**Electronic Supplementary Information**

# Electronic structures and optical spectra of all-boron fullerene $B_{40}$

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Figure S4. Computed optical spectra of quasi-planar isomer of $B_{40}$ fullerene: (a) IR, and (b) Raman.

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## I. Computational details

**Geometry optimizations:** In the present work, full geometry optimization and electronic structure computation of the ground state ($S_0$) of the gas-phase $B_{40}$ fullerene are performed based on the PBE0 and BHandHLYP functionals with 6-31G* basis set. To obtain relatively accurate electronic structures and profiles of the selected molecular orbitals and vertical excitation energies, the ground-state geometry is also re-optimized using a larger basis set 6-311G*. Frequency calculations at the same level were performed to confirm each stationary point to be a true local minimum. We note that the relative energies and frequency calculations at the PBE0/6-311G* level should be reliable for boron clusters, because this level has been tested in the previous studies.[1,2,3] Based on the optimized ground-state structure, the geometry of the first singlet excited state ($S_1$) of $B_{40}$ fullerene is computed using the TD-PBE0 and TD-BHandHLYP methods combined with 6-31G* and 6-311* basis sets. However, only the TD-PBE0/6-31* level gives rise to a convergent geometry of $S_1$ state. Therefore, the adiabatic energy, Huang-Rhys factor, and highly resolved electronic spectra are computed using the optimized $S_0$ and $S_1$ geometries at (TD)PBE0/6-31G* level. Note also that both the ground state and the first singlet excited state of $B_{40}$ fullerene are optimized with the $D_{2d}$ point group symmetry. All computations above are carried out using the Gaussian09 software package. [4]

**Simulation of highly resolved electronic spectra:** With the harmonic oscillator approximation, the absorption or emission coefficient for the electronic transition $b \rightarrow a$ in the Condon approximation can be expressed as:[5]

$$\alpha(\omega) = \frac{2\pi\omega}{3\hbar c}\left|\vec{\mu}_{ab}\right|^2 \int_{-\infty}^{\infty} dt \exp\left[it(\omega_{ab} - \omega) - \gamma_{ab}|t|\right] \prod_i G_i(t) \qquad (1),$$

where $\hbar$ is Planck's constant, $c$ is the speed of light, $\vec{\mu}_{ab}$ denotes the electronic transition dipole moment and $\omega_{ab}$ is the energy gap between the excited vibrational state and ground vibrational state. The time correlation function $G_i(t)$ is given by

$$G_i(t) = \exp\left[-S_i\left\{(2\bar{n}_i+1) - (\bar{n}_i+1)e^{it\omega_i} - \bar{n}_i e^{-it\omega_i}\right\}\right] \qquad (2)$$

Huang-Rhys factor $S_i = \omega_i d_i^2 / 2\hbar$. To obtain more reasonable electronic spectra, the transition dipole moment is expanded in a Taylor series in terms of the nuclear coordinate,

$$\vec{\mu}_{ab} = \vec{\mu}_{ab}(\vec{Q}) = \vec{\mu}_{ab}(0) + \sum_i \left(\frac{\partial \vec{\mu}_{ab}}{\partial Q_i}\right)_0 Q_i + \cdots \qquad (3)$$

The zero-order term of this expansion is the so-called FC spectrum for strongly allowed transitions, while the first-order term reflects the Herzberg-Teller effect[6] for weakly allowed or forbidden transition. Here, the vibrational highly-resolved absorption and emission spectra of $B_{40}$ fullerene including the Herzberg-Teller effect are obtained using the method presented in our previous reports.[7,8]

**Supplemental References**


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## II. Tables

**Table S1.** Predicted normal mode frequencies ($cm^{-1}$) of the ground state ($S_0$) of the boron fullerene $B_{40}$ based on PBE0 and BHandLYP functional with 6-311G* and 6-31G* basis sets. [a]

| *Sym* | frequency | | *Sym* | frequency | | *Sym* | frequency | |
|---|---|---|---|---|---|---|---|---|
| | PBE0 | BHandLYP | | PBE0 | BHandLYP | | PBE0 | BHandLYP |
| $a_1$ | 171 (171) | 176(176) | $b_1$ | 244 (244) | 256(256) | $e$ | 199 (198) | 203(201) |
| | 244 (241) | 250(248) | | 278 (278) | 292(293) | | 219 (219) | 230(230) |
| | 356 (354) | 388(389) | | 351 (347) | 360(356) | | 328 (326) | 348(347) |
| | 427 (429) | 434(435) | | 369 (369) | 387(384) | | 359 (358) | 363(366) |
| | 437 (437) | 442(443) | | 448 (454) | 446(452) | | 382 (382) | 392(392) |
| | 464 (466) | 481(482) | | 483 (486) | 494(496) | | 390 (393) | 395(397) |
| | 518 (524) | 532(539) | | 581 (585) | 583(588) | | 401 (400) | 423(423) |
| | 648 (654) | 648(655) | | 623 (632) | 624(634) | | 412 (413) | 427(427) |
| | 662 (669) | 676(683) | | 790 (792) | 791(794) | | 434 (436) | 446(448) |
| | 695 (699) | 698(704) | | 859 (864) | 862(869) | | 475 (482) | 480(486) |
| | 755 (762) | 749(758) | | 925 (930) | 939(945) | | 491 (494) | 505(508) |
| | 882 (888) | 880(887) | | 1188 (1193) | 1203(1210) | | 504 (505) | 514(517) |
| | 1028 (1031) | 1041(1045) | | 1256 (1261) | 1269(1278) | | 584 (590) | 595(603) |
| | 1149 (1154) | 1158(1166) | | 1299 (1305) | 1324(1334) | | 633 (636) | 633(638) |
| | 1195 (1200) | 1208(1216) | $b_2$ | 189 (188) | 196(196) | | 659 (664) | 653(660) |
| | 1327 (1333) | 1354(1363) | | 277 (273) | 290(286) | | 691 (696) | 681(689) |
| $a_2$ | 244 (243) | 257(255) | | 342 (340) | 360(359) | | 710 (715) | 727(732) |
| | 306 (305) | 308(308) | | 428 (432) | 440(444) | | 766 (773) | 767(774) |
| | 356 (359) | 353(356) | | 478 (480) | 491(494) | | 822 (826) | 826(832) |
| | 412 (412) | 420(419) | | 512 (514) | 525(527) | | 843 (849) | 849(856) |
| | 470 (473) | 470(476) | | 565 (567) | 571(575) | | 861 (867) | 866(873) |
| | 471 (477) | 495(496) | | 617 (625) | 620(630) | | 999 (1002) | 1007(1013) |
| | 614 (620) | 606(614) | | 709 (714) | 701(709) | | 1043 (1048) | 1050(1057) |

| | | | | | |
|---|---|---|---|---|---|
| 625 (624) | 637(637) | 713 (719) | 714(722) | 1154 (1159) | 1165(1173) |
| 772 (779) | 782(789) | 795 (802) | 797(805) | 1209 (1215) | 1224(1232) |
| 916 (919) | 919(923) | 817 (820) | 828(833) | 1252 (1259) | 1261(1271) |
| 1062 (1067) | 1075(1083) | 1103 (1108) | 1102(1109) | 1275 (1281) | 1294(1303) |
| 1247 (1253) | 1252(1261) | 1200 (1205) | 1215(1223) | 1314 (1321) | 1341(1351) |
| 1280 (1285) | 1292(1300) | 1264 (1271) | 1275(1283) | | |

[a] Data in parenthesis are calculated by 6-31G* basis set.

**Table S2.** Predicted infrared and Raman absorption peaks ($cm^{-1}$) of $B_{40}$ and the corresponding intensities and assignments (6-31G*). Note that the intensities less than 2.0 are not given.

| 6-31G* | | | | | | 6-311G* | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $V_{IR}$ | $I_{IR}$ | $V_{Raman}$ | $I_{Raman}$ | Assignment | | $V_{IR}$ | $I_{IR}$ | $V_{Raman}$ | $I_{Raman}$ | Assignment |
| | | 171 | 44.7 | $a_1$ | | | | 171 | 44.9 | $a_1$ |
| | | 188 | 47.3 | $b_2$ | | | | 189 | 48.1 | $b_2$ |
| | | 219 | 20.5 | $e$ | | | | 219 | 22.8 | $e$ |
| | | 244 | 23.5 | $b_1$ | | | | 244 | 23.7 | $b_1$ |
| 273 | 7.0 | | | $b_2$ | | 277 | 2.4 | | | $b_2$ |
| | | 278 | 5.2 | $b_1$ | | | | 278 | 8.4 | $b_1$ |
| 326 | 5.1 | 326 | 2.2 | $e$ | | | | 342 | 909 | $b_2$ |
| | | 340 | 12.5 | $b_2$ | | 359 | 4.7 | | | $e$ |
| | | 354 | 6.0 | $a_1$ | | | . | 369 | 11.7 | $b_1$ |
| | . | 369 | 11.5 | $b_1$ | | 382 | 19.6 | 382 | 6.2 | $e$ |
| 382 | 27.7 | 382 | 3.4 | $e$ | | 390 | 7.3 | | | $e$ |
| 393 | 7.6 | 393 | 1.9 | $e$ | | | | 412 | 11.0 | a2 |
| | | 413 | 12.4 | $e$ | | | | 427 | 82.3 | $a_1$ |
| | | 429 | 69.5 | $a_1$ | | 428 | 6.7 | 428 | 9.9 | $b_2$ |
| 432 | 5.6 | 432 | 15.0 | $b_2$ | | | | 437 | 31.2 | $a_1$ |
| | | 437 | 9.7 | $a_1$ | | | | 464 | 41.7 | $a_1$ |
| | | 466 | 28.7 | $a_1$ | | | | 483 | 16.3 | $b_1$ |
| | | 486 | 21.2 | $b_1$ | | | | 518 | 40.2 | $a_1$ |
| | | 494 | 5.6 | $e$ | | 565 | 5.8 | | | $b_2$ |
| | | 514 | 2.4 | $b_2$ | | | | 584 | 8.6 | $e$ |
| | | 524 | 51.2 | $a_1$ | | 617 | 13.1 | | | $b_2$ |
| 567 | 8.1 | 567 | 2.6 | $b_2$ | | | | 648 | 80.0 | $a_1$ |
| 590 | 3.5 | 590 | 13.1 | $e$ | | | | 662 | 63.5 | $a_1$ |
| 625 | 19.5 | | | $b_2$ | | | | 695 | 24.9 | $a_1$ |
| | | 654 | 71.2 | $a_1$ | | 709 | 6.7 | 709 | 14.3 | $b_2$ |
| | | 669 | 88.4 | $a_1$ | | 713 | 13.7 | 713 | 15.3 | $b_2$ |
| | | 699 | 44.1 | $a_1$ | | | | 755 | 10.4 | $a_1$ |
| 714 | 5.0 | 714 | 11.7 | $b_2$ | | 795 | 19.4 | 795 | 11.2 | $b_2$ |
| 719 | 9.6 | 719 | 21.6 | $b_2$ | | 817 | 10.6 | | | $b_2$ |
| | | 762 | 14.1 | $a_1$ | | 822 | 11.2 | 822 | 10.1 | $e$ |
| 773 | 3.9 | | | $e$ | | 843 | 5.4 | | | $e$ |
| 802 | 23.0 | 802 | 12.5 | $b_2$ | | | | 858 | 4.8 | $b_1$ |
| 820 | 7.7 | | | $b_2$ | | | | 882 | 11.7 | $a_1$ |
| 826 | 10.1 | 826 | 8.4 | $e$ | | | | 925 | 7.2 | $b_1$ |
| 849 | 3.5 | 849 | 2.1 | $e$ | | 999 | 4.4 | | | $e$ |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | 864 | 3.3 | $b_1$ | | 1043 | 10.2 | | | $e$ |
| | | 888 | 5.5 | $a_1$ | | 1103 | 15.8 | | | $b_2$ |
| | | 930 | 6.1 | $b_1$ | | | | 1149 | 36.9 | $a_1$ |
| 1002 | 4.7 | | | $e$ | | 1154 | 11.9 | | | $e$ |
| | | 1031 | 4.4 | $a_1$ | | | | 1195 | 26.0 | $a_1$ |
| 1048 | 10.1 | | | $e$ | | 1200 | 10.0 | 1200 | 8.9 | $b_2$ |
| 1108 | 14.6 | | | $b_2$ | | 1209 | 7.0 | | | $e$ |
| | | 1154 | 32.7 | $a_1$ | | | | | | |
| 1159 | 12.0 | | | $e$ | | | | | | |
| | | 1200 | 19.5 | $a_1$ | | 1252 | 38.7 | | | $e$ |
| 1205 | 9.1 | 1205 | 6.4 | $b_2$ | | | | 1256 | 16.5 | $b_1$ |
| 1215 | 5.4 | | | $e$ | | 1264 | 99.5 | 1264 | 32.1 | $b_2$ |
| 1259 | 35.9 | | | $e$ | | 1275 | 159.0 | 1275 | 10.9 | $e$ |
| | | 1261 | 12.1 | $b_1$ | | | | 1299 | 29.4 | $b_1$ |
| 1271 | 92.1 | 1271 | 29.0 | $b_2$ | | 1314 | 12.4 | 1314 | 16.6 | $e$ |
| 1281 | 152.8 | 1281 | 8.3 | $e$ | | | | 1327 | 164.8 | $a_1$ |
| | | 1305 | 22.8 | $b_1$ | | | | | | |
| 1321 | 9.7 | 1321 | 14.2 | $e$ | | | | | | |
| | | 1333 | 144.8 | $a_1$ | | | | | | |

**Table S3.** Normal modes and their incorporation with the electronic states in the absorption and emission spectra of $B_{40}$, computed at the PBE0/6-31G* level.

| Absorption | | | Emission | | |
|---|---|---|---|---|---|
| $n^a$ | $\omega^b$ | $i^c$ | $n$ | $\omega$ | $i$ |
| 0-0 | | 100.00 | 0-0 | | 100.00 |
| $2^1$ | 172.043 | 17.79 | $1^1$ | 170.697 | 18.95 |
| $1^2$ | 197.825 | 16.02 | $10^1$ | 273.138 | 2.52 |
| $12^1$ | 261.231 | 23.99 | $13^1$ | 325.625 | 2.23 |
| $17^1$ | 304.817 | 2.17 | $1^2$ | 341.394 | 1.71 |
| $22^1$ | 338.943 | 14.24 | $17^1$ | 354.458 | 17.95 |
| $25^1$ | 368.038 | 1.07 | $22^1$ | 381.699 | 9.41 |
| $1^2 2^1$ | 369.869 | 2.85 | $24^1$ | 392.763 | 2.20 |
| $27^1$ | 392.763 | 32.78 | $31^1$ | 428.696 | 7.89 |
| $31^1$ | 397.745 | 8.00 | $35^1$ | 437.142 | 6.07 |
| $32^1$ | 407.526 | 3.58 | $10^1 1^1$ | 443.835 | 0.48 |
| $35^1$ | 431.688 | 5.78 | $37^1$ | 465.890 | 2.53 |
| $12^1 2^1$ | 433.275 | 4.27 | $41^1$ | 481.527 | 0.70 |
| $37^1$ | 442.540 | 9.84 | $49^1$ | 523.981 | 22.91 |
| $38^1$ | 454.949 | 5.91 | $17^1 1^1$ | 525.155 | 3.10 |
| $41^1$ | 458.161 | 2.86 | $22^1 1^1$ | 552.396 | 1.78 |
| $12^1 1^2$ | 459.057 | 3.84 | $50^1$ | 566.795 | 1.54 |
| $42^1$ | 475.926 | 2.02 | $52^1$ | 590.374 | 0.83 |
| $46^1$ | 499.814 | 7.88 | $31^1 1^1$ | 599.393 | 1.40 |
| $22^1 2^1$ | 510.986 | 2.81 | $56^1$ | 624.675 | 3.55 |
| $49^1$ | 517.591 | 25.62 | $60^1$ | 654.246 | 6.02 |
| $50^1$ | 563.221 | 3.35 | $63^1$ | 668.618 | 2.08 |
| $27^1 2^1$ | 564.806 | 5.83 | $49^1 1^1$ | 694.678 | 4.28 |
| $27^1 1^2$ | 590.588 | 5.25 | $17^2$ | 708.916 | 1.94 |

| | | | | | |
|---|---|---|---|---|---|
| $22^{1}12^{1}$ | 600.174 | 3.42 | $70^{1}$ | 719.101 | 1.85 |
| $37^{1}2^{1}$ | 614.583 | 1.96 | $22^{1}17^{1}$ | 736.157 | 1.69 |
| $58^{1}$ | 627.184 | 2.95 | $28^{1}20^{1}$ | 770.656 | 2.91 |
| $37^{1}1^{2}$ | 640.365 | 1.57 | $31^{1}17^{1}$ | 783.154 | 1.34 |
| $60^{1}$ | 656.163 | 36.73 | $76^{1}$ | 801.925 | 3.74 |
| $63^{1}$ | 659.566 | 11.77 | $28^{2}$ | 823.560 | 2.01 |
| $65^{1}$ | 662.389 | 1.53 | $37^{1}18^{1}$ | 824.101 | 0.01 |
| $46^{1}2^{1}$ | 671.858 | 1.40 | $49^{1}17^{1}$ | 878.439 | 3.97 |
| $49^{1}2^{1}$ | 689.635 | 4.60 | $49^{1}22^{1}$ | 905.680 | 2.15 |
| $37^{1}12^{1}$ | 703.771 | 2.36 | $49^{1}31^{1}$ | 952.677 | 1.72 |
| $49^{1}1^{2}$ | 715.417 | 4.10 | $49^{1}35^{1}$ | 961.123 | 1.46 |
| $71^{1}$ | 731.036 | 2.64 | $60^{1}17^{1}$ | 1008.704 | 0.94 |
| $27^{1}22^{1}$ | 731.706 | 4.67 | $94^{1}$ | 1108.149 | 1.24 |
| $49^{1}12^{1}$ | 778.823 | 6.14 | $56^{1}49^{1}$ | 1148.656 | 0.81 |
| $60^{1}2^{1}$ | 828.206 | 6.53 | $96^{1}$ | 1159.349 | 1.10 |
| $37^{1}27^{1}$ | 835.303 | 3.22 | $60^{1}49^{1}$ | 1178.227 | 1.29 |
| $38^{1}27^{1}$ | 847.712 | 1.94 | $99^{1}$ | 1199.813 | 10.74 |
| $60^{1}1^{2}$ | 853.988 | 5.88 | $100^{1}$ | 1205.349 | 1.07 |
| $49^{1}22^{1}$ | 856.534 | 3.74 | $104^{1}$ | 1258.622 | 2.91 |
| $49^{1}27^{1}$ | 910.354 | 8.39 | $107^{1}$ | 1270.553 | 8.22 |
| $63^{1}12^{1}$ | 920.798 | 2.82 | $108^{1}$ | 1280.982 | 11.84 |
| $49^{1}37^{1}$ | 960.131 | 2.40 | $112^{1}$ | 1320.719 | 0.63 |
| $60^{1}22^{1}$ | 995.106 | 5.23 | $76^{1}49^{1}$ | 1325.906 | 0.85 |
| $63^{1}22^{1}$ | 998.509 | 1.90 | $114^{1}$ | 1333.313 | 4.48 |
| $49^{1}46^{1}$ | 1017.406 | 2.02 | $99^{1}1^{1}$ | 1370.510 | 2.16 |
| $49^{2}$ | 1035.182 | 3.10 | $107^{1}1^{1}$ | 1441.250 | 1.55 |
| $63^{1}27^{1}$ | 1052.329 | 3.85 | $108^{1}1^{1}$ | 1451.679 | 2.24 |
| $60^{1}35^{1}$ | 1087.850 | 2.12 | $114^{1}1^{1}$ | 1504.010 | 0.80 |
| $94^{1}$ | 1090.230 | 3.13 | $99^{1}17^{1}$ | 1554.271 | 2.00 |
| $60^{1}37^{1}$ | 1098.703 | 3.61 | $99^{1}22^{1}$ | 1581.512 | 1.01 |

| | | | | | |
|---|---|---|---|---|---|
| $97^1$ | 1109.746 | 4.59 | $107^1 17^1$ | 1625.011 | 1.47 |
| $60^1 38^1$ | 1111.112 | 2.17 | $109^1 17^1$ | 1635.440 | 2.11 |
| $99^1$ | 1148.334 | 17.08 | $110^1 28^1$ | 1696.934 | 1.49 |
| $60^1 49^1$ | 1173.754 | 9.40 | $99^1 49^1$ | 1723.794 | 2.54 |
| $63^1 49^1$ | 1177.158 | 3.15 | $107^1 49^1$ | 1794.534 | 1.87 |
| $102^1$ | 1180.846 | 13.56 | $108^1 49^1$ | 1804.963 | 2.69 |
| $103^1$ | 1189.546 | 4.11 | $114^1 49^1$ | 1857.294 | 0.97 |
| $108^1$ | 1243.965 | 1.43 | | | |
| $111^1$ | 1283.063 | 7.72 | | | |
| $63^1 60^1$ | 1315.729 | 4.32 | | | |
| $114^1$ | 1315.952 | 6.88 | | | |
| $99^1 2^1$ | 1320.378 | 3.04 | | | |
| $99^1 1^2$ | 1346.159 | 2.73 | | | |
| $102^1 2^1$ | 1352.890 | 2.24 | | | |
| $102^1 1^2$ | 1378.672 | 2.17 | | | |
| $102^1 12^1$ | 1442.078 | 3.25 | | | |
| $99^1 22^1$ | 1487.277 | 2.43 | | | |
| $102^1 22^1$ | 1519.789 | 1.83 | | | |
| $102^1 27^1$ | 1573.609 | 4.44 | | | |
| $99^1 37^1$ | 1590.874 | 1.68 | | | |
| $99^1 49^1$ | 1665.925 | 4.37 | | | |
| $102^1 49^1$ | 1698.437 | 3.34 | | | |
| $114^1 27^1$ | 1708.715 | 2.25 | | | |
| $111^1 49^1$ | 1800.654 | 1.97 | | | |
| $99^1 63^1$ | 1807.901 | 2.00 | | | |
| $102^1 60^1$ | 1837.009 | 4.97 | | | |

[a] Fundamental vibrations, assigned as $n^q$ (n is excited normal mode, *q* represents quantum number). [b] Frequencies ($cm^{-1}$) relative to the electronic origin band which is set as 0. [c] Relative peak intensity, the 0-0 origin band intensity is 100.

**Table S4.** Predicted normal mode frequencies ($cm^{-1}$) of the ground state ($S_0$) and the first excited state ($S_1$) [a] for $B_{40}$ fullerene (computed at the PBE0/6-31g* level).

| S0 | | | | | | S1 | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| mode | **freq** | *sym* | mode | **freq** | *sym* | mode | **freq** | sym | mode | **freq** | sym |
| 1 | **171** | $a_1$ | 58 | **636** | *e* | 1 | **99** | $a_2$ | 58 | **627** | $b_2$ |
| 2 | **188** | $b_2$ | 59 | **636** | *e* | 2 | **172** | $a_1$ | 59 | **642** | $b_1$ |
| 3 | **199** | *e* | 60 | **654** | $a_1$ | 3 | **175** | *e* | 60 | **656** | $b_2$ |
| 4 | **199** | *e* | 61 | **664** | *e* | 4 | **715** | *e* | 61 | **657** | *e* |
| 5 | **219** | *e* | 62 | **664** | *e* | 5 | **189** | $b_2$ | 62 | **657** | *e* |
| 6 | **219** | *e* | 63 | **669** | $a_1$ | 6 | **209** | $b_1$ | 63 | **660** | $a_1$ |
| 7 | **241** | $a_1$ | 64 | **696** | *e* | 7 | **210** | *e* | 64 | **662** | $a_1$ |
| 8 | **243** | $a_2$ | 65 | **696** | *e* | 8 | **210** | *e* | 65 | **662** | *e* |
| 9 | **244** | $b_1$ | 66 | **699** | $a_1$ | 9 | **247** | $a_1$ | 66 | **662** | *e* |
| 10 | **273** | $b_2$ | 67 | **714** | $b_2$ | 10 | **251** | $a_2$ | 67 | **683** | $a_1$ |
| 11 | **278** | $b_1$ | 68 | **715** | *e* | 11 | **254** | $b_1$ | 68 | **703** | $b_2$ |
| 12 | **305** | $a_2$ | 69 | **715** | *e* | 12 | **261** | $b_2$ | 69 | **709** | *e* |
| 13 | **326** | *e* | 70 | **719** | $b_2$ | 13 | **283** | *e* | 70 | **709** | *e* |
| 14 | **326** | *e* | 71 | **762** | $a_1$ | 14 | **283** | *e* | 71 | **731** | $b_2$ |
| 15 | **340** | $b_2$ | 72 | **773** | *e* | 15 | **291** | $b_2$ | 72 | **740** | $a_2$ |
| 16 | **347** | $b_1$ | 73 | **773** | *e* | 16 | **292** | $a_2$ | 73 | **757** | *e* |
| 17 | **354** | $a_1$ | 74 | **779** | $a_2$ | 17 | **305** | *e* | 74 | **757** | *e* |
| 18 | **358** | *e* | 75 | **792** | $b_1$ | 18 | **305** | *e* | 75 | **771** | $a_1$ |
| 19 | **358** | *e* | 76 | **802** | $b_2$ | 19 | **317** | $b_1$ | 76 | **773** | $b_1$ |
| 20 | **359** | $a_2$ | 77 | **820** | $b_2$ | 20 | **338** | *e* | 77 | **793** | $b_2$ |
| 21 | **369** | $b_1$ | 78 | **826** | *e* | 21 | **338** | *e* | 78 | **807** | *e* |
| 22 | **382** | *e* | 79 | **826** | *e* | 22 | **339** | $a_1$ | 79 | **807** | *e* |
| 23 | **382** | *e* | 80 | **849** | *e* | 23 | **347** | $b_1$ | 80 | **833** | *e* |
| 24 | **393** | *e* | 81 | **849** | *e* | 24 | **368** | *e* | 81 | **833** | *e* |
| 25 | **393** | *e* | 82 | **864** | $b_1$ | 25 | **368** | *e* | 82 | **840** | *e* |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 26 | **400** | *e* | 83 | **867** | *e* | 26 | **377** | $a_2$ | 83 | **840** | *e* |
| 27 | **400** | *e* | 84 | **867** | *e* | 27 | **393** | $b_2$ | 84 | **866** | $b_1$ |
| 28 | **412** | $a_2$ | 85 | **888** | $a_1$ | 28 | **395** | *e* | 85 | **879** | $a_1$ |
| 29 | **413** | *e* | 86 | **919** | $a_2$ | 29 | **395** | *e* | 86 | **897** | $a_2$ |
| 30 | **413** | *e* | 87 | **930** | $b_1$ | 30 | **398** | *e* | 87 | **921** | $b_1$ |
| 31 | **429** | $a_1$ | 88 | **1002** | *e* | 31 | **398** | *e* | 88 | **988** | *e* |
| 32 | **432** | $b_2$ | 89 | **1002** | *e* | 32 | **408** | *e* | 89 | **988** | *e* |
| 33 | **436** | *e* | 90 | **1031** | $a_1$ | 33 | **408** | *e* | 90 | **1014** | $a_2$ |
| 34 | **436** | *e* | 91 | **1048** | *e* | 34 | **415** | $b_1$ | 91 | **1016** | $a_1$ |
| 35 | **437** | $a_1$ | 92 | **1048** | *e* | 35 | **432** | $a_1$ | 92 | **1046** | *e* |
| 36 | **454** | $b_1$ | 93 | **1067** | $a_2$ | 36 | **442** | $a_2$ | 93 | **1046** | *e* |
| 37 | **466** | $a_1$ | 94 | **1108** | $b_2$ | 37 | **443** | $a_1$ | 94 | **1090** | *e* |
| 38 | **473** | $a_2$ | 95 | **1154** | $a_1$ | 38 | **455** | $a_1$ | 95 | **1090** | *e* |
| 39 | **477** | $a_2$ | 96 | **1159** | *e* | 39 | **458** | *e* | 96 | **1104** | $a_2$ |
| 40 | **480** | $b_2$ | 97 | **1159** | *e* | 40 | **458** | *e* | 97 | **1110** | $b_2$ |
| 41 | **482** | *e* | 98 | **1193** | $b_1$ | 41 | **458** | $b_2$ | 98 | **1139** | $a_1$ |
| 42 | **482** | *e* | 99 | **1200** | $a_1$ | 42 | **476** | *e* | 99 | **1148** | $b_2$ |
| 43 | **486** | $b_1$ | 100 | **1205** | $b_2$ | 43 | **476** | *e* | 100 | **1158** | *e* |
| 44 | **494** | *e* | 101 | **1215** | *e* | 44 | **486** | $b_1$ | 101 | **1158** | *e* |
| 45 | **494** | *e* | 102 | **1215** | *e* | 45 | **498** | $a_2$ | 102 | **1181** | $a_1$ |
| 46 | **505** | *e* | 103 | **1253** | $a_2$ | 46 | **500** | $b_2$ | 103 | **1190** | *e* |
| 47 | **505** | *e* | 104 | **1259** | *e* | 47 | **502** | *e* | 104 | **1190** | *e* |
| 48 | **514** | $b_2$ | 105 | **1259** | *e* | 48 | **502** | *e* | 105 | **1191** | $b_1$ |
| 49 | **524** | $a_1$ | 106 | **1261** | $b_1$ | 49 | **518** | $a_1$ | 106 | **1222** | $b_2$ |
| 50 | **567** | $b_2$ | 107 | **1271** | $b_2$ | 50 | **563** | $b_2$ | 107 | **1243** | $b_1$ |
| 51 | **585** | $b_1$ | 108 | **1281** | *e* | 51 | **578** | $b_1$ | 108 | **1244** | *e* |
| 52 | **590** | *e* | 109 | **1281** | *e* | 52 | **590** | *e* | 109 | **1244** | *e* |
| 53 | **590** | *e* | 110 | **1285** | $a_2$ | 53 | **590** | *e* | 110 | **1245** | $a_2$ |
| 54 | **620** | $a_2$ | 111 | **1305** | $b_1$ | 54 | **613** | $a_2$ | 111 | **1283** | *e* |
| 55 | **624** | $a_2$ | 112 | **1321** | *e* | 55 | **615** | *e* | 112 | **1283** | *e* |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 56 | **625** | $b_2$ | 113 | **1321** | $e$ | 56 | **615** | $e$ | 113 | **1296** | $b_1$ |
| 57 | **632** | $b_1$ | 114 | **1333** | $a_1$ | 57 | **617** | $a_2$ | 114 | **1316** | $a_1$ |

a. Both of the states $S_0$ and $S_1$ belong to $D_{2d}$ point group symmetry.

**Table S5.** Computed Huang-Rhys factors (*S*) of totally-symmetry normal modes ($a_1$) for absorption and emission spectra of $B_{40}$ at the PBE0/6-31g* level.

| Absorption | | | Emission | | |
|---|---|---|---|---|---|
| mode | frequency ($cm^{-1}$) | *S* | mode | frequency | *S* |
| 2 | 172 | 0.4118 | 1 | 171 | 0.4102 |
| 9 | 247 | 0.0022 | 7 | 241 | 0.0001 |
| 22 | 339 | 0.3235 | 17 | 354 | 0.4001 |
| 35 | 432 | 0.1251 | 31 | 429 | 0.1600 |
| 37 | 443 | 0.2213 | 35 | 437 | 0.1305 |
| 38 | 455 | 0.1306 | 37 | 466 | 0.0626 |
| 49 | 518 | 0.5401 | 49 | 524 | 0.5182 |
| 63 | 660 | 0.2417 | 60 | 654 | 0.1588 |
| 64 | 662 | 0.0027 | 63 | 669 | 0.0676 |
| 67 | 683 | 0.0000 | 66 | 699 | 0.0106 |
| 75 | 771 | 0.0000 | 71 | 762 | 0.0063 |
| 85 | 879 | 0.0019 | 85 | 888 | 0.0007 |
| 91 | 1016 | 0.0123 | 90 | 1031 | 0.0009 |
| 98 | 1139 | 0.0201 | 95 | 1154 | 0.0171 |
| 102 | 1181 | 0.2985 | 99 | 1200 | 0.3001 |
| 114 | 1316 | 0.1242 | 114 | 1333 | 0.1305 |

Table S6. Predicted normal mode frequencies ($cm^{-1}$) of ground state ($S_0$) and the infrared and Raman activities for the quasi-planar isomer of $B_{40}$ fullerene (at the PBE0/6-311G* level).

| Mode | Freq | Infrared | Raman Activity |
|---|---|---|---|
| 1 | 45.33 | 0.1610 | 33.8778 |
| 2 | 55.10 | 0.0297 | 16.9376 |
| 3 | 80.03 | 0.4359 | 18.2961 |
| 4 | 114.83 | 1.7551 | 8.2751 |
| 5 | 117.57 | 0.0103 | 0.0153 |
| 6 | 138.67 | 0.5791 | 2.8517 |
| 7 | 149.58 | 0.3851 | 0.6612 |
| 8 | 157.52 | 1.2937 | 22.5588 |
| 9 | 196.36 | 0.5322 | 0.3272 |
| 10 | 206.94 | 2.6741 | 14.5455 |
| 11 | 224.54 | 0.1662 | 18.5944 |
| 12 | 230.70 | 0.2293 | 11.6072 |
| 13 | 239.27 | 1.8819 | 8.3302 |
| 14 | 242.70 | 0.9247 | 13.2154 |
| 15 | 254.70 | 0.0263 | 13.1753 |
| 16 | 256.95 | 0.8497 | 50.0842 |
| 17 | 274.12 | 1.6131 | 1.0693 |
| 18 | 289.38 | 4.0123 | 27.0578 |
| 19 | 294.92 | 0.0523 | 4.8821 |
| 20 | 300.50 | 4.7480 | 10.3442 |
| 21 | 308.36 | 0.6832 | 1.2134 |
| 22 | 325.07 | 11.9989 | 45.7982 |
| 23 | 335.80 | 0.3652 | 94.5524 |
| 24 | 341.09 | 4.0747 | 6.3848 |
| 25 | 353.45 | 0.7995 | 2.7430 |
| 26 | 358.55 | 1.9001 | 104.4626 |
| 27 | 360.93 | 0.0100 | 1.9929 |
| 28 | 364.14 | 6.2650 | 11.1466 |
| 29 | 369.07 | 0.8006 | 1.5261 |
| 30 | 376.09 | 0.0298 | 3.4873 |
| 31 | 389.68 | 15.2098 | 16.0630 |
| 32 | 389.85 | 0.0500 | 0.7685 |
| 33 | 399.49 | 1.4195 | 10.7881 |
| 34 | 403.88 | 31.5299 | 0.7005 |
| 35 | 404.13 | 3.5671 | 3.3608 |
| 36 | 417.91 | 3.6048 | 27.1612 |
| 37 | 430.41 | 1.0098 | 0.0041 |
| 38 | 441.92 | 0.4941 | 14.1729 |
| 39 | 449.29 | 0.0281 | 0.2342 |
| 40 | 452.77 | 0.2461 | 3.5385 |
| 41 | 460.20 | 0.4483 | 0.6328 |
| 42 | 463.73 | 0.1887 | 1.4920 |
| 43 | 469.20 | 2.1075 | 1.4156 |
| 44 | 473.64 | 0.1938 | 1.4698 |
| 45 | 482.33 | 0.6594 | 2.6790 |
| 46 | 486.32 | 0.2938 | 0.1526 |
| 47 | 498.63 | 3.5598 | 4.2971 |
| 48 | 518.53 | 0.0007 | 9.6190 |
| 49 | 523.31 | 0.6206 | 7.7413 |

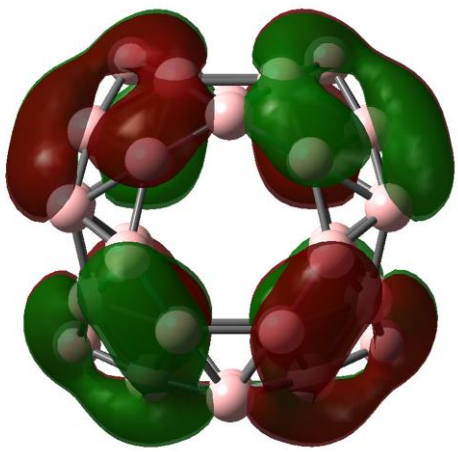
Continued Table S6

| Mode | Freq | Infrared | Raman Activity |
|---|---|---|---|
| 50 | 528.87 | 0.0154 | 3.5429 |
| 51 | 543.48 | 0.9693 | 9.8565 |
| 52 | 558.78 | 6.3007 | 0.6931 |
| 53 | 578.19 | 8.5971 | 34.5311 |
| 54 | 579.86 | 0.3774 | 4.5455 |
| 55 | 590.90 | 1.3787 | 0.7040 |
| 56 | 601.44 | 4.6609 | 9.5441 |
| 57 | 624.29 | 0.5285 | 2.6286 |
| 58 | 641.09 | 0.0080 | 1.2947 |
| 59 | 649.05 | 0.0178 | 39.5059 |
| 60 | 655.09 | 0.0396 | 21.0975 |
| 61 | 660.13 | 4.4277 | 13.5043 |
| 62 | 674.43 | 0.1009 | 38.9569 |
| 63 | 682.95 | 2.2575 | 6.7509 |
| 64 | 688.90 | 0.1008 | 2.6974 |
| 65 | 696.57 | 8.1939 | 2.6660 |
| 66 | 700.15 | 16.4606 | 59.6386 |
| 67 | 705.34 | 7.3834 | 50.2710 |
| 68 | 727.85 | 2.2611 | 12.2634 |
| 69 | 729.92 | 2.0207 | 24.9894 |
| 70 | 734.85 | 5.1010 | 11.0596 |
| 71 | 740.82 | 4.5895 | 9.8801 |
| 72 | 768.46 | 0.1169 | 263.8089 |
| 73 | 774.25 | 21.5890 | 21.4458 |
| 74 | 782.51 | 45.3856 | 6.5190 |
| 75 | 802.93 | 19.1296 | 73.9034 |
| 76 | 821.21 | 35.2320 | 0.3181 |
| 77 | 844.91 | 37.1814 | 60.9587 |
| 78 | 851.19 | 11.9368 | 0.5116 |
| 79 | 876.01 | 17.2026 | 68.1600 |
| 80 | 876.30 | 0.2040 | 17.2208 |
| 81 | 887.35 | 32.2464 | 6.1233 |
| 82 | 910.51 | 141.8112 | 9.7754 |
| 83 | 931.13 | 11.9881 | 4.7086 |
| 84 | 934.10 | 1.0265 | 2.6387 |
| 85 | 962.18 | 1.6934 | 37.2579 |
| 86 | 975.59 | 9.2432 | 7.0479 |
| 87 | 982.63 | 7.8473 | 1.2103 |
| 88 | 1009.48 | 18.1531 | 7.4461 |
| 89 | 1013.27 | 78.6948 | 38.3528 |
| 90 | 1034.68 | 18.6491 | 32.1426 |
| 91 | 1047.33 | 26.0133 | 23.6746 |
| 92 | 1064.95 | 13.0377 | 89.2184 |
| 93 | 1068.52 | 11.3796 | 0.3119 |
| 94 | 1081.83 | 74.5240 | 111.4712 |
| 95 | 1112.08 | 20.1803 | 38.7017 |
| 96 | 1128.54 | 14.5619 | 3.5485 |
| 97 | 1130.20 | 37.7634 | 55.0452 |
| 98 | 1141.21 | 129.1481 | 29.7817 |
| 99 | 1154.68 | 6.3795 | 29.6325 |

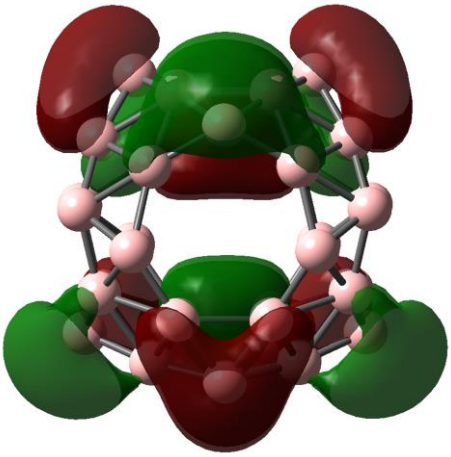
Continued Table S6

| Mode | Freq | Infrared | Raman Activity |
|---|---|---|---|
| 99 | 1154.68 | 6.3795 | 29.6325 |
| 100 | 1158.49 | 1.8903 | 52.7581 |
| 101 | 1163.35 | 9.2253 | 3.0448 |
| 102 | 1171.78 | 13.2525 | 27.6671 |
| 103 | 1184.55 | 0.4565 | 40.7742 |
| 104 | 1196.98 | 2.1626 | 102.1173 |
| 105 | 1216.43 | 12.8059 | 2.9580 |
| 106 | 1224.08 | 7.3154 | 253.6919 |
| 107 | 1246.93 | 7.7794 | 616.9933 |
| 108 | 1267.22 | 3.9655 | 11.9421 |
| 109 | 1269.42 | 0.2180 | 19.3292 |
| 110 | 1298.67 | 97.4346 | 37.2487 |
| 111 | 1305.79 | 0.4895 | 46.3490 |
| 112 | 1317.47 | 2.1039 | 10.6987 |
| 113 | 1319.00 | 14.3209 | 18.2733 |
| 114 | 1333.88 | 3.4470 | 243.2841 |

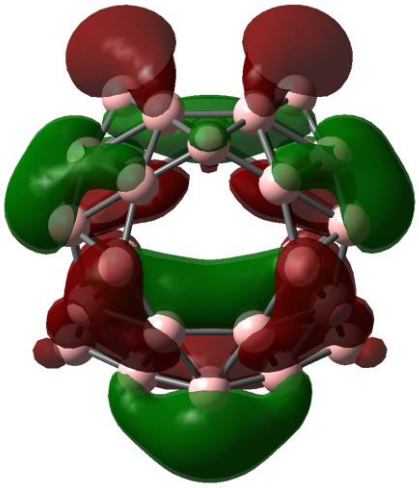
## III. Figures



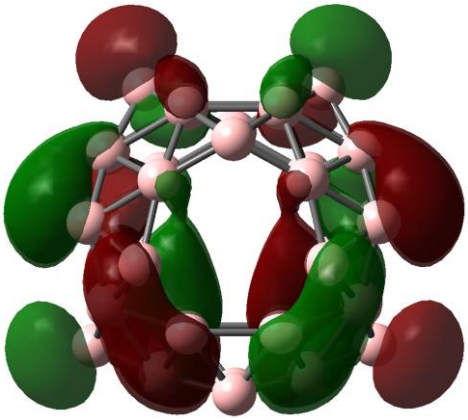
HOMO-1



HOMO

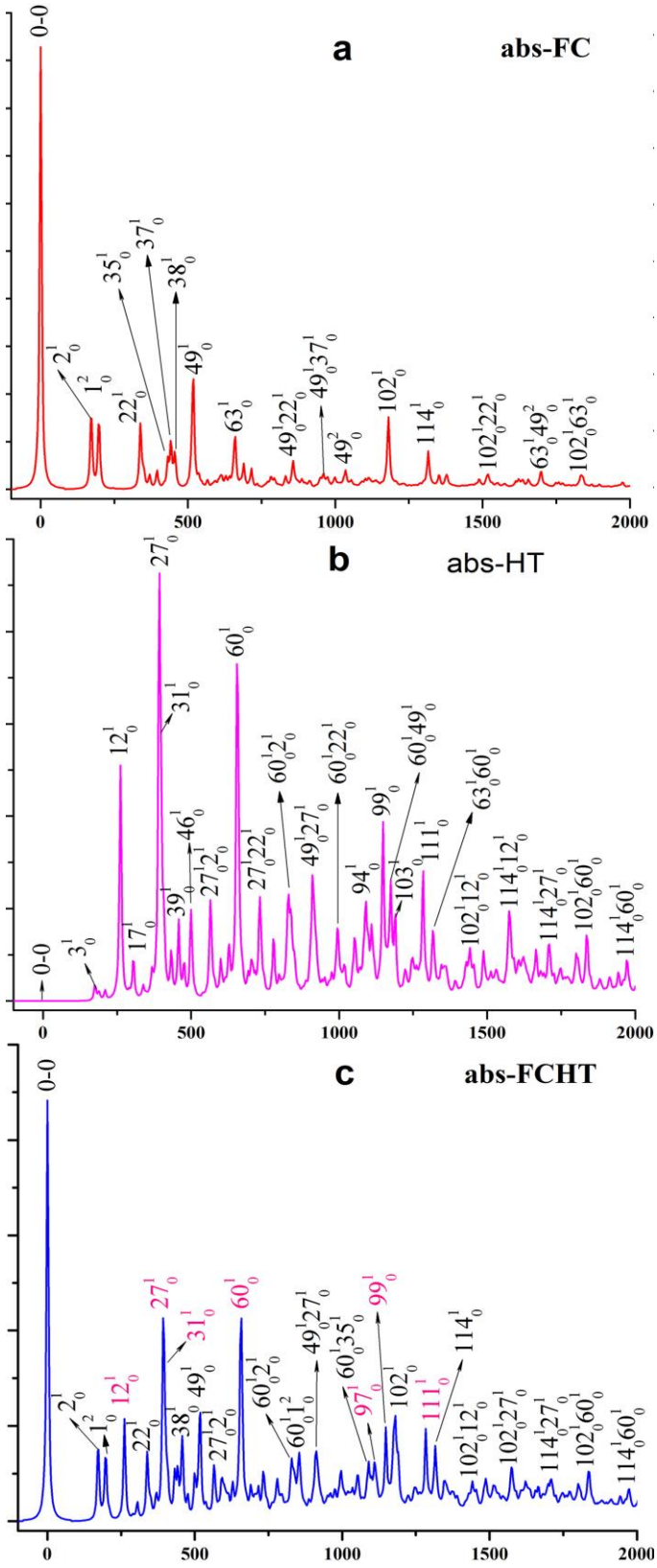


LUMO



LUMO-1

**Figure S1**. The frontier molecular orbitals of $B_{40}$ computed at PBE0/6-311G* level.


a
abs-FC
0-0
$2^1_0$
$1^2_0$
$1^1_0$
$22^1_0$
$35^1_0$
$37^1_0$
$38^1_0$
$49^1_0$
$63^1_0$
$49^1_0 22^1_0$
$49^1_0 37^1_0$
$49^2_0$
$102^1_0$
$114^1_0$
$102^1_0 22^1_0$
$63^1_0 49^2_0$
$102^1_0 63^1_0$
0
500
1000
1500
2000
b
abs-HT
$27^1_0$
$60^1_0$
$31^1_0$
$12^1_0$
$60^1_0 2^1_0$
$60^1_0 22^1_0$
$60^1_0 49^1_0$
$63^1_0 60^1_0$
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$114^1_0 12^1_0$
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$114^1_0 60^1_0$
$17^1_0$
$3^1_0$
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0
500
1000
1500
2000
c
abs-FCHT
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$1^2_0$
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$22^1_0$
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$38^1_0$
$49^1_0$
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$60^1_0 35^1_0$
$97^1_0$
$99^1_0$
$102^1_0$
$111^1_0$
$114^1_0$
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0
500
1000
1500
2000

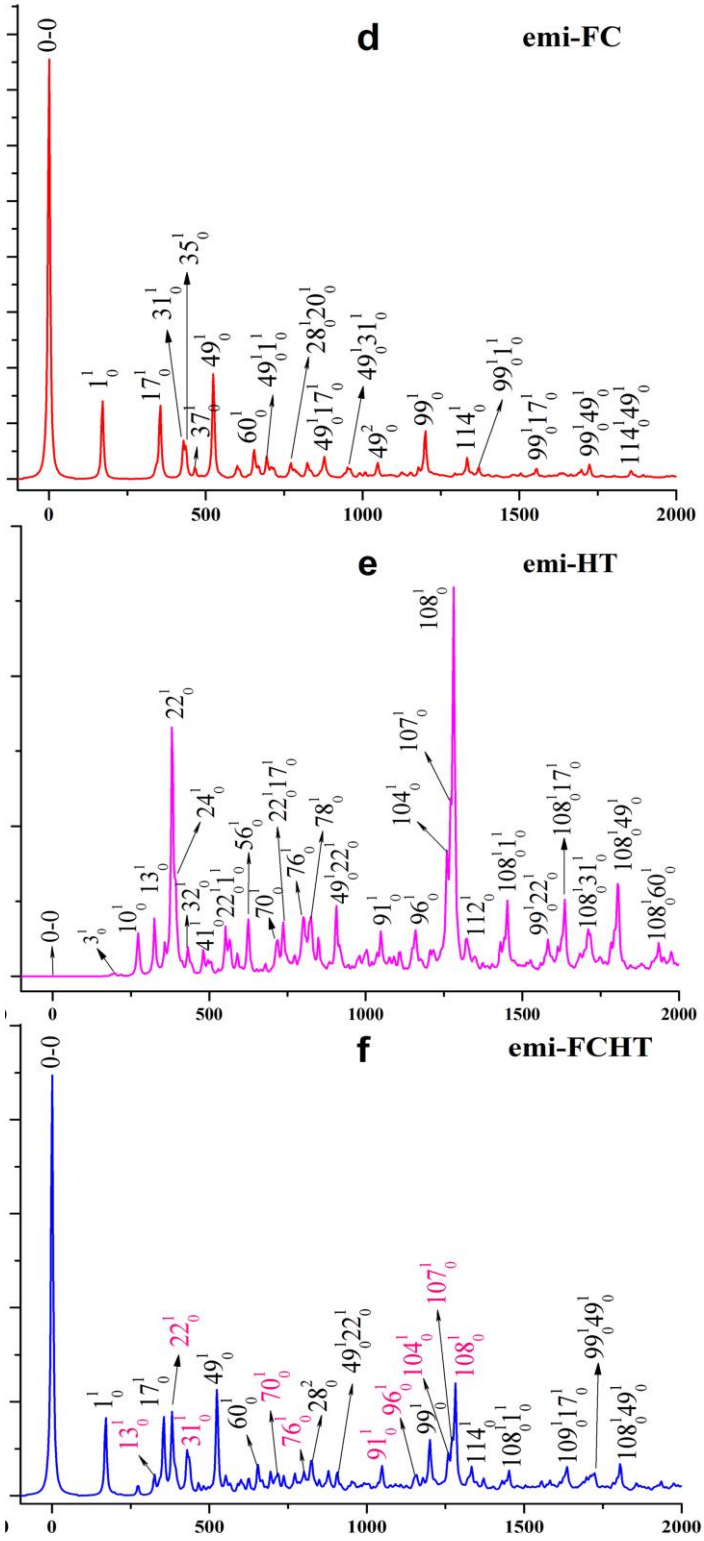
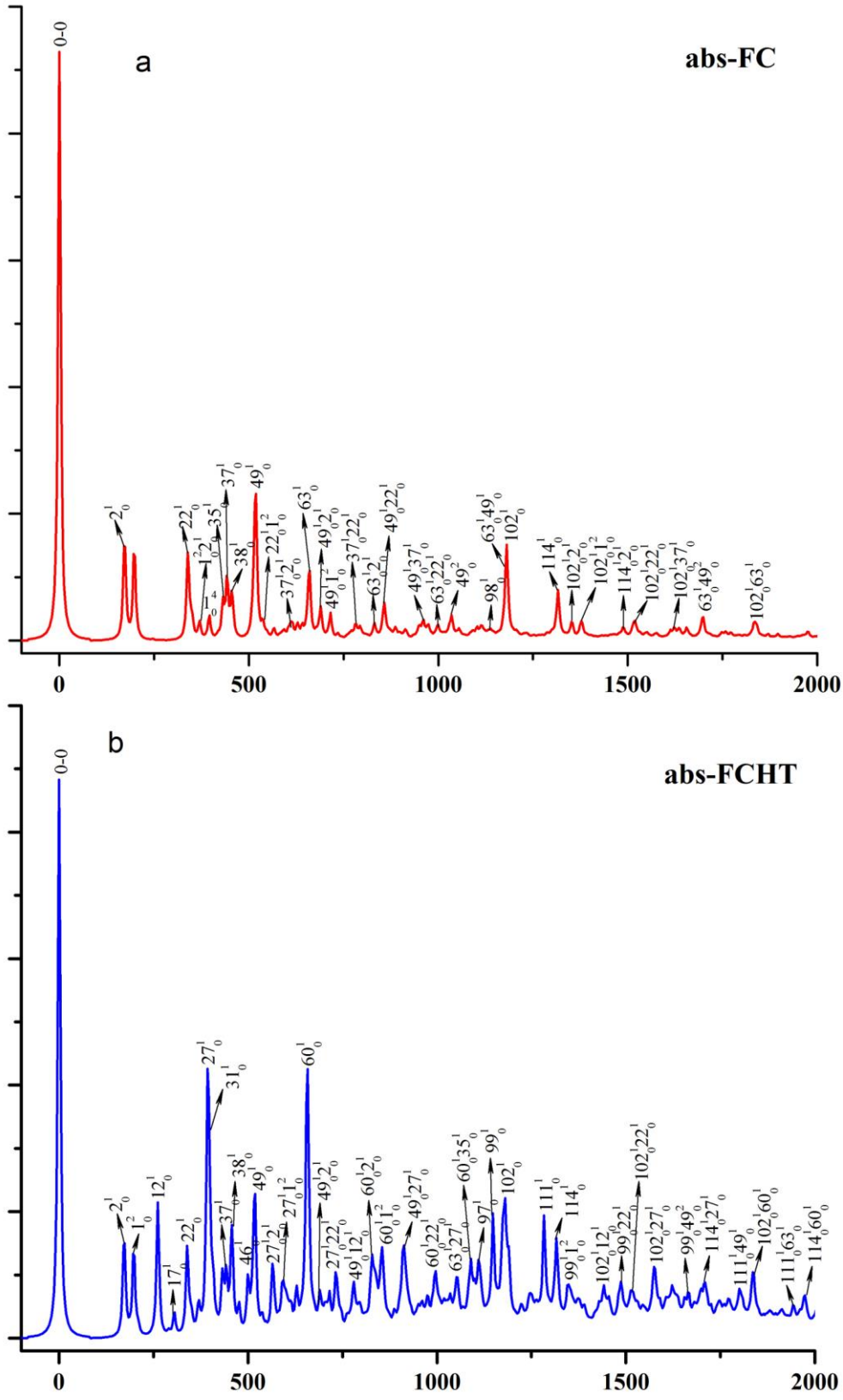



**Figure S2**. Simulated well-resolved absorption (left column, a-c) and emission (right column, d-f) spectra of $B_{40}$ within a range of 2000 $cm^{-1}$ (the 0-0 line is set to zero). FC represents the spectra simulated in Franck-Condon approximation; HT represents pure Herzberg-Teller spectra; and FCHT represents the total spectra with consideration of both FC and HT effects.


a
abs-FC
0-0
0
500
1000
1500
2000
b
abs-FCHT
0-0
0
500
1000
1500
2000

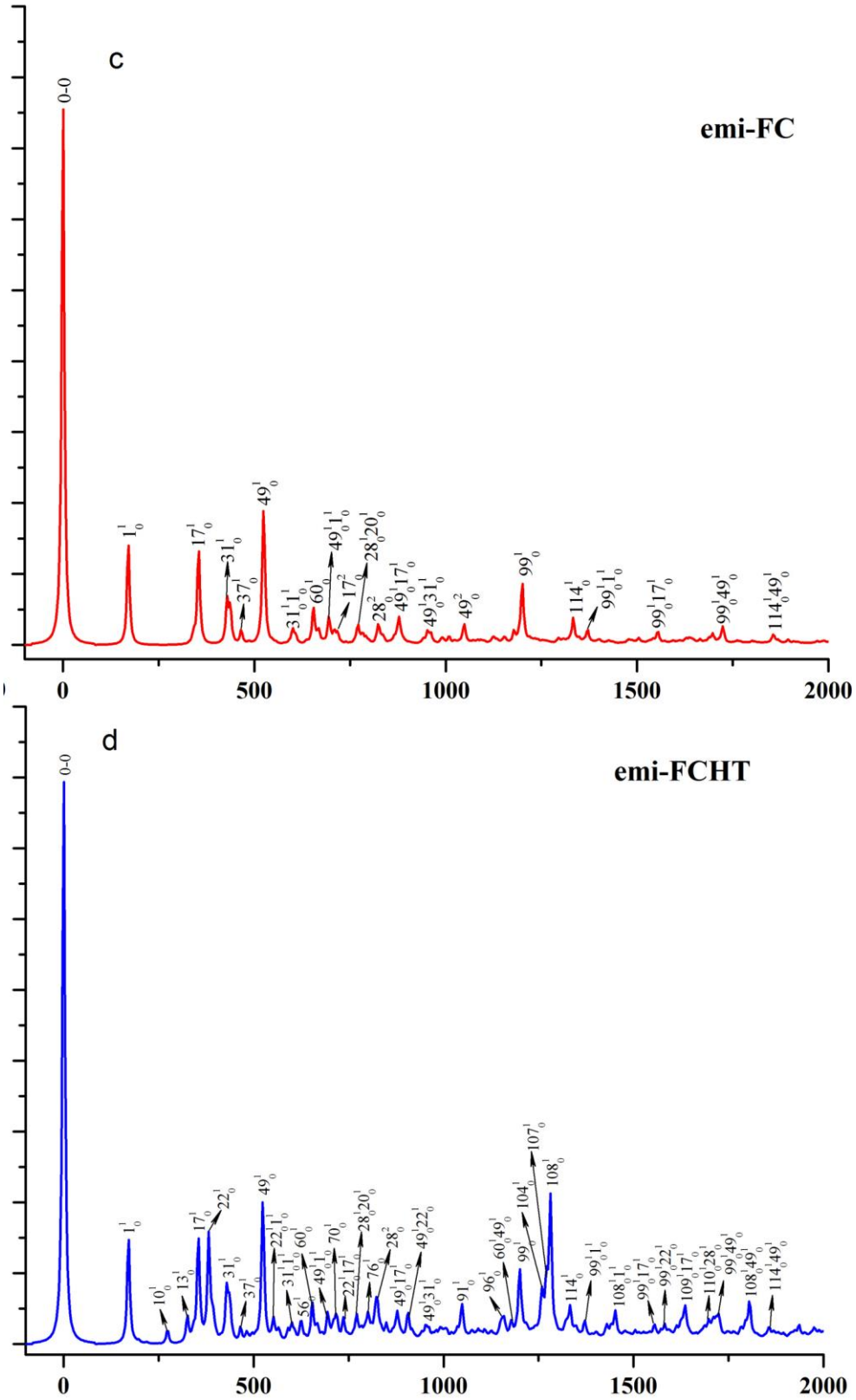



**Figure S3**. Simulated highly-resolved absorption and emission spectra of $B_{40}$ within a range of 2000 $cm^{-1}$, and detailed assignments of the normal modes and combinated bands.

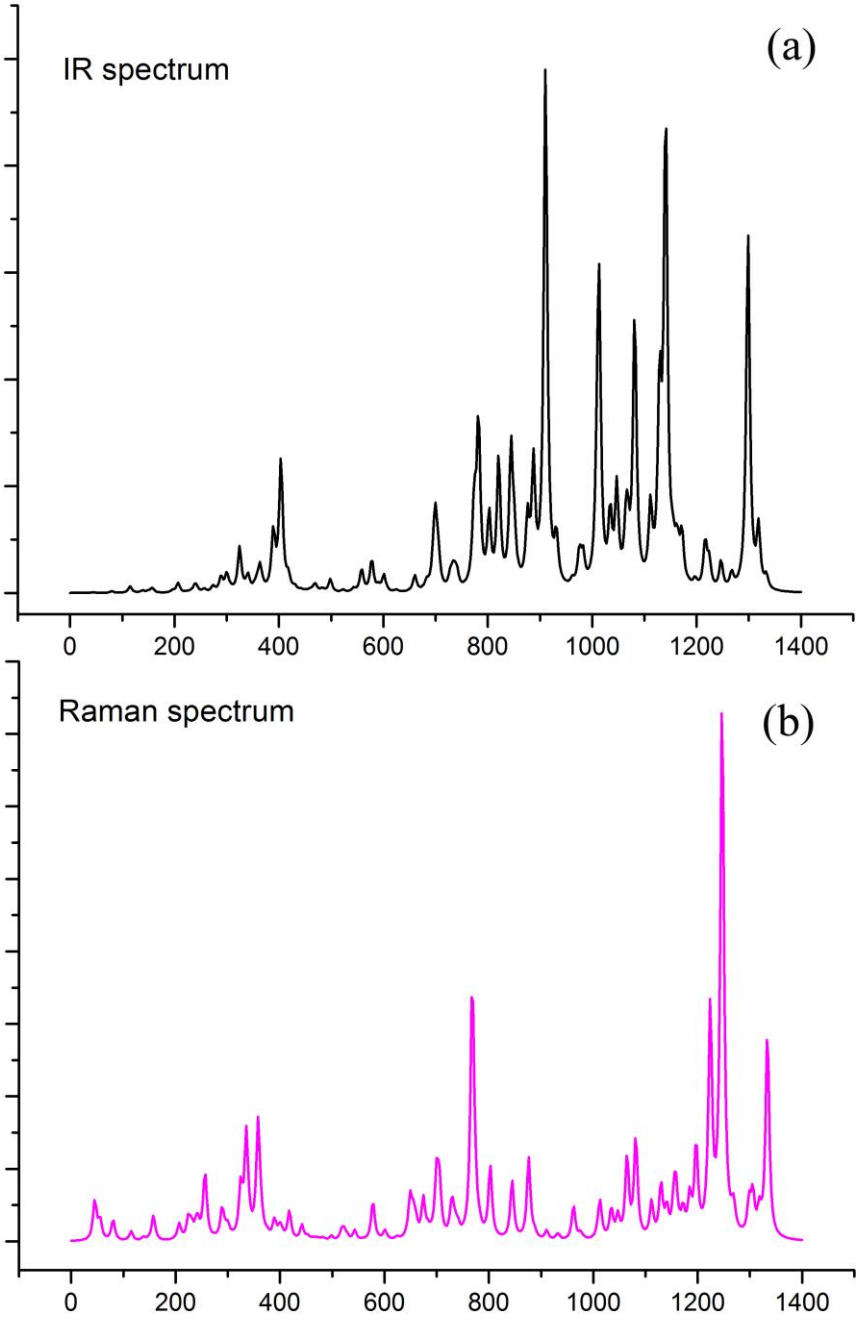



Figure S4. Computed optical spectra of quasi-planar isomer of $B_{40}$ fullerene: (a) IR, and (b) Raman.

## IV. Cartesian coordinates of ground and the first excited stated for B40 cluster optimized by different theoretical levels.

### Ground state

PBE0/6-311G*

| | | | |
|---|---|---|---|
| B | -0.87512400 | -2.36859900 | 1.67786000 |
| B | -1.38625700 | 2.36223600 | -1.20078600 |
| B | -2.36859900 | -0.87512400 | -1.67786000 |
| B | -0.87512400 | 2.36859900 | 1.67786000 |
| B | -2.63661500 | 0.00000000 | 1.98391700 |
| B | -2.36223600 | -1.38625700 | 1.20078600 |
| B | -0.88680500 | 1.38805600 | -2.53401000 |
| B | 1.38625700 | 2.36223600 | -1.20078600 |
| B | 1.68762200 | 0.00000000 | -2.86237900 |
| B | -1.38625700 | -2.36223600 | -1.20078600 |
| B | 0.00000000 | 1.68762200 | 2.86237900 |
| B | 0.00000000 | 2.63661500 | -1.98391700 |
| B | 0.00000000 | -1.68762200 | 2.86237900 |
| B | 0.88680500 | -1.38805600 | -2.53401000 |
| B | 1.38625700 | -2.36223600 | -1.20078600 |
| B | -1.68762200 | 0.00000000 | -2.86237900 |
| B | 1.38805600 | 0.88680500 | 2.53401000 |
| B | 2.36859900 | -0.87512400 | -1.67786000 |
| B | 0.00000000 | -2.63661500 | -1.98391700 |
| B | 0.88680500 | 1.38805600 | -2.53401000 |
| B | 2.36223600 | 1.38625700 | 1.20078600 |
| B | 2.36223600 | -1.38625700 | 1.20078600 |
| B | -2.36859900 | 0.87512400 | -1.67786000 |

| | | | |
|---|---|---|---|
| B | 2.63661500 | 0.00000000 | 1.98391700 |
| B | 0.87512400 | -2.36859900 | 1.67786000 |
| B | 1.38805600 | -0.88680500 | 2.53401000 |
| B | -1.38805600 | 0.88680500 | 2.53401000 |
| B | -1.38805600 | -0.88680500 | 2.53401000 |
| B | -2.36223600 | 1.38625700 | 1.20078600 |
| B | 0.87512400 | 2.36859900 | 1.67786000 |
| B | 2.36859900 | 0.87512400 | -1.67786000 |
| B | -0.88680500 | -1.38805600 | -2.53401000 |
| B | -2.72821200 | 1.74572000 | -0.38298800 |
| B | -1.74572000 | 2.72821200 | 0.38298800 |
| B | 1.74572000 | 2.72821200 | 0.38298800 |
| B | 2.72821200 | 1.74572000 | -0.38298800 |
| B | 1.74572000 | -2.72821200 | 0.38298800 |
| B | 2.72821200 | -1.74572000 | -0.38298800 |
| B | -1.74572000 | -2.72821200 | 0.38298800 |
| B | -2.72821200 | -1.74572000 | -0.38298800 |

BHandHLYP/6-311G*

| | | | |
|---|---|---|---|
| B | -0.877615 | -2.379870 | 1.662873 |
| B | -1.369099 | 2.356639 | -1.187279 |
| B | -2.379870 | -0.877615 | -1.662873 |
| B | -0.877615 | 2.379870 | 1.662873 |
| B | -2.618329 | 0.000000 | 1.979723 |
| B | -2.356639 | -1.369099 | 1.187279 |
| B | -0.890385 | 1.378081 | -2.513059 |
| B | 1.369099 | 2.356639 | -1.187279 |
| B | 1.697528 | 0.000000 | -2.829412 |
| B | -1.369099 | -2.356639 | -1.187279 |

| | | | |
|---|---|---|---|
| B | 0.000000 | 1.697528 | 2.829412 |
| B | 0.000000 | 2.618329 | -1.979723 |
| B | 0.000000 | -1.697528 | 2.829412 |
| B | 0.890385 | -1.378081 | -2.513059 |
| B | 1.369099 | -2.356639 | -1.187279 |
| B | -1.697528 | 0.000000 | -2.829412 |
| B | 1.378081 | 0.890385 | 2.513059 |
| B | 2.379870 | -0.877615 | -1.662873 |
| B | 0.000000 | -2.618329 | -1.979723 |
| B | 0.890385 | 1.378081 | -2.513059 |
| B | 2.356639 | 1.369099 | 1.187279 |
| B | 2.356639 | -1.369099 | 1.187279 |
| B | -2.379870 | 0.877615 | -1.662873 |
| B | 2.618329 | 0.000000 | 1.979723 |
| B | 0.877615 | -2.379870 | 1.662873 |
| B | 1.378081 | -0.890385 | 2.513059 |
| B | -1.378081 | 0.890385 | 2.513059 |
| B | -1.378081 | -0.890385 | 2.513059 |
| B | -2.356639 | 1.369099 | 1.187279 |
| B | 0.877615 | 2.379870 | 1.662873 |
| B | 2.379870 | 0.877615 | -1.662873 |
| B | -0.890385 | -1.378081 | -2.513059 |
| B | -2.729006 | 1.761978 | -0.384856 |
| B | -1.761978 | 2.729006 | 0.384856 |
| B | 1.761978 | 2.729006 | 0.384856 |
| B | 2.729006 | 1.761978 | -0.384856 |
| B | 1.761978 | -2.729006 | 0.384856 |
| B | 2.729006 | -1.761978 | -0.384856 |
| B | -1.761978 | -2.729006 | 0.384856 |

| | | | |
|---|---|---|---|
| B | -2.729006 | -1.761978 | -0.384856 |

PBE0/6-31G*

| | | | |
|---|---|---|---|
| B | -0.876448 | -2.367390 | 1.679316 |
| B | -1.385435 | 2.358613 | -1.201540 |
| B | -2.367390 | -0.876448 | -1.679316 |
| B | -0.876448 | 2.367390 | 1.679316 |
| B | -2.640146 | 0.000000 | 1.990059 |
| B | -2.358613 | -1.385435 | 1.201540 |
| B | -0.888227 | 1.388026 | -2.537266 |
| B | 1.385435 | 2.358613 | -1.201540 |
| B | 1.693408 | 0.000000 | -2.870169 |
| B | -1.385435 | -2.358613 | -1.201540 |
| B | 0.000000 | 1.693408 | 2.870169 |
| B | 0.000000 | 2.640146 | -1.990059 |
| B | 0.000000 | -1.693408 | 2.870169 |
| B | 0.888227 | -1.388026 | -2.537266 |
| B | 1.385435 | -2.358613 | -1.201540 |
| B | -1.693408 | 0.000000 | -2.870169 |
| B | 1.388026 | 0.888227 | 2.537266 |
| B | 2.367390 | -0.876448 | -1.679316 |
| B | 0.000000 | -2.640146 | -1.990059 |
| B | 0.888227 | 1.388026 | -2.537266 |
| B | 2.358613 | 1.385435 | 1.201540 |
| B | 2.358613 | -1.385435 | 1.201540 |
| B | -2.367390 | 0.876448 | -1.679316 |
| B | 2.640146 | 0.000000 | 1.990059 |
| B | 0.876448 | -2.367390 | 1.679316 |
| B | 1.388026 | -0.888227 | 2.537266 |

| | | | |
|---|---|---|---|
| B | -1.388026 | 0.888227 | 2.537266 |
| B | -1.388026 | -0.888227 | 2.537266 |
| B | -2.358613 | 1.385435 | 1.201540 |
| B | 0.876448 | 2.367390 | 1.679316 |
| B | 2.367390 | 0.876448 | -1.679316 |
| B | -0.888227 | -1.388026 | -2.537266 |
| B | -2.733784 | 1.749051 | -0.382624 |
| B | -1.749051 | 2.733784 | 0.382624 |
| B | 1.749051 | 2.733784 | 0.382624 |
| B | 2.733784 | 1.749051 | -0.382624 |
| B | 1.749051 | -2.733784 | 0.382624 |
| B | 2.733784 | -1.749051 | -0.382624 |
| B | -1.749051 | -2.733784 | 0.382624 |
| B | -2.733784 | -1.749051 | -0.382624 |

BHandHLYP/6-31G*

| | | | |
|---|---|---|---|
| B | -0.878839 | -2.378459 | 1.663191 |
| B | -1.366198 | 2.350406 | -1.186244 |
| B | -2.378459 | -0.878839 | -1.663191 |
| B | -0.878839 | 2.378459 | 1.663191 |
| B | -2.618983 | 0.000000 | 1.986141 |
| B | -2.350406 | -1.366198 | 1.186244 |
| B | -0.891595 | 1.375052 | -2.514210 |
| B | 1.366198 | 2.350406 | -1.186244 |
| B | 1.706083 | 0.000000 | -2.837228 |
| B | -1.366198 | -2.350406 | -1.186244 |
| B | 0.000000 | 1.706083 | 2.837228 |
| B | 0.000000 | 2.618983 | -1.986141 |
| B | 0.000000 | -1.706083 | 2.837228 |

| | | | |
|---|---|---|---|
| B | 0.891595 | -1.375052 | -2.514210 |
| B | 1.366198 | -2.350406 | -1.186244 |
| B | -1.706083 | 0.000000 | -2.837228 |
| B | 1.375052 | 0.891595 | 2.514210 |
| B | 2.378459 | -0.878839 | -1.663191 |
| B | 0.000000 | -2.618983 | -1.986141 |
| B | 0.891595 | 1.375052 | -2.514210 |
| B | 2.350406 | 1.366198 | 1.186244 |
| B | 2.350406 | -1.366198 | 1.186244 |
| B | -2.378459 | 0.878839 | -1.663191 |
| B | 2.618983 | 0.000000 | 1.986141 |
| B | 0.878839 | -2.378459 | 1.663191 |
| B | 1.375052 | -0.891595 | 2.514210 |
| B | -1.375052 | 0.891595 | 2.514210 |
| B | -1.375052 | -0.891595 | 2.514210 |
| B | -2.350406 | 1.366198 | 1.186244 |
| B | 0.878839 | 2.378459 | 1.663191 |
| B | 2.378459 | 0.878839 | -1.663191 |
| B | -0.891595 | -1.375052 | -2.514210 |
| B | -2.734401 | 1.766081 | -0.384588 |
| B | -1.766081 | 2.734401 | 0.384588 |
| B | 1.766081 | 2.734401 | 0.384588 |
| B | 2.734401 | 1.766081 | -0.384588 |
| B | 1.766081 | -2.734401 | 0.384588 |
| B | 2.734401 | -1.766081 | -0.384588 |
| B | -1.766081 | -2.734401 | 0.384588 |
| B | -2.734401 | -1.766081 | -0.384588 |

**The first singlet excited state**

PBE0/6-31G*

| | | | |
|---|---|---|---|
| B | -0.873781 | -2.340954 | 1.678356 |
| B | -1.407499 | 2.351049 | -1.220494 |
| B | -2.340954 | -0.873781 | -1.678356 |
| B | -0.873781 | 2.340954 | 1.678356 |
| B | -2.625510 | 0.000000 | 1.982163 |
| B | -2.351049 | -1.407499 | 1.220494 |
| B | -0.884010 | 1.377372 | -2.573638 |
| B | 1.407499 | 2.351049 | -1.220494 |
| B | 1.679873 | 0.000000 | -2.915431 |
| B | -1.407499 | -2.351049 | -1.220494 |
| B | 0.000000 | 1.679873 | 2.915431 |
| B | 0.000000 | 2.625510 | -1.982163 |
| B | 0.000000 | -1.679873 | 2.915431 |
| B | 0.884010 | -1.377372 | -2.573638 |
| B | 1.407499 | -2.351049 | -1.220494 |
| B | -1.679873 | 0.000000 | -2.915431 |
| B | 1.377372 | 0.884010 | 2.573638 |
| B | 2.340954 | -0.873781 | -1.678356 |
| B | 0.000000 | -2.625510 | -1.982163 |
| B | 0.884010 | 1.377372 | -2.573638 |
| B | 2.351049 | 1.407499 | 1.220494 |
| B | 2.351049 | -1.407499 | 1.220494 |
| B | -2.340954 | 0.873781 | -1.678356 |
| B | 2.625510 | 0.000000 | 1.982163 |
| B | 0.873781 | -2.340954 | 1.678356 |
| B | 1.377372 | -0.884010 | 2.573638 |
| B | -1.377372 | 0.884010 | 2.573638 |

| | | | |
|---|---|---|---|
| B | -1.377372 | -0.884010 | 2.573638 |
| B | -2.351049 | 1.407499 | 1.220494 |
| B | 0.873781 | 2.340954 | 1.678356 |
| B | 2.340954 | 0.873781 | -1.678356 |
| B | -0.884010 | -1.377372 | -2.573638 |
| B | -2.721543 | 1.732541 | -0.382007 |
| B | -1.732541 | 2.721543 | 0.382007 |
| B | 1.732541 | 2.721543 | 0.382007 |
| B | 2.721543 | 1.732541 | -0.382007 |
| B | 1.732541 | -2.721543 | 0.382007 |
| B | 2.721543 | -1.732541 | -0.382007 |
| B | -1.732541 | -2.721543 | 0.382007 |
| B | -2.721543 | -1.732541 | -0.382007 |