symmetry

MDPI

*Supporting Information*

# Chiroptical Symmetry Analysis of Trianglimines: A Case Study

**Ani Ozcelik [1], Raquel Pereira-Cameselle [1], Ricardo A. Mosquera [2], Ángeles Peña-Gallego [2,*] and J. Lorenzo Alonso-Gómez [1,*]**

[1] Departamento de Química Orgánica, Universidade de Vigo, Lagoas-Marcosende s/n, Vigo 36310, Spain; lorenzo@uvigo.es

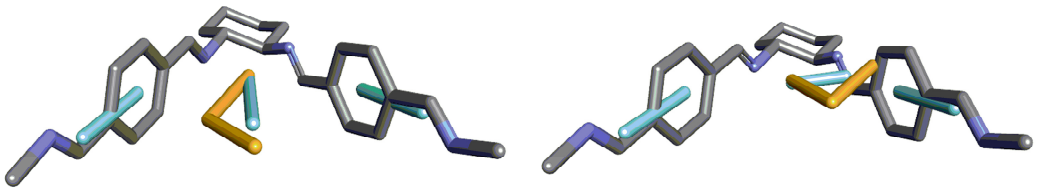
[2] Departamento de Química Física, Universidade de Vigo, Lagoas-Marcosende s/n, Vigo 36310, Spain; mpena@uvigo.es

* Correspondence: mpena@uvigo.es (A. P.-G.); lorenzo@uvigo.es (J.L. A-G.)

## Computational Details

### General Procedure and Analysis of Data

All calculations were carried out with the GAUSSIAN 09 program package. Structures of symmetry $D_3$ were optimized at cam-B3LYP level employing the 6-311G(d,p) basis set in gas phase. Harmonic frequency calculations were performed at the same level to confirm them as local minima. In order to obtain the UV-Vis and ECD spectra, a TDDFT calculation was performed at the same level obtaining the 50 first excited states.



**(a)** **(b)**

**Figure 1. Representation of the two allowed transitions, (a) in phase and (b) out of phase, for the exciton coupling of two chromophores in the truncated systems from 1.**

**coordinates (in Armstrong) are shown below**

**STRUCTURE 1**

| | | | |
|---|---|---|---|
| C | -0.706235 | 6.278465 | 0.303538 |
| H | -0.592600 | 6.255651 | 1.399027 |
| C | -1.463897 | 7.546123 | -0.099407 |
| H | -2.453966 | 7.527665 | 0.363259 |
| H | -1.624280 | 7.521776 | -1.182239 |
| C | -0.704995 | 8.811416 | 0.293536 |
| H | -1.257253 | 9.694496 | -0.037978 |
| H | -0.641394 | 8.874913 | 1.385941 |

| | | | |
|---|---|---|---|
| C | 0.704995 | 8.811416 | -0.293536 |
| H | 1.257253 | 9.694496 | 0.037978 |
| H | 0.641394 | 8.874913 | -1.385941 |
| C | 1.463897 | 7.546123 | 0.099407 |
| H | 1.624280 | 7.521776 | 1.182239 |
| H | 2.453966 | 7.527665 | -0.363259 |
| C | 0.706235 | 6.278465 | -0.303538 |
| H | 0.592600 | 6.255651 | -1.399027 |
| C | 1.868772 | 4.295903 | -0.684790 |
| H | 1.716046 | 4.452669 | -1.762164 |
| C | 2.603519 | 3.072799 | -0.320415 |
| C | 3.088971 | 2.236536 | -1.325988 |
| C | 3.765019 | 1.072488 | -1.012494 |
| C | 3.962881 | 0.718314 | 0.320415 |
| C | 3.481382 | 1.556859 | 1.325988 |
| C | 2.811311 | 2.724358 | 1.012494 |
| C | 4.654747 | -0.529547 | 0.684790 |
| H | 4.714147 | -0.740195 | 1.762164 |
| C | 5.790428 | -2.527615 | 0.303538 |
| H | 5.713853 | -2.614619 | 1.399027 |
| C | 7.267083 | -2.505289 | -0.099407 |
| H | 7.746132 | -1.638636 | 0.363259 |
| H | 7.326189 | -2.354220 | -1.182239 |
| C | 7.983408 | -3.795164 | 0.293536 |
| H | 9.024306 | -3.758435 | -0.037978 |
| H | 8.006597 | -3.881993 | 1.385941 |
| C | 7.278412 | -5.016252 | -0.293536 |
| H | 7.767053 | -5.936061 | 0.037978 |
| H | 7.365203 | -4.992920 | -1.385941 |
| C | 5.803186 | -5.040833 | 0.099407 |
| H | 5.292166 | -5.889029 | -0.363259 |
| H | 5.701909 | -5.167556 | 1.182239 |
| C | 5.084193 | -3.750850 | -0.303538 |
| H | 5.121253 | -3.641032 | -1.399027 |

| | | | |
|---|---|---|---|
| C | 2.785975 | -3.766355 | -0.684790 |
| H | 2.998101 | -3.712474 | -1.762164 |
| C | 1.359362 | -3.791113 | -0.320415 |
| C | 0.953708 | -3.796846 | 1.012494 |
| C | -0.392411 | -3.793395 | 1.325988 |
| C | -1.359362 | -3.791113 | 0.320415 |
| C | -0.953708 | -3.796846 | -1.012494 |
| C | 0.392411 | -3.793395 | -1.325988 |
| C | -2.785975 | -3.766355 | 0.684790 |
| H | -2.998101 | -3.712474 | 1.762164 |
| C | -5.084193 | -3.750850 | 0.303538 |
| H | -5.121253 | -3.641032 | 1.399027 |
| C | -5.803186 | -5.040833 | -0.099407 |
| H | -5.701909 | -5.167556 | -1.182239 |
| H | -5.292166 | -5.889029 | 0.363259 |
| C | -7.278412 | -5.016252 | 0.293536 |
| H | -7.365203 | -4.992920 | 1.385941 |
| H | -7.767053 | -5.936061 | -0.037978 |
| C | -7.983408 | -3.795164 | -0.293536 |
| H | -9.024306 | -3.758435 | 0.037978 |
| H | -8.006597 | -3.881993 | -1.385941 |
| C | -7.267083 | -2.505289 | 0.099407 |
| H | -7.746132 | -1.638636 | -0.363259 |
| H | -7.326189 | -2.354220 | 1.182239 |
| C | -5.790428 | -2.527615 | -0.303538 |
| H | -5.713853 | -2.614619 | -1.399027 |
| C | -4.654747 | -0.529547 | -0.684790 |
| H | -4.714147 | -0.740195 | -1.762164 |
| C | -3.962881 | 0.718314 | -0.320415 |
| C | -3.481382 | 1.556859 | -1.325988 |
| C | -2.811311 | 2.724358 | -1.012494 |
| C | -2.603519 | 3.072799 | 0.320415 |
| C | -3.088971 | 2.236536 | 1.325988 |
| C | -3.765019 | 1.072488 | 1.012494 |

| | | | |
|---|---|---|---|
| C | -1.868772 | 4.295903 | 0.684790 |
| H | -1.716046 | 4.452669 | 1.762164 |
| N | -1.427864 | 5.114822 | -0.168527 |
| N | 1.427864 | 5.114822 | 0.168527 |
| N | 5.143498 | -1.320844 | -0.168527 |
| N | 3.715634 | -3.793977 | 0.168527 |
| N | -3.715634 | -3.793977 | -0.168527 |
| N | -5.143498 | -1.320844 | 0.168527 |
| H | 4.144521 | 0.414733 | -1.783596 |
| H | 2.431430 | 3.381894 | 1.783596 |
| H | -1.713091 | -3.796627 | -1.783596 |
| H | 1.713091 | -3.796627 | 1.783596 |
| H | -2.431430 | 3.381894 | -1.783596 |
| H | -4.144521 | 0.414733 | 1.783596 |
| H | -0.704874 | -3.787703 | 2.364836 |
| H | 0.704874 | -3.787703 | -2.364836 |
| H | 3.632684 | 1.283413 | 2.364836 |
| H | 2.927810 | 2.504290 | -2.364836 |
| H | -3.632684 | 1.283413 | -2.364836 |
| H | -2.927810 | 2.504290 | 2.364836 |

## STRUCTURE 2

| | | | |
|---|---|---|---|
| C | 5.767477 | -2.521581 | 0.318144 |
| H | 5.679096 | -2.627472 | 1.410958 |
| C | 7.248849 | -2.493351 | -0.067436 |
| H | 7.722638 | -1.635183 | 0.416101 |
| H | 7.320049 | -2.322877 | -1.146791 |
| C | 7.961336 | -3.790157 | 0.309094 |
| H | 9.006246 | -3.747385 | -0.009336 |
| O | 7.971553 | -3.897709 | 1.399924 |
| C | 7.263041 | -4.999641 | -0.309094 |
| H | 7.748453 | -5.925945 | 0.009336 |
| H | 7.361292 | -4.954713 | -1.399924 |
| C | 5.783730 | -5.031012 | 0.067436 |
| H | 5.671695 | -5.177910 | 1.146791 |
| H | 5.277429 | -5.870409 | -0.416101 |
| C | 5.067492 | -3.733991 | -0.318144 |
| H | 5.115005 | -3.604505 | -1.410958 |
| C | 2.774996 | -3.742470 | -0.727645 |
| H | 2.990870 | -3.668778 | -1.797150 |
| C | 1.350117 | -3.771714 | -0.358982 |
| C | 0.359137 | -3.775868 | -1.350016 |
| C | -0.976094 | -3.777033 | -0.980883 |
| C | -1.350117 | -3.771714 | 0.358982 |
| C | -0.359137 | -3.775868 | 1.350016 |
| C | 0.976094 | -3.777033 | 0.980883 |
| C | -2.774996 | -3.742470 | 0.727645 |
| H | -2.990870 | -3.668778 | 1.797150 |
| C | -5.067492 | -3.733991 | 0.318144 |
| H | -5.115005 | -3.604505 | 1.410958 |
| C | -5.783730 | -5.031012 | -0.067436 |
| H | -5.277429 | -5.870409 | 0.416101 |
| H | -5.671695 | -5.177910 | -1.146791 |
| C | -7.263041 | -4.999641 | 0.309094 |
| H | -7.748453 | -5.925945 | -0.009336 |

| | | | |
|---|---|---|---|
| H | -7.361292 | -4.954713 | 1.399924 |
| C | -7.961336 | -3.790157 | -0.309094 |
| H | -9.006246 | -3.747385 | 0.009336 |
| H | -7.971553 | -3.897709 | -1.399924 |
| C | -7.248849 | -2.493351 | 0.067436 |
| H | -7.722638 | -1.635183 | -0.416101 |
| H | -7.320049 | -2.322877 | 1.146791 |
| C | -5.767477 | -2.521581 | -0.318144 |
| H | -5.679096 | -2.627472 | -1.410958 |
| C | -4.628572 | -0.531982 | -0.727645 |
| H | -4.672690 | -0.755780 | -1.797150 |
| C | -3.941459 | 0.716621 | -0.358982 |
| C | -3.759054 | 1.043194 | 0.980883 |
| C | -3.090429 | 2.198956 | 1.350016 |
| C | -2.591342 | 3.055093 | 0.358982 |
| C | -2.782960 | 2.733839 | -0.980883 |
| C | -3.449566 | 1.576912 | -1.350016 |
| C | -1.853576 | 4.274452 | 0.727645 |
| H | -1.681820 | 4.424558 | 1.797150 |
| C | -0.699985 | 6.255572 | 0.318144 |
| H | -0.564090 | 6.231977 | 1.410958 |
| C | -1.465119 | 7.524363 | -0.067436 |
| H | -1.648354 | 7.500787 | -1.146791 |
| H | -2.445209 | 7.505592 | 0.416101 |
| C | -0.698295 | 8.789798 | 0.309094 |
| H | -0.610261 | 8.852422 | 1.399924 |
| H | -1.257792 | 9.673330 | -0.009336 |
| C | 0.698295 | 8.789798 | -0.309094 |
| H | 1.257792 | 9.673330 | 0.009336 |
| H | 0.610261 | 8.852422 | -1.399924 |
| C | 1.465119 | 7.524363 | 0.067436 |
| H | 2.445209 | 7.505592 | -0.416101 |
| H | 1.648354 | 7.500787 | 1.146791 |
| C | 0.699985 | 6.255572 | -0.318144 |
| H | 0.564090 | 6.231977 | -1.410958 |

| | | | |
|---|---|---|---|
| C | 1.853576 | 4.274452 | -0.727645 |
| H | 1.681820 | 4.424558 | -1.797150 |
| C | 2.591342 | 3.055093 | -0.358982 |
| C | 3.090429 | 2.198956 | -1.350016 |
| C | 3.759054 | 1.043194 | -0.980883 |
| C | 3.941459 | 0.716621 | 0.358982 |
| C | 3.449566 | 1.576912 | 1.350016 |
| C | 2.782960 | 2.733839 | 0.980883 |
| C | 4.628572 | -0.531982 | 0.727645 |
| H | 4.672690 | -0.755780 | 1.797150 |
| N | 5.127955 | -1.305538 | -0.139393 |
| N | 3.694606 | -3.788170 | 0.139393 |
| N | -3.694606 | -3.788170 | -0.139393 |
| N | -5.127955 | -1.305538 | 0.139393 |
| N | -1.433348 | 5.093708 | -0.139393 |
| N | 1.433348 | 5.093708 | 0.139393 |
| H | -4.156513 | 0.349694 | 1.707701 |
| H | -2.381100 | 3.424799 | -1.707701 |
| H | -1.775413 | -3.774493 | -1.707701 |
| H | 1.775413 | -3.774493 | 1.707701 |
| H | 2.381100 | 3.424799 | 1.707701 |
| H | 4.156513 | 0.349694 | -1.707701 |
| O | 0.788071 | -3.775745 | -2.643245 |
| O | -0.788071 | -3.775745 | 2.643245 |
| O | 2.875856 | 2.570362 | -2.643245 |
| O | 3.663927 | 1.205383 | 2.643245 |
| O | -3.663927 | 1.205383 | -2.643245 |
| O | -2.875856 | 2.570362 | 2.643245 |
| C | -3.349923 | 1.722687 | 3.668588 |
| H | -2.888401 | 0.731867 | 3.614431 |
| H | -3.070666 | 2.200121 | 4.605490 |
| H | -4.438252 | 1.615446 | 3.628332 |
| C | -3.166852 | 2.039775 | -3.668588 |
| H | -2.078016 | 2.135495 | -3.614431 |
| H | -3.440694 | 1.559214 | -4.605490 |

| | | | |
|---|---|---|---|
| H | -3.618143 | 3.035916 | -3.628332 |
| C | -0.183071 | -3.762462 | -3.668588 |
| H | -0.810385 | -2.867362 | -3.614431 |
| H | 0.370028 | -3.759335 | -4.605490 |
| H | -0.820109 | -4.651362 | -3.628332 |
| C | 0.183071 | -3.762462 | 3.668588 |
| H | 0.810385 | -2.867362 | 3.614431 |
| H | -0.370028 | -3.759335 | 4.605490 |
| H | 0.820109 | -4.651362 | 3.628332 |
| C | 3.349923 | 1.722687 | -3.668588 |
| H | 2.888401 | 0.731867 | -3.614431 |
| H | 3.070666 | 2.200121 | -4.605490 |
| H | 4.438252 | 1.615446 | -3.628332 |
| C | 3.166852 | 2.039775 | 3.668588 |
| H | 2.078016 | 2.135495 | 3.614431 |
| H | 3.440694 | 1.559214 | 4.605490 |
| H | 3.618143 | 3.035916 | 3.628332 |

**STRUCTURE 3**

| | | | |
|---|---|---|---|
| C | -0.704834 | 6.272774 | 0.306756 |
| H | -0.589900 | 6.248184 | 1.401023 |
| C | -1.465721 | 7.539781 | -0.091622 |
| H | -2.452881 | 7.520816 | 0.376494 |
| H | -1.631969 | 7.518662 | -1.173844 |
| C | -0.703202 | 8.804171 | 0.297777 |
| H | -1.257313 | 9.686847 | -0.030534 |
| H | -0.634126 | 8.867572 | 1.389727 |
| C | 0.703202 | 8.804171 | -0.297777 |
| H | 1.257313 | 9.686847 | 0.030534 |
| H | 0.634126 | 8.867572 | -1.389727 |
| C | 1.465721 | 7.539781 | 0.091622 |
| H | 1.631969 | 7.518662 | 1.173844 |
| H | 2.452881 | 7.520816 | -0.376494 |
| C | 0.704834 | 6.272774 | -0.306756 |
| H | 0.589900 | 6.248184 | -1.401023 |
| C | 1.863915 | 4.267219 | -0.703863 |
| H | 1.704595 | 4.422037 | -1.777828 |
| C | 2.588194 | 3.058625 | -0.326232 |
| C | 3.072364 | 2.219240 | -1.328171 |
| C | 3.755715 | 1.052468 | -1.029461 |
| C | 3.942944 | 0.712129 | 0.326232 |
| C | 3.458100 | 1.551125 | 1.328171 |
| C | 2.789322 | 2.726311 | 1.029461 |
| C | 4.627477 | -0.519412 | 0.703863 |
| H | 4.681894 | -0.734796 | 1.777828 |
| C | 5.784799 | -2.525983 | 0.306756 |
| H | 5.706036 | -2.613223 | 1.401023 |
| C | 7.262502 | -2.500539 | -0.091622 |
| H | 7.739658 | -1.636150 | 0.376494 |
| H | 7.327337 | -2.346004 | -1.173844 |
| C | 7.976237 | -3.793094 | 0.297777 |
| H | 9.017712 | -3.754558 | -0.030534 |
| H | 7.996606 | -3.884616 | 1.389727 |
| C | 7.273034 | -5.011077 | -0.297777 |

| | | | |
|---|---|---|---|
| H | 7.760399 | -5.932289 | 0.030534 |
| H | 7.362479 | -4.982956 | -1.389727 |
| C | 5.796781 | -5.039242 | 0.091622 |
| H | 5.286777 | -5.884665 | -0.376494 |
| H | 5.695368 | -5.172658 | 1.173844 |
| C | 5.079964 | -3.746791 | -0.306756 |
| H | 5.116136 | -3.634961 | -1.401023 |
| C | 2.763563 | -3.747807 | -0.703863 |
| H | 2.977299 | -3.687241 | -1.777828 |
| C | 1.354750 | -3.770754 | -0.326232 |
| C | 0.966393 | -3.778779 | 1.029461 |
| C | -0.385736 | -3.770365 | 1.328171 |
| C | -1.354750 | -3.770754 | 0.326232 |
| C | -0.966393 | -3.778779 | -1.029461 |
| C | 0.385736 | -3.770365 | -1.328171 |
| C | -2.763563 | -3.747807 | 0.703863 |
| H | -2.977299 | -3.687241 | 1.777828 |
| C | -5.079964 | -3.746791 | 0.306756 |
| H | -5.116136 | -3.634961 | 1.401023 |
| C | -5.796781 | -5.039242 | -0.091622 |
| H | -5.695368 | -5.172658 | -1.173844 |
| H | -5.286777 | -5.884665 | 0.376494 |
| C | -7.273034 | -5.011077 | 0.297777 |
| H | -7.362479 | -4.982956 | 1.389727 |
| H | -7.760399 | -5.932289 | -0.030534 |
| C | -7.976237 | -3.793094 | -0.297777 |
| H | -9.017712 | -3.754558 | 0.030534 |
| H | -7.996606 | -3.884616 | -1.389727 |
| C | -7.262502 | -2.500539 | 0.091622 |
| H | -7.739658 | -1.636150 | -0.376494 |
| H | -7.327337 | -2.346004 | 1.173844 |
| C | -5.784799 | -2.525983 | -0.306756 |
| H | -5.706036 | -2.613223 | -1.401023 |
| C | -4.627477 | -0.519412 | -0.703863 |
| H | -4.681894 | -0.734796 | -1.777828 |

| | | | |
|---|---|---|---|
| C | -3.942944 | 0.712129 | -0.326232 |
| C | -3.458100 | 1.551125 | -1.328171 |
| C | -2.789322 | 2.726311 | -1.029461 |
| C | -2.588194 | 3.058625 | 0.326232 |
| C | -3.072364 | 2.219240 | 1.328171 |
| C | -3.755715 | 1.052468 | 1.029461 |
| C | -1.863915 | 4.267219 | 0.703863 |
| H | -1.704595 | 4.422037 | 1.777828 |
| N | -1.426309 | 5.101997 | -0.149618 |
| N | 1.426309 | 5.101997 | 0.149618 |
| N | 5.131614 | -1.315778 | -0.149618 |
| N | 3.705304 | -3.786218 | 0.149618 |
| N | -3.705304 | -3.786218 | -0.149618 |
| N | -5.131614 | -1.315778 | 0.149618 |
| H | -0.679455 | -3.761209 | 2.371215 |
| H | 0.679455 | -3.761209 | -2.371215 |
| H | 3.597030 | 1.292179 | 2.371215 |
| H | 2.917575 | 2.469030 | -2.371215 |
| H | -3.597030 | 1.292179 | -2.371215 |
| H | -2.917575 | 2.469030 | 2.371215 |
| O | 4.208340 | 0.284266 | -2.034895 |
| H | 4.673441 | -0.483672 | -1.629216 |
| O | 2.350352 | 3.502396 | 2.034895 |
| H | 1.917848 | 4.289155 | 1.629216 |
| O | -1.857988 | -3.786662 | -2.034895 |
| H | -2.755593 | -3.805483 | -1.629216 |
| O | 1.857988 | -3.786662 | 2.034895 |
| H | 2.755593 | -3.805483 | 1.629216 |
| O | -2.350352 | 3.502396 | -2.034895 |
| H | -1.917848 | 4.289155 | -1.629216 |
| O | -4.208340 | 0.284266 | 2.034895 |
| H | -4.673441 | -0.483672 | 1.629216 |