3 | 50.0 | 124.9 |
| cq2 | ct2 | cqq | 50.0 | 112.0 |
| ct2 | ct2 | cqq | 50.0 | 112.0 |
| olc | ct2 | cqq | 50.0 | 109.6 |
| cq2 | cqq | ct2 | 50.0 | 125.9 |
| cqq | cq2 | ct2 | 50.0 | 120.2 |
| cqq | cq2 | ct3 | 50.0 | 123.7 |
| ct2 | cq2 | ct3 | 50.0 | 116.0 |
| ct3 | cq2 | ct3 | 50.0 | 116.0 |
| cq2 | ct2 | ct2 | 50.0 | 114.5 |
| cq2 | ct2 | ct3 | 50.0 | 114.5 |
| hc | ct2 | cq2 | 35.0 | 109.5 |
| hc | ct3 | cq2 | 35.0 | 109.5 |
| hc | ct2 | cqq | 35.0 | 109.5 |
| on | no | ct2 | 80.0 | 109.5 |
| on | no | ct3 | 80.0 | 109.5 |
| ct3 | no | ct2 | 60.0 | 109.5 |
| ct3 | no | ct3 | 60.0 | 109.5 |
| no | ct2 | ct2 | 67.7 | 115.0 |
| no | ct2 | hc | 40.0 | 109.5 |
| no | ct3 | hc | 40.0 | 109.5 |
| ct2 | ct2 | ct2 | 58.0 | 109.5 |
| ct2 | ct2 | ct3 | 58.0 | 109.5 |
| ct2 | ct1 | ct3 | 58.0 | 111.5 |
| ct2 | ct1 | ct2 | 58.0 | 111.5 |
| ct3 | ct1 | ct2 | 58.0 | 111.5 |
| ct3 | ct1 | ct3 | 58.0 | 111.5 |
| olc | c3 | c2 | 50.0 | 109.6 # Same as olc - ct2 - cqq |
| cbb | cbb | cf | 65.490 | 124.050 # Same as ce - ce - cf |
| cnb | cbb | cf | 65.490 | 124.050 # Same as ce - ce - cf |
| cbb | cf | c2 | 65.420 | 124.330 # Same as ce - cf - cf |
| cbb | cf | ha | 50.240 | 117.980 # Same as ce - cf - ha |

DIHE

| | | | | | | | |
|-----|-----|-----|---|---|-------|---------|-------------------------------|
| X | nmh | mgc | X | 1 | 0.000 | 180.000 | 2.000 |
| X | ns | mgc | X | 1 | 0.000 | 180.000 | 2.000 |
| X | nmh | cnb | X | 1 | 2.500 | 180.000 | 2.000 |
| X | nmh | crb | X | 1 | 2.500 | 180.000 | 2.000 |
| X | ns | ccs | X | 1 | 2.500 | 180.000 | 2.000 |
| X | ns | cnb | X | 1 | 2.500 | 180.000 | 2.000 # Same with X-nmh-cnb-X |
| X | ns | crb | X | 1 | 2.500 | 180.000 | 2.000 # Same with X-nmh-crb-X |
| X | nmh | cpb | X | 1 | 0.000 | 180.000 | 2.000 |
| X | nmh | cqb | X | 1 | 2.500 | 180.000 | 2.000 |
| X | cnb | cbb | X | 1 | 3.50 | 180.000 | 2.000 |
| X | crb | cbb | X | 1 | 3.50 | 180.000 | 2.000 |
| X | cpb | cbb | X | 1 | 3.50 | 180.000 | 2.000 |
| X | cqb | cbb | X | 1 | 3.50 | 180.000 | 2.000 |
| X | cbb | cbb | X | 1 | 5.00 | 180.000 | 2.000 |
| ct1 | ct1 | ccs | X | 1 | 1.575 | 180.000 | 2.000 |
| hc | ct1 | ccs | X | 1 | 0.00 | 180.000 | 2.000 |
| ct2 | ct1 | ccs | X | 1 | 0.00 | 180.000 | 2.000 |
| ct3 | ct1 | ccs | X | 1 | 0.00 | 180.000 | 2.000 |
| X | ct1 | ct1 | X | 1 | 0.00 | 180.000 | 3.000 |
| X | cbb | c2k | X | 1 | 5.000 | 180.000 | 2.000 |
| csb | ct1 | c2k | X | 1 | 1.575 | 180.000 | 2.000 |
| hc | ct1 | c2k | X | 1 | 0.000 | 180.000 | 2.000 |
| c2a | ct1 | c2k | X | 1 | 0.000 | 180.000 | 2.000 |
| c2k | ct1 | csb | X | 1 | 1.575 | 180.000 | 2.000 |
| hc | ct1 | csb | X | 1 | 0.000 | 180.000 | 2.000 |
| c2a | ct1 | csb | X | 1 | 0.000 | 180.000 | 2.000 |
| X | cab | ccs | X | 1 | 3.500 | 180.000 | 2.000 |
| X | csb | ccs | X | 1 | 3.500 | 180.000 | 2.000 |

| | | | | | | | |
|-----|-----|-----|-----|---|--------|---------|-----------------------------|
| X | cab | cnb | X | 1 | 3.500 | 180.000 | 2.000 |
| X | cab | crb | X | 1 | 3.500 | 180.000 | 2.000 |
| X | cab | cpb | X | 1 | 3.500 | 180.000 | 2.000 |
| X | csb | cqb | X | 1 | 3.500 | 180.000 | 2.000 |
| o2c | c2a | olc | X | 1 | 1.000 | 180.000 | 1.000 |
| o2c | c2a | olc | c3 | 1 | 1.000 | 180.000 | 1.000 |
| o2c | c2a | olc | ct3 | 1 | 1.000 | 180.000 | 1.000 |
| o2c | c2a | olc | c3 | 1 | 6.000 | 180.000 | 2.000 |
| o2c | c2a | olc | X | 1 | 6.000 | 180.000 | 2.000 |
| ct1 | c2a | olc | X | 1 | 1.500 | 180.000 | 2.000 |
| ct1 | c2a | olc | ct3 | 1 | 1.500 | 180.000 | 2.000 |
| ct2 | c2a | olc | X | 1 | 1.500 | 180.000 | 2.000 |
| ct2 | c2a | olc | c3 | 1 | 1.500 | 180.000 | 2.000 |
| olc | c2a | ct2 | X | 1 | 0.030 | 0.000 | 3.000 |
| olc | c2a | ct2 | hc | 1 | 0.030 | 0.000 | 3.000 |
| olc | c2a | ct2 | ct2 | 1 | 0.030 | 0.000 | 3.000 |
| o2c | c2a | ct2 | hc | 1 | 0.030 | 180.000 | 3.000 |
| o2c | c2a | ct2 | ct2 | 1 | 0.030 | 180.000 | 3.000 |
| X | c2a | ct1 | X | 1 | 0.000 | 180.000 | 3.000 |
| X | olc | ct2 | X | 1 | 0.180 | 0.000 | 3.000 |
| c2a | olc | c3 | c2 | 1 | 0.180 | 0.000 | 3.000 |
| X | olc | ct3 | hc | 1 | 0.180 | 0.000 | 3.000 |
| c2a | olc | c3 | h1 | 1 | 0.180 | 0.000 | 3.000 |
| c2a | olc | ct3 | h1 | 1 | 0.180 | 0.000 | 3.000 |
| X | cbb | c2e | X | 1 | 5.000 | 180.000 | 2.000 |
| X | cbb | ct3 | X | 1 | 0.000 | 180.000 | 2.000 |
| X | ct1 | ct2 | X | 1 | 0.156 | 0.000 | 3.000 |
| X | ct1 | ct3 | X | 1 | 0.156 | 0.000 | 3.000 |
| X | ct2 | ct2 | X | 1 | 0.156 | 0.000 | 3.000 |
| X | ct2 | ct3 | X | 1 | 0.156 | 0.000 | 3.000 |
| X | ct3 | ct3 | X | 1 | 0.156 | 0.000 | 3.000 |
| X | c2e | ct3 | X | 1 | 0.000 | 180.000 | 2.000 |
| X | cbb | cf | X | 4 | 26.600 | 180.000 | 2.000 # Same with X-ce-cf-X |
| X | cbb | ct2 | X | 2 | 0.000 | 180.000 | 2.000 # Same with X-c3-ca-X |

IMPROPER

| | | | | | | |
|---|---|-----|-----|--------|-------|-----|
| X | X | csb | X | 1.100 | 180.0 | 2.0 |
| X | X | ns | X | 1.100 | 180.0 | 2.0 |
| X | X | nmh | X | 1.100 | 180.0 | 2.0 |
| X | X | cab | X | 1.100 | 180.0 | 2.0 |
| X | X | cbb | X | 1.100 | 180.0 | 2.0 |
| X | X | ccs | X | 1.100 | 180.0 | 2.0 |
| X | X | cnb | X | 1.100 | 180.0 | 2.0 |
| X | X | crb | X | 1.100 | 180.0 | 2.0 |
| X | X | ccs | X | 1.100 | 180.0 | 2.0 |
| X | X | cpb | X | 1.100 | 180.0 | 2.0 |
| X | X | cqb | X | 1.100 | 180.0 | 2.0 |
| X | X | c2k | o2c | 10.500 | 180.0 | 2.0 |

NONBON

| | | |
|-----|--------|--------|
| mgc | 0.650 | 0.250 |
| cab | 1.908 | 0.086 |
| csb | 1.908 | 0.086 |
| cbb | 1.908 | 0.086 |
| ccs | 1.908 | 0.086 |
| cnb | 1.908 | 0.086 |
| cpb | 1.908 | 0.086 |
| cqb | 1.908 | 0.086 |
| crb | 1.908 | 0.086 |
| c2k | 1.908 | 0.086 |
| c2a | 1.908 | 0.086 |
| olc | 1.6637 | 0.170 |
| o2c | 1.6612 | 0.210 |
| nmh | 1.824 | 0.170 |
| ns | 1.824 | 0.170 |
| ct1 | 1.908 | 0.1094 |
| ct2 | 1.908 | 0.1094 |
| ct3 | 1.908 | 0.1094 |

Definition of the GAFF2 based atoms types, bond connectivity and RESP charges for β -carotene

@<TRIPOS>MOLECULE

BCR

96 97 1 0 0

SMALL

No Charge or Current Charge

@<TRIPOS>ATOM

| | | | | | | | | |
|----|------|---------|---------|---------|----|------|-----|-----------|
| 1 | C1 | 5.2430 | 34.2110 | 7.1440 | c3 | 2741 | BCR | 0.520876 |
| 2 | C2 | 4.3100 | 34.8670 | 8.1640 | c3 | 2741 | BCR | -0.153725 |
| 3 | C3 | 4.2420 | 34.3760 | 9.5990 | c3 | 2741 | BCR | 0.057544 |
| 4 | C4 | 4.2390 | 32.8230 | 9.7110 | c3 | 2741 | BCR | -0.129668 |
| 5 | C5 | 4.8880 | 32.1110 | 8.5550 | c2 | 2741 | BCR | 0.189555 |
| 6 | C6 | 5.3500 | 32.7170 | 7.3970 | ce | 2741 | BCR | -0.406682 |
| 7 | C7 | 5.9500 | 31.8730 | 6.3290 | ce | 2741 | BCR | 0.118700 |
| 8 | C8 | 7.0420 | 31.0820 | 6.5130 | cf | 2741 | BCR | -0.350037 |
| 9 | C9 | 7.4690 | 30.2260 | 5.4030 | cf | 2741 | BCR | 0.188330 |
| 10 | C10 | 8.4190 | 29.3240 | 5.6480 | ce | 2741 | BCR | -0.316233 |
| 11 | C11 | 8.8860 | 28.3120 | 4.6990 | ce | 2741 | BCR | -0.008810 |
| 12 | C12 | 9.7950 | 27.4720 | 5.2180 | cf | 2741 | BCR | -0.376308 |
| 13 | C13 | 10.3210 | 26.2840 | 4.4570 | cf | 2741 | BCR | 0.221509 |
| 14 | C14 | 11.1310 | 25.4070 | 5.1140 | ce | 2741 | BCR | -0.341417 |
| 15 | C15 | 11.6470 | 24.1590 | 4.5150 | ce | 2741 | BCR | -0.112451 |
| 16 | C16 | 12.3400 | 23.2780 | 5.2460 | cf | 2741 | BCR | -0.126191 |
| 17 | C17 | 12.7450 | 21.9790 | 4.6920 | cf | 2741 | BCR | -0.332899 |
| 18 | C18 | 13.2860 | 20.9250 | 5.3860 | ce | 2741 | BCR | 0.206356 |
| 19 | C19 | 13.5180 | 19.6680 | 4.6210 | ce | 2741 | BCR | -0.365331 |
| 20 | C20 | 14.1140 | 18.5980 | 5.1740 | cf | 2741 | BCR | -0.007725 |
| 21 | C21 | 14.1690 | 17.3900 | 4.3260 | cf | 2741 | BCR | -0.336895 |
| 22 | C22 | 14.7030 | 16.1910 | 4.6980 | ce | 2741 | BCR | 0.170995 |
| 23 | C23 | 14.5980 | 15.0460 | 3.7480 | ce | 2741 | BCR | -0.315312 |
| 24 | C24 | 14.6160 | 13.7720 | 4.2080 | cf | 2741 | BCR | 0.054632 |
| 25 | C25 | 14.3950 | 12.5470 | 3.3440 | cf | 2741 | BCR | -0.300273 |
| 26 | C26 | 13.1670 | 12.3560 | 2.8240 | c2 | 2741 | BCR | 0.178004 |
| 27 | C27 | 12.8460 | 11.1670 | 1.9330 | c3 | 2741 | BCR | -0.100874 |
| 28 | C28 | 14.0880 | 10.8480 | 1.1190 | c3 | 2741 | BCR | 0.041870 |
| 29 | C29 | 15.0930 | 10.3820 | 2.1360 | c3 | 2741 | BCR | -0.174348 |
| 30 | C30 | 15.4560 | 11.5200 | 3.0820 | c3 | 2741 | BCR | 0.517469 |
| 31 | C31 | 6.6780 | 34.7870 | 7.0350 | c3 | 2741 | BCR | -0.417696 |
| 32 | C32 | 4.5400 | 34.5790 | 5.8530 | c3 | 2741 | BCR | -0.456532 |
| 33 | C33 | 4.9680 | 30.5960 | 8.7790 | c3 | 2741 | BCR | -0.379835 |
| 34 | C34 | 6.8390 | 30.3420 | 4.0290 | c3 | 2741 | BCR | -0.258093 |
| 35 | C35 | 9.9310 | 26.0930 | 3.0060 | c3 | 2741 | BCR | -0.204429 |
| 36 | C36 | 13.6120 | 20.9330 | 6.8650 | c3 | 2741 | BCR | -0.168116 |
| 37 | C37 | 15.3170 | 16.0070 | 6.0540 | c3 | 2741 | BCR | -0.235548 |
| 38 | C38 | 12.0740 | 13.3510 | 3.0770 | c3 | 2741 | BCR | -0.415232 |
| 39 | C39 | 16.6330 | 12.2520 | 2.4630 | c3 | 2741 | BCR | -0.454504 |
| 40 | C40 | 15.6970 | 10.9170 | 4.4460 | c3 | 2741 | BCR | -0.431307 |
| 41 | HC21 | 3.3000 | 34.8060 | 7.7580 | hc | 2741 | BCR | 0.033746 |
| 42 | HC22 | 4.5730 | 35.9250 | 8.2030 | hc | 2741 | BCR | 0.033746 |
| 43 | HC31 | 3.3410 | 34.7700 | 10.0700 | hc | 2741 | BCR | -0.005016 |
| 44 | HC32 | 5.0910 | 34.7730 | 10.1540 | hc | 2741 | BCR | -0.005016 |
| 45 | HC41 | 3.2090 | 32.4800 | 9.8000 | hc | 2741 | BCR | 0.049649 |
| 46 | HC42 | 4.7510 | 32.5380 | 10.6300 | hc | 2741 | BCR | 0.049649 |
| 47 | HC7 | 5.4890 | 31.8890 | 5.3410 | ha | 2741 | BCR | 0.089803 |
| 48 | HC8 | 7.5830 | 31.0840 | 7.4600 | ha | 2741 | BCR | 0.196276 |
| 49 | H10C | 8.8850 | 29.3400 | 6.6330 | ha | 2741 | BCR | 0.158878 |
| 50 | H11C | 8.5300 | 28.2450 | 3.6710 | ha | 2741 | BCR | 0.163465 |
| 51 | H12C | 10.1660 | 27.6560 | 6.2270 | ha | 2741 | BCR | 0.206724 |
| 52 | H14C | 11.4150 | 25.6400 | 6.1410 | ha | 2741 | BCR | 0.159668 |
| 53 | H15C | 11.4610 | 23.9520 | 3.4610 | ha | 2741 | BCR | 0.182949 |
| 54 | H16C | 12.6090 | 23.5290 | 6.2720 | ha | 2741 | BCR | 0.182269 |
| 55 | H17C | 12.6010 | 21.8380 | 3.6210 | ha | 2741 | BCR | 0.155445 |
| 56 | H19C | 13.1950 | 19.6140 | 3.5820 | ha | 2741 | BCR | 0.202424 |
| 57 | H20C | 14.5290 | 18.6200 | 6.1810 | ha | 2741 | BCR | 0.160907 |
| 58 | H21C | 13.7500 | 17.4630 | 3.3230 | ha | 2741 | BCR | 0.170255 |
| 59 | H23C | 14.5070 | 15.2350 | 2.6790 | ha | 2741 | BCR | 0.181715 |
| 60 | H24C | 14.8020 | 13.6180 | 5.2710 | ha | 2741 | BCR | 0.106958 |
| 61 | H271 | 12.0080 | 11.3970 | 1.2760 | hc | 2741 | BCR | 0.037749 |
| 62 | H272 | 12.5530 | 10.3080 | 2.5350 | hc | 2741 | BCR | 0.037749 |
| 63 | H281 | 14.4460 | 11.7250 | 0.5800 | hc | 2741 | BCR | 0.000153 |
| 64 | H282 | 13.8880 | 10.0760 | 0.3760 | hc | 2741 | BCR | 0.000153 |
| 65 | H291 | 15.9900 | 10.0210 | 1.6310 | hc | 2741 | BCR | 0.040575 |
| 66 | H292 | 14.6860 | 9.5450 | 2.7020 | hc | 2741 | BCR | 0.040575 |
| 67 | H311 | 7.2350 | 34.2350 | 6.2790 | hc | 2741 | BCR | 0.094143 |
| 68 | H312 | 7.1800 | 34.6930 | 7.9980 | hc | 2741 | BCR | 0.094143 |

| | | | | | | | | |
|----|------|---------|---------|--------|----|------|-----|----------|
| 69 | H313 | 6.6270 | 35.8390 | 6.7540 | hc | 2741 | BCR | 0.094143 |
| 70 | H321 | 5.0960 | 34.1720 | 5.0080 | hc | 2741 | BCR | 0.102362 |
| 71 | H322 | 4.4860 | 35.6630 | 5.7650 | hc | 2741 | BCR | 0.102362 |
| 72 | H323 | 3.5330 | 34.1630 | 5.8570 | hc | 2741 | BCR | 0.102362 |
| 73 | H331 | 5.4430 | 30.1270 | 7.9180 | hc | 2741 | BCR | 0.101612 |
| 74 | H332 | 3.9630 | 30.1950 | 8.9040 | hc | 2741 | BCR | 0.101612 |
| 75 | H333 | 5.5550 | 30.3920 | 9.6740 | hc | 2741 | BCR | 0.101612 |
| 76 | H341 | 7.2990 | 29.6190 | 3.3560 | hc | 2741 | BCR | 0.076108 |
| 77 | H342 | 6.9930 | 31.3490 | 3.6410 | hc | 2741 | BCR | 0.076108 |
| 78 | H343 | 5.7690 | 30.1410 | 4.1010 | hc | 2741 | BCR | 0.076108 |
| 79 | H351 | 10.4000 | 25.1890 | 2.6200 | hc | 2741 | BCR | 0.062642 |
| 80 | H352 | 10.2640 | 26.9520 | 2.4240 | hc | 2741 | BCR | 0.062642 |
| 81 | H353 | 8.8470 | 26.0010 | 2.9290 | hc | 2741 | BCR | 0.062642 |
| 82 | H361 | 14.0300 | 19.9680 | 7.1510 | hc | 2741 | BCR | 0.054733 |
| 83 | H362 | 12.7030 | 21.1180 | 7.4370 | hc | 2741 | BCR | 0.054733 |
| 84 | H363 | 14.3380 | 21.7190 | 7.0750 | hc | 2741 | BCR | 0.054733 |
| 85 | H371 | 15.6820 | 14.9840 | 6.1520 | hc | 2741 | BCR | 0.071622 |
| 86 | H372 | 14.5670 | 16.1990 | 6.8210 | hc | 2741 | BCR | 0.071622 |
| 87 | H373 | 16.1470 | 16.7030 | 6.1760 | hc | 2741 | BCR | 0.071622 |
| 88 | H381 | 11.1620 | 13.0250 | 2.5780 | hc | 2741 | BCR | 0.105731 |
| 89 | H382 | 12.3730 | 14.3250 | 2.6890 | hc | 2741 | BCR | 0.105731 |
| 90 | H383 | 11.8940 | 13.4290 | 4.1490 | hc | 2741 | BCR | 0.105731 |
| 91 | H391 | 17.4330 | 11.5420 | 2.2530 | hc | 2741 | BCR | 0.100119 |
| 92 | H392 | 16.9940 | 13.0120 | 3.1560 | hc | 2741 | BCR | 0.100119 |
| 93 | H393 | 16.3180 | 12.7270 | 1.5350 | hc | 2741 | BCR | 0.100119 |
| 94 | H401 | 16.4630 | 10.1450 | 4.3720 | hc | 2741 | BCR | 0.090657 |
| 95 | H402 | 14.7720 | 10.4750 | 4.8180 | hc | 2741 | BCR | 0.090657 |
| 96 | H403 | 16.0300 | 11.6940 | 5.1340 | hc | 2741 | BCR | 0.090657 |

@<TRIPOS>BOND

| | | | |
|----|----|----|---|
| 1 | 1 | 2 | 1 |
| 2 | 1 | 6 | 1 |
| 3 | 1 | 31 | 1 |
| 4 | 1 | 32 | 1 |
| 5 | 2 | 3 | 1 |
| 6 | 2 | 41 | 1 |
| 7 | 2 | 42 | 1 |
| 8 | 3 | 4 | 1 |
| 9 | 3 | 43 | 1 |
| 10 | 3 | 44 | 1 |
| 11 | 4 | 5 | 1 |
| 12 | 4 | 45 | 1 |
| 13 | 4 | 46 | 1 |
| 14 | 5 | 6 | 2 |
| 15 | 5 | 33 | 1 |
| 16 | 6 | 7 | 1 |
| 17 | 7 | 8 | 2 |
| 18 | 7 | 47 | 1 |
| 19 | 8 | 9 | 1 |
| 20 | 8 | 48 | 1 |
| 21 | 9 | 10 | 2 |
| 22 | 9 | 34 | 1 |
| 23 | 10 | 11 | 1 |
| 24 | 10 | 49 | 1 |
| 25 | 11 | 12 | 2 |
| 26 | 11 | 50 | 1 |
| 27 | 12 | 13 | 1 |
| 28 | 12 | 51 | 1 |
| 29 | 13 | 14 | 2 |
| 30 | 13 | 35 | 1 |
| 31 | 14 | 15 | 1 |
| 32 | 14 | 52 | 1 |
| 33 | 15 | 16 | 2 |
| 34 | 15 | 53 | 1 |
| 35 | 16 | 17 | 1 |
| 36 | 16 | 54 | 1 |
| 37 | 17 | 18 | 2 |
| 38 | 17 | 55 | 1 |
| 39 | 18 | 19 | 1 |
| 40 | 18 | 36 | 1 |
| 41 | 19 | 20 | 2 |
| 42 | 19 | 56 | 1 |
| 43 | 20 | 21 | 1 |
| 44 | 20 | 57 | 1 |
| 45 | 21 | 22 | 2 |
| 46 | 21 | 58 | 1 |
| 47 | 22 | 23 | 1 |
| 48 | 22 | 37 | 1 |
| 49 | 23 | 24 | 2 |
| 50 | 23 | 59 | 1 |
| 51 | 24 | 25 | 1 |

| | | | |
|----|----|----|---|
| 52 | 24 | 60 | 1 |
| 53 | 25 | 26 | 2 |
| 54 | 25 | 30 | 1 |
| 55 | 26 | 27 | 1 |
| 56 | 26 | 38 | 1 |
| 57 | 27 | 28 | 1 |
| 58 | 27 | 61 | 1 |
| 59 | 27 | 62 | 1 |
| 60 | 28 | 29 | 1 |
| 61 | 28 | 63 | 1 |
| 62 | 28 | 64 | 1 |
| 63 | 29 | 30 | 1 |
| 64 | 29 | 65 | 1 |
| 65 | 29 | 66 | 1 |
| 66 | 30 | 39 | 1 |
| 67 | 30 | 40 | 1 |
| 68 | 31 | 67 | 1 |
| 69 | 31 | 68 | 1 |
| 70 | 31 | 69 | 1 |
| 71 | 32 | 70 | 1 |
| 72 | 32 | 71 | 1 |
| 73 | 32 | 72 | 1 |
| 74 | 33 | 73 | 1 |
| 75 | 33 | 74 | 1 |
| 76 | 33 | 75 | 1 |
| 77 | 34 | 76 | 1 |
| 78 | 34 | 77 | 1 |
| 79 | 34 | 78 | 1 |
| 80 | 35 | 79 | 1 |
| 81 | 35 | 80 | 1 |
| 82 | 35 | 81 | 1 |
| 83 | 36 | 82 | 1 |
| 84 | 36 | 83 | 1 |
| 85 | 36 | 84 | 1 |
| 86 | 37 | 85 | 1 |
| 87 | 37 | 86 | 1 |
| 88 | 37 | 87 | 1 |
| 89 | 38 | 88 | 1 |
| 90 | 38 | 89 | 1 |
| 91 | 38 | 90 | 1 |
| 92 | 39 | 91 | 1 |
| 93 | 39 | 92 | 1 |
| 94 | 39 | 93 | 1 |
| 95 | 40 | 94 | 1 |
| 96 | 40 | 95 | 1 |
| 97 | 40 | 96 | 1 |

@<TRIPOS>SUBSTRUCTURE
1 BCR 1 TEMP 0 **** **** 0 ROOT

GAFF2 based bonded and LJ parameters for β -carotene

Remark line goes here
MASS

BOND #Associated parameters for the bonded atoms can be found in the AMBER GAFF2 force-field library.

ANGLE #Associated parameters for the angles can be found in the AMBER GAFF2 force-field library.

| DIHE | | | | | |
|-------------|---|-------|---------|--------|---------------------|
| c3-c3-ce-c2 | 6 | 0.000 | 0.000 | 3.000 | same as X -c3-cc-X |
| c3-c3-ce-ce | 6 | 0.000 | 0.000 | 3.000 | same as X -c3-cc-X |
| hc-c3-cf-cf | 1 | 0.380 | 180.000 | -3.000 | same as hc-c3-c2-c2 |
| hc-c3-cf-cf | 1 | 0.000 | 0.000 | -2.000 | same as hc-c3-c2-c2 |
| hc-c3-cf-cf | 1 | 1.150 | 0.000 | 1.000 | same as hc-c3-c2-c2 |
| hc-c3-cf-ce | 1 | 0.380 | 180.000 | -3.000 | same as hc-c3-c2-c2 |
| hc-c3-cf-ce | 1 | 0.000 | 0.000 | -2.000 | same as hc-c3-c2-c2 |
| hc-c3-cf-ce | 1 | 1.150 | 0.000 | 1.000 | same as hc-c3-c2-c2 |
| hc-c3-ce-cf | 1 | 0.380 | 180.000 | -3.000 | same as hc-c3-c2-c2 |
| hc-c3-ce-cf | 1 | 0.000 | 0.000 | -2.000 | same as hc-c3-c2-c2 |
| hc-c3-ce-cf | 1 | 1.150 | 0.000 | 1.000 | same as hc-c3-c2-c2 |
| hc-c3-ce-ce | 1 | 0.380 | 180.000 | -3.000 | same as hc-c3-c2-c2 |

| | | | | | |
|-------------|---|-------|-------|--------|-------------------------|
| hc-c3-ce-ce | 1 | 0.000 | 0.000 | -2.000 | same as hc-c3-c2-c2 |
| hc-c3-ce-ce | 1 | 1.150 | 0.000 | 1.000 | same as hc-c3-c2-c2 |
| c3-c3-cf-cf | 6 | 0.000 | 0.000 | 3.000 | same as X -c3-cd-X |
| c3-c3-cf-c2 | 6 | 0.000 | 0.000 | 3.000 | same as X -c3-cd-X |
| IMPROPER | | | | | |
| c3-c3-c2-ce | | 1.1 | 180.0 | 2.0 | Using the default value |
| c2-c3-ce-ce | | 1.1 | 180.0 | 2.0 | Using the default value |
| ce-cf-ce-ha | | 1.1 | 180.0 | 2.0 | Same as X -X -ca-ha |
| ce-cf-cf-ha | | 1.1 | 180.0 | 2.0 | Same as X -X -ca-ha |
| c3-ce-cf-cf | | 1.1 | 180.0 | 2.0 | Using the default value |
| c3-ce-ce-cf | | 1.1 | 180.0 | 2.0 | Using the default value |
| c2-c3-cf-cf | | 1.1 | 180.0 | 2.0 | Using the default value |
| c3-c3-c2-cf | | 1.1 | 180.0 | 2.0 | Using the default value |

NONBON

#LJ parameters for the assigned atom types can be found in the AMBER GAFF2 force-field library.

References

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