

First observable CD spectra from n- σ^* excitation: TD-DFT calculation and determination of absolute configuration of 2,6-dithiaspiro[3.3]heptane 2,6-dioxide

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Dedicated to Professor Manfred Schlosser in honor of his scientific achievements

Table 1. Bond angles and dihedral angles in the optimized structure of **1a** (B3LYP/6-31G(d)) and the estimated coupling constants for W-shape coupling

Intra-ring $\theta_2(\text{C1-C4-C3}) = 94.7^\circ$							$^4J_{HH}/\text{Hz}$		
H _{1eq} -C1-C4- C3-H _{3eq}	$\varphi_1(\text{H}_{1eq}\text{-C1-}$ $\text{C4-C3})$	145.2°	$\varphi_2(\text{C1-C4-C3-}$ $\text{H}_{3eq})$	-145.2°	$\theta_1(\text{H}_{1eq}\text{-C1-}$ $\text{C4})$	119.0°	$\theta_3(\text{C4-C3-}$ $\text{H}_{3eq})$	119.5°	ca. 3-4
H _{1eq} -C1-C4- C3-H _{3ax}			$\varphi_2(\text{C1-C4-C3-}$ $\text{H}_{3ax})$	83.4°			$\theta_3(\text{C4-C3-}$ $\text{H}_{3ax})$	112.4°	<1.0
H _{1ax} -C1-C4- C3-H _{3eq}	$\varphi_1(\text{H}_{1ax}\text{-C1-}$ $\text{C4-C3})$	-83.1°	$\varphi_2(\text{C1-C4-C3-}$ $\text{H}_{3eq})$	-145.3°	$\theta_1(\text{H}_{1ax}\text{-C1-}$ $\text{C4})$	112.5°	$\theta_3(\text{C4-C3-}$ $\text{H}_{3eq})$	119.5°	<1.0
H _{1ax} -C1-C4- C3-H _{3ax}			$\varphi_2(\text{C1-C4-C3-}$ $\text{H}_{3ax})$	83.4°			$\theta_3(\text{C4-C3-}$ $\text{H}_{3ax})$	112.4°	<1.0

Inter-ring $\theta_2(\text{C1-C4-C5}) = 114.2^\circ$							$^4J_{HH}/\text{Hz}$		
H _{1eq} -C1-C4-C5-H _{5eq}	$\varphi_1(\text{H}_{1eq}\text{-C1-C4-C5})$	22.6°	$\varphi_2(\text{C1-C4-C5-H}_{5eq})$	22.5°	$\theta_1(\text{H}_{1eq}\text{-C1-C4})$	119.0°	$\theta_3(\text{C4-C5-H}_{5eq})$	119.0°	<1.0
H _{1eq} -C1-C4-C5-H _{5ax}			$\varphi_2(\text{C1-C4-C5-H}_{5ax})$	154.2°			$\theta_3(\text{C4-C5-H}_{5ax})$	112.5°	<1.0
H _{1ax} -C1-C4-C5-H _{5eq}	$\varphi_1(\text{H}_{1ax}\text{-C1-C4-C5})$	154.2°	$\varphi_2(\text{C1-C4-C5-H}_{5eq})$	22.5°	$\theta_1(\text{H}_{1ax}\text{-C1-C4})$	112.5°	$\theta_3(\text{C4-C5-H}_{5eq})$	119.0°	<1.0
H _{1ax} -C1-C4-C5-H _{5ax}			$\varphi_2(\text{C1-C4-C5-H}_{5ax})$	154.2°			$\theta_3(\text{C4-C5-H}_{5ax})$	112.5°	<1.0
H _{1eq} -C1-C4-C7-H _{7eq}	$\varphi_1(\text{H}_{1eq}\text{-C1-C4-C7})$	22.6°	$\varphi_2(\text{C1-C4-C7-H}_{7eq})$	-86.8°	$\theta_1(\text{H}_{1eq}\text{-C1-C4})$	119.0°	$\theta_3(\text{C4-C7-H}_{7eq})$	119.5°	<1.0
H _{1eq} -C1-C4-C7-H _{7ax}			$\varphi_2(\text{C1-C4-C7-H}_{7ax})$	44.9°			$\theta_3(\text{C4-C7-H}_{7ax})$	112.4°	<1.0
H _{1ax} -C1-C4-C7-H _{7eq}	$\varphi_1(\text{H}_{1ax}\text{-C1-C4-C7})$	154.2°	$\varphi_2(\text{C1-C4-C7-H}_{7eq})$	-86.8°	$\theta_1(\text{H}_{1ax}\text{-C1-C4})$	112.5°	$\theta_3(\text{C4-C7-H}_{7eq})$	119.5°	<1.0
H _{1ax} -C1-C4-C7-H _{7ax}			$\varphi_2(\text{C1-C4-C7-H}_{7ax})$	44.9°			$\theta_3(\text{C4-C7-H}_{7ax})$	112.4°	<1.0