Data Article

Data from X-ray crystallographic analysis and DFT calculations on isomeric azo disperse dyes

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ARTICLE INFO

Article history:
Received 9 February 2018
Accepted 4 October 2018
Available online 9 October 2018

ABSTRACT

X-ray crystallography and DFT calculations were used to characterize the molecular nature and excited state properties of isomeric photo-stable azo dyes for textile fibers undergoing extensive sunlight exposure. Structural data in CIF files arising from X-ray analysis are reported and the complete files are deposited with the Cambridge Crystallographic Data Centre as CCDC 1548989 (https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=1548989) and CCDC 1548990 (https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=1548990).

Data from calculating the vertical electronic excitation of 20 excited states for each dye and from calculating excited state oxidation potential (ESOP) and Frontier HOMO/LUMO isosurfaces are also presented. This data is related to the article “Molecular and excited state properties of isomeric scarlet disperse dyes” (Lim et al., 2018) [1].

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Specifications table

| Subject area               | Chemistry, Photophysics                                      |
|----------------------------|---------------------------------------------------------------|
| More specific subject area | Inkjet printing, Azo Dyes, Excited State Properties, X-ray   |
|                            | Crystallography.                                              |
| Type of data               | Table, Image (x-ray, TD-DFT calculations), Figure             |
| How data was acquired      | X-ray Diffraction Analysis: Bruker-Nonius X8 Apex2 Diffractometer; DFT Calculations: Gaussian 09 (B3LYP and DGDZVP). |
| Data format                | Raw, analyzed.                                                |
| Experimental factors       | Slow evaporation of CH₂Cl₂ solutions of dyes at room temperature gave thin plate-like single crystals that for X-ray analysis |
| Experimental features      | Excited structures determined using single point energy calculations. Vertical electronic excitations of 20 excited states were solved and excited state oxidation potentials were extracted. |
| Data source location       | North Carolina State University, Raleigh, NC, USA.           |
| Data accessibility         | Data is with this article. X-ray: Cambridge Crystallographic Data Centre as CCDC 1548989 (https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=1548989) and CCDC 1548990 (https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=1548990). |
| Related research article   | Jihye Lim, Malgorzata Szymczyk, Nahid Mehraban, Yi Ding, Lisa Parrillo-Chapman, Ahmed El-Shafei, Harold S. Freeman, Molecular and excited state properties of isomeric scarlet disperse dyes, J. Molec. Struc., Vol. 1161, 254–261. |

Value of the data

- The data illustrate the reliability of current day molecular modeling methods for generating equilibrium geometries of monoazo dyes that are comparable to X-ray crystal structures.
- The data show essential calculations for predicting the molecular and excited state properties of organic dyes.
- The data are useful for further studies on the development of synthetic dyes having high photostability.
- The data show key vertical electronic excitations of 20 excited states for each dye along with the oscillator strength and molecular orbitals involved.

1. Data

The data arise from X-ray crystallographic analysis and computational methods in the characterization of isomeric monoazo dyes Sc2 and Sc3 for textile fibers. The data are Supplementary material for the study describing the “Molecular and excited state properties of isomeric scarlet disperse dyes” [1].

The overlay of data from X-ray and computational analysis of dyes Sc2 and Sc3 is shown in Fig. 1, to demonstrate the ability of DFT-based calculations to accurately predict the structures of these monoazo dyes. Root-mean squared (RMS) values were 0.0053 for Sc2 and 0.0001 for Sc3. Other key crystallographic data for the two dyes are summarized in Tables 1 and 2, including the associated crystal systems, space groups, molecular volumes, number of molecules per unit cell, 2θmax values, and bond lengths. The latter values are especially helpful in establishing the tautomeric form (azo vs.
Table 1
Crystallographic data for the major components of the scarlet disperse dye.

|                  | Sc2                          | Sc3                          |
|------------------|------------------------------|------------------------------|
| Composition      | $\text{C}_{20}\text{H}_{14}\text{F}_3\text{N}_7\text{O}_2 \cdot 0.5(\text{CH}_2\text{Cl}_2)$ | $\text{C}_{20}\text{H}_{14}\text{F}_3\text{N}_7\text{O}_2$ |
| Formula Weight   | 483.84                       | 441.38                       |
| Temperature (K)  | 100.01                       | 100.04                       |
| Crystal system   | Monoclinic                   | Triclinic                    |
| Space group      | $\text{P}2_1/c$              | $P\overline{1}$              |
| $a$ (Å)          | 20.753(2)                    | 7.5946(2)                    |
| $b$ (Å)          | 6.5429(8)                    | 11.0682(3)                   |
| $c$ (Å)          | 16.9106(19)                  | 11.3236(13)                  |
| $\alpha$ (°)     | 90                           | 80.9900(10)                  |
| $\beta$ (°)      | 113.308(5)                   | 88.6460(10)                  |
| $\gamma$ (°)     | 90                           | 81.4210(4)                   |
| Volume (Å³)      | 2108.8(4)                    | 929.59(4)                    |
| $Z$              | 4                            | 2                            |
| $\rho$calc (g/cm³) | 1.524                         | 1.577                         |
| $\mu$ (mm⁻¹)    | 0.243                        | 0.128                         |
| $f$(000)         | 988                          | 452                          |
| Crystal dimension (mm) | 0.142 × 0.105 × 0.057 | 0.518 × 0.309 × 0.247 |
| $\theta$max (°)  | 4.818–46.51                  | 3.642–72.86                  |
| Reflections collected | 7750                         | 28,451                       |
| Independent reflections | 2984                         | 9000                         |
| Reflections observed | 1711                         | 7465                         |
| Number of variables | 323                          | 299                          |
| $R1$ [$|F| > 2\sigma(|F|)]$ | 0.0542                        | 0.0405                        |
| $wR2$ [$|F| > 2\sigma(|F|)]$ | 0.1127                        | 0.1152                        |
| $wR1$ [all data] | 0.1171                       | 0.0506                        |
| $wR2$ [all data] | 0.1341                       | 0.1241                        |
| Largest Diffraction peak/ hole (e⁻/Å³) | 0.31/– 0.25                  | 0.70/– 0.46                  |
| Max. shift in final cycles | < 0.001                     | < 0.001                      |

Fig. 1. The X-ray structures (top) of Sc2 (a) and Sc3 (b) superimposed on the calculated structures (bottom).
hydrazone) of the dyes analyzed (cf. N1–N2, N2–C8, N4–C12 data) (Table 3).

Data for intermolecular H-bonding interactions between layers of molecules positioned parallel to each other are given in Fig. 2. The unit cell for Sc2 shows intermolecular H-bond distances between the NH2 and CN groups (2.418 Å). Also seen are short contacts corresponding to intermolecular hydrogen bonds for Sc3, namely the NO2 and NH2 groups (2.188 Å), and the NH2 and CN groups (2.512 Å).

Calculation of vertical electronic excitation energies for 20 excited states along with the oscillator strength (f) and molecular orbitals involved for each dye led to the raw data shown in Tables 4 and 5 for Sc2 and Sc3. From these data the excited state oxidation potential (ESOP) for each dye can be extracted.

### Table 2
Bond lengths for Sc2.

| Atom | Atom | Length/ Å |
|------|------|-----------|
| F1   | C7   | 1.341(5)  |
| F2   | C7   | 1.343(5)  |
| F3   | C7   | 1.346(4)  |
| O1   | N3   | 1.226(5)  |
| O2   | N3   | 1.236(4)  |
| N1   | N2   | 1.284(4)  |
| N1   | C1   | 1.419(5)  |
| N2   | C8   | 1.380(4)  |
| N3   | C4   | 1.464(5)  |
| N4   | C12  | 1.344(4)  |
| N5   | C11  | 1.326(4)  |
| N6   | C12  | 1.349(4)  |
| N6   | C15  | 1.413(5)  |
| N7   | C14  | 1.154(5)  |
| C1   | C2   | 1.400(5)  |
| C1   | C6   | 1.397(5)  |
| C2   | C3   | 1.384(5)  |

| Atom | Atom | Length/ Å |
|------|------|-----------|
| C2   | C7   | 1.503(5)  |
| C3   | C4   | 1.379(6)  |
| C4   | C5   | 1.383(5)  |
| C5   | C6   | 1.375(5)  |
| C8   | C9   | 1.419(5)  |
| C8   | C12  | 1.426(5)  |
| C9   | C10  | 1.377(5)  |
| C9   | C13  | 1.499(5)  |
| C10  | C11  | 1.430(5)  |
| C10  | C14  | 1.428(5)  |
| C15  | C16  | 1.389(5)  |
| C15  | C20  | 1.387(5)  |
| C16  | C17  | 1.383(6)  |
| C17  | C18  | 1.377(6)  |
| C18  | C19  | 1.384(6)  |
| C19  | C20  | 1.386(5)  |
| C20  | C15  | 1.730(11) |
| C20  | C15  | 1.765(11) |

### Table 3
Bond lengths for Sc3.

| Atom | Atom | Length/ Å |
|------|------|-----------|
| F1   | C7   | 1.3451(9) |
| F2   | C7   | 1.3380(9) |
| F3   | C7   | 1.3399(8) |
| O1   | N3   | 1.2248(10) |
| O2   | N3   | 1.2243(10) |
| N1   | N2   | 1.2848(8) |
| N1   | C1   | 1.4134(9) |
| N1   | C8   | 1.3675(8) |
| N3   | C4   | 1.4579(9) |
| N4   | C11  | 1.3222(9) |
| N4   | C12  | 1.3351(8) |
| N5   | C14  | 1.1546(9) |
| N6   | C11  | 1.3341(9) |
| N7   | C12  | 1.3503(9) |
| N7   | C15  | 1.4127(9) |
| C7   | C2   | 1.5026(10) |
| C1   | C2   | 1.4084(9) |
| C1   | C6   | 1.4057(10) |
| C2   | C3   | 1.3868(9) |
| C3   | C4   | 1.3838(10) |
| C4   | C5   | 1.3910(10) |
| C5   | C6   | 1.3829(10) |
| C6   | C7   | 1.4176(9) |
| C7   | C8   | 1.4501(9) |
| C8   | C9   | 1.3852(9) |
| C9   | C10  | 1.5007(10) |
| C10  | C11  | 1.4326(10) |
| C10  | C12  | 1.4233(10) |
| C11  | C14  | 1.4013(10) |
| C12  | C15  | 1.3990(10) |
| C15  | C17  | 1.3991(10) |
| C16  | C18  | 1.3868(11) |
| C17  | C19  | 1.3910(11) |
| C18  | C20  | 1.3868(10) |
Fig. 2. Unit cells showing intermolecular interactions (Å) between molecules of Sc2 (a) and Sc3 (b).

Table 4
Calculated excitation energies and oscillator strengths for the 20 excited states of Sc2.

| Excited State | Singlet-A | Excitation Energy (eV) | Oscillator Strength (nm) | Oscillator Strength (a.u.) |
|---------------|-----------|------------------------|--------------------------|----------------------------|
| 111 - > 114   | 0.16845   | 2.3593                 | 525.52                   | 1.0963                     |
| 113 - > 114   | 0.68009   |                        |                          |                            |
| Excited State 2: | Singlet-A | 2.4599                 | 504.02                   | 0.0772                     |
| 111 - > 114   | 0.61550   |                        |                          |                            |
| 111 - > 115   | - 0.18095 |                        |                          |                            |
| 112 - > 114   | - 0.19991 |                        |                          |                            |
| 113 - > 114   | - 0.19321 |                        |                          |                            |
| Excited State 3: | Singlet-A | 3.0046                 | 412.65                   | 0.0698                     |
| 111 - > 114   | 0.22058   |                        |                          |                            |
| 112 - > 114   | 0.66351   |                        |                          |                            |
| Excited State 4: | Singlet-A | 3.3435                 | 370.82                   | 0.2245                     |
| 109 - > 114   | 0.12672   |                        |                          |                            |
| 111 - > 115   | 0.88917   |                        |                          |                            |
| Excited State 5: | Singlet-A | 3.4878                 | 355.48                   | 0.0107                     |
| 110 - > 114   | 0.70043   |                        |                          |                            |
| Excited State 6: | Singlet-A | 3.6637                 | 338.41                   | 0.0109                     |
| 105 - > 114   | 0.14783   |                        |                          |                            |
| 111 - > 114   | 0.18820   |                        |                          |                            |
| 111 - > 115   | 0.60693   |                        |                          |                            |
| 112 - > 115   | - 0.22758 |                        |                          |                            |
| Excited State 7: | Singlet-A | 3.7276                 | 332.61                   | 0.0050                     |
| 105 - > 114   | 0.59143   |                        |                          |                            |
| 105 - > 115   | 0.31989   |                        |                          |                            |
| 109 - > 114   | 0.10910   |                        |                          |                            |
| 111 - > 115   | - 0.13494 |                        |                          |                            |
| Excited State 8: | Singlet-A | 3.7570                 | 330.01                   | 0.0971                     |
| 109 - > 114   | 0.65678   |                        |                          |                            |
| 113 - > 115   | - 0.11278 |                        |                          |                            |
| Excited State 9: | Singlet-A | 3.9326                 | 315.28                   | 0.0126                     |
| 108 - > 114   | 0.54817   |                        |                          |                            |
| 112 - > 115   | - 0.11815 |                        |                          |                            |
| 113 - > 116   | 0.23227   |                        |                          |                            |
| 113 - > 117   | - 0.31543 |                        |                          |                            |
Table 4 (continued)

| Excited State 10: | Singlet-A | 3.9699 eV | 312.31 nm | $f = 0.0747$ |
|------------------|-----------|-----------|-----------|-------------|
| 108 -> 114       | 0.12487   |           |           |             |
| 109 -> 114       | -0.13850  |           |           |             |
| 111 -> 115       | 0.14977   |           |           |             |
| 112 -> 115       | 0.42170   |           |           |             |
| 113 -> 116       | 0.36207   |           |           |             |
| 113 -> 117       | 0.32511   |           |           |             |

| Excited State 11: | Singlet-A | 4.0260 eV | 307.96 nm | $f = 0.0300$ |
|------------------|-----------|-----------|-----------|-------------|
| 111 -> 115       | 0.17399   |           |           |             |
| 112 -> 115       | 0.47223   |           |           |             |
| 113 -> 116       | -0.27249  |           |           |             |
| 113 -> 117       | -0.39237  |           |           |             |

| Excited State 12: | Singlet-A | 4.0562 eV | 305.67 nm | $f = 0.0019$ |
|------------------|-----------|-----------|-----------|-------------|
| 107 -> 114       | 0.66738   |           |           |             |
| 107 -> 115       | -0.17285  |           |           |             |

| Excited State 13: | Singlet-A | 4.2097 eV | 294.52 nm | $f = 0.0568$ |
|------------------|-----------|-----------|-----------|-------------|
| 108 -> 114       | -0.39065  |           |           |             |
| 113 -> 116       | 0.46544   |           |           |             |
| 113 -> 117       | -0.34136  |           |           |             |

| Excited State 14: | Singlet-A | 4.2568 eV | 291.26 nm | $f = 0.0003$ |
|------------------|-----------|-----------|-----------|-------------|
| 103 -> 114       | 0.62259   |           |           |             |
| 103 -> 115       | 0.32497   |           |           |             |

| Excited State 15: | Singlet-A | 4.4996 eV | 275.54 nm | $f = 0.0045$ |
|------------------|-----------|-----------|-----------|-------------|
| 110 -> 115       | 0.67093   |           |           |             |
| 113 -> 119       | -0.15611  |           |           |             |

| Excited State 16: | Singlet-A | 4.5874 eV | 270.27 nm | $f = 0.0100$ |
|------------------|-----------|-----------|-----------|-------------|
| 106 -> 114       | 0.54991   |           |           |             |
| 111 -> 116       | -0.24554  |           |           |             |
| 113 -> 118       | 0.31130   |           |           |             |

| Excited State 17: | Singlet-A | 4.5933 eV | 269.92 nm | $f = 0.0026$ |
|------------------|-----------|-----------|-----------|-------------|
| 106 -> 114       | 0.17037   |           |           |             |
| 111 -> 116       | 0.44354   |           |           |             |
| 111 -> 117       | 0.40398   |           |           |             |
| 112 -> 116       | -0.20839  |           |           |             |
| 112 -> 117       | -0.20558  |           |           |             |

| Excited State 18: | Singlet-A | 4.6084 eV | 269.04 nm | $f = 0.0008$ |
|------------------|-----------|-----------|-----------|-------------|
| 106 -> 114       | -0.11476  |           |           |             |
| 111 -> 116       | -0.40558  |           |           |             |
| 111 -> 117       | 0.50411   |           |           |             |
| 112 -> 116       | 0.16311   |           |           |             |
| 112 -> 117       | -0.15477  |           |           |             |

| Excited State 19: | Singlet-A | 4.6379 eV | 267.33 nm | $f = 0.1619$ |
|------------------|-----------|-----------|-----------|-------------|
| 106 -> 114       | -0.30153  |           |           |             |
| 113 -> 118       | 0.60206   |           |           |             |

| Excited State 20: | Singlet-A | 4.7032 eV | 263.62 nm | $f = 0.0287$ |
|------------------|-----------|-----------|-----------|-------------|
| 109 -> 115       | 0.63757   |           |           |             |
| 111 -> 116       | 0.10091   |           |           |             |
| 112 -> 117       | 0.14383   |           |           |             |

2. Experimental design, materials, and methods

Single crystal X-ray diffraction analysis was conducted using a Bruker–Nonius X8 Apex2 diffractometer. The frame integration was performed with the program SAINT. The resulting raw data
Table 5
Calculated excitation energies and oscillator strengths for the 20 excited states of Sc3.

| Excited State 1: Singlet-A | 2.3700 eV | 523.13 nm | \( f = 0.5373 \) |
|---------------------------|----------|-----------|-----------------|
| 111 - > 114              | 0.11383  |           |                 |
| 112 - > 114              | - 0.18480|           |                 |
| 113 - > 114              | 0.66822  |           |                 |
| Excited State 2: Singlet-A | 2.4473 eV | 506.61 nm | \( f = 0.1416 \) |
| 111 - > 114              | 0.50266  |           |                 |
| 111 - > 115              | - 0.16373|           |                 |
| 112 - > 114              | - 0.39149|           |                 |
| 113 - > 114              | - 0.21595|           |                 |
| Excited State 3: Singlet-A | 3.0048 eV | 412.61 nm | \( f = 0.4636 \) |
| 111 - > 114              | 0.42774  |           |                 |
| 112 - > 114              | 0.54660  |           |                 |
| Excited State 4: Singlet-A | 3.3508 eV | 370.01 nm | \( f = 0.0122 \) |
| 110 - > 114              | 0.64733  |           |                 |
| 111 - > 114              | - 0.10057|           |                 |
| 113 - > 115              | 0.24591  |           |                 |
| Excited State 5: Singlet-A | 3.3624 eV | 368.74 nm | \( f = 0.0530 \) |
| 110 - > 114              | - 0.24661|           |                 |
| 113 - > 115              | 0.64269  |           |                 |
| Excited State 6: Singlet-A | 3.6418 eV | 340.45 nm | \( f = 0.0038 \) |
| 111 - > 114              | - 0.17595|           |                 |
| 111 - > 115              | - 0.44934|           |                 |
| 112 - > 115              | 0.47335  |           |                 |
| Excited State 7: Singlet-A | 3.7276 eV | 332.61 nm | \( f = 0.0003 \) |
| 105 - > 114              | 0.60898  |           |                 |
| 105 - > 115              | 0.33006  |           |                 |
| Excited State 8: Singlet-A | 3.8726 eV | 320.16 nm | \( f = 0.0456 \) |
| 107 - > 114              | - 0.17843|           |                 |
| 109 - > 114              | 0.61937  |           |                 |
| 111 - > 115              | - 0.15064|           |                 |
| 113 - > 116              | - 0.15214|           |                 |
| 113 - > 117              | - 0.10277|           |                 |
| Excited State 9: Singlet-A | 3.9310 eV | 315.40 nm | \( f = 0.0241 \) |
| 107 - > 114              | 0.39742  |           |                 |
| 108 - > 114              | 0.35278  |           |                 |
| 111 - > 115              | - 0.11320|           |                 |
| 112 - > 115              | - 0.10887|           |                 |
| 113 - > 116              | - 0.27464|           |                 |
| 113 - > 117              | 0.30370  |           |                 |
| Excited State 10: Singlet-A | 3.9832 eV | 311.27 nm | \( f = 0.0557 \) |
| 108 - > 114              | 0.20907  |           |                 |
| 109 - > 114              | 0.26135  |           |                 |
| 111 - > 115              | 0.33755  |           |                 |
| 112 - > 115              | 0.32994  |           |                 |
| 113 - > 116              | 0.35017  |           |                 |
| 113 - > 117              | 0.13756  |           |                 |
| Excited State 11: Singlet-A | 4.0392 eV | 306.95 nm | \( f = 0.5148 \) |
| 107 - > 114              | 0.13790  |           |                 |
| 111 - > 115              | - 0.29550|           |                 |
| 112 - > 115              | - 0.32129|           |                 |
| 113 - > 116              | 0.49368  |           |                 |
| 113 - > 117              | 0.12655  |           |                 |
| Excited State 12: Singlet-A | 4.1265 eV | 300.46 nm | \( f = 0.0008 \) |
| 106 - > 114              | 0.64834  |           |                 |
| 106 - > 115              | - 0.17133|           |                 |
was scaled and absorption corrected using a multi-scan averaging of symmetry equivalent data using SIRPOW [2]. Structures were solved using the program SHELXT [3]. Slow evaporation of CH$_2$Cl$_2$ solutions of Sc$_2$ and Sc$_3$ at room temperature gave thin plate-like single crystals that were suitable for X-ray crystallographic analysis. The equilibrium molecular geometries (EMGs) of Sc$_1$, Sc$_2$ and Sc$_3$ were calculated in the neutral forms using density functional theory (DFT) employing the generalized gradient approximation (GGA) at the hybrid exchange-correlation energy functional 3-Parameter (Exchange), Lee et al. (B3LYP) [4,5] and the full-electron basis set Density Gauss double-zeta with polarization functions (DGDZVP) [6,7], implemented in Gaussian 09. The X-ray structures of Sc$_2$ and Sc$_3$ were superimposed on the corresponding calculated molecular geometries and the RMS was calculated in each case. The isosurfaces of the HOMO and LUMO were extracted for each dye from the corresponding checkpoint files. In addition, TD-DFT calculations were performed on the EMGs and the geometry of the excited state structure was calculated using single point energy calculations for each dye. Vertical electronic excitation energies for 20 excited states were calculated for each dye and the excited state oxidation potential (ESOP) for each dye was extracted.

### Table 5 (continued)

| Excited State 13: | Singlet-A | 4.1991 eV | 295.27 nm | $f = 0.0884$ |
|------------------|-----------|-----------|-----------|--------------|
| 108 -> 114       | 0.12260   |           |           |              |
| 113 -> 116       | 0.40583   |           |           |              |
| 113 -> 117       | 0.53076   |           |           |              |
| Excited State 14: | Singlet-A | 4.2585 eV | 291.14 nm | $f = 0.0006$ |
| 103 -> 114       | 0.62158   |           |           |              |
| 103 -> 115       | 0.32547   |           |           |              |
| Excited State 15: | Singlet-A | 4.2974 eV | 288.51 nm | $f = 0.0161$ |
| 106 -> 114       | 0.10519   |           |           |              |
| 107 -> 114       | 0.48658   |           |           |              |
| 108 -> 114       | 0.34478   |           |           |              |
| 109 -> 114       | 0.10188   |           |           |              |
| 113 -> 117       | 0.26919   |           |           |              |
| Excited State 16: | Singlet-A | 4.3887 eV | 282.51 nm | $f = 0.0007$ |
| 106 -> 114       | 0.10513   |           |           |              |
| 110 -> 115       | 0.65507   |           |           |              |
| 111 -> 116       | 0.10839   |           |           |              |
| 112 -> 116       | 0.15738   |           |           |              |
| Excited State 17: | Singlet-A | 4.4058 eV | 281.41 nm | $f = 0.0203$ |
| 110 -> 115       | 0.19596   |           |           |              |
| 111 -> 116       | 0.33235   |           |           |              |
| 112 -> 116       | 0.57520   |           |           |              |
| Excited State 18: | Singlet-A | 4.5811 eV | 270.64 nm | $f = 0.0046$ |
| 111 -> 117       | 0.46157   |           |           |              |
| 112 -> 117       | 0.51752   |           |           |              |
| Excited State 19: | Singlet-A | 4.6346 eV | 267.52 nm | $f = 0.1259$ |
| 111 -> 116       | 0.59135   |           |           |              |
| 112 -> 116       | 0.32627   |           |           |              |
| Excited State 20: | Singlet-A | 4.8246 eV | 256.98 nm | $f = 0.0022$ |
| 110 -> 116       | 0.43307   |           |           |              |
| 110 -> 120       | 0.13187   |           |           |              |
| 112 -> 118       | 0.16383   |           |           |              |
| 113 -> 118       | 0.48759   |           |           |              |
Acknowledgments

The authors thank the Walmart Innovation Fund (Grant no. 558811) for financial support and the Department of Chemistry at North Carolina State University for use of the Apex2 diffractometer.

Transparency document. Supplementary material

Transparency document associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.10.010.

References

[1] J. Lim, M. Szymczyk, N. Mehraban, Y. Ding, L. Parrillo-Chapman, A. El-Shafei, H. Freeman, Molecular and excited state properties of isomeric scarlet disperse dyes, J. Mol. Struct. 1161 (2018) 254–261.
[2] A. Altomare, G. Cascarano, C. Giacovazzo, A. Guagliardi, M. Burla, G. Polidori, et al., SIRPOW, 92—a program for automatic solution of crystal structures by direct methods optimized for powder data, J. Appl. Cryst. 27 (1994) 435–436.
[3] Bruker, Structure Determination Programs. Version 6.10, SHELXTL, Bruker Analytical X-ray Instruments Inc., Madison, Wisconsin, USA, 2000.
[4] C.T. Lee, W.T. Yang, R.G. Parr, Development of the Colle–Salvetti correlation-energy formula into a functional of the electron density, Phys. Rev. B Condens Matter. 37 (1988) 785–789.
[5] A.D. Becke, Density-functional exchange-energy approximation with correct asymptotic behavior, Phys. Rev. A 38 (1988) 3098–3100.
[6] N. Godbout, D.R. Salahub, J. Andzelm, E. Wimmer, Optimization of Gaussian-type basis sets for local spin density functional calculations. Part I. Boron through neon, optimization technique and validation, Can. J. Chem. 70 (1992) 560–571.
[7] C. Sosa, J. Andzelm, B.C. Elkin, E. Wimmer, K.D. Dobbs, D.A. Dixon, A local density functional study of the structure and vibrational frequencies of molecular transition-metal compounds, J. Phys. Chem. 96 (1992) 6630–6636.