RSC Advances

Rational design of near-infrared dyes based on boron dipyrromethene derivatives for application in organic solar cells

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Figure S1. Geometries of PPB.
Table S1  Calculated the longest absorption and fluorescence wavelengths ($\lambda_{\text{abs}}$ and $\lambda_{\text{fl}}$) of parent molecule 1 by various methods with 6-31G(d,p) basis set, along with available experimental data.

| Methods       | $\lambda_{\text{abs}}$ | $\lambda_{\text{fl}}$ |
|---------------|-------------------------|------------------------|
| TD-B3LYP      | 658                     | 697                    |
| TD-PBE0       | 639                     | 677                    |
| TD-LC-ωPBE   | 531                     | 569                    |
| TD-ωB97XD    | 569                     | 627                    |
| TD-M062X      | 589                     | 642                    |
| TD-CAM-B3LYP | 576                     | 634                    |
| Exp$^a$       | 655                     | 672                    |

$^a$Experimental data for parent molecule in CHCl$_3$ taken from ref. 9.
Table S2 Calculated the longest absorption wavelengths ($\lambda_{\text{abs}}$ and $\lambda_{\text{fl}}$) of PPB by various methods with 6-31G(d,p) basis set, along with available experimental data.

| Methods          | $\lambda_{\text{abs}}$ | $\lambda_{\text{fl}}$ |
|------------------|------------------------|------------------------|
| TD-B3LYP         | 634.6                  | 679.8                  |
| TD-PBE0          | 617.3                  | 662.5                  |
| TD-LCoPBE        | 515.6                  | 600.9                  |
| TD-mB97XD        | 553.9                  | 617.4                  |
| TD-M062X         | 569.3                  | 629.6                  |
| TD-CAM-B3LYP     | 558.5                  | 620.9                  |
| Exp\textsuperscript{a} | 638                   | 661                   |

\textsuperscript{a}Experimental data for parent molecule in CHCl\textsubscript{3} taken from ref. 18.
Table S3 The $\lambda_{abs}$ and corresponding oscillator strength $f$ (in parenthesis) and absorption region $R$ of the first fifteen excited states for the designed compounds obtained by the TD-B3LYP/6-31G(d,p) level.

| Species | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   |
|---------|-----|-----|-----|-----|-----|-----|-----|-----|
| $S_1$   | 659(0.94) | 672(0.93) | 623(0.94) | 638(0.96) | 677(0.81) | 719(0.80) | 719(0.74) | 667(0.87) |
| $S_2$   | 482(0.00) | 489(0.00) | 456(0.00) | 464(0.00) | 539(0.00) | 614(0.00) | 599(0.00) | 500(0.00) |
| $S_3$   | 473(0.71) | 480(0.78) | 446(0.70) | 458(0.76) | 509(0.54) | 553(0.41) | 527(0.48) | 486(0.63) |
| $S_4$   | 417(0.00) | 432(0.00) | 401(0.00) | 416(0.00) | 422(0.00) | 455(0.00) | 431(0.00) | 443(0.00) |
| $S_5$   | 320(0.02) | 413(0.00) | 373(0.00) | 408(0.00) | 418(0.00) | 449(0.08) | 421(0.13) | 406(0.01) |
| $S_6$   | 390(0.00) | 396(0.02) | 369(0.03) | 373(0.00) | 391(0.07) | 429(0.00) | 415(0.00) | 405(0.00) |
| $S_7$   | 388(0.00) | 395(0.00) | 366(0.00) | 373(0.01) | 383(0.00) | 423(0.00) | 395(0.00) | 399(0.00) |
| $S_8$   | 380(0.00) | 373(0.00) | 362(0.00) | 369(0.39) | 379(0.02) | 403(0.20) | 385(0.00) | 388(0.00) |
| $S_9$   | 377(0.01) | 372(0.27) | 352(0.01) | 363(0.00) | 378(0.00) | 392(0.00) | 370(0.01) | 354(0.09) |
| $S_{10}$| 373(0.00) | 363(0.00) | 350(0.00) | 340(0.00) | 375(0.00) | 382(0.03) | 368(0.00) | 347(0.15) |
| $S_{11}$| 336(0.04) | 362(0.00) | 328(0.03) | 339(0.02) | 355(0.06) | 382(0.00) | 355(0.10) | 332(0.00) |
| $S_{12}$| 318(0.76) | 339(0.00) | 309(0.72) | 322(0.04) | 326(0.55) | 342(0.30) | 336(0.29) | 332(0.01) |
| $S_{13}$| 309(0.01) | 327(0.00) | 290(0.01) | 315(0.00) | 324(0.03) | 339(0.00) | 321(0.36) | 326(0.00) |
| $S_{14}$| 303(0.00) | 315(0.44) | 285(0.00) | 308(0.47) | 319(0.00) | 334(0.29) | 320(0.09) | 306(0.51) |
| $S_{15}$| 297(0.49) | 313(0.02) | 283(0.38) | 300(0.00) | 313(0.30) | 324(0.02) | 315(0.00) | 303(0.62) |
| $R$     | 362   | 359   | 340   | 330   | 364   | 395   | 399   | 364   |
**Table S4** The Cartesian coordinates of 1–8 in $S_0$ at the B3LYP/6-31G(d,p) level.

| Atom | X    | Y    | Z    |
|------|------|------|------|
| C    | 0.00000000 | 0.00000000 | 0.00000000 |
| C    | 2.28580192  | 0.00000000 | 0.00000000 |
| C    | 1.85214988  | 1.33315016 | 0.00000000 |
| C    | 0.43103567   | 1.35703579 | 0.02394175 |
| C    | 2.28361575   | 2.68992476 | 0.02495778 |
| C    | -0.00218179  | 2.69061767 | 0.01640964 |
| N    | 1.14329898   | 3.49349582 | 0.01922489 |
| N    | 1.14058129   | -0.80326090 | 0.00123249 |
| C    | 3.65385781   | -0.49847040 | -0.01356528 |
| C    | 4.04435194   | -1.69248360 | 0.62194604 |
| C    | 4.65386877   | 0.26592269 | -0.65890421 |
| C    | 5.36758431   | -2.11771332 | 0.60591234 |
| H    | 3.31411373   | -2.28274542 | 1.15810204 |
| C    | 5.96745415   | -0.16135564 | -0.69474253 |
| H    | 4.38793917   | 1.19857930  | -1.13901916 |
| C    | 6.33953850   | -1.36150275 | -0.06580355 |
| H    | 5.63042445   | -3.03453832 | 1.11869400 |
| H    | 6.73104226   | 0.41423402  | -1.20661249 |
| C    | -1.37027388  | 3.18864936  | 0.00487621 |
| C    | -2.38319267  | 2.42509840  | 0.63083778 |
| C    | -1.74925706  | 4.37708936  | -0.64808876 |
| C    | -3.70019542  | 2.84323127  | 0.62358547 |
| H    | -2.12564650  | 1.49793025  | 1.12584418 |
| C    | -3.07514106  | 4.79330964  | -0.67458637 |
| H    | -1.00776941  | 4.96860605  | -1.16705918 |
| C    | -4.06259584  | 4.03226893  | -0.03230429 |
| H    | -4.47500169  | 2.26564762  | 1.11600327 |
| H    | -3.32801151  | 5.70609441  | -1.19942488 |
| B    | 1.04652075   | -2.36608754 | -0.02238722 |
| N    | -0.46105004  | -2.68951791 | -0.35063567 |
| N    | 3.53422787   | 3.14662736  | 0.08786082 |
| C    | 3.70386197   | 4.44504650  | 0.28296441 |
| S    | 5.32596086   | 5.10646209  | 0.47572929 |
| N    | -1.25073179  | -0.45755624 | -0.05512076 |
| C    | -1.42119549  | -1.75686324 | -0.24295416 |
| S    | -3.04437106  | -2.41979062 | -0.42166890 |
| B    | 1.23884332   | 5.05622018  | 0.04436796 |
| N    | 2.74317796   | 5.37738420  | 0.38954798 |
| C    | 3.23442030   | 6.66035305  | 0.64335723 |
| C    | 2.47584511   | 7.82143760  | 0.82802198 |
| C    | 4.64035959   | 6.71217834  | 0.71620782 |
| C    | 3.14738336   | 9.01687304  | 1.06535603 |
|    | x      | y      | z      |
|----|--------|--------|--------|
| H  | -5.61618368 | 5.45622221 | -1.66177779 |
| H  | -5.37562808 | 6.38184006 | -0.16343862 |
| C  | -7.99534176 | 6.79953382 | -1.07796910 |
| H  | -7.82476626 | 4.65369343 | -0.79969006 |
| H  | -7.59340428 | 5.58366455 | 0.67600318 |
| C  | -9.51755124 | 6.87931634 | -0.90772364 |
| H  | -7.53707838 | 7.13032724 | -0.67360808 |
| H  | -7.75256570 | 6.78638444 | -2.14995532 |
| H  | -9.97422838 | 5.96292277 | -1.30711353 |
| H  | -9.76226163 | 6.89785251 | 0.16352094 |
| C  | 8.10273398 | -2.92836267 | 0.25703485 |
| C  | 9.57734087 | -3.06261964 | -0.09244678 |
| H  | 7.52030128 | -3.74779289 | -0.18575347 |
| H  | 7.95238321 | -2.95500819 | 1.34525880 |
| C  | 10.17745358 | -4.38557933 | 0.39938115 |
| H  | 9.68576029 | -2.98194214 | -1.18081356 |
| H  | 10.12181440 | -2.2158575 | 0.34152861 |
| C  | 11.65811905 | -4.54671238 | 0.03321817 |
| H  | 10.06317871 | -4.45935821 | 1.49002919 |
| H  | 9.60798730 | -5.2253215 | -0.02357676 |
| H  | 11.77114588 | -4.46301071 | -1.05675823 |
| H  | 12.23101086 | -3.71258103 | 0.46205247 |
| C  | -10.14425702 | 8.09903138 | -1.59395300 |
| C  | -11.66730074 | 8.17693798 | -1.43405419 |
| H  | -9.89274602 | 8.08135740 | -2.66404621 |
| H  | -9.68950408 | 9.01554633 | -1.19179383 |
| C  | -12.29534707 | 9.39333180 | -2.12545958 |
| H  | -12.12199040 | 7.25918296 | -1.83380786 |
| H  | -11.92044326 | 8.19781629 | -0.3643966 |
| C  | -13.81692401 | 9.46173076 | -1.96493491 |
| H  | -11.84298942 | 10.31056665 | -1.72452491 |
| H  | -12.04056113 | 9.37271134 | -3.19383568 |
| H  | -14.23433883 | 10.33872513 | -2.47013568 |
| H  | -14.30006241 | 8.57341646 | -2.38750178 |
| H  | -14.10192358 | 9.51998754 | -0.90831024 |
| C  | 12.26243252 | -5.87480309 | 0.50479125 |
| C  | 13.73904566 | -6.04378283 | 0.12764140 |
| H  | 11.68267385 | -6.70702616 | 0.08055252 |
| H  | 12.15436485 | -5.95654979 | 1.59574716 |
| C  | 14.34223742 | -7.37577456 | 0.59027991 |
| H  | 13.84726809 | -5.95744379 | -0.96306115 |
| H  | 14.32138127 | -5.21485876 | 0.55505116 |
| C  | 15.81546687 | -7.53911907 | 0.20508498 |
| H  | 14.23712177 | -7.46108138 | 1.68042281 |
|   |         |         |         |
|---|---------|---------|---------|
| H | 13.75860484 | -8.20348719 | 0.16474018 |
| H | 16.21510849 | -8.49923472 | 0.54723080 |
| H | 15.94856025 | -7.49210084 | -0.88172720 |
| H | 16.43100096 | -6.74696467 | 0.64639688 |
| N | -0.25786354 | -5.07220709 | -0.58704199 |
| N | -3.09569328 | -5.11643339 | -0.75372597 |
| N | 5.34419710 | 7.81399533 | 0.81137078 |
| N | 2.50801070 | 7.76527088 | 0.61981751 |
| 3 | 0.00000000 | 0.00000000 | 0.00000000 |
| C | 2.28758777 | 0.00000000 | 0.00000000 |
| C | 1.85985195 | 1.33089606 | 0.00000000 |
| C | 0.43773291 | 1.35780675 | 0.02368367 |
| C | 2.29813257 | 2.68835274 | 0.02454116 |
| C | 0.01048884 | 2.68920546 | 0.01655536 |
| N | 1.15430408 | 3.49524722 | 0.01657838 |
| N | 1.14413554 | -0.80646893 | 0.00372114 |
| C | 3.65902483 | -0.49882270 | -0.02081096 |
| C | 4.06150926 | -1.67477951 | 0.63767513 |
| C | 4.64616395 | 0.25028123 | -0.70010037 |
| C | 5.38700594 | -2.09637465 | 0.61441291 |
| H | 3.33821405 | -2.25633750 | 1.19285785 |
| C | 5.96182619 | -0.17325437 | -0.74271953 |
| H | 4.36794839 | 1.16799413 | -1.20211758 |
| C | 6.34704542 | -1.35427817 | -0.08691974 |
| H | 5.65894046 | -3.0099631 | 1.14405412 |
| H | 6.71599938 | 0.38890969 | -1.28323308 |
| C | -1.36110739 | 3.18755906 | 0.01356385 |
| C | -2.36146303 | 2.43794970 | 0.67275109 |
| C | -1.75218919 | 4.35940150 | -0.65927988 |
| C | -3.68072579 | 2.85230317 | 0.67488753 |
| H | -2.09179108 | 1.52463972 | 1.18718494 |
| C | -3.08050762 | 4.77220201 | -0.67564944 |
| H | -1.01777656 | 4.94320759 | -1.19713478 |
| C | -4.05625455 | 4.02375402 | -0.00334797 |
| H | -4.44646877 | 2.28706188 | 1.19558971 |
| H | -3.34248106 | 5.67410031 | -1.21486459 |
| B | 1.06399956 | -2.37793982 | 0.00222594 |
| N | -0.43005981 | -2.68972937 | -0.32009145 |
| N | 3.55038488 | 3.13454558 | 0.09188477 |
| C | 3.69879426 | 4.44362328 | 0.27708311 |
| N | -1.25227380 | -0.44735768 | -0.06004678 |
| C | -1.40109822 | -1.75727933 | -0.23844947 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| B    | 1.23639010| 5.06663756| 0.02022804|
| N    | 2.72753448| 5.37597173| 0.35800913|
| C    | 3.32612449| 6.60780700| 0.61291254|
| C    | 2.77454897| 7.87271169| 0.80437207|
| C    | 4.72076292| 6.40386513| 0.67877476|
| C    | 3.65875931| 8.92301231| 1.05121213|
| H    | 1.70133606| 8.01615334| 0.77177522|
| C    | 5.60376235| 7.45034850| 0.92774256|
| C    | 5.04676361| 8.71730403| 1.11104531|
| H    | 3.26417116| 9.92234475| 1.20516974|
| H    | 6.67582409| 7.29051284| 0.97877640|
| H    | 5.70257012| 9.55954583| 1.30743720|
| C    | -2.42475506| -3.71990153| -0.62400472|
| C    | -1.02968698| -3.92303940| -0.56526055|
| C    | -3.30886017| -4.76794194| -0.86226043|
| C    | -0.47883905| -5.18874664| -0.75349953|
| C    | -2.75253180| -6.03568889| -1.04226294|
| H    | -4.38126045| -4.60870709| -0.90775451|
| C    | -1.36412207| -6.24059327| -0.98967368|
| H    | 0.59458704| -5.33175269| -0.72654518|
| H    | -3.40919844| -6.87912270| -1.23036029|
| H    | -0.97010473| -7.24058519| -1.14078271|
| F    | 1.87425557| -2.94231867| -0.96274271|
| F    | 1.35554580| -2.88575020| 1.26985522|
| F    | 0.95954324| 5.57638413| -1.25004010|
| F    | 0.41638497| 5.63074950| 0.97692621|
| O    | -5.37710109| 4.33819071| 0.04536945|
| O    | 7.66074503| -1.68545754| -0.18803206|
| C    | -5.83703577| 5.50975254| -0.63360789|
| C    | -7.34420026| 5.59609475| -0.44190687|
| H    | -5.58449943| 5.44459074| -1.70138313|
| H    | -5.33807040| 6.39896833| -0.22336653|
| C    | -7.95396054| 6.81886592| -1.13822009|
| H    | -7.79881092| 4.67615495| -0.82951580|
| H    | -7.56144399| 5.62525246| 0.63273803|
| C    | -9.47699072| 6.90595844| -0.97937014|
| H    | -7.49499937| 7.73500865| -0.74071636|
| H    | -7.70411185| 6.79354876| -2.20839845|
| H    | -9.93434432| 5.98864403| -1.37604997|
| H    | -9.72952858| 6.93236064| 0.08992854|
| C    | 8.12311303| -2.88982656| 0.42919488|
| C    | 9.60154015| -3.04004081| 0.10150506|
| H    | 7.55107309| -3.74745415| 0.04866540|
| H    | 7.96592289| -2.83586912| 1.51597381|
| Element | X        | Y        | Z        |
|---------|---------|---------|---------|
| C       | 10.2179 | -4.2958 | 0.7298  |
| H       | 9.7163  | -3.0686 | -0.9889 |
| C       | 10.1316 | -2.1451 | 0.4496  |
| C       | 11.6992 | -4.4794 | 0.3769  |
| H       | 10.1082 | -4.2512 | 1.8226  |
| H       | 9.6569  | -5.1832 | 0.4040  |
| H       | 11.8056 | -4.5340 | -0.7156 |
| H       | 12.2601 | -3.5881 | 0.6916  |
| C       | -10.0944| 8.1234  | -1.6779 |
| C       | -11.6189| 8.2045  | -1.5346 |
| H       | -9.8317 | 8.1004  | -2.7452 |
| H       | -9.6424 | 9.0411  | -1.2753 |
| H       | -12.2376| 8.2455  | -2.2361 |
| H       | -12.0708| 7.2863  | -1.9366 |
| H       | -11.8836| 8.2289  | -0.4677 |
| H       | -13.7609| 9.4900  | -2.0942 |
| H       | -11.7893| 10.3376 | -1.8318 |
| H       | -11.9699| 9.3967  | -3.3014 |
| H       | -14.1715| 10.3663 | -2.6069 |
| C       | 12.3286 | -5.7255 | 1.0112  |
| C       | 13.8047 | -5.9198 | 0.6441  |
| H       | 11.7592 | -6.6153 | 0.7062  |
| H       | 12.2313 | -5.6647 | 2.1046  |
| C       | 14.4378 | -7.1623 | 1.2826  |
| H       | 13.9013 | -5.9858 | -0.4490 |
| H       | 14.3746 | -5.0288 | 0.9440  |
| C       | 15.9100 | -7.3524 | 0.9058  |
| H       | 14.3450 | -7.0941 | 2.3750  |
| H       | 13.8657 | -8.0520 | 0.9857  |
| H       | 16.3324 | -8.2456 | 1.3772  |
| H       | 16.0309 | -7.4601 | -0.1781 |
| H       | 16.5138 | -6.4935 | 1.2204  |
| N       | -2.6171 | -2.3590 | -0.4084 |
| H       | -3.4821 | -1.8423 | -0.4313 |
| N       | 4.9140 | 5.0440  | 0.4571  |
| H       | 5.7785 | 4.5267  | 0.4831  |

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| Element | X        | Y        | Z        |
|---------|---------|---------|---------|
| C       | 0.0000  | 0.0000  | 0.0000  |
| C       | 2.2832 | 0.0000  | 0.0000  |
| C       | 1.8498 | 1.3343  | 0.0000  |
| C       | 0.4295 | 1.3562  | 0.0222  |
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | 2.27856251 | 2.69109376 | 0.02024855 |
| C       | -0.00424047| 2.69009424 | 0.00980683 |
| N       | 1.13780137 | 3.49595650 | 0.00090001 |
| N       | 1.14027074 | -0.80566898| 0.01143779 |
| C       | 3.65362033 | -0.49239396| -0.03909849|
| C       | 4.06679167 | -1.68607994| 0.58252836 |
| C       | 4.63297342 | 0.27721214 | -0.70953304|
| C       | 5.39113862 | -2.10472270| 0.53021080 |
| H       | 3.35287188 | -2.28433864| 1.13117844 |
| C       | 5.94758136 | -0.14250711| -0.78003078|
| H       | 4.34764449 | 1.20512019 | -1.18760507|
| C       | 6.34196855 | -1.34253697| -0.16348282|
| H       | 5.67025362 | -3.02369388| 1.03028642 |
| H       | 6.69393526 | 0.43379956 | -1.31628881|
| C       | -1.37593507| 3.18043054 | 0.01712096 |
| C       | -2.36721793| 2.42090830 | 0.68098709 |
| C       | -1.77965874| 4.35564366 | -0.64444353|
| C       | -3.68772101| 2.82767586 | 0.69766252 |
| H       | -2.08775732| 1.50885258 | 1.19201284 |
| C       | -3.10965293| 4.75970195 | -0.64780178|
| H       | -1.05357021| 4.94885129 | -1.18270354|
| C       | -4.07585258| 4.00134881 | 0.02860132 |
| H       | -4.44554002| 2.25678133 | 1.22355672 |
| H       | -3.38113793| 5.66370879 | -1.17839902|
| B       | 1.07247596 | -2.38755392| -0.01848780|
| N       | -0.44517417| -2.70346349| -0.28690245|
| N       | 3.53295887 | 3.14359147 | 0.09579853 |
| C       | 3.68656653 | 4.44697419 | 0.25631246 |
| N       | -1.25557128| -0.45046183| -0.06706680|
| C       | -1.41268459| -1.75378473| -0.22346387|
| B       | 1.20362698 | 5.07796945 | 0.02355985 |
| N       | 2.71704764 | 5.39515330 | 0.31421793 |
| C       | 3.33984928 | 6.61864526 | 0.51218423 |
| C       | 4.73878395 | 6.39303960 | 0.58330580 |
| C       | 3.71563764 | 8.79576803 | 0.81638231 |
| C       | 5.09257462 | 8.56351767 | 0.88991910 |
| H       | 3.32864187 | 9.80590297 | 0.91588367 |
| H       | 5.78111391 | 9.38834101 | 1.04765960 |
| C       | -2.47053869| -3.69919685| -0.53568698|
| C       | -1.07134200| -3.92663130| -0.47615898|
| C       | -2.83011164| -5.87005246| -0.83281507|
| C       | -1.45291654| -6.10405298| -0.77092434|
| H       | -3.52119747| -6.69433910| -0.98198441|
| H       | -1.06825054| -7.11502779| -0.87100790|
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| F    | 1.85293003 | -2.89277637| -1.02644866|
| F    | 1.39830303 | -2.90874218| 1.22892602 |
| F    | 0.89839605 | 5.59212934 | -1.23024906|
| F    | 0.40584771 | 5.58709359 | 1.01531151 |
| O    | -5.39543110| 4.30745374 | 0.09086295 |
| O    | 7.65113513 | -1.67051603| -0.29335409|
| C    | -5.87094700| 5.48173068 | -0.57603152|
| C    | -7.37576137| 5.55818525 | -0.36438383|
| H    | -5.63106167| 5.42262993 | -1.64684903|
| H    | -5.37100172| 6.37017607 | -0.16618637|
| C    | -8.00117150| 6.77922718 | -1.04994492|
| H    | -7.83001751| 4.63665008 | -0.74846546|
| H    | -7.57910401| 5.58373108 | 0.71303457 |
| C    | -9.52168768| 6.86044851 | -0.86581065|
| H    | -7.53917729| 7.69680676 | -0.65941731|
| H    | -7.76879381| 6.75526486 | -2.12405629|
| H    | -9.98209457| 5.94083544 | -1.25347695|
| H    | -9.75622730| 6.88752006 | 0.20754038 |
| C    | 8.11550265 | -2.91407303| 0.24368685 |
| C    | 9.58424585 | -3.05821100| -0.12651311|
| H    | 7.52482087 | -3.74057625| -0.17418497|
| H    | 7.98286176 | -2.92139827| 1.33469599 |
| C    | 10.18968977| -4.37386240| 0.37824589 |
| H    | 9.67551624 | -2.99661841| -1.21772125|
| H    | 10.13761498| -2.20478492| 0.28393663 |
| C    | 11.66475301| -4.54322238| -0.00636533|
| H    | 10.09098623| -4.42975638| 1.47148484 |
| H    | 9.61302671 | -5.21932311| -0.02271554|
| H    | 11.76249160| -4.47593386| -1.09896797|
| H    | 12.24502132| -3.70379306| 0.40182849 |
| C    | -10.15528063| 8.07457365 | -1.55561544|
| C    | -11.67704759| 8.15208980 | -1.38375525|
| H    | -9.91255008| 8.04954028 | -2.62758904|
| H    | -9.69817113| 8.99434966 | -1.16376280|
| C    | -12.31200570| 9.36356673 | -2.07746973|
| H    | -12.13407481| 7.23142884 | -1.77411716|
| H    | -11.92150577| 8.17933002 | -0.31216048|
| C    | -13.83240243| 9.43093690 | -1.90567764|
| H    | -11.85783318| 10.28372163| -1.68540718|
| H    | -12.06536567| 9.33701125 | -3.14762269|
| H    | -14.25486963| 10.30447676| -2.41266675|
| H    | -14.31759332| 8.53957930 | -2.31942085|
| H    | -14.10936878| 9.49489362 | -0.84724231|
| C    | 12.27380743 | -5.86518061| 0.47619030 |
C  8.09886915   -2.93445519    0.38929926
C  9.57911607   -3.08042694    0.06874682
H  7.52533632   -3.77384003   -0.02748612
H  7.93213487   -2.91791279    1.47565074
C 10.18270407   -4.36229024    0.65565517
H  9.70317428   -3.06952576   -1.02097496
H 10.11085992   -2.20201405    0.45426579
C 11.66559598   -4.54247272    0.30758970
H 10.06460173   -3.5679315   1.74841522
H  9.61890024   -5.23352913    0.29330501
H 11.78016066   -4.55810664   -0.78536319
H 12.22947556   -3.6687190  0.65864414
C 11.06359395   8.19758398  -1.66399885
C 11.58873411   8.28389217  -1.53112784
H  9.79265120   8.18990557  -2.72948074
H  9.61029282   9.10664196  -1.24362562
C 12.19612782   9.51204178  -2.22019704
H 12.04183228   7.37368045  -1.94952901
H 11.86146711   8.29446324  -0.46607869
C 13.72008160   9.58801547  -2.08807078
H 11.74608524  10.42179103  -1.80006515
H 11.92097666   9.50215236  -3.2836526
H 14.12249745  10.47336511  -2.59087700
H 14.20025637   8.70763540  -2.53017764
H 14.0250927    9.63578322  -1.03648819
C 12.28201781  -5.81487371   0.90106868
C 13.75914467  -6.00670700  0.53685761
H 11.70850806  -6.68892614   0.56082232
H 12.17767587  -5.79234477  1.99525727
C 14.37914821  -7.27555561  1.13481318
H 13.86251545  -6.03465362  -0.55739914
H 14.33325695  -5.13087154   0.87175517
C 15.85218725  -7.46355039  0.76015392
H 14.28037987  -7.24510653   2.22847640
H 13.80260769  -8.15001551   0.80355348
H 16.26502934  -8.37603549  1.20235348
H 15.97920797  -7.53406725  -0.32618171
H 16.46047418  -6.62098476   1.10825290
C  2.79608634  -2.40041249  -0.44046547
H  3.31708342  -1.93690324  -1.28627199
H  3.41625842  -2.23297515   0.44876992
C  5.07938589   5.08873723   0.49460499
H  5.59463666   4.62024886   1.34117958
H  5.70565189   4.92649747  -0.39132421
| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| S       | -3.10641791 | -5.36107405 | -0.98573403 |
| S       | 5.38571127  | 8.04625447  | 1.05961452  |
| C       | 0.00000000  | 0.00000000  | 0.00000000  |
| C       | 2.28615254  | 0.00000000  | 0.00000000  |
| C       | 1.85200175  | 1.33479344  | 0.00000000  |
| C       | 0.43186470  | 1.35662362  | 0.02643596  |
| C       | 2.28385321  | 2.69142538  | 0.02646530  |
| C       | -0.00229562 | 2.69140733  | 0.02643620  |
| N       | 1.14259587  | 3.49532017  | 0.02773193  |
| N       | 1.14124763  | -0.80390461 | -0.00124842 |
| C       | 3.65309508  | -0.49981048 | -0.00463715 |
| C       | 4.03460659  | -1.70383349 | 0.61868479  |
| C       | 4.66302449  | 0.27321885  | -0.62456055 |
| C       | 5.35842400  | -2.12690864 | 0.61932143  |
| H       | 3.29751586  | -2.30295281 | 1.13506722  |
| C       | 5.97760966  | 0.0141323   | -0.6426067  |
| H       | 4.40430705  | 1.21320980  | -1.09378137 |
| C       | 6.34157754  | -1.3578474  | -0.02008844 |
| H       | 5.61279986  | -3.05219249 | 1.12111612  |
| H       | 6.74941934  | 0.43173844  | -1.1333352  |
| C       | -1.36924911 | 3.19119577  | 0.03101678  |
| C       | -2.37920050 | 2.41811174  | 0.65082927  |
| C       | -1.75073917 | 4.39522359  | -0.59230727 |
| C       | -3.69380363 | 2.84269524  | 0.66877526  |
| H       | -2.12048775 | 1.47810791  | 1.1202965  |
| C       | -3.07457155 | 4.81825333  | -0.59305140 |
| H       | -1.01361619 | 4.99437785  | -1.1086458  |
| C       | -4.05775434 | 4.04917083  | 0.04624136  |
| H       | -4.46564252 | 2.25950016  | 1.15939072  |
| H       | -3.32894507 | 5.74352284  | -1.09487284 |
| B       | 1.04261831  | -2.37175647 | -0.02612286 |
| N       | -0.44906452 | -2.66048103 | -0.36224330 |
| N       | 3.54096472  | 3.14507953  | 0.08957303  |
| C       | 3.71225079  | 4.44140766  | 0.29005442  |
| N       | -1.25712056 | -0.45363273 | -0.06307075 |
| C       | -1.42842911 | -1.74996359 | -0.26350666 |
| B       | 1.24120953  | 5.06317409  | 0.05260253  |
| N       | 2.73287303  | 5.35191203  | 0.38880655  |
| C       | 3.30510974  | 6.60707269  | 0.66880499  |
| C       | 2.81721457  | 7.91850903  | 0.91221196  |
| C       | 4.67081760  | 6.51302572  | 0.72703004  |
| C       | 3.86522687  | 8.81371177  | 1.14235773  |
| Atoms | x     | y     | z     |
|-------|-------|-------|-------|
| C     | -2.38703799 | -3.82158565 | -0.70032511 |
| C     | -1.02132826  | -3.91564621  | -0.64216665  |
| C     | -0.53346348  | -5.22709633  | -0.88553205  |
| C     | -1.57949845  | -6.12228468  | -1.11560773  |
| F     | 1.85096583   | -2.93471536  | -0.99604259  |
| F     | 0.96570687   | 5.59528896   | -1.20759095  |
| F     | 0.43281379   | 5.62613646   | 1.02248106   |
| O     | -5.37245246  | 4.37425493   | 0.11175271   |
| O     | 7.65624941   | -1.68303933  | -0.08575228  |
| C     | -5.82146055  | 5.59284812   | -0.49052492  |
| C     | -7.32337498  | 5.69171643   | -0.26795844  |
| H     | -5.58491086  | 5.58614698   | -1.56370136  |
| H     | -5.3005003   | 6.44615631   | -0.03502706  |
| C     | -7.92328637  | 6.97044857   | -0.86521030  |
| H     | -7.89156584  | 4.80875008   | -0.70927914  |
| H     | -7.52106644  | 5.65027774   | 0.81002870   |
| C     | -9.43942334  | 7.07527082   | -0.65808726  |
| H     | -7.43514175  | 7.84827698   | -0.41889311  |
| H     | -7.70160736  | 7.01323218   | -1.94096558  |
| H     | -9.92698189  | 6.19902570   | -1.10813185  |
| H     | -9.66186468  | 7.02650148   | 0.41710402   |
| C     | 8.10531192   | -2.90152875  | 0.51669928   |
| C     | 9.60719086   | -2.90152875  | 0.51669928   |
| C     | 7.58381967   | -3.75491182  | 0.06143550   |
| H     | 7.86890756   | -2.89461455  | 1.58990501   |
| C     | 10.20713589  | -4.27913642  | 0.89133328   |
| H     | 9.80472695   | -2.95926572  | -0.78408648  |
| H     | 10.80547984  | -2.11745324  | 0.73501688   |
| C     | 11.72324981  | -4.38403158  | 0.68407328   |
| H     | 9.98555691   | -4.32175839  | 1.96711569   |
| H     | 9.71893286   | -5.15702012  | 0.44519128   |
| H     | 11.94558115  | -4.33538522  | -0.39114638  |
| H     | 12.21080028  | -3.50775876  | 1.13397479   |
| C     | -10.05019858 | 8.35328608   | -1.24521960  |
| C     | -11.56701104 | 8.45433769   | -1.04395640  |
| H     | -9.82267658  | 8.40412496   | -2.31960572  |
| H     | -9.56467937  | 9.22919244   | -0.79170707  |
| C     | -12.18074968 | 9.73236177   | -1.62854383  |
| H     | -12.05287438 | 7.57907698   | -1.49867467  |
| H     | -11.79542173 | 8.40183258   | 0.03025795   |
| C     | -13.69609106 | 9.82303009   | -1.42568294  |
| H     | -11.69727094 | 10.60699137  | -1.17245139  |
| H     | -11.95116729 | 9.78531625   | -2.70151031  |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | -14.10357977 | 10.74439245 | -1.85421709 |
| H    | -14.21060335 | 8.97979583  | -1.90043035 |
| H    | -13.95503179 | 9.80895527  | -0.36083386 |
| C    | 12.33402895  | -5.66201481 | 1.27127018  |
| C    | 13.85081662  | -5.76315325 | 1.06987166  |
| H    | 11.84843161  | -6.53794212 | 0.81788154  |
| H    | 12.10660319  | -5.71274783 | 2.34568261  |
| C    | 14.46454281  | -7.04117316 | 1.65447888  |
| H    | 14.07912515  | -5.71072835 | -0.00436972 |
| H    | 14.33677117  | -4.88788926 | 1.52448446  |
| C    | 15.97985765  | -7.13194363 | 1.45146995  |
| H    | 14.23506418  | -7.09404864 | 2.72747251  |
| H    | 13.98096690  | -7.91580255 | 1.19848940  |
| H    | 16.38733499  | -8.05330820 | 1.88000997  |
| H    | 16.23868730  | -7.11794089 | 0.38659285  |
| H    | 16.49447039  | -6.28871473 | 1.92611783  |
| C    | -2.79344029  | -2.40068711 | -0.45643845 |
| H    | -3.32214139  | -1.92534856 | -1.29112740 |
| H    | -3.40807602  | -2.24871414 | 0.43984289  |
| C    | 5.07724970   | 5.09213826  | 0.48306208  |
| H    | 5.60593982   | 4.61673666  | 1.31772130  |
| H    | 5.69190938   | 4.94024501  | -0.41321789 |
| S    | -3.1563876   | -5.34348898 | -1.04453087 |
| S    | 5.44012812   | 8.03491975  | 1.07132451  |
| C    | -1.15044661  | -7.45666457 | -1.36645055 |
| H    | -1.80635684  | -8.29506215 | -1.56573458 |
| C    | 0.21361729   | -7.54716100 | -1.32519867 |
| H    | 0.81731872   | -8.43085191 | -1.48024027 |
| S    | 1.00738657   | -6.02524497 | -0.99126805 |
| C    | 2.07008276   | 10.23854107 | 1.35183412  |
| H    | 1.46636941   | 11.12222808 | 1.50686176  |
| C    | 3.43414077   | 10.14808925 | 1.59312727  |
| H    | 4.09001735   | 10.98652128 | 1.59238254  |
| S    | 1.27635501   | 8.71665134  | 1.01781480  |

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 0.00000000 | 0.00000000 | 0.00000000 |
| C    | 2.28571348 | 0.00000000 | 0.00000000 |
| C    | 1.85507844 | 1.33389590 | 0.00000000 |
| C    | 0.43465279 | 1.35829353 | 0.02184873 |
| C    | 2.28871142 | 2.69290925 | 0.01971904 |
| C    | 0.00346349 | 2.69160377 | 0.00883348 |
| N    | 1.14780037 | 3.49709202 | 0.00603505 |
| N    | 1.14027395 | -0.80518629 | 0.00536477 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 3.65492208 | -0.50012268 | -0.02745849 |
| C    | 4.04752602  | -1.71073274 | 0.57379834  |
| C    | 4.65304653  | 0.27658486  | -0.66056835 |
| C    | 5.36907538  | -2.14138165 | 0.53287049  |
| H    | 3.31995927  | -2.31279049 | 1.09983953  |
| C    | 5.96546405  | -0.15383505 | -0.71767749 |
| H    | 4.38713558  | 1.22383378  | -1.11081587 |
| C    | 6.33795924  | -1.37226395 | -0.12601291 |
| H    | 5.63138442  | -3.07393796 | 1.01695016  |
| H    | 6.72681181  | 0.43191781  | -1.22170773 |
| C    | -1.36679232 | 3.18962567  | 0.00306663  |
| C    | -2.37610875 | 2.42046002  | 0.63209744  |
| C    | -1.74992841 | 4.38030753  | -0.64225322 |
| C    | -3.69383305 | 2.84268363  | 0.63352646  |
| H    | -2.11554172 | 1.49401188  | 1.11875175  |
| C    | -3.0760942  | 4.79682905  | -0.65915389 |
| H    | -1.01044229 | 4.95757228  | -1.15935767 |
| C    | -4.06010271 | 4.03653636  | -0.01518183 |
| H    | -4.46589617 | 2.26366958  | 1.12897958  |
| H    | -3.33136149 | 5.71315796  | -1.1701732  |
| B    | 1.04421277  | -2.37613111 | -0.02592266 |
| N    | -0.45736017 | -2.67127558 | -0.30089497 |
| N    | 3.54276713  | 3.14568475  | 0.09221776  |
| C    | 3.71236166  | 4.44973033  | 0.26611043  |
| N    | -1.25538755 | -0.45024312 | -0.06335745 |
| C    | -1.42908034 | -1.75423941 | -0.23250257 |
| B    | 1.24163456  | 5.06804919  | 0.02896190  |
| N    | 2.73831827  | 5.36493622  | 0.32819836  |
| C    | 3.3179360   | 6.63003739  | 0.56926492  |
| C    | 2.94933421  | 7.98417772  | 0.76164179  |
| C    | 4.68341865  | 6.5147582  | 0.64971196  |
| C    | 4.14440495  | 8.65631160  | 0.95484680  |
| H    | 1.96022211  | 8.41496370  | 0.76440095  |
| H    | 4.33034478  | 9.70376045  | 1.13729494  |
| C    | -2.40752737 | -3.81543379 | -0.59957499 |
| C    | -1.04103509 | -3.93627300 | -0.53160354 |
| C    | -0.67745273 | -5.29196215 | -0.72156258 |
| C    | -1.87556928 | -5.96258230 | -0.90064000 |
| H    | 0.31071086  | -5.72480946 | -0.73160290 |
| H    | -2.06521058 | -7.01042407 | -1.07691711 |
| F    | 1.82337969  | -2.91966621 | -1.02702706 |
| F    | 1.36830959  | -2.91692050 | 1.22182332  |
| F    | 0.93990083  | 5.60008072  | -1.22819589 |
| F    | 0.44383488  | 5.61682561  | 1.01194321  |
|   |   |   |   |
|---|---|---|---|
| O | -5.38020530 | 4.35142095 | 0.03104655 |
| O | 7.64842661 | -1.71059824 | -0.24166690 |
| C | -5.83136661 | 5.53826590 | -0.62657106 |
| C | -7.33916290 | 5.62800015 | -0.44115397 |
| H | -5.57348075 | 5.49316662 | -1.69413115 |
| H | -5.33099700 | 6.41710911 | -0.19627878 |
| C | -7.93981738 | 6.86291500 | -1.12379463 |
| H | -7.79557514 | 4.71550936 | -0.84388750 |
| H | -7.56182509 | 5.64317937 | 0.63269272 |
| C | -9.46214822 | 6.96025770 | -0.96430003 |
| H | -7.47408522 | 7.77123108 | -0.71629190 |
| H | -7.6877057 | 6.84737065 | -2.19410728 |
| H | -9.92662300 | 6.04927793 | -1.36727572 |
| H | -9.71435448 | 6.98124249 | 0.10516698 |
| C | 8.08893649 | -2.96880199 | 0.27612579 |
| C | 9.56275863 | -3.12226635 | -0.07041096 |
| H | 7.49786343 | -3.78110270 | -0.16925404 |
| H | 7.93702414 | -2.99952295 | 1.36445545 |
| C | 10.14476148 | -4.45449243 | 0.41770371 |
| H | 9.67464044 | -3.03902322 | -1.15830626 |
| H | 10.11779380 | -2.28355504 | 0.36744210 |
| C | 11.62411561 | -4.63417055 | 0.05503543 |
| H | 10.02656656 | -4.53109876 | 1.50777638 |
| H | 9.56537303 | -5.28502250 | -0.00979379 |
| H | 11.74141142 | -4.54774890 | -1.03431355 |
| H | 12.20705104 | -3.80941707 | 0.48862906 |
| C | -10.07012577 | 8.18723838 | -1.65447297 |
| C | -11.59337324 | 8.28244501 | -1.50626952 |
| H | -9.81066472 | 8.16737657 | -2.72264068 |
| H | -9.60812924 | 9.09837359 | -1.24837954 |
| C | -12.20323525 | 9.50624768 | -2.20167295 |
| H | -12.05534203 | 7.37012604 | -1.91008904 |
| H | -11.85454515 | 8.3059514 | -0.43851736 |
| C | -13.72426696 | 9.59178717 | -2.05310163 |
| H | -11.74281693 | 10.41807742 | -1.79657476 |
| H | -11.93941100 | 9.48349475 | -3.26804110 |
| H | -14.12786648 | 10.47337358 | -2.56095798 |
| H | -14.21404788 | 8.70918985 | -2.48033192 |
| H | -14.01690684 | 9.65260005 | -0.99869896 |
| C | 12.20960939 | -5.97193963 | 0.52299040 |
| C | 13.68514241 | -6.15892540 | 0.15014851 |
| H | 11.62039086 | -6.79474580 | 0.09345803 |
| H | 12.09680235 | -6.05681305 | 1.61324622 |
| C | 14.26937697 | -7.50049415 | 0.60940271 |
| Atom | X-Coordinate | Y-Coordinate | Z-Coordinate |
|------|--------------|--------------|--------------|
| H    | -1.03566217  | 4.99437337   | -1.12042727  |
| C    | -4.07776506  | 4.02886424   | 0.02194704   |
| H    | -4.47840696  | 2.23959421   | 1.13957492   |
| H    | -3.35409674  | 5.72866682   | -1.11547019  |
| B    | 1.04924788   | -2.38192041  | -0.04739695  |
| N    | 3.52263723   | 3.15326123   | 0.09624001   |
| C    | 3.70192633   | 4.44374551   | 0.27361898   |
| N    | -1.26206787  | -0.45635507  | -0.06774715  |
| C    | -1.44541825  | -1.74665903  | -0.24126513  |
| B    | 1.20910445   | 5.07520149   | 0.05232342   |
| N    | 2.72089125   | 5.37149574   | 0.34584924   |
| C    | 3.30439799   | 6.62191741   | 0.56966838   |
| C    | 4.73094245   | 6.50033353   | 0.64543481   |
| C    | -2.48117457  | -3.80226085  | -0.59924187  |
| C    | -1.05425498  | -3.92627680  | -0.53486835  |
| F    | 1.82355017   | -2.88078750  | -1.06382620  |
| F    | 1.36783283   | -2.92866403  | 1.19104736   |
| F    | 0.91057307   | 5.61373648   | -1.19484188  |
| F    | 0.41735397   | 5.57896021   | 1.05225102   |
| O    | -5.39178285  | 4.34423491   | 0.08081546   |
| O    | 7.63185181   | -1.70247558  | -0.27567004  |
| C    | -5.85356355  | 5.54831542   | -0.54580914  |
| C    | -7.35872093  | 5.62963436   | -0.34059084  |
| H    | -5.60626932  | 5.52492375   | -1.61602465  |
| H    | -5.34793273  | 6.41511209   | -0.09914962  |
| C    | -7.96949924  | 6.87744332   | -0.99047603  |
| H    | -7.81784034  | 4.72487718   | -0.75718213  |
| H    | -7.56857423  | 5.62226860   | 0.73581288   |
| C    | -9.48964596  | 6.96811629   | -0.80761615  |
| H    | -7.49957179  | 7.77809133   | -0.57110983  |
| H    | -7.73427762  | 6.88343827   | -2.06419611  |
| H    | -9.95782735  | 6.06381314   | -1.22105831  |
| H    | -9.72644426  | 6.96847164   | 0.26555989   |
| C    | 8.08073493   | -2.97104827  | 0.22000465   |
| C    | 9.55246360   | -3.11321216  | -0.13766588  |
| H    | 7.48800472   | -3.77493223  | -0.23679019  |
| H    | 7.93366365   | -3.01650681  | 1.30789844   |
| C    | 10.13996294  | -4.45177678  | 0.32670604   |
| H    | 9.65781115   | -3.01302681  | -1.22468982  |
| H    | 10.10748387  | -2.28011764  | 0.31052191   |
| C    | 11.61740732  | -4.62198672  | -0.04825282  |
| H    | 10.02889252  | -4.54493149  | 1.41618187   |
| H    | 9.55978012   | -5.27691865  | -0.10987208  |
|  | X       | Y       | Z       |
|---|---------|---------|---------|
| H | 11.72722330 | -4.51956740 | -1.13694840 |
| H | 12.20101493 | -3.80218326 | 0.39359965  |
| C | -10.10968505 | 8.20649708  | -1.46588673 |
| C | -11.63067657 | 8.29541246  | -1.29276957 |
| H | -9.86636223 | 8.20672785  | -2.53801306 |
| H | -9.64326423 | 9.11088905  | -1.04996768 |
| C | -12.25252821 | 9.53002213  | -1.95694496 |
| H | -12.09692641 | 7.38935622  | -1.70572007 |
| H | -11.87545392 | 8.29898133  | -0.22091488 |
| C | -13.77212326 | 9.60937915  | -1.78334681 |
| H | -11.78860543 | 10.43553312 | -1.54284398 |
| H | -12.0604069 | 9.52662470  | -3.02745201 |
| H | -14.18511381 | 10.49926226 | -2.26922615 |
| H | -14.26674347 | 8.7334183  | -2.21826919 |
| H | -14.04850753 | 9.65097297  | 0.72365254  |
| C | -13.20866161 | -9.65097297 | 0.39662017  |
| C | -13.68177644 | 6.14360499  | 0.01033620  |
| H | 11.61792845 | 6.78290299  | -0.04023154 |
| H | 12.10396993 | 6.06541268  | 1.48634494  |
| C | -3.21782490 | -7.49018117 | 0.44700683  |
| H | -13.78657593 | -6.03929502 | -1.07912589 |
| H | -14.27503023 | -5.32885063 | 0.44978569  |
| C | -1.574149250 | -7.66317761 | 0.05259159  |
| H | -14.17026116 | -7.59337727 | 1.53593197  |
| H | -13.67713948 | -8.30369254 | 0.00960037  |
| H | -16.13168004 | -8.63349198 | 0.37631342  |
| H | -15.87054749 | -7.59883411 | -1.03381243 |
| H | -16.36774629 | -6.88574899 | 0.50487784  |
| C | -2.83488760 | -2.35834572 | 0.40661887  |
| H | -3.35326692 | -1.90844087 | -1.25968563 |
| H | -3.44506309 | -2.16761868 | 0.48286026  |
| C | 5.08887373  | 5.05760000  | 0.45178286  |
| H | 5.60138477  | 4.60637173  | 1.30767981  |
| H | 5.70646221  | 4.87043627  | 0.43334467  |
| N | -3.12097240 | -4.91984513 | -0.79949047 |
| N | 5.36704264  | 7.61859336  | 0.85366421  |
| N | -0.56686267 | -5.12757431 | -0.68143697 |
| N | 2.81359423  | 7.82195097  | 0.71524910  |
| S | -1.92040286 | -6.10766629 | -0.90270256 |
| S | 4.16334808  | 8.80396222  | 0.94998871  |
Table S5: The Cartesian coordinates of 1–8 in S₁ at the TD-B3LYP/6-31G(d,p) level

|  | C                  | 0.00000000 | 0.00000000 | 0.00000000 |
|  | C                  | 2.28014064 | 0.00000000 | 0.00000000 |
|  | C                  | 1.82601486 | 1.35466384 | 0.00000000 |
|  | C                  | 0.41913259 | 1.36446777 | 0.04021943 |
|  | C                  | 2.24518382 | 2.71910812 | 0.04021473 |
|  | C                  | -0.03497060 | 2.71914973 | 0.04021861 |
|  | N                  | 1.10271813 | 3.51613145 | 0.04354061 |
|  | N                  | 1.14249870 | -0.79699341 | -0.00331805 |
|  | C                  | 3.64904528 | -0.46862917 | 0.03036134 |
|  | C                  | 4.66968409 | 0.34295794 | -0.53200148 |
|  | C                  | 5.36693666 | -2.09102047 | 0.64838416 |
|  | H                  | 3.29877398 | -2.31475153 | 1.10702065 |
|  | C                  | 5.99092179 | -0.05696977 | -0.52024678 |
|  | H                  | 4.41032290 | 1.29360354 | -0.9792090 |
|  | C                  | 6.35761595 | -1.28081364 | 0.06796122 |
|  | H                  | 5.62479241 | -3.02755020 | 1.12730954 |
|  | H                  | 6.76701138 | 0.55811850 | -0.96312622 |
|  | C                  | -1.40387172 | 3.18779926 | 0.00998693 |
|  | C                  | -2.42441132 | 2.37635890 | 0.57276099 |
|  | C                  | -1.79402609 | 4.40897900 | -0.58622340 |
|  | C                  | -3.74563879 | 2.77632168 | 0.56125666 |
|  | H                  | -2.16497826 | 1.42583011 | 1.02017407 |
|  | C                  | -3.12189434 | 4.81009504 | -0.60796793 |
|  | H                  | -1.05387767 | 5.03308587 | -1.06722891 |
|  | C                  | -4.11245151 | 4.00004166 | -0.02713130 |
|  | H                  | -4.52162531 | 2.16136085 | 1.00449430 |
|  | H                  | -3.37983100 | 5.74656962 | -1.08696263 |
|  | B                  | 1.04640834 | -2.36010340 | -0.06017851 |
|  | N                  | -0.45339968 | -2.68159072 | -0.42219380 |
|  | N                  | 3.49942921 | 3.18094752 | 0.13217629 |
|  | C                  | 3.67035361 | 4.46890078 | 0.34178372 |
|  | S                  | 5.29137661 | 5.14260696 | 0.54596780 |
|  | B                  | 1.19888412 | 5.07923260 | 0.10039945 |
|  | N                  | 2.69880330 | 5.40067122 | 0.46217311 |
|  | C                  | 3.18233131 | 6.67490957 | 0.73890089 |
|  | B                  | 2.41752377 | 7.83073953 | 0.94465427 |
|  | C                  | 4.59189463 | 6.73594905 | 0.81268914 |
|  | C                  | 3.08158168 | 9.02521712 | 1.20108991 |
| Atom | x         | y         | z         |
|------|-----------|-----------|-----------|
| H    | 1.33728618| 7.77265685| 0.91493901|
| C    | 5.25053069| 7.93627153| 1.07275974|
| C    | 4.48246404| 9.08350428| 1.26346201|
| H    | 2.50191583| 9.92896945| 1.36104419|
| H    | 6.33354058| 7.97536518| 1.12668329|
| H    | 4.97539997| 10.0289204| 1.46661971|
| C    | -2.34638529| -4.01695837| -0.77295638|
| C    | -0.93683081| -3.95583152| -0.69907187|
| C    | -3.00492107| -5.21730009| -1.03318847|
| C    | -0.17193083| -5.11158826| -0.90489337|
| C    | -2.23676494| -6.36446166| -1.22395996|
| H    | -4.08792577| -5.2564052| -1.08718602|
| C    | -0.83589138| -6.3008607| -1.16149357|
| H    | 0.90830033| -5.05342893| -0.87509698|
| H    | -2.72962429| -7.30981646| -1.42724646|
| H    | -0.25615314| -2.0978263| -1.32150363|
| F    | 1.87620628| -2.88373565| -1.03327629|
| F    | 1.30970888| -2.92070519| 1.1882072 |
| F    | 0.93525931| 5.63989229| -1.14850540|
| F    | 0.36938028| 5.60288811| 1.07373479|
| O    | -5.43279037| 4.30109812| 0.00866505|
| O    | 7.67798951| -1.58177350| 0.03252012|
| C    | -5.88778235| 5.53032185| -0.56816020|
| C    | -7.39714530| 5.59644466| -0.38841927|
| H    | -5.61968042| 5.56117008| -1.63338346|
| H    | -5.39514630| 6.37720921| -0.07066482|
| C    | -7.99854277| 6.88201657| -0.96963527|
| H    | -7.84603509| 4.71873826| -0.86914285|
| H    | -7.62738627| 5.52160132| 0.68122365|
| C    | -9.52257653| 6.95758683| -0.81476962|
| H    | -7.54112700| 7.75432264| -0.48183434|
| H    | -7.73953549| 6.95894071| -2.03512035|
| H    | -9.97945745| 6.08700457| -1.30592802|
| H    | -9.78348733| 6.87637907| 0.24974417|
| C    | 8.13281788| -2.81139121| 0.60864590|
| C    | 9.64216525| -2.87767024| 0.42882116|
| H    | 7.64003550| -3.65794866| 0.11074240|
| H    | 7.86475720| -2.84274045| 1.67386635|
| C    | 10.2435402| -4.16365315| 1.00934769|
| H    | 9.87238499| -2.80228289| -0.64078938|
| H    | 10.09122150| -2.00030579| 0.91001010|
| C    | 11.76737241| -4.23941667| 0.85440833|
| H    | 9.98437918| -4.24105903| 2.07480351|
| H    | 9.78575601| -5.03563406| 0.52113403|
| Atoms | x       | y       | z        |
|-------|---------|---------|----------|
| H     | 4.37346197 | 1.30801939 | -1.01666093 |
| C     | 6.35303370  | -1.27553663 | -0.05836607  |
| H     | 5.65649943  | -3.03347184 | 1.00889692   |
| H     | 6.72967742  | 0.57492790  | -1.08315579  |
| C     | -1.39629127 | 3.19157834  | 0.00521688   |
| C     | -2.41378622 | 2.37661358  | 0.57026958   |
| C     | -1.78869151 | 4.41653838  | -0.58415259  |
| C     | -3.73424817 | 2.77602714  | 0.56782929   |
| H     | -2.15161877 | 1.42521684  | 1.01370460   |
| C     | -3.11541876 | 4.81690378  | -0.59786074  |
| H     | -1.05013958 | 5.04516403  | -1.06124880  |
| C     | -4.10375216 | 4.00324575  | -0.01489174  |
| H     | -4.50836669 | 2.16011008  | 1.01276792   |
| H     | -3.37555649 | 5.75659006  | -1.06883428  |
| B     | 1.05789983  | -2.37273280 | -0.05947813  |
| N     | -0.46978057 | -2.69505878 | -0.34335845  |
| N     | 3.50299377  | 3.17742723  | 0.14996526   |
| C     | 3.68576920  | 4.46517752  | 0.33365813   |
| S     | 5.32506256  | 5.10403976  | 0.54452437   |
| N     | -1.25453171 | -0.45785579 | -0.09749794  |
| C     | -1.43743081 | -1.74740754 | -0.26760020  |
| S     | -3.07790699 | -2.39007602 | -0.45713320  |
| B     | 1.19429040  | 5.09512646  | 0.10178527   |
| N     | 2.71831656  | 5.41283446  | 0.41067281   |
| C     | 3.22590675  | 6.68016149  | 0.63074046   |
| C     | 4.64064945  | 6.71879671  | 0.73463890   |
| C     | 3.17982910  | 8.90672613  | 0.94639945   |
| C     | 4.57330645  | 8.93804515  | 1.05111509   |
| H     | 2.60132594  | 9.82264846  | 1.03554512   |
| H     | 5.10045097  | 9.87189271  | 1.22349431   |
| C     | -2.39362419 | -4.00621545 | -0.63592444  |
| C     | -0.97805613 | -3.96510357 | -0.54533416  |
| C     | -2.32680966 | -6.22868546 | -0.92912350  |
| C     | -0.93250541 | -6.19488025 | -0.83768285  |
| H     | -2.85454391 | -7.16483525 | -1.08655720  |
| H     | -0.35385951 | -7.11113237 | -0.92241007  |
| F     | 1.84185533  | -2.85026223 | -1.17721342  |
| F     | 1.37273077  | -2.92556815 | 1.17574647   |
| F     | 0.90226711  | 5.65236270  | -1.13731008  |
| F     | 0.39504529  | 5.57204689  | 1.10747077   |
| O     | -5.42044068 | 4.30347641  | 0.02786566   |
| O     | 7.66690157  | -1.57644219 | -0.14684024  |
| C     | -5.88218497 | 5.53635685  | -0.54177237  |
| C     | -7.39058329 | 5.59789185  | -0.35540000  |
| Symbol | X         | Y         | Z         |
|--------|-----------|-----------|-----------|
| H      | 14.05941999 | -7.83206604 | 0.48905402 |
| H      | 16.51228979 | -7.98948467 | 0.97112796 |
| H      | 16.2444370  | -7.00000511 | -0.47007344|
| H      | 16.62444370 | -6.22761354 | 1.07380559 |
| N      | -0.23859951 | -5.06381768 | 0.64530876 |
| N      | -3.07826001 | -5.11695419 | -0.82598573|
| N      | 5.32458381  | 7.82674154  | 0.94286086 |
| N      | 2.48665635  | 7.77856257  | 0.73553350 |
| C      | 0.00000000  | 0.00000000  | 0.00000000 |
| C      | 2.28266614  | 0.00000000  | 0.00000000 |
| C      | 1.82609150  | 1.35484134  | 0.00000000 |
| C      | 0.41952461  | 1.36284564  | 0.03990451 |
| C      | 2.24561569  | 2.71768530  | 0.03993849 |
| C      | -0.03705164 | 2.71768281  | 0.03990460 |
| N      | 1.09998320  | 3.51734652  | 0.03875301 |
| N      | 1.14564134  | -0.79965907 | 0.00114805 |
| C      | 3.65288324  | -0.46601416 | 0.01586880 |
| C      | 4.05741594  | -1.67841374 | 0.61927075 |
| C      | 4.66228615  | 0.33921047  | -0.57456676|
| C      | 5.38780229  | -2.07533163 | 0.62474005 |
| H      | 3.32645109  | -2.29984345 | 1.11766419 |
| C      | 5.98564358  | -0.05674156 | -0.57833828|
| H      | 4.39079291  | 1.28070901  | -1.03407056|
| C      | 6.36637818  | -1.27043685 | 0.01986266 |
| H      | 5.65518877  | -3.00612056 | 1.10973133 |
| H      | 6.75225947  | 0.55181231  | -1.04680792|
| C      | -1.40727358 | 3.18369360  | 0.02405822 |
| C      | -2.41665106 | 2.37847816  | 0.61455085 |
| C      | -1.81183868 | 4.39607528  | -0.57935778|
| C      | -3.74001228 | 2.77441929  | 0.61835470 |
| H      | -2.14513574 | 1.43699239  | 1.07406660 |
| C      | -3.14222983 | 4.79298097  | -0.58479381|
| H      | -1.08089635 | 5.01750301  | -1.07778671|
| C      | -4.12078011 | 3.98809203  | 0.02013055 |
| H      | -4.50660676 | 2.16586838  | 1.08686447 |
| H      | -3.40963741 | 5.72375785  | -1.06993848|
| B      | 1.06395601  | -2.37188583 | -0.03880828 |
| N      | -0.42439713 | -2.68275264 | -0.39183794 |
| N      | 3.50426623  | 3.17175850  | 0.14185350 |
| C      | 3.65032394  | 4.46868922  | 0.34267004 |
| N      | -1.25864273 | -0.45408968 | -0.10188623|
| C      | -1.40469486 | -1.75102810 | -0.30266384|
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| B    | 1.18166990 | 5.08957001 | 0.07869095 |
| N    | 2.67003640 | 5.40042330 | 0.43182245 |
| C    | 3.2579843  | 6.62626139 | 0.70940143 |
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N  2.71024161  5.38762076  0.42949899
C  3.28602892  6.62875822  0.68145494
C  4.71589962  6.51254644  0.75803993
C  -2.46566438  -3.80183704  -0.65740557
C  -1.03499442  -3.91583402  -0.59424868
F  1.84492516  -2.85923296  -1.08079105
F  1.36361466  -2.9378051  1.16630591
F  0.91961425  5.65856652  -1.13221380
F  0.39479622  5.58162564  1.10539936
O  -5.40421928  4.33982574  0.00293763
O  7.65518268  -1.6134657  -0.14812141
C  -5.85398390  5.58199981  -0.55914214
C  -7.36187659  5.65723043  -0.37518008
H  -5.58684058  5.62048890  -1.62384523
H  -5.35206251  6.41652252  -0.05153384
C  -7.95081994  6.95441610  -0.94400615
H  -7.81935121  4.78857693  -0.86411110
H  -7.59118584  5.57480056  0.69401558
C  -9.47403845  7.04370527  -0.78838698
H  -7.48465650  7.81727426  -0.44799277
H  -7.69112639  7.03866883  -2.00873282
H  -9.93970770  6.18204942  -1.28695919
H  -9.73592767  6.95600139  0.27537316
C  8.12647673  -2.87108246  0.35442980
C  9.61411349  -2.95687968  0.04916856
H  7.57638495  -3.68839034  -0.13046378
H  7.94049652  -2.92817727  1.43549777
C  10.24026510  -4.27141551  0.53149165
H  9.75436918  -2.84862293  -1.03314639
H  10.11908073  -2.10399345  0.51870899
C  11.73724916  -4.36882679  0.21150983
H  10.09288368  -4.37441257  1.61573733
H  9.71524051  -5.11967509  0.07026606
Fig. S1. Geometries of PPB.