Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Electronic Supplementary Information

# Excited-State Non-Radiative Decay in Stilbenoid Compounds: An *ab initio* Quantum-Chemistry Study on Size and Substituent Effects

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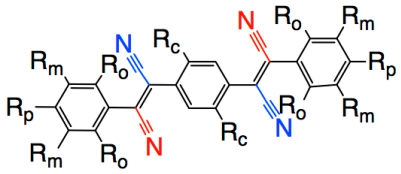


α- DCS

| Label | $R_c$ | $R_o$ | $R_m$ | $R_p$ |
|---|---|---|---|---|
| 1 | | | | |
| 2 | | | | $OC_4H_9$ |
| 3 | $C_6H_{13}$ | | | |
| 4 | $OCH_3$ | | | |
| 5 | $OCH_3$ | | | $OC_4H_9$ |
| 6 | | | $CF_3$ | |
| 7 | $OCH_3$ | $OCH_3$ | | |
| 8 | | | $OC_{12}H_{25}$ | $OC_{12}H_{25}$ |
| 9 | | | | CONHR |
| 10 | | | | $N(C_4H_9)_2$ |
| 11 | $OCH_3$ | | | $N(CH_3)_2$ |
| 12 | | | | $NPh_2$ |

β- DCS

| Label | $R_c$ | $R_o$ | $R_m$ | $R_p$ |
|---|---|---|---|---|
| 13 | | | | |
| 14 | $C_6H_{13}$ | | | |
| 15 | $C_6H_{13}$ | $C_6H_{13}$ | $C_6H_{13}$ | |
| 16 | Ph | | | |
| 17 | | | $CF_3$ | |
| 18 | | | | $OC_4H_9$ |
| 19 | $OCH_3$ | | | |
| 20 | $OCH_3$ | $CH_3O$ | | |
| 21 | $OCH_3$ | | | $OC_4H_9$ |
| 22 | | | | OPh |
| 23 | | | $CF_3$ | |
| 24 | | | | CONHR |
| 25 | Ph | | | $NPh_2$ |
| 26 | $OCH_3$ | | | $N(CH_3)_2$ |
| 27 | $NPh_2$ | | $CF_3$ | |
| 28 | $PhNPh_2$ | | $OCH_3$ | |
| 29 | PCz | | | $OC_6H_{13}$ |
| 30 | PCz | | $CH_3$ | |
| 31 | PCz | | $CF_3$ | |
| 32 | CzR | | | $CF_3$ |
| 33 | CzR | | $CF_3$ | |

**Figure S1.** Chemical structures of the $\alpha,\beta$-DCS-family reported in Shi, J.; Izquierdo, Maria A.; Oh, S; Park, S. Y.; Milián-Medina, Begoña; Roca-Sanjuán, Daniel; Gierschner, J. Inverted Energy Gap Law for the Nonradiative Decay in Fluorescent Floppy Molecules: Larger Fluorescence Quantum Yields for Smaller Energy Gaps. *Org. Chem. Front.* **2019**, DOI: 10.1039/c9qo00259f. $R_x$ represents a functional group substitution in the position *o, m*, and *p* (ortho, meta, and para), respectively, Ph=phenyl, Cz=carbazole, R=alkyl.

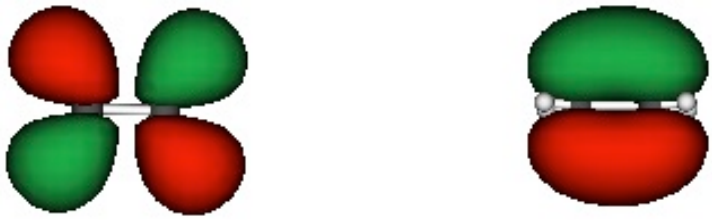

**Figure S2.** Contour plots of the natural orbitals that compose the CAS(2,2) for CASPT2 PESs of ethene. Density value of the isosurfaces of 0.04 a. u.

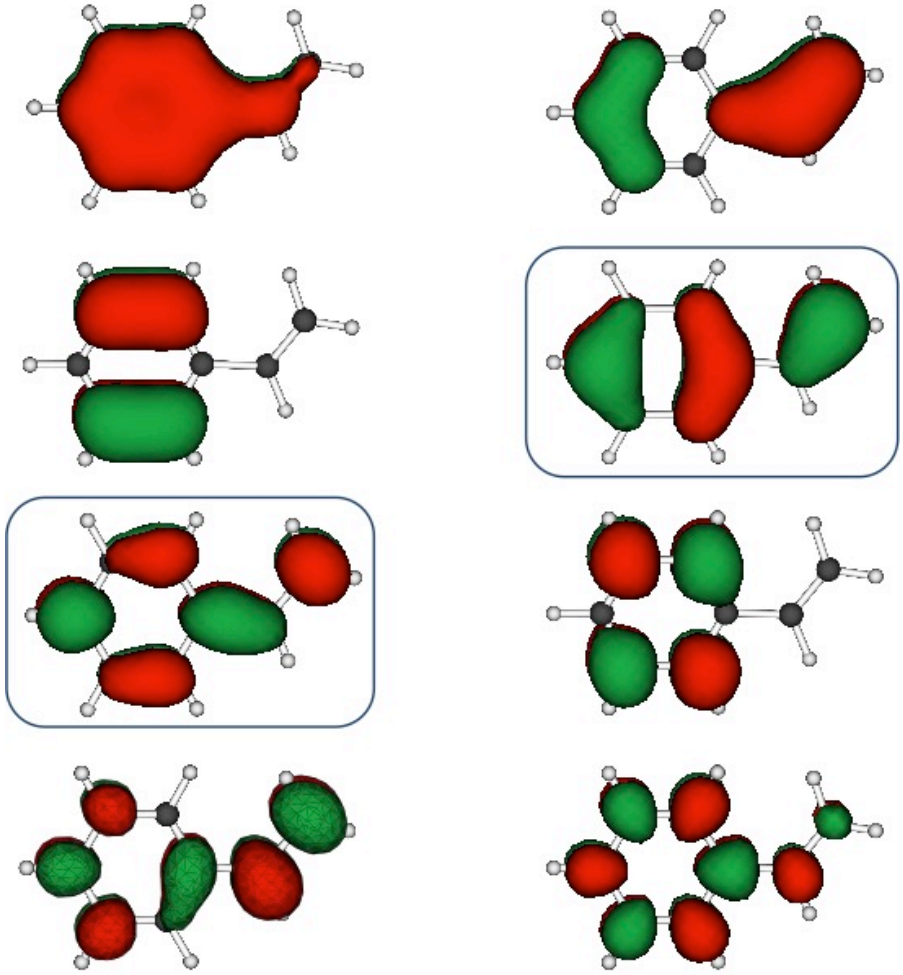

**Figure S3.** Contour plots of the natural orbitals that compose the CAS(2,2) and CAS(8,8) for CASPT2 PESs of styrene. Density value of the isosurfaces of 0.04 a. u.

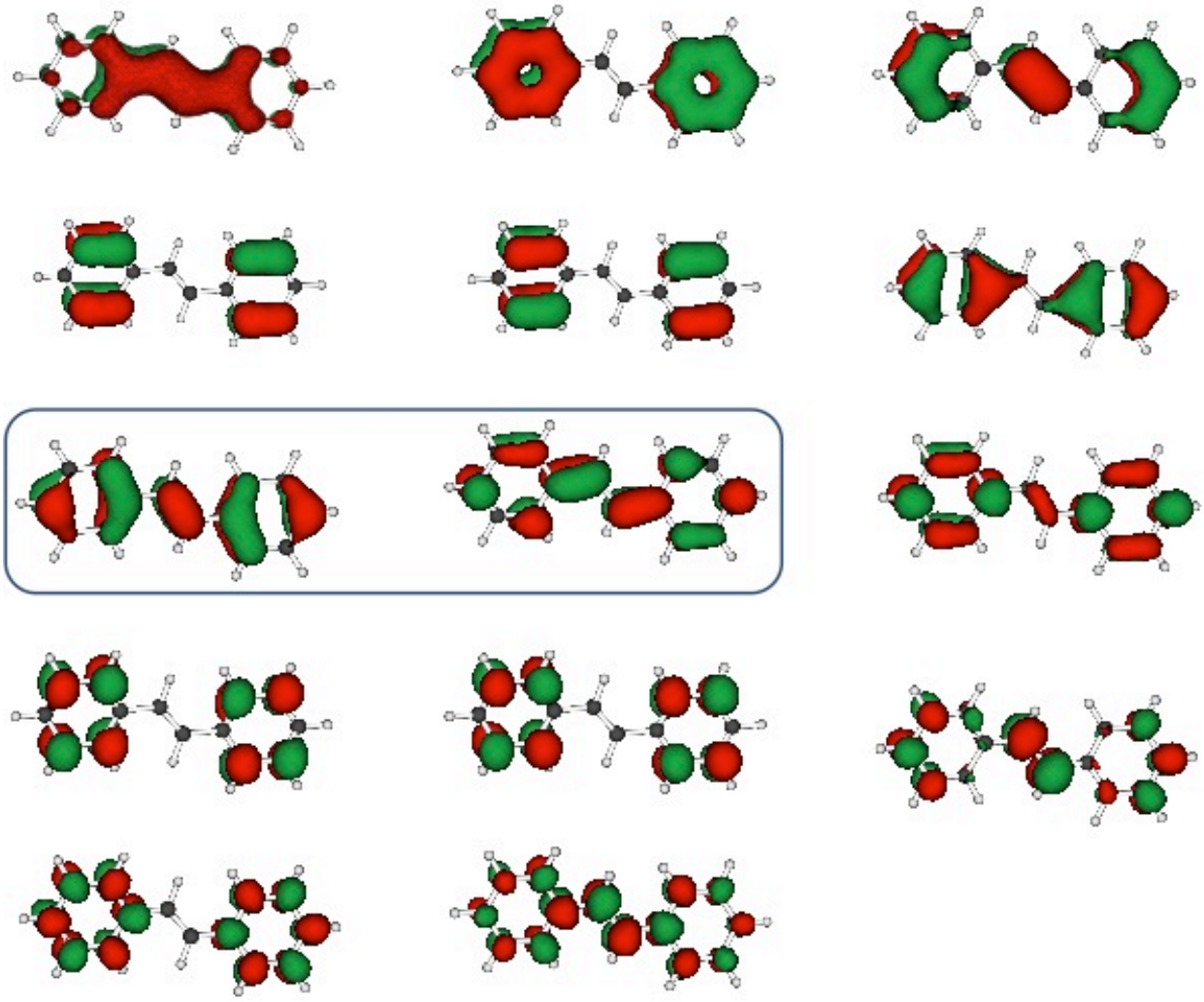

**Figure S4.** Contour plots of the natural orbitals that compose the CAS(2,2) and CAS(14,14) for CASPT2 PESs of stilbene. Density value of the isosurfaces of 0.04 a. u.

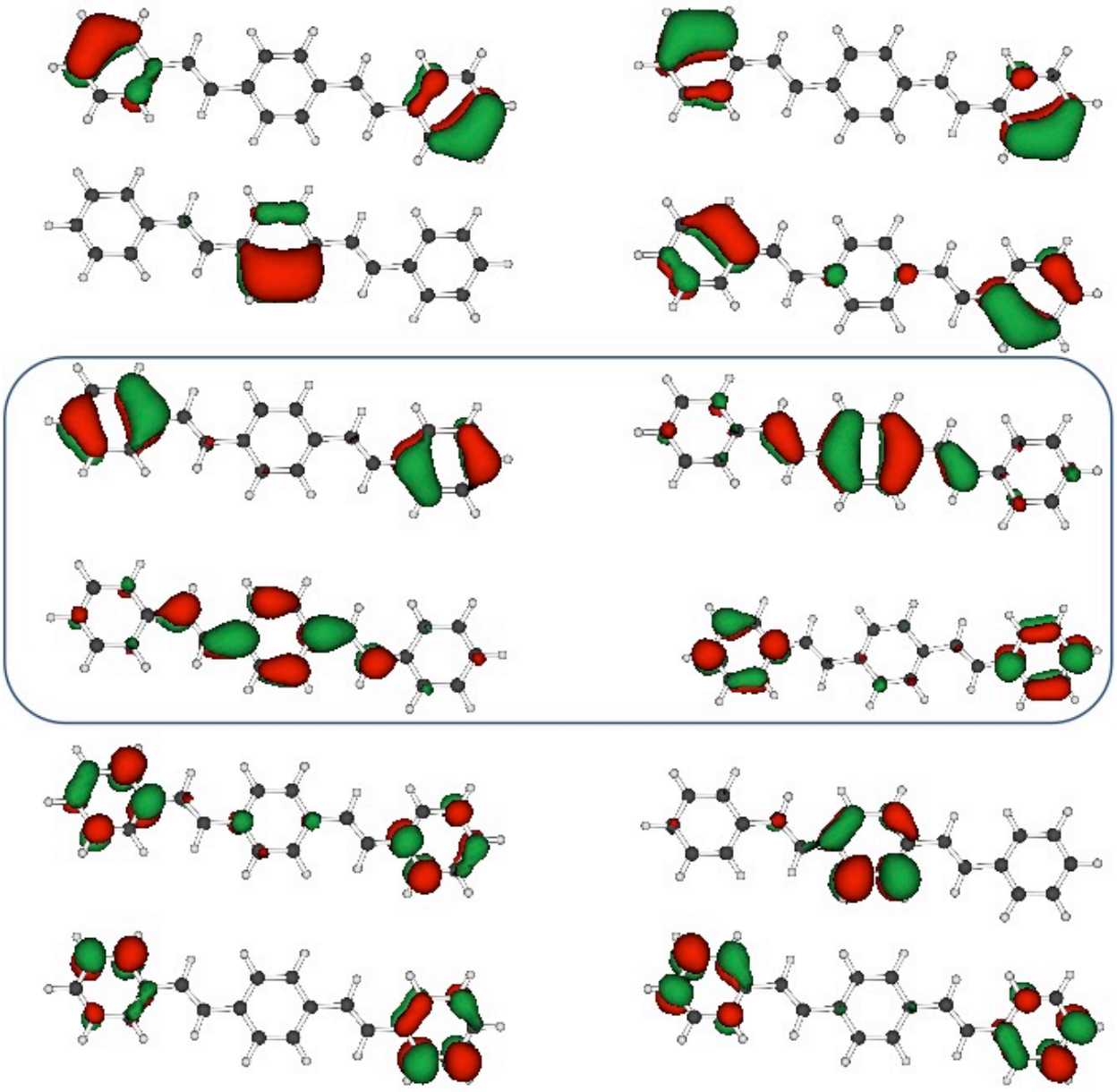

**Figure S5.** Contour plots of the natural orbitals that compose the CAS(4,4) and CAS(12,12) for CASPT2 PESs of DSB. Density value of the isosurfaces of 0.04 a. u.

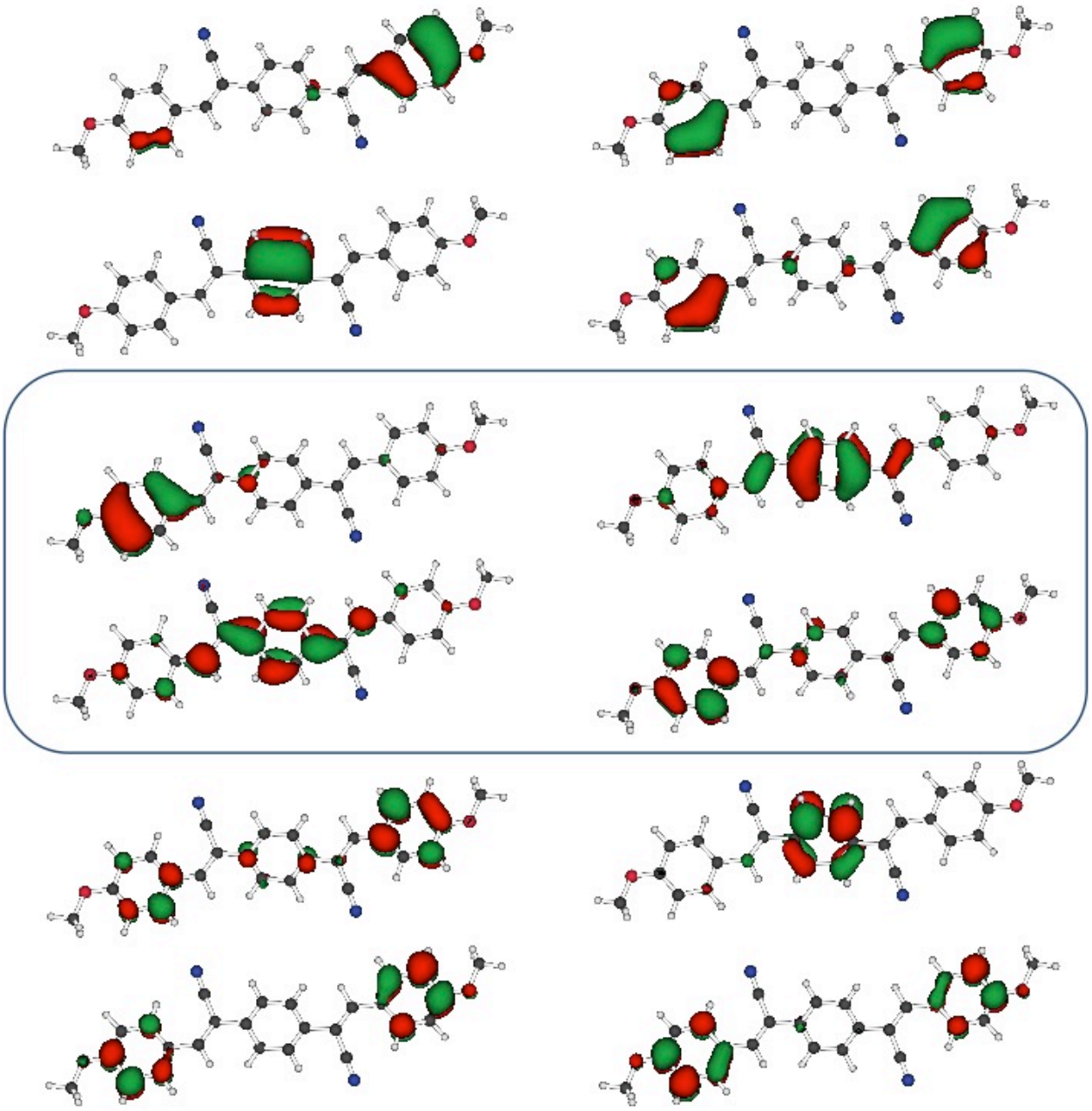

**Figure S6.** Contour plots of the natural orbitals that compose the CAS(4,4) and CAS(12,12) for CASPT2 PESs of $\alpha$-DMDCS. Density value of the isosurfaces of 0.04 a. u.

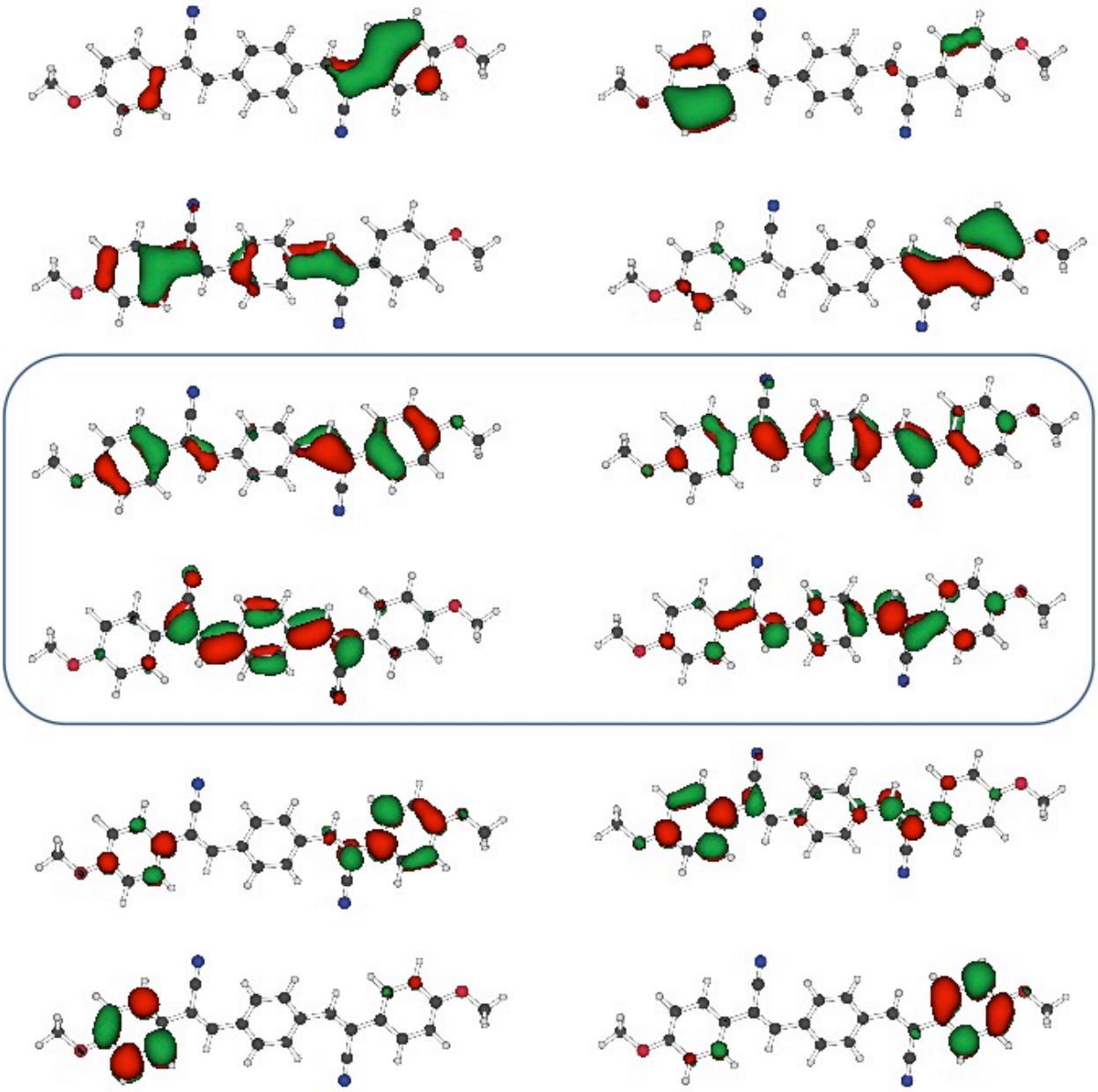

**Figure S7.** Contour plots of the natural orbitals that compose the CAS(4,4) and CAS(12,12) for CASPT2 PESs of $\beta$-DMDCS. Density value of the isosurfaces of 0.04 a. u.

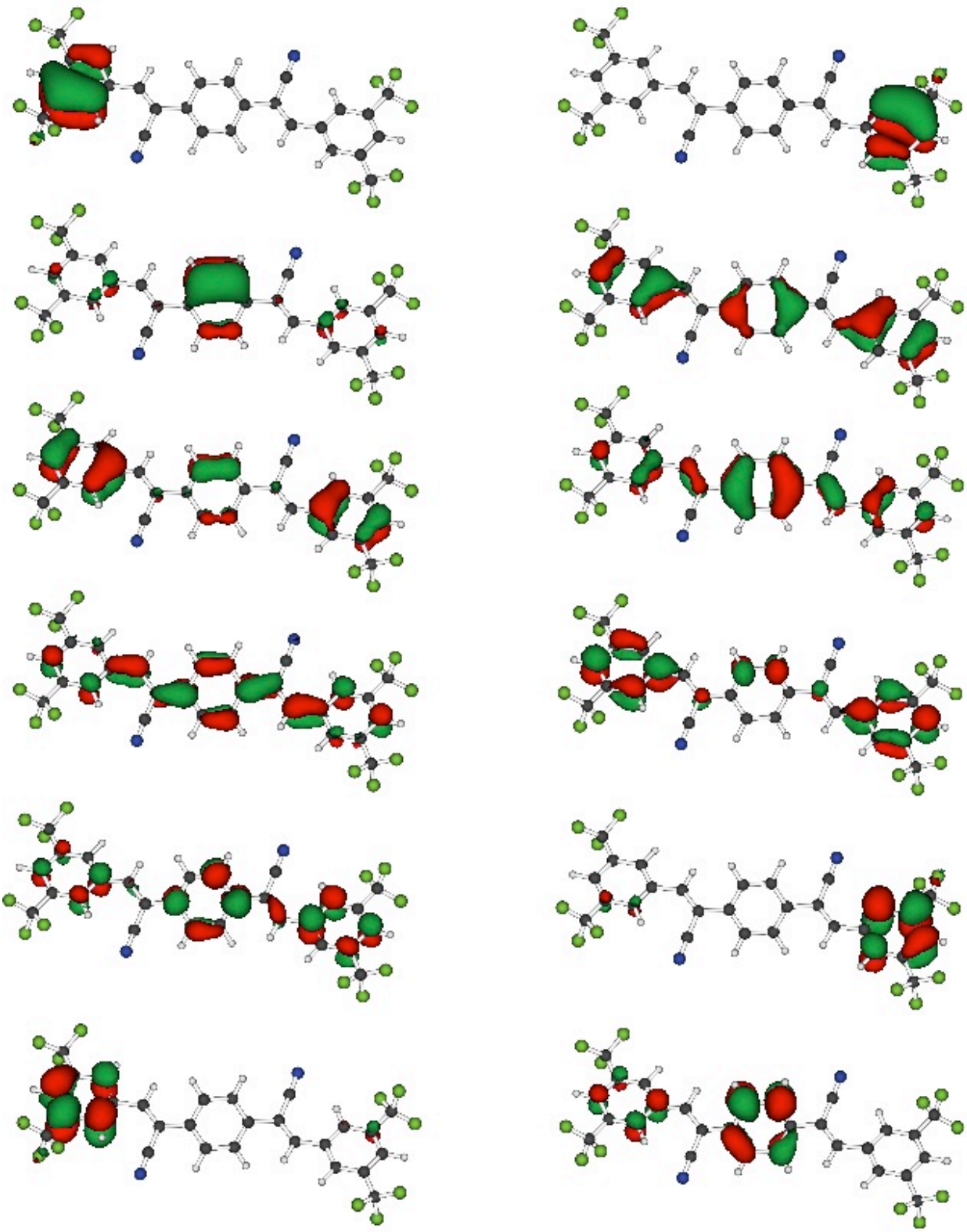

**Figure S8.** Contour plots of the natural orbitals that compose the CAS(12,12) for CASPT2 PESs of $\alpha$-TFDCS. Density value of the isosurfaces of 0.04 a. u.

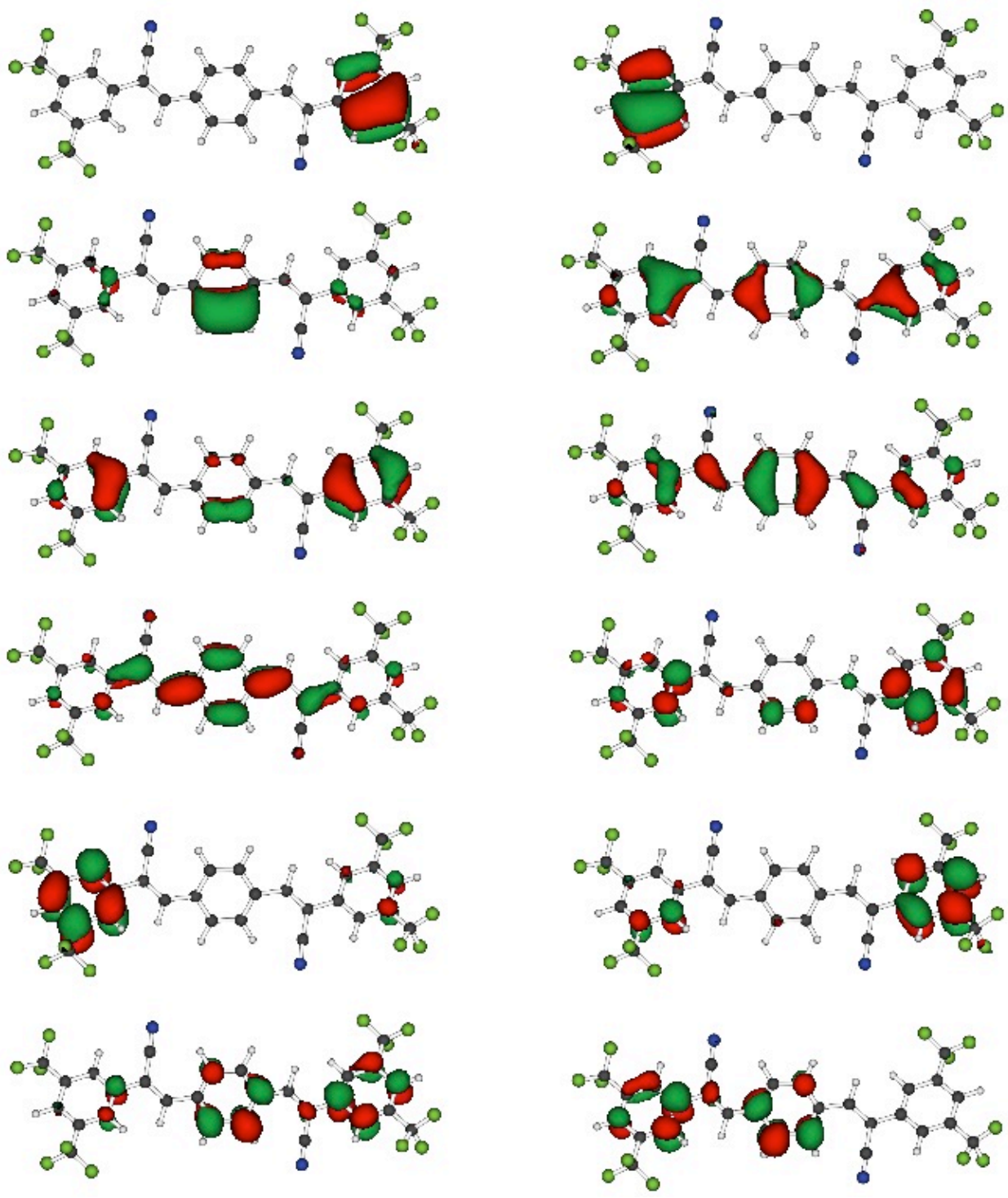

**Figure S9.** Contour plots of the natural orbitals that compose the CAS(12,12) for CASPT2 PESs of $\beta$-TFDCS. Density value of the isosurfaces of 0.04 a. u.

**Cartesian coordinates (in Å) of optimized structures of the $S_0$ obtained with CAM-B3LYP/cc-pVTZ**

**Ethene**

| | | | |
|---|---|---|---|
| C | 0.000000 | 0.000000 | -0.659472 |
| C | 0.000000 | 0.000000 | 0.659472 |
| H | -0.920856 | 0.000000 | -1.226963 |
| H | 0.920856 | 0.000000 | -1.226963 |
| H | -0.920856 | 0.000000 | 1.226963 |
| H | 0.920856 | 0.000000 | 1.226963 |

**Styrene**

| | | | |
|---|---|---|---|
| C | -0.110483 | -0.300265 | -1.747081 |
| C | -0.435103 | -0.978412 | -0.656298 |
| C | -1.659410 | -0.844390 | 0.144802 |
| C | -2.674568 | 0.059480 | -0.164823 |
| C | -3.806812 | 0.147788 | 0.619736 |
| C | -3.953392 | -0.665135 | 1.733991 |
| C | -2.955330 | -1.566754 | 2.054374 |
| C | -1.821178 | -1.652954 | 1.265714 |
| H | -0.750931 | 0.458218 | -2.175318 |
| H | 0.823913 | -0.485868 | -2.256103 |
| H | -1.042832 | -2.360404 | 1.520888 |
| H | 0.262879 | -1.723545 | -0.290211 |
| H | -2.579188 | 0.701630 | -1.028757 |
| H | -4.582750 | 0.855571 | 0.362342 |
| H | -4.841277 | -0.593615 | 2.346456 |
| H | -3.057947 | -2.205854 | 2.920442 |

**Stilbene**

| | | | |
|---|---|---|---|
| C | 0.100072 | -0.285468 | -1.505066 |
| C | -0.507446 | -1.173785 | -0.721102 |
| C | -1.699693 | -0.947517 | 0.098819 |
| C | -2.252306 | 0.315346 | 0.315468 |
| C | -3.383785 | 0.470197 | 1.090769 |
| C | -3.991634 | -0.630976 | 1.674842 |
| C | -3.451875 | -1.888940 | 1.477161 |
| C | -2.317844 | -2.041944 | 0.699977 |
| C | 1.292223 | -0.511806 | -2.325111 |

| | | | |
|---|---|---|---|
| C | 2.074684 | -1.663900 | -2.238100 |
| C | 3.184180 | -1.829376 | -3.042438 |
| C | 3.545488 | -0.847046 | -3.952206 |
| C | 2.785664 | 0.304867 | -4.045259 |
| C | 1.674264 | 0.468807 | -3.238192 |
| H | -0.314224 | 0.712892 | -1.583947 |
| H | 1.084104 | 1.372668 | -3.316306 |
| H | -1.900824 | -3.029243 | 0.549353 |
| H | -0.118273 | -2.184252 | -0.675431 |
| H | -1.786822 | 1.189584 | -0.116611 |
| H | -3.793570 | 1.458661 | 1.246819 |
| H | -4.876256 | -0.505645 | 2.283249 |
| H | -3.913625 | -2.755345 | 1.930157 |
| H | 1.821497 | -2.435800 | -1.525550 |
| H | 3.777156 | -2.729557 | -2.956468 |
| H | 4.416299 | -0.979052 | -4.578853 |
| H | 3.058712 | 1.080310 | -4.747548 |

**DSB**

| | | | |
|---|---|---|---|
| C | -1.386965 | -5.071803 | -0.042109 |
| C | -2.610713 | -5.675103 | -0.325525 |
| C | -2.742171 | -7.051581 | -0.361557 |
| C | -1.647641 | -7.858661 | -0.109682 |
| C | -0.423668 | -7.274731 | 0.180792 |
| C | -0.294536 | -5.901047 | 0.216250 |
| C | -1.310225 | -3.610074 | -0.025925 |
| C | -0.208637 | -2.869310 | 0.087849 |
| C | -0.134508 | -1.409651 | 0.104643 |
| C | 1.118658 | -0.795749 | 0.084154 |
| C | 1.254399 | 0.575392 | 0.091499 |
| C | 0.135470 | 1.406302 | 0.120081 |
| C | -1.117305 | 0.792291 | 0.155060 |
| C | -1.253052 | -0.578865 | 0.147586 |
| C | 0.209258 | 2.866069 | 0.122717 |
| C | 1.303701 | 3.608990 | -0.036785 |
| C | 1.380161 | 5.070821 | -0.033657 |
| C | 2.587714 | 5.679014 | -0.370911 |
| C | 2.717752 | 7.055952 | -0.391810 |
| C | 1.638243 | 7.858502 | -0.070320 |
| C | 0.430818 | 7.269555 | 0.274302 |
| C | 0.303080 | 5.895445 | 0.294551 |
| H | -3.471386 | -5.049527 | -0.523640 |

| | | | |
|---|---|---|---|
| H | -3.702945 | -7.493807 | -0.586087 |
| H | -1.745198 | -8.934884 | -0.134630 |
| H | 0.436072 | -7.897713 | 0.385887 |
| H | 0.666255 | -5.469541 | 0.457562 |
| H | -2.244761 | -1.006260 | 0.185668 |
| H | -2.266420 | -3.111811 | -0.134981 |
| H | 0.751284 | -3.366760 | 0.162558 |
| H | 2.005549 | -1.415784 | 0.062992 |
| H | 2.246914 | 1.002559 | 0.084758 |
| H | -0.644007 | 5.459787 | 0.578759 |
| H | -2.003849 | 1.412200 | 0.189966 |
| H | -0.745217 | 3.361879 | 0.255514 |
| H | 2.252641 | 3.112896 | -0.203736 |
| H | 3.436589 | 5.057002 | -0.623628 |
| H | 3.665706 | 7.502042 | -0.659109 |
| H | 1.734846 | 8.935025 | -0.083169 |
| H | -0.416750 | 7.888879 | 0.533891 |

**$\alpha$-DMDCS**

| | | | |
|---|---|---|---|
| C | -6.090606 | 0.406441 | -0.291380 |
| C | -7.389110 | -0.080895 | -0.156831 |
| C | -7.675384 | -1.433148 | -0.157048 |
| C | -6.639139 | -2.345515 | -0.300317 |
| C | -5.332159 | -1.881055 | -0.442365 |
| C | -5.061926 | -0.535783 | -0.438052 |
| C | -5.921704 | 1.849645 | -0.274639 |
| C | -4.828877 | 2.633851 | -0.295869 |
| C | -3.505006 | 2.095400 | -0.287048 |
| C | -4.908165 | 4.113221 | -0.293807 |
| C | -3.881628 | 4.876708 | 0.255417 |
| C | -3.958958 | 6.253304 | 0.291768 |
| C | -5.055593 | 6.925872 | -0.239284 |
| C | -6.082132 | 6.162383 | -0.788505 |
| C | -6.004801 | 4.785787 | -0.824858 |
| C | -5.134877 | 8.405246 | -0.237220 |
| C | -6.458734 | 8.943733 | -0.245985 |
| C | -4.042075 | 9.189471 | -0.258451 |
| C | -3.873322 | 10.632684 | -0.241690 |
| C | -2.574884 | 11.120201 | -0.376210 |
| C | -2.288811 | 12.472498 | -0.375966 |
| C | -3.325194 | 13.384710 | -0.232702 |
| C | -4.632111 | 12.920058 | -0.090690 |

| | | | |
|---|---|---|---|
| C | -4.902146 | 11.574748 | -0.095030 |
| C | -8.098460 | -4.215868 | -0.180975 |
| C | -1.866149 | 15.255282 | -0.351986 |
| H | -8.204512 | 0.621999 | -0.046483 |
| H | -8.697044 | -1.759852 | -0.047811 |
| H | -4.539294 | -2.605766 | -0.556721 |
| H | -4.038897 | -0.217286 | -0.552261 |
| H | -6.801933 | 4.231902 | -1.299303 |
| H | -6.861311 | 2.384821 | -0.218512 |
| H | -3.016899 | 4.384958 | 0.678337 |
| H | -3.161827 | 6.807188 | 0.766216 |
| H | -5.925132 | 11.256082 | 0.019145 |
| H | -6.946863 | 6.654133 | -1.211422 |
| H | -3.102433 | 8.654357 | -0.314590 |
| H | -1.759379 | 10.417427 | -0.486553 |
| H | -1.267196 | 12.799353 | -0.485178 |
| H | -5.425084 | 13.644652 | 0.023658 |
| H | -8.747807 | -3.888583 | -0.995151 |
| H | -1.975330 | 16.334307 | -0.311820 |
| H | -1.216768 | 14.928083 | 0.462198 |
| H | -8.545180 | -3.934010 | 0.774353 |
| H | -7.989441 | -5.294909 | -0.221126 |
| H | -1.419369 | 14.973507 | -1.307310 |
| O | -6.796651 | -3.684738 | -0.316683 |
| O | -3.167880 | 14.723956 | -0.216310 |
| N | -7.537342 | 9.334400 | -0.261043 |
| N | -2.426309 | 1.704982 | -0.271955 |

**$\beta$-DMDCS**

| | | | |
|---|---|---|---|
| C | 3.882177 | 3.513790 | -0.828433 |
| C | 5.269845 | 3.513790 | -0.828433 |
| C | 5.997012 | 4.692586 | -0.828433 |
| C | 5.332909 | 5.910030 | -0.839366 |
| C | 3.940213 | 5.927054 | -0.862418 |
| C | 3.232171 | 4.749835 | -0.861548 |
| C | 3.125281 | 2.242316 | -0.792734 |
| C | 3.821698 | 1.107098 | -1.316412 |
| C | 1.885886 | 2.142837 | -0.282139 |
| C | 0.965627 | 1.018665 | -0.170859 |
| C | -0.211255 | 1.233890 | 0.552658 |
| C | -1.155815 | 0.247951 | 0.727340 |
| C | -0.965551 | -1.018756 | 0.170868 |

| | | | |
|---|---|---|---|
| C | 0.211331 | -1.233981 | -0.552649 |
| C | 1.155890 | -0.248041 | -0.727332 |
| C | -1.885820 | -2.142916 | 0.282147 |
| C | -3.125228 | -2.242353 | 0.792718 |
| C | -3.821613 | -1.107094 | 1.316347 |
| C | -3.882171 | -3.513800 | 0.828428 |
| C | -5.269838 | -3.513750 | 0.828386 |
| C | -5.997049 | -4.692518 | 0.828394 |
| C | -5.332994 | -5.909988 | 0.839383 |
| C | -3.940299 | -5.927064 | 0.862477 |
| C | -3.232211 | -4.749874 | 0.861596 |
| C | 7.352743 | 7.159149 | -0.832185 |
| C | -7.352877 | -7.159033 | 0.832219 |
| O | 5.941563 | 7.116605 | -0.842233 |
| O | -5.941693 | -7.116539 | 0.842259 |
| N | 4.419314 | 0.222984 | -1.736697 |
| N | -4.419165 | -0.222935 | 1.736628 |
| H | 5.804519 | 2.574197 | -0.822562 |
| H | 7.074240 | 4.645383 | -0.821526 |
| H | 3.436211 | 6.881903 | -0.897163 |
| H | 2.153767 | 4.792481 | -0.914292 |
| H | 2.039847 | -0.473187 | -1.300132 |
| H | 1.492934 | 3.056579 | 0.144646 |
| H | -0.384905 | 2.206528 | 0.993536 |
| H | -2.039777 | 0.473096 | 1.300137 |
| H | -2.153811 | -4.792563 | 0.914375 |
| H | 0.384980 | -2.206618 | -0.993529 |
| H | -1.492879 | -3.056671 | -0.144625 |
| H | -5.804477 | -2.574136 | 0.822473 |
| H | -7.074275 | -4.645275 | 0.821453 |
| H | -3.436335 | -6.881931 | 0.897265 |
| H | -7.772008 | -6.677205 | 1.717725 |
| H | -7.758938 | -6.684593 | -0.063338 |
| H | 7.771895 | 6.677380 | -1.717713 |
| H | 7.623293 | 8.210294 | -0.834506 |
| H | -7.623467 | -8.210167 | 0.834589 |
| H | 7.758820 | 6.684684 | 0.063351 |

**$\alpha$-TFDCS**

| | | | |
|---|---|---|---|
| C | 5.227899 | 0.143694 | 0.042335 |
| C | 5.952786 | 1.332652 | -0.026481 |
| C | 7.333090 | 1.326526 | -0.044824 |

| | | | |
|---|---|---|---|
| C | 8.027749 | 0.133460 | 0.017300 |
| C | 7.317079 | -1.050862 | 0.100520 |
| C | 5.935989 | -1.056065 | 0.113342 |
| C | 8.083148 | 2.627689 | -0.074579 |
| C | 8.063100 | -2.356391 | 0.133891 |
| C | 3.771575 | 0.260908 | 0.053066 |
| C | 2.808414 | -0.657592 | -0.116348 |
| C | 3.105500 | -2.024719 | -0.417407 |
| C | 1.366553 | -0.324795 | -0.050158 |
| C | 0.438722 | -1.063777 | -0.778460 |
| C | -0.901870 | -0.742064 | -0.750342 |
| C | -1.366683 | 0.316082 | 0.024310 |
| C | -0.438873 | 1.055030 | 0.752660 |
| C | 0.901688 | 0.733287 | 0.724577 |
| C | -2.808479 | 0.648915 | 0.090556 |
| C | -3.105893 | 2.015907 | 0.392269 |
| C | -3.772009 | -0.269246 | -0.078252 |
| C | -5.228122 | -0.149186 | -0.064730 |
| C | -5.955895 | -1.335019 | 0.023991 |
| C | -7.336194 | -1.325035 | 0.039996 |
| C | -8.027646 | -0.131291 | -0.043716 |
| C | -7.314008 | 1.049536 | -0.147545 |
| C | -5.932831 | 1.050900 | -0.157466 |
| C | -8.089446 | -2.616525 | 0.186436 |
| C | -8.056532 | 2.355828 | -0.214105 |
| H | 5.427062 | 2.275595 | -0.075262 |
| H | 5.421565 | -1.999637 | 0.189621 |
| H | 1.587271 | 1.300654 | 1.336975 |
| H | 3.424026 | 1.275760 | 0.195219 |
| H | 0.771319 | -1.890292 | -1.390287 |
| H | -1.587538 | -1.309521 | -1.362581 |
| H | -5.415559 | 1.991036 | -0.254471 |
| H | -0.771496 | 1.881513 | 1.364517 |
| H | -3.425750 | -1.284689 | -0.219452 |
| H | -5.432816 | -2.279288 | 0.074647 |
| H | -9.106825 | -0.121505 | -0.049750 |
| H | 9.106927 | 0.125455 | 0.007628 |
| F | -9.283968 | -2.567017 | -0.413762 |
| F | -8.309349 | -2.910174 | 1.476946 |
| F | -9.245854 | 2.217938 | -0.815158 |
| F | -7.370865 | 3.286389 | -0.885469 |
| F | -8.291737 | 2.844140 | 1.012437 |
| F | -7.415272 | -3.647978 | -0.339397 |
| F | 7.381492 | -3.304357 | 0.784451 |

| | | | |
|---|---|---|---|
| F | 9.253578 | -2.229577 | 0.735203 |
| F | 8.296800 | -2.814680 | -1.104555 |
| F | 7.397835 | 3.582346 | -0.717267 |
| F | 9.269665 | 2.504908 | -0.679758 |
| F | 8.319134 | 3.083646 | 1.165476 |
| N | -3.300478 | 3.117265 | 0.644082 |
| N | 3.299881 | -3.126182 | -0.668960 |

**$\beta$-TFDCS**

| | | | |
|---|---|---|---|
| C | -5.278031 | -0.299060 | 0.197778 |
| C | -6.235373 | -1.290865 | 0.012727 |
| C | -7.565564 | -0.957477 | -0.156717 |
| C | -7.973017 | 0.363597 | -0.133193 |
| C | -7.026153 | 1.349762 | 0.070426 |
| C | -5.693754 | 1.026093 | 0.242517 |
| C | -8.589259 | -2.045240 | -0.326220 |
| C | -7.449813 | 2.788034 | 0.166804 |
| C | -3.845711 | -0.657205 | 0.339123 |
| C | -3.595572 | -1.953002 | 0.888201 |
| C | -2.857881 | 0.163678 | -0.054109 |
| C | -1.408110 | 0.030598 | -0.000205 |
| C | -0.659910 | 1.025708 | -0.635849 |
| C | 0.716187 | 1.005993 | -0.651702 |
| C | 1.411932 | -0.024359 | -0.016098 |
| C | 0.663703 | -1.019164 | 0.620025 |
| C | -0.712385 | -0.999543 | 0.635712 |
| C | 2.861650 | -0.158202 | 0.037251 |
| C | 3.850113 | 0.659448 | -0.361111 |
| C | 3.600933 | 1.952457 | -0.917025 |
| C | 5.281961 | 0.300062 | -0.217899 |
| C | 6.241616 | 1.290482 | -0.043415 |
| C | 7.572740 | 0.955430 | 0.121583 |
| C | 7.977440 | -0.365778 | 0.105045 |
| C | 7.027216 | -1.351751 | -0.088799 |
| C | 5.695194 | -1.026863 | -0.255756 |
| C | 8.580549 | 2.042162 | 0.372540 |
| C | 7.453125 | -2.789226 | -0.187010 |
| H | -5.939592 | -2.329626 | -0.012868 |
| H | -4.981252 | 1.815963 | 0.426187 |
| H | -1.236321 | -1.789957 | 1.146404 |
| H | -3.183228 | 1.087492 | -0.515280 |
| H | -1.176335 | 1.835329 | -1.133728 |

| | | | |
|---|---|---|---|
| H | 1.240108 | 1.796565 | -1.162149 |
| H | 4.981159 | -1.816041 | -0.435758 |
| H | 1.180117 | -1.828596 | 1.118217 |
| H | 3.186456 | -1.080142 | 0.502526 |
| H | 5.950345 | 2.330998 | -0.037285 |
| H | 9.017764 | -0.622610 | 0.230484 |
| H | -9.011262 | 0.620266 | -0.275463 |
| N | -3.440918 | -3.002002 | 1.324525 |
| N | 3.446480 | 2.999140 | -1.358944 |
| F | -9.629679 | -1.635729 | -1.062706 |
| F | -9.078331 | -2.442419 | 0.857763 |
| F | -8.073904 | -3.126864 | -0.921552 |
| F | -6.512135 | 3.614186 | -0.318615 |
| F | -7.665726 | 3.150199 | 1.440306 |
| F | -8.580874 | 3.022180 | -0.506887 |
| F | 8.272959 | 3.166474 | -0.283469 |
| F | 9.811328 | 1.676568 | -0.004764 |
| F | 8.644915 | 2.353179 | 1.676587 |
| F | 7.717895 | -3.136074 | -1.455502 |
| F | 6.498412 | -3.620823 | 0.253048 |
| F | 8.558490 | -3.031346 | 0.526002 |

**Cartesian coordinates (in Å) of optimized structures of the $S_1$ obtained with CAM-B3LYP/cc-pVTZ**

**Ethene**

| | | | |
|---|---|---|---|
| C | 0.000000 | 0.000000 | -0.704332 |
| C | 0.000000 | 0.000000 | 0.704332 |
| H | -1.004212 | 0.000000 | -1.180818 |
| H | 1.004212 | 0.000000 | -1.180818 |
| H | -1.004212 | 0.000000 | 1.180818 |
| H | 1.004212 | 0.000000 | 1.180818 |

**Styrene**

| | | | |
|---|---|---|---|
| C | -0.204418 | -0.268276 | -1.751008 |
| C | -0.432767 | -1.014991 | -0.598821 |
| C | -1.582905 | -0.889418 | 0.176049 |
| C | -2.620114 | 0.080756 | -0.187192 |
| C | -3.761986 | 0.162774 | 0.575476 |
| C | -3.947427 | -0.654298 | 1.680501 |
| C | -2.943680 | -1.593476 | 2.063435 |

| | | | |
|---|---|---|---|
| C | -1.803489 | -1.699044 | 1.332425 |
| H | -0.938300 | 0.417834 | -2.142981 |
| H | 0.713231 | -0.384520 | -2.308394 |
| H | -1.035784 | -2.410384 | 1.608527 |
| H | 0.318795 | -1.728564 | -0.284504 |
| H | -2.460940 | 0.745523 | -1.019782 |
| H | -4.530496 | 0.877124 | 0.312515 |
| H | -4.855954 | -0.579616 | 2.261382 |
| H | -3.098175 | -2.215932 | 2.932524 |

**Stilbene**

| | | | |
|---|---|---|---|
| C | -0.007461 | -0.296056 | -1.669194 |
| C | -0.620612 | -1.269757 | -0.847973 |
| C | -1.697741 | -1.024376 | 0.011494 |
| C | -2.247236 | 0.280650 | 0.205115 |
| C | -3.305481 | 0.475651 | 1.060939 |
| C | -3.868054 | -0.588811 | 1.753702 |
| C | -3.346019 | -1.878085 | 1.585867 |
| C | -2.292016 | -2.092128 | 0.742378 |
| C | 1.187044 | -0.484814 | -2.373917 |
| C | 1.962260 | -1.680970 | -2.270009 |
| C | 3.131139 | -1.822533 | -2.979953 |
| C | 3.584295 | -0.810780 | -3.816909 |
| C | 2.846002 | 0.374165 | -3.934144 |
| C | 1.683282 | 0.535699 | -3.234003 |
| H | -0.502940 | 0.657845 | -1.793068 |
| H | 1.113506 | 1.451120 | -3.328139 |
| H | -1.892071 | -3.089480 | 0.612633 |
| H | -0.258953 | -2.288192 | -0.900527 |
| H | -1.814345 | 1.124437 | -0.310932 |
| H | -3.705259 | 1.471712 | 1.195768 |
| H | -4.704413 | -0.424473 | 2.418380 |
| H | -3.780170 | -2.707501 | 2.126923 |
| H | 1.636639 | -2.473086 | -1.612594 |
| H | 3.704923 | -2.734658 | -2.885411 |
| H | 4.501042 | -0.936278 | -4.375589 |
| H | 3.198804 | 1.164382 | -4.582409 |

**DSB**

| | | | |
|---|---|---|---|
| C | -1.390784 | -5.018528 | -0.002636 |

| | | | |
|---|---|---|---|
| C | -2.651980 | -5.645845 | 0.020208 |
| C | -2.772826 | -7.016403 | 0.013582 |
| C | -1.638866 | -7.818993 | -0.016150 |
| C | -0.383640 | -7.224221 | -0.039086 |
| C | -0.254739 | -5.853801 | -0.032634 |
| C | -1.322608 | -3.591877 | 0.005504 |
| C | -0.178392 | -2.830379 | -0.013957 |
| C | -0.115476 | -1.423008 | -0.005795 |
| C | 1.147263 | -0.773229 | -0.028589 |
| C | 1.267377 | 0.579315 | -0.022019 |
| C | 0.110766 | 1.421382 | 0.008587 |
| C | -1.151967 | 0.771611 | 0.031361 |
| C | -1.272088 | -0.580936 | 0.024792 |
| C | 0.173682 | 2.828769 | 0.016792 |
| C | 1.317871 | 3.590271 | -0.002603 |
| C | 1.386037 | 5.016941 | 0.005658 |
| C | 2.647219 | 5.644259 | -0.017139 |
| C | 2.768055 | 7.014827 | -0.010412 |
| C | 1.634095 | 7.817400 | 0.019373 |
| C | 0.378869 | 7.222612 | 0.042275 |
| C | 0.249986 | 5.852193 | 0.035730 |
| H | -3.539786 | -5.027278 | 0.043418 |
| H | -3.754847 | -7.468895 | 0.031608 |
| H | -1.732044 | -8.895832 | -0.021381 |
| H | 0.503288 | -7.842814 | -0.062288 |
| H | 0.733664 | -5.418681 | -0.050913 |
| H | -2.255943 | -1.024618 | 0.042970 |
| H | -2.278447 | -3.084444 | 0.029439 |
| H | 0.777280 | -3.338676 | -0.037965 |
| H | 2.037073 | -1.389169 | -0.051938 |
| H | 2.251230 | 1.023002 | -0.040224 |
| H | -0.738410 | 5.417058 | 0.053997 |
| H | -2.041780 | 1.387547 | 0.054667 |
| H | -0.782002 | 3.337046 | 0.040760 |
| H | 2.273723 | 3.082865 | -0.026602 |
| H | 3.535035 | 5.025710 | -0.040400 |
| H | 3.750075 | 7.467321 | -0.028398 |
| H | 1.727255 | 8.894241 | 0.024677 |
| H | -0.508064 | 7.841194 | 0.065509 |

**$\alpha$-DMDCS**

| | | | |
|---|---|---|---|
| C | -6.117820 | 0.426424 | -0.260688 |

| | | | |
|---|---|---|---|
| C | -7.429384 | -0.091530 | -0.295261 |
| C | -7.694251 | -1.439598 | -0.292494 |
| C | -6.634092 | -2.345494 | -0.254174 |
| C | -5.322729 | -1.864765 | -0.219325 |
| C | -5.065604 | -0.520941 | -0.222280 |
| C | -5.976719 | 1.842170 | -0.267596 |
| C | -4.854882 | 2.661755 | -0.240915 |
| C | -3.540784 | 2.108129 | -0.197962 |
| C | -4.927689 | 4.090961 | -0.254051 |
| C | -3.755667 | 4.883346 | -0.225993 |
| C | -3.799859 | 6.243660 | -0.237694 |
| C | -5.036607 | 6.948310 | -0.279091 |
| C | -6.208628 | 6.155927 | -0.307158 |
| C | -6.164436 | 4.795613 | -0.295457 |
| C | -5.109415 | 8.377513 | -0.292204 |
| C | -6.423525 | 8.931116 | -0.335096 |
| C | -3.987558 | 9.197079 | -0.265565 |
| C | -3.846355 | 10.612822 | -0.272375 |
| C | -2.534733 | 11.130645 | -0.238017 |
| C | -2.269727 | 12.478685 | -0.240709 |
| C | -3.329801 | 13.384694 | -0.278720 |
| C | -4.641219 | 12.904100 | -0.313337 |
| C | -4.898481 | 11.560302 | -0.310462 |
| C | -8.076847 | -4.234063 | -0.282082 |
| C | -1.886847 | 15.273113 | -0.250923 |
| H | -8.259081 | 0.602464 | -0.325135 |
| H | -8.716889 | -1.781018 | -0.319916 |
| H | -4.515858 | -2.582809 | -0.189946 |
| H | -4.039758 | -0.194388 | -0.194639 |
| H | -7.098523 | 4.258203 | -0.318500 |
| H | -6.920905 | 2.363784 | -0.299514 |
| H | -2.794131 | 4.391988 | -0.194270 |
| H | -2.865773 | 6.781072 | -0.214647 |
| H | -5.924366 | 11.233867 | -0.337911 |
| H | -7.170164 | 6.647287 | -0.338885 |
| H | -3.043393 | 8.675418 | -0.233803 |
| H | -1.705100 | 10.436565 | -0.208382 |
| H | -1.247049 | 12.819998 | -0.213465 |
| H | -5.448023 | 13.622229 | -0.342465 |
| H | -8.605788 | -3.943562 | -1.191542 |
| H | -2.016419 | 16.350468 | -0.262876 |
| H | -1.357755 | 14.982479 | 0.658406 |
| H | -8.658452 | -3.929937 | 0.590004 |
| H | -7.947168 | -5.311403 | -0.270009 |

| | | | |
|---|---|---|---|
| H | -1.305447 | 14.969004 | -1.123152 |
| O | -6.775465 | -3.682698 | -0.247827 |
| O | -3.188292 | 14.721884 | -0.284965 |
| N | -7.494643 | 9.344516 | -0.369697 |
| N | -2.469733 | 1.694562 | -0.163284 |

**$\beta$-DMDCS**

| | | | |
|---|---|---|---|
| C | 4.03104642 | 3.39449944 | -0.15898823 |
| C | 5.43456542 | 3.39449944 | -0.15898823 |
| C | 6.16839214 | 4.55965668 | -0.15898823 |
| C | 5.51507087 | 5.78951121 | -0.16309191 |
| C | 4.11932761 | 5.81901648 | -0.17338083 |
| C | 3.39820597 | 4.65521701 | -0.17300524 |
| C | 3.28926766 | 2.14777632 | -0.14893962 |
| C | 4.06873210 | 0.96746479 | -0.27414802 |
| C | 1.90831786 | 2.09525571 | -0.00228498 |
| C | 1.00493564 | 1.01725434 | -0.00874921 |
| C | -0.37010583 | 1.30933369 | 0.21827833 |
| C | -1.33445344 | 0.35439287 | 0.23014065 |
| C | -1.00497088 | -1.01719758 | 0.00884078 |
| C | 0.37007152 | -1.30927573 | -0.21818263 |
| C | 1.33441957 | -0.35433536 | -0.23004539 |
| C | -1.90834844 | -2.09520409 | 0.00236348 |
| C | -3.28930012 | -2.14774928 | 0.14898204 |
| C | -4.06880350 | -0.96745865 | 0.27415645 |
| C | -4.03105234 | -3.39449075 | 0.15900239 |
| C | -5.43456934 | -3.39452517 | 0.15888580 |
| C | -6.16836747 | -4.55970047 | 0.15884788 |
| C | -5.51501422 | -5.78953773 | 0.16303226 |
| C | -4.11927206 | -5.81900607 | 0.17343979 |
| C | -3.39818301 | -4.65518640 | 0.17309899 |
| C | 7.54734495 | 7.02070973 | -0.16063066 |
| C | -7.54725795 | -7.02078611 | 0.16046195 |
| O | 6.13371653 | 6.98425313 | -0.16286226 |
| O | -6.13362890 | -6.98429681 | 0.16277506 |
| N | 4.74141960 | 0.03939807 | -0.37439899 |
| N | -4.74155872 | -0.03944827 | 0.37446291 |
| H | 5.96110586 | 2.45122252 | -0.15353397 |
| H | 7.24531639 | 4.50277751 | -0.15465150 |
| H | 3.62598323 | 6.78009441 | -0.18884963 |
| H | 2.32227959 | 4.72638484 | -0.20243238 |
| H | 2.35533161 | -0.64490062 | -0.41056367 |

| | | | |
|---|---|---|---|
| H | 1.43277451 | 3.05123321 | 0.15999653 |
| H | -0.65054879 | 2.34028053 | 0.39062288 |
| H | -2.35536363 | 0.64496093 | 0.41065894 |
| H | -2.32225601 | -4.72631964 | 0.20262360 |
| H | 0.65051606 | -2.34022320 | -0.39052718 |
| H | -1.43279229 | -3.05117656 | -0.15991692 |
| H | -5.96113410 | -2.45126225 | 0.15335926 |
| H | -7.24529383 | -4.50284967 | 0.15441398 |
| H | -3.62590329 | -6.78007155 | 0.18897354 |
| H | -7.95674603 | -6.53807794 | 1.04946632 |
| H | -7.95392518 | -6.54309837 | -0.73258775 |
| H | 7.95676936 | 6.53802396 | -1.04967653 |
| H | 7.82078003 | 8.07087712 | -0.16308015 |
| H | -7.82066752 | -8.07096011 | 0.16293215 |
| H | 7.95405222 | 6.54297990 | 0.73237706 |

**$\alpha$-TFDCS**

| | | | |
|---|---|---|---|
| C | 5.210772 | 0.148345 | 0.007030 |
| C | 5.957969 | 1.346148 | 0.002337 |
| C | 7.329345 | 1.332950 | 0.005965 |
| C | 8.024721 | 0.129742 | 0.015340 |
| C | 7.308526 | -1.055169 | 0.023074 |
| C | 5.930211 | -1.062877 | 0.019283 |
| C | 8.111749 | 2.615005 | 0.028384 |
| C | 8.054789 | -2.361314 | -0.015410 |
| C | 3.790208 | 0.279977 | 0.001401 |
| C | 2.777493 | -0.668070 | -0.011594 |
| C | 3.071866 | -2.064515 | -0.031889 |
| C | 1.389189 | -0.323567 | -0.010713 |
| C | 0.391247 | -1.328869 | -0.034872 |
| C | -0.934094 | -1.027504 | -0.034493 |
| C | -1.389184 | 0.323403 | -0.009164 |
| C | -0.391239 | 1.328733 | 0.013793 |
| C | 0.934098 | 1.027360 | 0.013611 |
| C | -2.777484 | 0.667813 | -0.006405 |
| C | -3.071978 | 2.064294 | 0.008675 |
| C | -3.790145 | -0.280402 | -0.011216 |
| C | -5.210695 | -0.148786 | -0.015826 |
| C | -5.957968 | -1.346350 | 0.005997 |
| C | -7.329335 | -1.333156 | 0.000718 |
| C | -8.024616 | -0.130148 | -0.026642 |
| C | -7.308355 | 1.054524 | -0.050304 |

| | | | |
|---|---|---|---|
| C | -5.930044 | 1.062192 | -0.045209 |
| C | -8.111955 | -2.614546 | 0.044932 |
| C | -8.054580 | 2.361198 | -0.035382 |
| H | 5.437045 | 2.292382 | -0.006243 |
| H | 5.417958 | -2.009911 | 0.032594 |
| H | 1.639285 | 1.841883 | 0.034504 |
| H | 3.459010 | 1.306649 | 0.004147 |
| H | 0.693537 | -2.365462 | -0.055236 |
| H | -1.639295 | -1.841967 | -0.057353 |
| H | -5.417683 | 2.008825 | -0.073867 |
| H | -0.693533 | 2.365342 | 0.033322 |
| H | -3.458886 | -1.307045 | -0.004827 |
| H | -5.437073 | -2.292489 | 0.022591 |
| H | -9.104134 | -0.119560 | -0.042783 |
| H | 9.104345 | 0.118926 | 0.021118 |
| F | -9.060736 | -2.640876 | -0.900673 |
| F | -8.733646 | -2.765326 | 1.223615 |
| F | -9.233302 | 2.263410 | -0.664651 |
| F | -7.362649 | 3.340557 | -0.623786 |
| F | -8.312895 | 2.756478 | 1.220389 |
| F | -7.335587 | -3.689598 | -0.134541 |
| F | 7.364341 | -3.350214 | 0.558509 |
| F | 9.235109 | -2.273759 | 0.612365 |
| F | 8.310017 | -2.735847 | -1.278203 |
| F | 7.337230 | 3.685684 | -0.182237 |
| F | 9.068994 | 2.620037 | -0.909012 |
| F | 8.722915 | 2.792259 | 1.208927 |
| N | -3.270995 | 3.194546 | 0.021923 |
| N | 3.270743 | -3.194731 | -0.049464 |

**$\beta$-TFDCS**

| | | | |
|---|---|---|---|
| C | 5.256140 | 0.322425 | 0.021807 |
| C | 6.265486 | 1.297875 | -0.016378 |
| C | 7.593700 | 0.940245 | -0.058150 |
| C | 7.974090 | -0.392852 | -0.056961 |
| C | 6.988703 | -1.364469 | -0.007821 |
| C | 5.655043 | -1.023541 | 0.034212 |
| C | 8.659556 | 2.000948 | -0.066413 |
| C | 7.392533 | -2.811429 | 0.051320 |
| C | 3.856928 | 0.712693 | 0.048294 |
| C | 3.606909 | 2.101580 | 0.200959 |
| C | 2.821123 | -0.202641 | -0.095229 |
| C | 1.424802 | -0.044134 | -0.042421 |

| | | | |
|---|---|---|---|
| C | 0.625641 | -1.196740 | -0.297381 |
| C | -0.729523 | -1.168573 | -0.270498 |
| C | -1.426408 | 0.044342 | 0.024897 |
| C | -0.627238 | 1.196911 | 0.280059 |
| C | 0.727934 | 1.168745 | 0.253162 |
| C | -2.822753 | 0.202904 | 0.077131 |
| C | -3.858498 | -0.712332 | -0.067469 |
| C | -3.608348 | -2.101207 | -0.219947 |
| C | -5.257738 | -0.322088 | -0.040752 |
| C | -6.267187 | -1.297409 | -0.007092 |
| C | -7.595705 | -0.939822 | 0.028791 |
| C | -7.976239 | 0.393104 | 0.027485 |
| C | -6.990521 | 1.364750 | -0.016365 |
| C | -5.656708 | 1.023945 | -0.052524 |
| C | -8.656696 | -2.001283 | 0.122150 |
| C | -7.393626 | 2.811480 | -0.084277 |
| H | 5.999237 | 2.344120 | -0.027797 |
| H | 4.927822 | -1.816674 | 0.086100 |
| H | 1.274255 | 2.072992 | 0.459813 |
| H | 3.131483 | -1.216658 | -0.298802 |
| H | 1.128271 | -2.127119 | -0.525122 |
| H | -1.275814 | -2.072861 | -0.477005 |
| H | -4.929481 | 1.817110 | -0.104225 |
| H | -1.129869 | 2.127260 | 0.507922 |
| H | -3.133169 | 1.216895 | 0.280761 |
| H | -6.001504 | -2.343915 | -0.007959 |
| H | -9.019774 | 0.667787 | 0.054706 |
| H | 9.016873 | -0.667859 | -0.104392 |
| N | 3.446246 | 3.233689 | 0.322376 |
| N | -3.447460 | -3.233318 | -0.341029 |
| F | 9.698496 | 1.646127 | -0.834123 |
| F | 9.140691 | 2.214529 | 1.167484 |
| F | 8.202287 | 3.171270 | -0.521061 |
| F | 6.407852 | -3.624925 | -0.352347 |
| F | 7.716292 | -3.176354 | 1.300600 |
| F | 8.459500 | -3.058044 | -0.717692 |
| F | -8.237479 | -3.175036 | -0.359469 |
| F | -9.758880 | -1.655104 | -0.555688 |
| F | -9.028612 | -2.204478 | 1.395241 |
| F | -7.700328 | 3.173743 | -1.338680 |
| F | -6.414305 | 3.625641 | 0.330898 |
| F | -8.470874 | 3.059936 | 0.669620 |

**Cartesian coordinates (in Å) of optimized structures of the $^{S_0}/_{S_1}$CI obtained with CASSCF(2,2)/ANO-S-VDZP**

**Ethene**

| | | | |
|---|---|---|---|
| C | -0.15404814 | -0.68287291 | -1.90744046 |
| C | 0.14085062 | -0.90151628 | -0.56230210 |
| H | -1.16550253 | -0.67275800 | -2.33661183 |
| H | 0.61226547 | -0.34292842 | -2.60811240 |
| H | -0.46117207 | -1.60797511 | 0.01637236 |
| H | -0.58280446 | 0.01381106 | -0.46360756 |

**Styrene**

| | | | |
|---|---|---|---|
| C | 0.23998049 | -0.46345193 | -1.61418477 |
| C | -0.44397570 | -1.30422060 | -0.72685365 |
| H | 0.28659686 | 0.24589979 | -0.70709612 |
| H | -0.37216287 | 0.20071040 | -2.23244125 |
| H | -0.98587683 | -2.35287127 | 1.67914727 |
| H | 0.02307379 | -2.26193822 | -0.46957609 |
| C | -1.64331981 | -1.05731444 | 0.09857338 |
| C | -2.66189756 | -0.20989227 | -0.34753291 |
| C | -3.78576379 | -0.00203832 | 0.43265151 |
| C | -3.88043558 | -0.60492252 | 1.68488610 |
| C | -2.86956129 | -1.44106082 | 2.14395758 |
| C | -1.76850190 | -1.68943342 | 1.33679751 |
| H | -2.57326957 | 0.25958655 | -1.31407440 |
| H | -4.58626434 | 0.62884174 | 0.07311814 |
| H | -4.75077272 | -0.42546438 | 2.30157827 |
| H | -2.94481415 | -1.89993996 | 3.11955265 |

**Stilbene**

| | | | |
|---|---|---|---|
| C | -0.65973797 | 0.07145573 | -1.65587116 |
| C | -1.08090652 | -0.91906297 | -0.76503149 |
| H | 0.36438003 | -0.14128092 | -1.16959429 |
| H | 1.46799108 | 0.79005967 | -3.19656982 |
| H | -1.71636739 | -2.74063000 | 1.07414020 |
| H | -0.59908156 | -1.91215773 | -0.73263450 |
| C | -2.06398799 | -0.77025896 | 0.28667848 |
| C | -2.81227457 | 0.41036004 | 0.39664332 |
| C | -3.79609592 | 0.51018500 | 1.36151098 |
| C | -4.02598719 | -0.56049932 | 2.22440972 |

| | | | |
|---|---|---|---|
| C | -3.28509576 | -1.73595084 | 2.13156804 |
| C | -2.30248563 | -1.83653246 | 1.16328150 |
| H | -2.58065070 | 1.21325216 | -0.28314211 |
| H | -4.38107708 | 1.41370601 | 1.45382839 |
| H | -4.79234937 | -0.47570820 | 2.98363616 |
| H | -3.47599125 | -2.55543232 | 2.80888019 |
| C | -0.39667911 | -0.27187811 | -3.06570095 |
| C | -1.31941800 | -1.01898285 | -3.81465678 |
| C | -1.10266695 | -1.29441588 | -5.15937339 |
| C | 0.03622340 | -0.83708555 | -5.80639446 |
| C | 0.95727413 | -0.08823172 | -5.07567237 |
| C | 0.74766483 | 0.19202938 | -3.73750771 |
| H | -2.22864682 | -1.36825838 | -3.34482357 |
| H | -1.83764229 | -1.87369263 | -5.70407604 |
| H | 0.20247285 | -1.05022332 | -6.85273017 |
| H | 1.85152829 | 0.28415267 | -5.55932821 |

**Cartesian coordinates (in Å) of approximated structures of the $S_0/S_1$ CI obtained with the methodology presented in the main text**

**Ethene**

| | | | |
|---|---|---|---|
| C | -0.17431802 | -0.70826425 | -1.92588226 |
| C | 0.12791458 | -0.91810168 | -0.55122893 |
| H | -1.17957770 | -0.67281467 | -2.39533707 |
| H | 0.63545905 | -0.32560032 | -2.56907535 |
| H | -0.44186270 | -1.60205560 | 0.09071540 |
| H | -0.57802632 | 0.03259686 | -0.51089379 |

**Styrene**

| | | | |
|---|---|---|---|
| C | 0.10944432 | -1.23265347 | -1.71341339 |
| C | -0.14140728 | -0.70340908 | -0.40805820 |
| H | -0.72367768 | -0.45382964 | -2.01331820 |
| H | -0.54681538 | -2.09387327 | -1.98828881 |
| H | -1.05110415 | -2.53099934 | 1.35017234 |
| H | 0.66672388 | -0.15899453 | 0.12493327 |
| C | -1.46692620 | -0.68359724 | 0.27781640 |
| C | -2.40532075 | 0.34618879 | 0.04078169 |
| C | -3.65348812 | 0.32491443 | 0.69580180 |
| C | -3.96520096 | -0.71701132 | 1.59455888 |
| C | -3.02588290 | -1.74212192 | 1.83330833 |
| C | -1.77907826 | -1.73056530 | 1.17471705 |
| H | -2.15804986 | 1.15868944 | -0.65250910 |

| | | | |
|---|---|---|---|
| H | -4.37875460 | 1.12473084 | 0.50748715 |
| H | -4.93340184 | -0.72958564 | 2.10579423 |
| H | -3.26402520 | -2.55539240 | 2.52871978 |

**Stilbene**

| | | | |
|---|---|---|---|
| C | -0.28326430 | 1.10760134 | -1.42096754 |
| C | -0.44387990 | -0.16923800 | -0.71818760 |
| H | 0.73651488 | 1.52215232 | -1.35145104 |
| H | 1.76472163 | 0.30702234 | -3.16369399 |
| H | -1.25726081 | -2.62307324 | 0.06229453 |
| H | 0.28358804 | -1.00756101 | -0.78191756 |
| C | -1.65478456 | -0.48408982 | 0.00017318 |
| C | -2.57133565 | 0.55670094 | 0.31179607 |
| C | -3.77834619 | 0.25064456 | 0.95734664 |
| C | -4.10342690 | -1.09806817 | 1.24028067 |
| C | -3.19861417 | -2.13984352 | 0.92353704 |
| C | -1.96800225 | -1.83186802 | 0.32531571 |
| H | -2.29778146 | 1.56743298 | -0.00739921 |
| H | -4.48463012 | 1.04654187 | 1.21738866 |
| H | -5.06689017 | -1.34147889 | 1.70259486 |
| H | -3.46394937 | -3.17997227 | 1.14153180 |
| C | -0.36021746 | 0.25146583 | -2.67375803 |
| C | -1.61110592 | -0.32083200 | -3.04976746 |
| C | -1.71860847 | -1.20176727 | -4.14376887 |
| C | -0.57110690 | -1.53794946 | -4.88740054 |
| C | 0.68518778 | -0.97765301 | -4.54229574 |
| C | 0.79259547 | -0.11550537 | -3.44225556 |
| H | -2.49672849 | -0.05038735 | -2.46993820 |
| H | -2.69193435 | -1.62741654 | -4.40939281 |
| H | -0.64598490 | -2.23153594 | -5.73204115 |
| H | 1.57563709 | -1.23640378 | -5.12655389 |

**DSB**

| | | | |
|---|---|---|---|
| C | -2.10721986 | 2.59288154 | 4.97367360 |
| C | -2.08503967 | 2.43069578 | 6.37291187 |
| C | -2.23042310 | 3.50292609 | 7.22277297 |
| C | -2.40419696 | 4.78314522 | 6.71116750 |
| C | -2.42959945 | 4.96911452 | 5.33470734 |
| C | -2.28482429 | 3.90136098 | 4.47817401 |
| C | -1.95165421 | 1.44557011 | 4.13729985 |
| C | -1.95009392 | 1.43303791 | 2.76277080 |
| C | -1.79635116 | 0.29887711 | 1.94133389 |
| C | -1.81604807 | 0.44326227 | 0.52853336 |

| | | | |
|---|---|---|---|
| C | -1.67268790 | -0.61441926 | -0.31087313 |
| C | -1.49292536 | -1.93969117 | 0.19815086 |
| C | -1.47320639 | -2.08407528 | 1.61094209 |
| C | -1.61656941 | -1.02639509 | 2.45035654 |
| C | -1.33922200 | -3.07387400 | -0.62329100 |
| C | -2.70294900 | -3.24615000 | -0.62325500 |
| C | -3.54324100 | -3.35223600 | 0.52685700 |
| C | -4.92988700 | -3.52739200 | 0.35034000 |
| C | -5.78286200 | -3.63510300 | 1.42455400 |
| C | -5.28706400 | -3.57244800 | 2.72114000 |
| C | -3.92321400 | -3.40016000 | 2.92144300 |
| C | -3.06367400 | -3.29161000 | 1.85181200 |
| H | -1.95008907 | 1.43651645 | 6.77881588 |
| H | -2.20910154 | 3.34678953 | 8.29263505 |
| H | -2.51856665 | 5.62654448 | 7.37741642 |
| H | -2.56447854 | 5.96284189 | 4.92955526 |
| H | -2.30857079 | 4.07537269 | 3.41245404 |
| H | -1.59417273 | -1.19084479 | 3.51694346 |
| H | -1.82422048 | 0.50679984 | 4.66090243 |
| H | -2.07754250 | 2.37244629 | 2.23977905 |
| H | -1.95073884 | 1.43636426 | 0.11951413 |
| H | -1.69505705 | -0.44997160 | -1.37746274 |
| H | -2.00799800 | -3.15824300 | 2.03719100 |
| H | -1.33847545 | -3.07716840 | 2.01996675 |
| H | -1.21173446 | -4.01326452 | -0.10027666 |
| H | -3.21379700 | -3.31073900 | -1.57538400 |
| H | -5.32345500 | -3.57713600 | -0.65663000 |
| H | -6.84281200 | -3.76898300 | 1.25716200 |
| H | -5.95576400 | -3.65690900 | 3.56612500 |
| H | -3.53039300 | -3.35051800 | 3.92795100 |

**$\alpha$-DMDCS**

| | | | |
|---|---|---|---|
| C | -2.99630759 | 2.64367275 | 5.43327639 |
| C | -2.91784338 | 2.48581103 | 6.82312098 |
| C | -3.27528912 | 3.48196987 | 7.70670701 |
| C | -3.73420485 | 4.69804468 | 7.21256143 |
| C | -3.82333591 | 4.88376119 | 5.83300367 |
| C | -3.46545970 | 3.88597506 | 4.96347189 |
| C | -2.58980914 | 1.52077124 | 4.62714643 |
| C | -2.54246246 | 1.32171992 | 3.27965645 |
| C | -2.94892142 | 2.34701307 | 2.36962820 |
| C | -2.09176674 | 0.08158235 | 2.66550596 |
| C | -2.07575545 | -0.06650778 | 1.27177471 |

| | | | |
|---|---|---|---|
| C | -1.66916370 | -1.22973055 | 0.67021917 |
| C | -1.21862440 | -2.33295794 | 1.42843740 |
| C | -1.24000555 | -2.18388795 | 2.83188201 |
| C | -1.65987029 | -1.02715064 | 3.42376427 |
| C | -0.78014000 | -3.54126400 | 0.80729400 |
| C | -0.42270100 | -4.63428694 | 1.62413223 |
| C | -2.15818800 | -3.88453100 | 0.76385300 |
| C | -2.97089000 | -3.98880600 | -0.37185900 |
| C | -4.37270500 | -4.05790700 | -0.21110100 |
| C | -5.22366400 | -4.12254400 | -1.28295300 |
| C | -4.69473000 | -4.10677100 | -2.57862800 |
| C | -3.30850800 | -4.04838200 | -2.76711100 |
| C | -2.46472000 | -4.01571900 | -1.69478000 |
| C | -4.04064388 | 5.61309870 | 9.38385597 |
| C | -6.84239900 | -4.25498700 | -3.58828100 |
| H | -2.56170408 | 1.54348199 | 7.21862624 |
| H | -3.19446372 | 3.30632050 | 8.76762163 |
| H | -4.18146558 | 5.83507779 | 5.46672995 |
| H | -3.54954709 | 4.07343268 | 3.90652202 |
| H | -1.64775178 | -0.97983903 | 4.50215900 |
| H | -2.26233950 | 0.67806765 | 5.21931224 |
| H | -2.40732264 | 0.75431298 | 0.65176735 |
| H | -1.70200167 | -1.29209871 | -0.40799023 |
| H | -1.39795400 | -4.00897600 | -1.85908500 |
| H | -0.90709589 | -3.00410238 | 3.45237234 |
| H | -2.69905900 | -3.90413500 | 1.70736300 |
| H | -4.78318400 | -4.04616600 | 0.78980900 |
| H | -6.28771800 | -4.17453500 | -1.11722600 |
| H | -2.92762300 | -4.06016200 | -3.77784100 |
| H | -3.01676679 | 5.43005735 | 9.71524803 |
| H | -7.21584600 | -4.29794000 | -4.60590100 |
| H | -7.14550100 | -5.15582600 | -3.05304100 |
| H | -4.68697289 | 4.80918443 | 9.74107130 |
| H | -4.38585211 | 6.55862254 | 9.78966356 |
| H | -7.25357400 | -3.37691000 | -3.08845100 |
| O | -4.11004400 | 5.74124620 | 7.97873109 |
| O | -5.43178200 | -4.17162400 | -3.69277100 |
| N | -0.14614019 | -5.53094913 | 2.29526893 |
| N | -3.26718553 | 3.14820599 | 1.61213837 |

***β*-DMDCS**

| | | | |
|---|---|---|---|
| C | 4.11510621 | 2.52333119 | 0.48137463 |

| | | | |
|---|---|---|---|
| C | 5.50986821 | 2.52333119 | 0.48137463 |
| C | 6.24767445 | 3.69173869 | 0.48137463 |
| C | 5.59778297 | 4.91794595 | 0.47714382 |
| C | 4.20397171 | 4.94397361 | 0.46635485 |
| C | 3.48446335 | 3.77682820 | 0.46637997 |
| C | 3.37035032 | 1.25931043 | 0.49160457 |
| C | 4.15904511 | 0.08018576 | 0.35166995 |
| C | 2.01968890 | 1.18208808 | 0.64410271 |
| C | 1.11594414 | 0.07460456 | 0.64533037 |
| C | -0.24618877 | 0.36007796 | 0.87745446 |
| C | -1.20968117 | -0.60725127 | 0.89709330 |
| C | -0.87005588 | -1.96525956 | 0.68099237 |
| C | 0.50132982 | -2.25520443 | 0.44712685 |
| C | 1.45502101 | -1.28453486 | 0.42688817 |
| C | -1.80423938 | -2.99657565 | 0.68696895 |
| C | -3.21578193 | -2.89693842 | 0.87323225 |
| C | -3.12672982 | -3.72921068 | 2.01317905 |
| C | -3.42076813 | -3.52130765 | -0.40237376 |
| C | -3.63009423 | -4.90513911 | -0.52024996 |
| C | -3.84090612 | -5.50262176 | -1.74143767 |
| C | -3.84320604 | -4.73060727 | -2.90283772 |
| C | -3.62903358 | -3.35484878 | -2.81107533 |
| C | -3.42448043 | -2.76422467 | -1.59199784 |
| C | 7.62906101 | 6.14792481 | 0.47941449 |
| C | -4.25824577 | -6.60675820 | -4.30045274 |
| O | 6.21630493 | 6.11559107 | 0.47679250 |
| O | -4.04091216 | -5.21858743 | -4.14145165 |
| N | 4.82836233 | -0.84497939 | 0.24321840 |
| N | -2.97968733 | -4.40349275 | 2.93906980 |
| H | 6.03718265 | 1.58026545 | 0.48680298 |
| H | 7.32449199 | 3.63393179 | 0.48551484 |
| H | 3.70823392 | 5.90375111 | 0.45030619 |
| H | 2.40817122 | 3.84791638 | 0.43621324 |
| H | 2.47775710 | -1.56476671 | 0.24106207 |
| H | 1.53150568 | 2.13196349 | 0.80644157 |
| H | -0.53075596 | 1.39060795 | 1.04628714 |
| H | -2.23995131 | -0.33727898 | 1.07838420 |
| H | -3.25347552 | -1.69798804 | -1.54971737 |
| H | 0.78700325 | -3.28479553 | 0.27660903 |
| H | -1.39567792 | -3.99248739 | 0.52340470 |
| H | -3.63186918 | -5.51862364 | 0.36924199 |
| H | -4.00283300 | -6.56800016 | -1.78297456 |
| H | -3.62777649 | -2.77234774 | -3.72090906 |
| H | -3.40192580 | -7.18438138 | -3.94854426 |

| | | | |
|---|---|---|---|
| H | -5.15670518 | -6.93011943 | -3.77186628 |
| H | 8.03811080 | 5.66348032 | -0.40904345 |
| H | 7.90605963 | 7.19719852 | 0.47666139 |
| H | -4.38901089 | -6.77033033 | -5.36519989 |
| H | 8.03449476 | 5.66922712 | 1.37262110 |

**$\alpha$-TFDCS**

| | | | |
|---|---|---|---|
| C | 4.04894339 | 0.37457731 | 3.51447762 |
| C | 5.44020437 | 0.14381104 | 3.59679621 |
| C | 6.32604472 | 1.18908096 | 3.65367327 |
| C | 5.87336354 | 2.50394739 | 3.63167963 |
| C | 4.51196341 | 2.74398028 | 3.54967741 |
| C | 3.60509387 | 1.70835626 | 3.49155109 |
| C | 7.80653192 | 0.94077355 | 3.71293727 |
| C | 4.01408984 | 4.16371190 | 3.57463150 |
| C | 3.18320162 | -0.74324591 | 3.45717319 |
| C | 1.76598300 | -0.76746600 | 3.39134700 |
| C | 2.04109134 | -1.08584405 | 4.74712344 |
| C | 1.39586492 | -1.88819229 | 2.58606428 |
| C | 1.42959631 | -3.21160687 | 3.08186073 |
| C | 1.07505530 | -4.27588653 | 2.30663555 |
| C | 0.65594967 | -4.11156959 | 0.96722465 |
| C | 0.62557046 | -2.79454614 | 0.47557956 |
| C | 0.97903808 | -1.72302440 | 1.24747039 |
| C | 0.27009523 | -5.22358852 | 0.11594943 |
| C | -0.11461497 | -4.88135801 | -1.21737903 |
| C | 0.25596187 | -6.52325549 | 0.52565478 |
| C | -0.08560450 | -7.74337501 | -0.16120542 |
| C | -0.01087571 | -8.92692071 | 0.59143277 |
| C | -0.31135877 | -10.14877648 | 0.03864539 |
| C | -0.69929665 | -10.24389864 | -1.28864426 |
| C | -0.77580645 | -9.08838664 | -2.04389690 |
| C | -0.47740525 | -7.85434858 | -1.50240721 |
| C | -0.24685621 | -11.40422888 | 0.86123903 |
| C | -1.23794177 | -9.17795246 | -3.47312379 |
| H | 5.80864293 | -0.87124516 | 3.61682195 |
| H | 2.55124801 | 1.93104124 | 3.42207400 |
| H | 0.93418857 | -0.73314749 | 0.81750828 |
| H | 3.69069116 | -1.70449897 | 3.48012211 |
| H | 1.74454538 | -3.38295618 | 4.10067210 |
| H | 1.12620153 | -5.25846564 | 2.74670717 |
| H | -0.54246506 | -6.98371418 | -2.13249384 |

| | | | |
|---|---|---|---|
| H | 0.31148129 | -2.62407084 | -0.54377429 |
| H | 0.54664068 | -6.68173119 | 1.55225466 |
| H | 0.29416974 | -8.87450434 | 1.62629516 |
| H | -0.92445035 | -11.20376982 | -1.72859079 |
| H | 6.57238306 | 3.32552884 | 3.67410699 |
| F | 0.44872709 | -12.36360839 | 0.23630289 |
| F | -1.47165229 | -11.89922064 | 1.09177295 |
| F | -0.87887138 | -10.33976117 | -4.03538751 |
| F | -0.73718770 | -8.19351345 | -4.22425019 |
| F | -2.57471383 | -9.09983299 | -3.55518652 |
| F | 0.32936053 | -11.20040216 | 2.05159012 |
| F | 2.84803826 | 4.29628637 | 2.93512184 |
| F | 4.88701428 | 5.00311695 | 3.00271509 |
| F | 3.82623961 | 4.58968509 | 4.83258627 |
| F | 8.09569836 | -0.34753509 | 3.92790656 |
| F | 8.38206283 | 1.65228741 | 4.69117291 |
| F | 8.40512784 | 1.29806944 | 2.56735000 |
| N | -0.41869590 | -4.57279691 | -2.27919021 |
| N | 2.25650759 | -1.33254526 | 5.85034939 |

**$\beta$-TFDCS**

| | | | |
|---|---|---|---|
| C | 4.14275321 | -0.46578850 | 1.78082817 |
| C | 4.40814977 | -1.12779430 | 0.56890032 |
| C | 5.01505253 | -0.46521137 | -0.47227910 |
| C | 5.37706984 | 0.86991069 | -0.35899165 |
| C | 5.11359465 | 1.53180574 | 0.82737992 |
| C | 4.50639000 | 0.88507019 | 1.88266794 |
| C | 5.26083870 | -1.17606270 | -1.77430916 |
| C | 5.45445871 | 2.99149648 | 0.94018917 |
| C | 3.52509500 | -1.14607200 | 2.89466600 |
| C | 3.06170482 | -2.46422391 | 2.69194655 |
| C | 2.11545400 | -1.16294000 | 3.07149700 |
| C | 1.11676900 | -1.12488700 | 2.09678000 |
| C | -0.24526000 | -1.20412800 | 2.49626400 |
| C | -1.26589500 | -1.17139900 | 1.59792000 |
| C | -1.00380600 | -1.05244400 | 0.20869500 |
| C | 0.35328800 | -0.97570400 | -0.18602900 |
| C | 1.37915700 | -1.00781000 | 0.70823300 |
| C | -1.97867200 | -1.01368200 | -0.82897300 |
| C | -3.34453900 | -1.01347700 | -0.79434900 |
| C | -4.04911900 | -0.97261000 | 0.44148400 |
| C | -4.17741300 | -1.02221200 | -2.00178900 |

| | | | |
|---|---|---|---|
| C | -5.55820000 | -0.82489200 | -1.90341100 |
| C | -6.35701100 | -0.82007800 | -3.02736400 |
| C | -5.81596000 | -1.01561300 | -4.28493400 |
| C | -4.45220200 | -1.22284500 | -4.39303300 |
| C | -3.64333900 | -1.23062100 | -3.27730800 |
| C | -7.83076800 | -0.54926400 | -2.90050400 |
| C | -3.86080000 | -1.50174100 | -5.74672500 |
| H | 4.14567774 | -2.16887429 | 0.45626781 |
| H | 4.31035767 | 1.43578663 | 2.78991083 |
| H | 2.39923300 | -0.94473200 | 0.35970000 |
| H | 1.74761400 | -1.23345900 | 4.09404500 |
| H | -0.46742000 | -1.29817200 | 3.55072700 |
| H | -2.27860200 | -1.24009300 | 1.95601200 |
| H | -2.59091900 | -1.41560400 | -3.41413500 |
| H | 0.57546100 | -0.88574700 | -1.24104800 |
| H | -1.55061200 | -0.96150900 | -1.81905400 |
| H | -6.01001100 | -0.67274600 | -0.93463300 |
| H | -6.44473300 | -1.01242700 | -5.16219300 |
| H | 5.86665899 | 1.37824061 | -1.17561780 |
| N | 2.65471504 | -3.53375207 | 2.55653564 |
| N | -4.65281400 | -0.93105700 | 1.41716200 |
| F | 6.41584003 | -0.79081587 | -2.33350246 |
| F | 4.29072302 | -0.91143977 | -2.66268569 |
| F | 5.30812284 | -2.50304487 | -1.62467599 |
| F | 5.57825570 | 3.38318095 | 2.21517850 |
| F | 4.50438399 | 3.75959887 | 0.38554487 |
| F | 6.60307939 | 3.28162489 | 0.31767210 |
| F | -8.29484600 | -0.85615300 | -1.68560900 |
| F | -8.53840600 | -1.25162700 | -3.79470400 |
| F | -8.10539000 | 0.74637700 | -3.11488700 |
| F | -4.00561400 | -2.79119500 | -6.08577700 |
| F | -2.54960600 | -1.23032200 | -5.78684100 |