

Table S1. Atomic charges on atoms in Chlorophyll C2 and Na+ quadruplex G4 caclulated with selected populational schemes.

File G4Na.out

Molecule Na+ Quadruplex G4

OPT G4 Na complex B3LYP/Def2TZVP VAC.

1 65

| Dipole | 0.0117 | -0.0189 | 0.0000 | 0.0222 | | | | | | | | |
|--------------------|---------|---------|-----------|---------|---------|---------|----------|---------|---------|---------|---------|---------|
| Quadrupole | 51.8905 | 51.0612 | -102.9516 | 0.4223 | -0.0000 | -0.0000 | | | | | | |
| Atomic coordinates | | | | Mul. | Lowdin | Hirsch. | I-Hirsch | CM5 | ESP | NPA | AIM | ACP |
| 7 | -3.5341 | -0.7683 | -0.0000 | -0.2368 | 0.2287 | -0.0567 | -0.7189 | -0.3887 | -0.6445 | -0.5806 | -1.1675 | -0.3873 |
| 6 | -4.7774 | -1.3537 | -0.0000 | 0.3425 | -0.3799 | 0.1681 | 0.8905 | 0.3785 | 0.8516 | 0.5915 | 1.4851 | 0.4803 |
| 7 | -4.8325 | -2.6904 | -0.0000 | -0.4024 | 0.0358 | -0.1360 | -0.9009 | -0.5797 | -0.8901 | -0.7623 | -1.1894 | -0.4987 |
| 7 | -5.9033 | -0.6673 | -0.0000 | -0.2884 | 0.1195 | -0.2203 | -0.6616 | -0.3905 | -0.7690 | -0.5247 | -1.1236 | -0.4477 |
| 6 | -5.7011 | 0.6556 | 0.0000 | 0.1802 | -0.2601 | 0.0815 | 0.5088 | 0.2339 | 0.6097 | 0.3425 | 0.9160 | 0.3012 |
| 6 | -4.5043 | 1.3490 | 0.0000 | 0.0553 | -0.2178 | -0.0343 | -0.2099 | 0.0547 | -0.1187 | -0.1040 | 0.3716 | 0.0889 |
| 6 | -3.2961 | 0.6062 | 0.0000 | 0.3751 | -0.3567 | 0.1648 | 0.7738 | 0.2604 | 0.5893 | 0.6293 | 1.3069 | 0.3951 |
| 8 | -2.1411 | 1.0398 | 0.0000 | -0.6241 | 0.0848 | -0.2638 | -0.7290 | -0.3900 | -0.6584 | -0.7354 | -1.2432 | -0.3951 |
| 7 | -4.7244 | 2.7117 | 0.0000 | -0.3672 | 0.1152 | -0.1448 | -0.3315 | -0.3408 | -0.3632 | -0.4682 | -1.1110 | -0.3875 |
| 6 | -6.0157 | 2.8382 | 0.0000 | 0.0840 | -0.2615 | 0.0704 | 0.2737 | 0.1696 | 0.1014 | 0.2057 | 0.9749 | 0.2102 |
| 7 | -6.6619 | 1.6252 | 0.0000 | -0.2361 | 0.2226 | -0.0377 | -0.5114 | -0.3843 | -0.4215 | -0.5033 | -1.1765 | -0.3583 |
| 1 | -2.6926 | -1.3651 | -0.0000 | 0.2740 | 0.2106 | 0.1066 | 0.3704 | 0.3190 | 0.4272 | 0.4507 | 0.4967 | 0.1948 |
| 1 | -6.5524 | 3.7733 | 0.0000 | 0.1612 | 0.1363 | 0.0707 | 0.1090 | 0.1435 | 0.1573 | 0.2064 | 0.1011 | 0.1316 |
| 1 | -7.6519 | 1.4588 | 0.0000 | 0.2386 | 0.1976 | 0.1630 | 0.3803 | 0.3604 | 0.3729 | 0.4272 | 0.4534 | 0.2877 |
| 1 | -4.0218 | -3.3186 | -0.0000 | 0.2750 | 0.1627 | 0.0861 | 0.3508 | 0.2927 | 0.3258 | 0.4357 | 0.5002 | 0.2277 |
| 1 | -5.7538 | -3.0903 | -0.0000 | 0.2431 | 0.1797 | 0.1354 | 0.3976 | 0.3335 | 0.4298 | 0.4044 | 0.4285 | 0.2665 |
| 7 | 0.7614 | -3.5245 | -0.0000 | -0.2364 | 0.2302 | -0.0562 | -0.7195 | -0.3892 | -0.7894 | -0.5800 | -1.1675 | -0.3873 |
| 6 | 1.3458 | -4.7648 | -0.0000 | 0.3425 | -0.3815 | 0.1681 | 0.8914 | 0.3790 | 0.9735 | 0.5917 | 1.4853 | 0.4803 |
| 7 | 2.6827 | -4.8178 | -0.0000 | -0.4027 | 0.0365 | -0.1357 | -0.9014 | -0.5801 | -0.9353 | -0.7622 | -1.1894 | -0.4987 |
| 7 | 0.6579 | -5.8895 | -0.0000 | -0.2885 | 0.1200 | -0.2207 | -0.6628 | -0.3910 | -0.7985 | -0.5252 | -1.1235 | -0.4477 |
| 6 | -0.6650 | -5.6899 | -0.0000 | 0.1812 | -0.2601 | 0.0816 | 0.5097 | 0.2340 | 0.5970 | 0.3423 | 0.9160 | 0.3012 |
| 6 | -1.3572 | -4.4965 | -0.0000 | 0.0548 | -0.2169 | -0.0342 | -0.2097 | 0.0548 | -0.2036 | -0.1041 | 0.3714 | 0.0889 |
| 6 | -0.6129 | -3.2890 | -0.0000 | 0.3750 | -0.3585 | 0.1654 | 0.7749 | 0.2612 | 0.6686 | 0.6298 | 1.3057 | 0.3951 |
| 8 | -1.0457 | -2.1366 | -0.0000 | -0.6213 | 0.0889 | -0.2625 | -0.7282 | -0.3893 | -0.6320 | -0.7333 | -1.2432 | -0.3952 |
| 7 | -2.7205 | -4.7189 | -0.0000 | 0.3681 | 0.1154 | -0.1449 | -0.3326 | -0.3415 | -0.2587 | -0.4691 | -1.1109 | -0.3875 |
| 6 | -2.8486 | -6.0079 | -0.0000 | 0.0852 | -0.2630 | 0.0710 | 0.2749 | 0.1710 | 0.0107 | 0.2064 | 0.9749 | 0.2102 |
| 7 | -1.6360 | -6.6506 | -0.0000 | -0.2354 | 0.2235 | -0.0377 | -0.5125 | -0.3861 | -0.3502 | -0.5027 | -1.1765 | -0.3583 |
| 1 | 1.3589 | -2.6842 | -0.0000 | 0.2744 | 0.2109 | 0.1069 | 0.3708 | 0.3195 | 0.5010 | 0.4506 | 0.4967 | 0.1948 |
| 1 | -3.7849 | -6.5453 | -0.0000 | 0.1616 | 0.1370 | 0.0713 | 0.1097 | 0.1439 | 0.1754 | 0.2068 | 0.1011 | 0.1316 |
| 1 | -1.4716 | -7.6376 | -0.0000 | 0.2366 | 0.1958 | 0.1620 | 0.3798 | 0.3611 | 0.3558 | 0.4261 | 0.4534 | 0.2877 |
| 1 | 3.3127 | -4.0093 | -0.0000 | 0.2749 | 0.1627 | 0.0867 | 0.3519 | 0.2932 | 0.3469 | 0.4360 | 0.5002 | 0.2277 |
| 1 | 3.0821 | -5.7385 | -0.0000 | 0.2428 | 0.1795 | 0.1351 | 0.3974 | 0.3336 | 0.4297 | 0.4041 | 0.4285 | 0.2665 |
| 7 | 3.5342 | 0.7682 | 0.0000 | -0.2367 | 0.2288 | -0.0567 | -0.7189 | -0.3887 | -0.7282 | -0.5805 | -1.1675 | -0.3873 |
| 6 | 4.7777 | 1.3536 | 0.0000 | 0.3424 | -0.3799 | 0.1681 | 0.8905 | 0.3785 | 0.9025 | 0.5915 | 1.4851 | 0.4803 |
| 7 | 4.8329 | 2.6902 | 0.0000 | -0.4024 | 0.0359 | -0.1359 | -0.9008 | -0.5795 | -0.9309 | -0.7623 | -1.1894 | -0.4987 |
| 7 | 5.9034 | 0.6673 | 0.0000 | -0.2883 | 0.1196 | -0.2203 | -0.6616 | -0.3905 | -0.7922 | -0.5246 | -1.1236 | -0.4477 |
| 6 | 5.7012 | -0.6555 | -0.0000 | 0.1802 | -0.2601 | 0.0815 | 0.5088 | 0.2339 | 0.6560 | 0.3424 | 0.9160 | 0.3012 |
| 6 | 4.5042 | -1.3489 | -0.0000 | 0.0553 | -0.2178 | -0.0343 | -0.2098 | 0.0547 | -0.1613 | -0.1040 | 0.3716 | 0.0889 |
| 6 | 3.2960 | -0.6061 | -0.0000 | 0.3751 | -0.3566 | 0.1648 | 0.7737 | 0.2604 | 0.6219 | 0.6293 | 1.3069 | 0.3951 |
| 8 | 2.1409 | -1.0399 | -0.0000 | -0.6242 | 0.0846 | -0.2638 | -0.7291 | -0.3901 | -0.6556 | -0.7354 | -1.2432 | -0.3951 |
| 7 | 4.7244 | -2.7115 | -0.0000 | -0.3673 | 0.1152 | -0.1448 | -0.3317 | -0.3409 | -0.3217 | -0.4682 | -1.1110 | -0.3875 |
| 6 | 6.0157 | -2.8380 | -0.0000 | 0.0840 | -0.2615 | 0.0704 | 0.2737 | 0.1695 | 0.0884 | 0.2056 | 0.9749 | 0.2102 |
| 7 | 6.6619 | -1.6251 | -0.0000 | -0.2360 | 0.2227 | -0.0376 | -0.5113 | -0.3843 | -0.4472 | -0.5033 | -1.1765 | -0.3583 |
| 1 | 2.6931 | 1.3650 | 0.0000 | 0.2739 | 0.2106 | 0.1066 | 0.3704 | 0.3191 | 0.4869 | 0.4506 | 0.4967 | 0.1948 |
| 1 | 6.5523 | -3.7730 | -0.0000 | 0.1612 | 0.1363 | 0.0707 | 0.1089 | 0.1435 | 0.1605 | 0.2064 | 0.1011 | 0.1316 |
| 1 | 7.6519 | -1.4585 | -0.0000 | 0.2386 | 0.1976 | 0.1630 | 0.3804 | 0.3604 | 0.3812 | 0.4273 | 0.4533 | 0.2877 |
| 1 | 4.0222 | 3.3185 | 0.0000 | 0.2750 | 0.1628 | 0.0862 | 0.3509 | 0.2927 | 0.3433 | 0.4358 | 0.5002 | 0.2277 |
| 1 | 5.7544 | 3.0902 | 0.0000 | 0.2432 | 0.1799 | 0.1354 | 0.3976 | 0.3335 | 0.4379 | 0.4044 | 0.4285 | 0.2665 |
| 7 | -0.7609 | 3.5244 | 0.0000 | -0.2365 | 0.2305 | -0.0562 | -0.7197 | -0.3894 | -0.8639 | -0.5800 | -1.1675 | -0.3873 |
| 6 | -1.3459 | 4.7636 | 0.0000 | 0.3423 | -0.3822 | 0.1681 | 0.8917 | 0.3792 | 1.0230 | 0.5917 | 1.4853 | 0.4803 |
| 7 | -2.6827 | 4.8161 | 0.0000 | -0.4026 | 0.0367 | -0.1358 | -0.9018 | -0.5807 | -0.9905 | -0.7621 | -1.1894 | -0.4987 |
| 7 | -0.6584 | 5.8880 | 0.0000 | -0.2884 | 0.1202 | -0.2208 | -0.6631 | -0.3912 | -0.8192 | -0.5254 | -1.1235 | -0.4477 |
| 6 | 0.6645 | 5.6894 | 0.0000 | 0.1814 | -0.2602 | 0.0816 | 0.5100 | 0.2340 | 0.6359 | 0.3423 | 0.9160 | 0.3012 |
| 6 | 1.3573 | 4.4971 | 0.0000 | 0.0547 | -0.2170 | -0.0342 | -0.2099 | 0.0548 | -0.2276 | -0.1043 | 0.3714 | 0.0889 |
| 6 | 0.6135 | 3.2900 | 0.0000 | 0.3746 | -0.3596 | 0.1654 | 0.7752 | 0.2613 | 0.7195 | 0.6299 | 1.3057 | 0.3951 |
| 8 | 1.0465 | 2.1387 | 0.0000 | -0.6202 | 0.0900 | -0.2623 | -0.7278 | -0.3888 | -0.6703 | -0.7328 | -1.2432 | -0.3951 |
| 7 | 2.7205 | 4.7203 | 0.0000 | -0.3680 | 0.1157 | -0.1450 | -0.3329 | -0.3418 | -0.2693 | -0.4690 | -1.1109 | -0.3875 |
| 6 | 2.8480 | 6.0086 | 0.0000 | 0.0852 | -0.2634 | 0.0710 | 0.2752 | 0.1712 | 0.0385 | 0.2065 | 0.9749 | 0.2102 |

| | | | | | | | | | | | | |
|----|---------|--------|--------|---------|--------|---------|---------|---------|---------|---------|---------|---------|
| 7 | 1.6351 | 6.6501 | 0.0000 | -0.2352 | 0.2239 | -0.0377 | -0.5127 | -0.3866 | -0.3957 | -0.5026 | -1.1765 | -0.3583 |
| 1 | -1.3581 | 2.6839 | 0.0000 | 0.2744 | 0.2109 | 0.1069 | 0.3708 | 0.3196 | 0.5399 | 0.4505 | 0.4967 | 0.1948 |
| 1 | 3.7840 | 6.5461 | 0.0000 | 0.1616 | 0.1370 | 0.0713 | 0.1097 | 0.1439 | 0.1704 | 0.2068 | 0.1011 | 0.1316 |
| 1 | 1.4702 | 7.6362 | 0.0000 | 0.2361 | 0.1955 | 0.1618 | 0.3797 | 0.3612 | 0.3688 | 0.4259 | 0.4534 | 0.2877 |
| 1 | -3.3127 | 4.0078 | 0.0000 | 0.2747 | 0.1626 | 0.0866 | 0.3518 | 0.2933 | 0.3883 | 0.4359 | 0.5002 | 0.2277 |
| 1 | -3.0821 | 5.7360 | 0.0000 | 0.2424 | 0.1790 | 0.1349 | 0.3974 | 0.3338 | 0.4408 | 0.4039 | 0.4285 | 0.2665 |
| 11 | 0.0000 | 0.0000 | 0.0000 | 0.6990 | 0.1246 | 0.3821 | 1.0294 | 0.7076 | 0.7792 | 0.9358 | 0.9072 | 0.5627 |

Dipole moment (in D) 0.02 (DEN) 0.03 0.04 0.02 0.02 0.02 0.06 0.02 0.01 0.00

 File Mg_Chlorophyll_C2.out
 Molecule Mg_Chlorophyll_C2
 OPT Mg Chlorophyll c2 B3LYP/Def2TZVP VAC.
 0 73

| Dipole | -9.2760 | 4.6537 | -0.9894 | 10.4250 | | | | | | | | |
|--------------------|----------|---------|---------|---------|---------|----------|---------|---------|---------|---------|---------|---------|
| Quadrupole | -31.9324 | 25.0152 | 6.9172 | 23.4103 | -5.1827 | -10.4527 | | | | | | |
| Atomic coordinates | | | Mu1. | Lowdin | Hirsch. | I-Hirsch | CM5 | ESP | NPA | AIM | ACP | |
| 6 | 1.7665 | 0.5238 | -0.1715 | 0.3055 | -0.1218 | 0.0363 | 0.2947 | 0.1009 | 0.0296 | 0.1634 | 0.3966 | 0.1407 |
| 6 | 0.6196 | 2.4085 | -0.1334 | 0.2308 | -0.1673 | 0.0356 | 0.3272 | 0.0983 | 0.2483 | 0.1434 | 0.4158 | 0.1503 |
| 7 | 0.4963 | 1.0541 | -0.1409 | -0.3970 | 0.1843 | -0.1610 | -0.8673 | -0.4408 | -0.5419 | -0.6697 | -1.2379 | -0.4615 |
| 6 | -0.4335 | 3.3320 | -0.1109 | -0.3292 | -0.0791 | -0.0500 | -0.2847 | -0.0924 | -0.3339 | -0.2210 | -0.0322 | -0.0913 |
| 1 | -0.1433 | 4.3763 | -0.1260 | 0.1262 | 0.1576 | 0.0371 | 0.1111 | 0.0980 | 0.1747 | 0.2114 | 0.0323 | 0.0781 |
| 6 | -1.7991 | 3.0770 | -0.0669 | 0.2700 | -0.1637 | 0.0372 | 0.3406 | 0.0987 | 0.0615 | 0.1510 | 0.4079 | 0.1512 |
| 6 | -2.8455 | 4.0844 | -0.0463 | -0.0235 | -0.0925 | -0.0025 | 0.0681 | -0.0077 | 0.2495 | -0.0012 | -0.0236 | 0.0252 |
| 7 | -2.3562 | 1.8320 | -0.0376 | -0.3600 | 0.1800 | -0.1669 | -0.9232 | -0.4687 | -0.3766 | -0.7028 | -1.2773 | -0.4726 |
| 6 | -4.0351 | 3.4086 | 0.0024 | 0.0494 | -0.0821 | -0.0193 | -0.0405 | -0.0188 | -0.1484 | -0.0876 | -0.0243 | 0.0029 |
| 6 | -3.7094 | 1.9868 | -0.0021 | 0.2507 | -0.1526 | 0.0415 | 0.3612 | 0.1039 | 0.2048 | 0.1733 | 0.4191 | 0.1568 |
| 6 | 1.9760 | -0.8522 | -0.2702 | -0.0847 | -0.0234 | -0.0014 | 0.0107 | 0.0033 | 0.1829 | 0.0028 | -0.0167 | 0.0164 |
| 6 | -4.6306 | 0.9460 | 0.0330 | -0.3119 | -0.0761 | -0.0491 | -0.2957 | -0.0911 | -0.2833 | -0.2218 | -0.0299 | -0.0912 |
| 1 | -5.6766 | 1.2280 | 0.0755 | 0.1226 | 0.1577 | 0.0374 | 0.1075 | 0.0980 | 0.1551 | 0.2128 | 0.0339 | 0.0771 |
| 6 | 0.9301 | -1.7848 | -0.2578 | 0.2419 | -0.1401 | 0.0326 | 0.3285 | 0.1030 | 0.0992 | 0.1808 | 0.4625 | 0.1445 |
| 6 | 1.3335 | -3.1265 | -0.4677 | 0.0118 | -0.0660 | -0.0429 | -0.2842 | -0.0354 | -0.2769 | -0.1996 | -0.0602 | -0.0330 |
| 7 | -0.3983 | -1.6939 | -0.1206 | -0.3856 | 0.1903 | -0.1624 | -0.8929 | -0.4705 | -0.4712 | -0.6870 | -1.2909 | -0.4666 |
| 6 | 0.2021 | -3.9095 | -0.4556 | -0.0835 | -0.0744 | 0.0179 | 0.1501 | 0.0132 | 0.1650 | 0.0462 | -0.0043 | 0.0465 |
| 6 | -0.8848 | -2.9742 | -0.2382 | 0.2798 | -0.1502 | 0.0384 | 0.3274 | 0.0993 | 0.2609 | 0.1328 | 0.3884 | 0.1502 |
| 6 | -4.3657 | -0.4289 | 0.0213 | 0.2361 | -0.1642 | 0.0383 | 0.3414 | 0.1012 | 0.1122 | 0.1545 | 0.4159 | 0.1533 |
| 7 | -3.1255 | -0.9830 | -0.0216 | -0.3623 | 0.1823 | -0.1632 | -0.8776 | -0.4510 | -0.5749 | -0.6814 | -1.2480 | -0.4627 |
| 6 | -3.2848 | -2.3439 | -0.0342 | 0.2306 | -0.1472 | 0.0402 | 0.3487 | 0.1024 | 0.3905 | 0.1576 | 0.4082 | 0.1549 |
| 6 | -2.2514 | -3.2661 | -0.1722 | -0.3226 | -0.0678 | -0.0406 | -0.2655 | -0.0821 | -0.4273 | -0.2011 | -0.0241 | -0.0832 |
| 1 | -2.5387 | -4.3071 | -0.2619 | 0.1768 | 0.1624 | 0.0376 | 0.1111 | 0.0987 | 0.1758 | 0.2238 | 0.0516 | 0.0742 |
| 6 | -4.7063 | -2.6619 | 0.0330 | 0.0861 | -0.0810 | -0.0181 | -0.0344 | -0.0176 | -0.1530 | -0.0837 | -0.0254 | 0.0047 |
| 6 | -5.3742 | -1.4673 | 0.0470 | -0.0604 | -0.1017 | -0.0077 | 0.0493 | -0.0128 | 0.2105 | -0.0075 | -0.0281 | 0.0211 |
| 6 | -5.3963 | 3.9397 | 0.0150 | -0.1640 | -0.1567 | -0.0332 | -0.0472 | -0.0899 | -0.0791 | -0.2041 | -0.0159 | -0.0730 |
| 1 | -6.1450 | 3.3392 | -0.4986 | 0.1072 | 0.1471 | 0.0386 | 0.0918 | 0.0955 | 0.1283 | 0.2002 | 0.0225 | 0.0794 |
| 6 | -5.7906 | 5.0739 | 0.5955 | -0.2683 | -0.1883 | -0.0750 | -0.2694 | -0.1769 | -0.3743 | -0.3594 | -0.0673 | -0.1841 |
| 1 | -5.1110 | 5.7026 | 1.1611 | 0.1294 | 0.1239 | 0.0389 | 0.1172 | 0.0929 | 0.1728 | 0.1901 | 0.0340 | 0.0854 |
| 1 | -6.8244 | 5.3989 | 0.5414 | 0.1173 | 0.1221 | 0.0388 | 0.1111 | 0.0912 | 0.1508 | 0.1977 | 0.0359 | 0.0879 |
| 6 | -2.6191 | 5.5596 | -0.1123 | -0.4395 | -0.2550 | -0.0805 | -0.4102 | -0.2236 | -0.3885 | -0.6287 | 0.0178 | -0.2484 |
| 1 | -1.7554 | 5.8031 | -0.7376 | 0.1186 | 0.1271 | 0.0355 | 0.1155 | 0.0879 | 0.0973 | 0.2140 | 0.0088 | 0.0853 |
| 1 | -3.4930 | 6.0653 | -0.5308 | 0.1501 | 0.1351 | 0.0359 | 0.1217 | 0.0892 | 0.1184 | 0.2282 | 0.0290 | 0.0816 |
| 1 | -2.4354 | 5.9902 | 0.8794 | 0.1396 | 0.1314 | 0.0382 | 0.1205 | 0.0896 | 0.1137 | 0.2186 | 0.0180 | 0.0873 |
| 6 | -6.8493 | -1.2334 | 0.1140 | -0.3868 | -0.2524 | -0.0794 | -0.4024 | -0.2222 | -0.4115 | -0.6248 | 0.0178 | -0.2481 |
| 1 | -7.1312 | -0.7184 | 1.0393 | 0.1345 | 0.1329 | 0.0396 | 0.1218 | 0.0912 | 0.1227 | 0.2209 | 0.0216 | 0.0875 |
| 1 | -7.1967 | -0.6144 | -0.7204 | 0.1292 | 0.1300 | 0.0370 | 0.1173 | 0.0887 | 0.1045 | 0.2167 | 0.0151 | 0.0857 |
| 1 | -7.4031 | -2.1742 | 0.0849 | 0.1165 | 0.1287 | 0.0375 | 0.1171 | 0.0903 | 0.1263 | 0.2186 | 0.0165 | 0.0874 |
| 6 | 2.0192 | 2.7810 | -0.1482 | 0.0434 | -0.0891 | 0.0003 | 0.0770 | -0.0048 | 0.0696 | 0.0124 | -0.0259 | 0.0279 |
| 6 | 2.7330 | 1.6103 | -0.1577 | -0.0373 | -0.0803 | -0.0203 | -0.0593 | -0.0188 | 0.0319 | -0.1073 | -0.0228 | 0.0006 |
| 6 | 2.5391 | 4.1803 | -0.0850 | -0.4321 | -0.2528 | -0.0811 | -0.4134 | -0.2241 | -0.3214 | -0.6310 | 0.0160 | -0.2498 |
| 1 | 2.4718 | 4.6807 | -1.0583 | 0.1379 | 0.1319 | 0.0378 | 0.1207 | 0.0892 | 0.0963 | 0.2191 | 0.0132 | 0.0853 |
| 1 | 1.9730 | 4.7845 | 0.6301 | 0.1262 | 0.1298 | 0.0381 | 0.1203 | 0.0904 | 0.0937 | 0.2179 | 0.0139 | 0.0874 |
| 1 | 3.5877 | 4.1930 | 0.2202 | 0.1501 | 0.1344 | 0.0348 | 0.1227 | 0.0886 | 0.1069 | 0.2280 | 0.0308 | 0.0806 |
| 6 | 4.1709 | 1.4696 | 0.0288 | -0.2488 | -0.0597 | 0.0000 | 0.0390 | -0.0519 | 0.0883 | -0.1065 | -0.0112 | -0.0476 |
| 1 | 4.4905 | 0.7870 | 0.8095 | 0.1657 | 0.1731 | 0.0406 | 0.1047 | 0.1122 | 0.0861 | 0.2336 | 0.1253 | 0.0522 |
| 6 | 5.1425 | 2.1379 | -0.5988 | -0.2199 | -0.1558 | -0.0557 | -0.3841 | -0.1071 | -0.5459 | -0.3367 | -0.0502 | -0.1091 |
| 1 | 4.9276 | 2.8198 | -1.4183 | 0.1180 | 0.1403 | 0.0395 | 0.1192 | 0.0987 | 0.1811 | 0.1988 | 0.0144 | 0.0764 |
| 6 | 6.5513 | 1.9241 | -0.1740 | 0.3780 | -0.5008 | 0.1965 | 0.8490 | 0.2489 | 0.8320 | 0.7298 | 1.5573 | 0.4237 |

| | | | | | | | | | | | | |
|----|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| 8 | 7.4966 | 2.4684 | -0.9738 | -0.3443 | 0.1065 | -0.1726 | -0.6465 | -0.3667 | -0.5935 | -0.6441 | -1.0835 | -0.3645 |
| 1 | 7.0883 | 2.8698 | -1.7551 | 0.3085 | 0.1872 | 0.1713 | 0.4325 | 0.3441 | 0.4064 | 0.4725 | 0.5702 | 0.2597 |
| 8 | 6.8759 | 1.3246 | 0.8190 | -0.3115 | 0.1178 | -0.2598 | -0.5542 | -0.3083 | -0.5091 | -0.5605 | -1.1600 | -0.3885 |
| 6 | 2.7794 | -3.1487 | -0.6633 | 0.0699 | -0.2451 | 0.1521 | 0.6017 | 0.1861 | 0.7159 | 0.5729 | 1.0567 | 0.2911 |
| 8 | 3.5241 | -4.0803 | -0.8516 | -0.2631 | 0.1462 | -0.2473 | -0.4684 | -0.2915 | -0.4984 | -0.5030 | -1.1391 | -0.3743 |
| 6 | 0.0962 | -5.3872 | -0.6392 | -0.4210 | -0.2475 | -0.0764 | -0.4240 | -0.2186 | -0.3542 | -0.6311 | 0.0201 | -0.2455 |
| 1 | -0.5409 | -5.6408 | -1.4933 | 0.1298 | 0.1328 | 0.0409 | 0.1254 | 0.0925 | 0.1055 | 0.2209 | 0.0235 | 0.0896 |
| 1 | 1.0855 | -5.8159 | -0.8099 | 0.1568 | 0.1398 | 0.0462 | 0.1443 | 0.0998 | 0.1234 | 0.2385 | 0.0472 | 0.0851 |
| 1 | -0.3375 | -5.8698 | 0.2437 | 0.1282 | 0.1329 | 0.0408 | 0.1253 | 0.0924 | 0.1078 | 0.2207 | 0.0201 | 0.0883 |
| 12 | -1.3505 | 0.0757 | -0.0590 | 0.6548 | 0.3051 | 0.4649 | 1.7724 | 1.0136 | 1.0832 | 1.7609 | 1.7175 | 0.7045 |
| 6 | -5.3125 | -3.9941 | 0.0752 | -0.1889 | -0.1553 | -0.0312 | -0.0452 | -0.0880 | -0.0514 | -0.2011 | -0.0182 | -0.0699 |
| 1 | -6.2381 | -4.1097 | -0.4865 | 0.1137 | 0.1479 | 0.0404 | 0.0960 | 0.0970 | 0.1188 | 0.2016 | 0.0277 | 0.0824 |
| 6 | -4.8541 | -5.0444 | 0.7570 | -0.2930 | -0.1925 | -0.0762 | -0.2762 | -0.1781 | -0.4095 | -0.3648 | -0.0695 | -0.1846 |
| 1 | -3.9662 | -4.9868 | 1.3784 | 0.1358 | 0.1238 | 0.0378 | 0.1131 | 0.0917 | 0.1842 | 0.1922 | 0.0335 | 0.0823 |
| 1 | -5.3746 | -5.9962 | 0.7342 | 0.1181 | 0.1221 | 0.0390 | 0.1124 | 0.0914 | 0.1595 | 0.1983 | 0.0362 | 0.0883 |
| 6 | 3.2481 | -1.6417 | -0.5899 | 0.0574 | -0.1025 | -0.0294 | -0.4975 | -0.0711 | -0.7112 | -0.4142 | 0.0148 | -0.0739 |
| 1 | 3.6360 | -1.3818 | -1.5802 | 0.0993 | 0.1817 | 0.0514 | 0.1496 | 0.1171 | 0.2186 | 0.2544 | 0.0694 | 0.0802 |
| 6 | 4.4502 | -1.5855 | 0.3294 | 0.2346 | -0.4884 | 0.1995 | 0.8068 | 0.2554 | 0.8474 | 0.7763 | 1.5843 | 0.4569 |
| 8 | 5.5838 | -1.6929 | -0.0599 | -0.2832 | 0.1388 | -0.2524 | -0.5403 | -0.3044 | -0.5295 | -0.5584 | -1.1755 | -0.3507 |
| 8 | 4.1073 | -1.4551 | 1.6201 | -0.2771 | 0.2464 | -0.1196 | -0.3481 | -0.2084 | -0.3594 | -0.4888 | -1.0792 | -0.2495 |
| 6 | 5.2183 | -1.4321 | 2.5308 | -0.2080 | -0.3019 | 0.0039 | -0.1190 | -0.1176 | -0.0676 | -0.2680 | 0.4389 | -0.1062 |
| 1 | 4.7817 | -1.2847 | 3.5176 | 0.1192 | 0.1099 | 0.0433 | 0.1007 | 0.1038 | 0.0889 | 0.1854 | 0.0403 | 0.0965 |
| 1 | 5.7585 | -2.3796 | 2.4856 | 0.1317 | 0.1146 | 0.0442 | 0.1061 | 0.1060 | 0.0956 | 0.1907 | 0.0539 | 0.0890 |
| 1 | 5.8981 | -0.6170 | 2.2741 | 0.1698 | 0.1189 | 0.0417 | 0.1210 | 0.1068 | 0.0952 | 0.2134 | 0.0468 | 0.0860 |

Dipole moment (in D) 10.42 (DEN) 8.25 5.80 8.41 11.14 10.22 10.48 12.97 19.89 10.21

Table S2. Quadrupole moments for set on non-polar, neutral molecules:

| | Population analysis schemes | | | | | | | | | |
|---|-----------------------------|---------|---------|---------|---------------------|---------|---------|---------|---------|---------|
| | Density | Mull | Lowdin | Hirsh. | Hirsh. Iterative | CM5 | ESP | NPA | AIM | ACP |
| Ethene (C2H4) | | | | | | | | | | |
| Q _{xx} | -2.206 | -2.084 | -2.188 | -0.708 | -2.023 | -1.68 | -2.963 | -3.492 | -0.585 | -1.615 |
| Q _{yy} | 1.081 | 0.667 | 0.7 | 0.227 | 0.648 | 0.538 | 0.949 | 1.118 | 0.187 | 0.517 |
| Q _{zz} | 1.125 | 1.417 | 1.487 | 0.481 | 1.375 | 1.142 | 2.014 | 2.374 | 0.398 | 1.098 |
| Cyclopropane (C3H6) | | | | | | | | | | |
| Q _{zz} | 1.551 | 0.417 | 0.5 | 0.145 | 0.433 | 0.366 | 0.538 | 0.834 | 0.091 | 0.351 |
| Ethyne (C2H2) | | | | | | | | | | |
| Q _{zz} | 4.47 | 4.386 | 2.884 | 2.131 | 4.704 | 3.371 | 6.463 | 5.291 | 3.872 | 3.234 |
| Carbon dioxide (CO2) | | | | | | | | | | |
| Q _{zz} | -3.002 | -2.411 | 2.672 | -2.145 | -6.252 | -2.68 | -4.658 | -6.382 | -14.723 | -3.897 |
| boron trihydride (BH3) | | | | | | | | | | |
| Q _{zz} | 1.487 | -0.105 | -0.325 | 0.574 | 1.57 | -0.456 | 2.055 | 1.078 | 6.395 | 0.649 |
| Boron trifluoride (BF3) | | | | | | | | | | |
| Q _{zz} | 2.687 | 2.742 | -4.427 | 1.719 | 5.424 | 1.038 | 4.02 | 5.979 | 10.271 | 3.174 |
| Boron trichloride (BCl3) | | | | | | | | | | |
| Q _{zz} | 0.648 | 2.027 | -13.074 | 1.268 | 4.035 | -0.356 | 1.634 | 1.957 | 14.725 | 3.229 |
| trans- SC12F4 | | | | | | | | | | |
| Q _{zz} | 3.199 | 0.302 | 5.89 | 0.523 | 0.348 | 1.457 | 3.619 | 4.904 | 9.758 | 0.241 |
| trans- SF2Cl4 | | | | | | | | | | |
| Q _{zz} | -3.131 | -0.761 | -5.475 | -0.383 | -0.276 | -1.219 | -3.576 | -6.079 | -9.257 | -0.322 |
| Benzene (C6H6) | | | | | | | | | | |
| Q _{zz} | -5.149 | -6.566 | -8.526 | -2.418 | -5.569 | -5.793 | -7.446 | -12.495 | -1.733 | -5.071 |
| Naphthalene (C10H8) | | | | | | | | | | |
| Q _{xx} | -7.929 | -9.032 | -16.039 | -4.11 | -8.732 | -10.008 | -10.676 | -22.262 | -3.158 | -8.286 |
| Q _{yy} | 4.074 | 5.791 | 8.432 | 2.145 | 4.594 | 5.234 | 5.324 | 12.16 | 2.014 | 4.425 |
| Q _{zz} | 3.856 | 3.241 | 7.606 | 1.964 | 4.137 | 4.774 | 5.352 | 10.102 | 1.144 | 3.861 |
| Anthracene (C14H10) | | | | | | | | | | |
| Q _{xx} | -10.736 | -10.736 | -23.614 | -5.843 | -12.04 | -14.273 | -14.517 | -32.011 | -4.729 | -11.55 |
| Q _{yy} | 5.574 | 7.732 | 12.651 | 3.152 | 6.626 | 7.64 | 7.032 | 18.239 | 3.36 | 6.397 |
| Q _{zz} | 5.162 | 3.004 | 10.964 | 2.692 | 5.414 | 6.633 | 7.485 | 13.772 | 1.369 | 5.153 |
| Pyrene (C16H10) | | | | | | | | | | |
| Q _{xx} | -11.806 | -11.908 | -28.239 | -6.697 | -12.82 | -16.51 | -16.206 | -37.576 | -5.374 | -13.023 |
| Q _{yy} | 5.868 | 2.404 | 14.036 | 3.534 | 6.524 | 8.294 | 8.075 | 18.06 | 2.438 | 6.523 |
| Q _{zz} | 5.938 | 9.504 | 14.203 | 3.163 | 6.296 | 8.216 | 8.131 | 19.516 | 2.936 | 6.5 |
| Coronene (C24H12) | | | | | | | | | | |
| Q _{zz} | -16.784 | -14.198 | -45.152 | -10.277 | -17.908 | -25.372 | -24.724 | -58.436 | -8.517 | -19.37 |
| Standard deviation for set of 14 molecule | | | | | | | | | | |
| | ref | 2.421 | 13.131 | 3.898 | 2.369 | 3.74 | 3.614 | 18.392 | 8.561 | 2.01 |