

**Supporting Information**  
**for**  
**Conformational analysis, stereoelectronic interactions and**  
**NMR properties of 2-fluorobicyclo[2.2.1]heptan-7-ols**

Fátima M. P. de Rezende<sup>1</sup>, Marilua A. Moreira<sup>1</sup>, Rodrigo A. Cormanich<sup>2</sup> and Matheus P. Freitas<sup>\*1</sup>

Address: <sup>1</sup>Department of Chemistry, Federal University of Lavras, P.O. Box 3037, 37200-000, Lavras, MG, Brazil and <sup>2</sup>Chemistry Institute, State University of Campinas, P.O. Box 6154, 13083-970, Campinas, SP, Brazil

Email: Matheus P. Freitas - matheus@dqi.ufla.br

\* Corresponding author

**Angular dependences of SSCCs and energies in 5–8**

**Figure S1:** Angular dependence of  $J_{F,H(O)}$  and its components FC (*Fermi Contact*), SD (*Spin Dipolar*), PSO (*Paramagnetic Spin-Orbit*) and DSO (*Diamagnetic Spin-Orbit*) in **5**.

**Figure S2:** Angular dependence of  $J_{F,H(O)}$  and its components FC (*Fermi Contact*), SD (*Spin Dipolar*), PSO (*Paramagnetic Spin-Orbit*) and DSO (*Diamagnetic Spin-Orbit*) in **6**.

**Figure S3:** Angular dependence of  $J_{F,H(O)}$  and its components FC (*Fermi Contact*), SD (*Spin Dipolar*), PSO (*Paramagnetic Spin-Orbit*) and DSO (*Diamagnetic Spin-Orbit*) in **7**.

**Figure S4:** Angular dependence of  $J_{F,H(O)}$  and its components FC (*Fermi Contact*), SD (*Spin Dipolar*), PSO (*Paramagnetic Spin-Orbit*) and DSO (*Diamagnetic Spin-Orbit*) in **8**.

**Figure S5:** Angular dependence of total hyperconjugation in **5–8**.

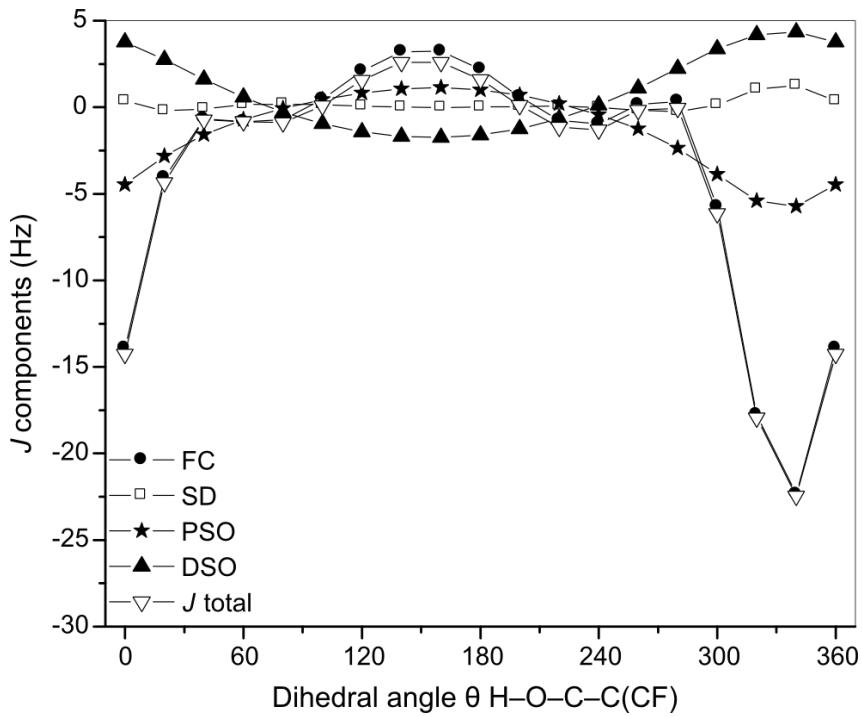
**Figure S6:** Angular dependence of Lewis-type energies in **5–8**.

**Figure S7:** Angular dependence of  ${}^1J_{F,H(O)}$  and  $n_{F \rightarrow \sigma^*_{OH}}$  in **5**.

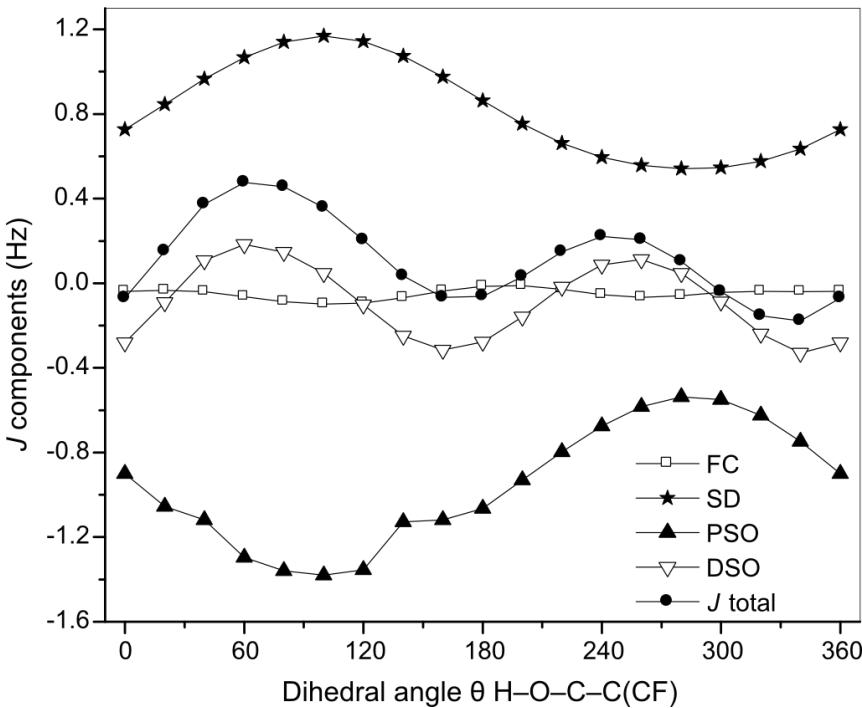
**Figure S8:** Angular dependence of  ${}^1J_{F,H(O)}$  and  $n_{F \rightarrow \sigma^*_{OH}}$  in **6**.

**Figure S9:** Angular dependence of  ${}^1J_{F,H(O)}$  and  $n_{F \rightarrow \sigma^*_{OH}}$  in **7**.

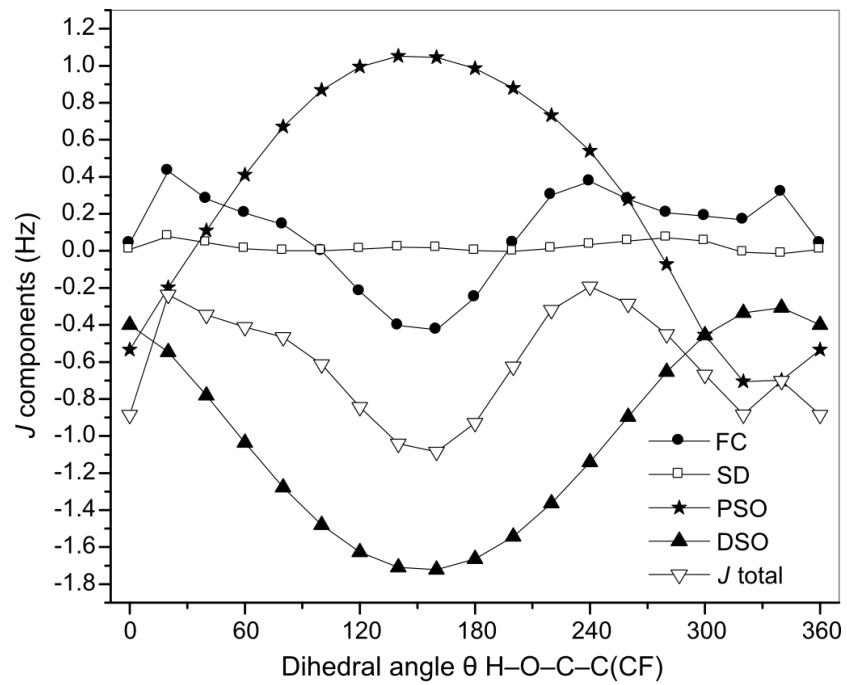
**Figure S10:** Angular dependence of  ${}^1J_{F,H(O)}$  and  $n_{F \rightarrow \sigma^*_{OH}}$  in **8**.



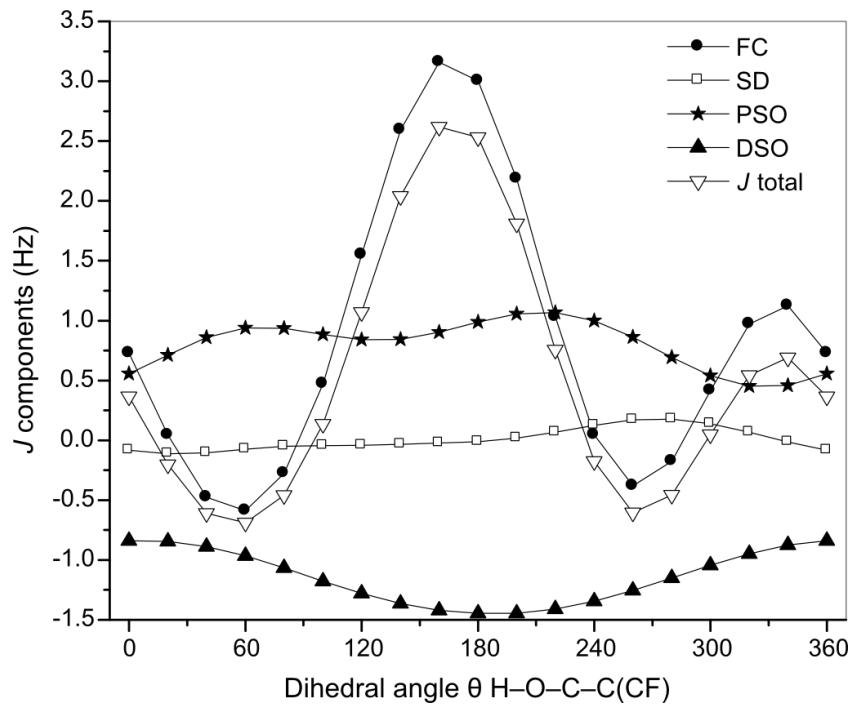
**Figure S1:** Angular dependence of  $J_{F,H(O)}$  and its components FC (*Fermi Contact*), SD (*Spin Dipolar*), PSO (*Paramagnetic Spin-Orbit*) and DSO (*Diamagnetic Spin-Orbit*) in 5.



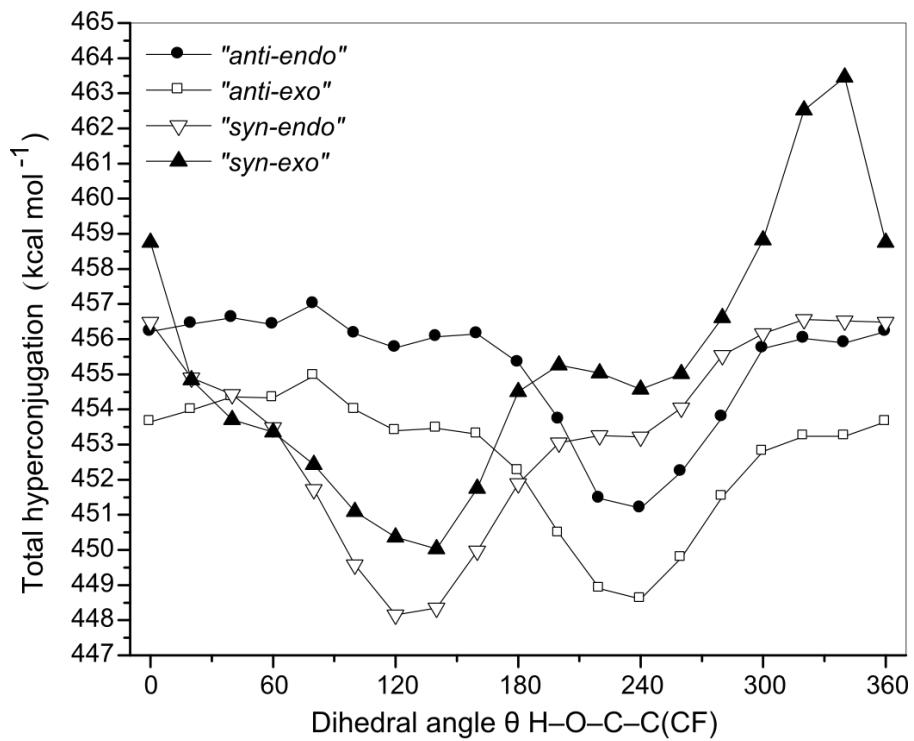
**Figure S2:** Angular dependence of  $J_{F,H(O)}$  and its components FC (*Fermi Contact*), SD (*Spin Dipolar*), PSO (*Paramagnetic Spin-Orbit*) and DSO (*Diamagnetic Spin-Orbit*) in 6.



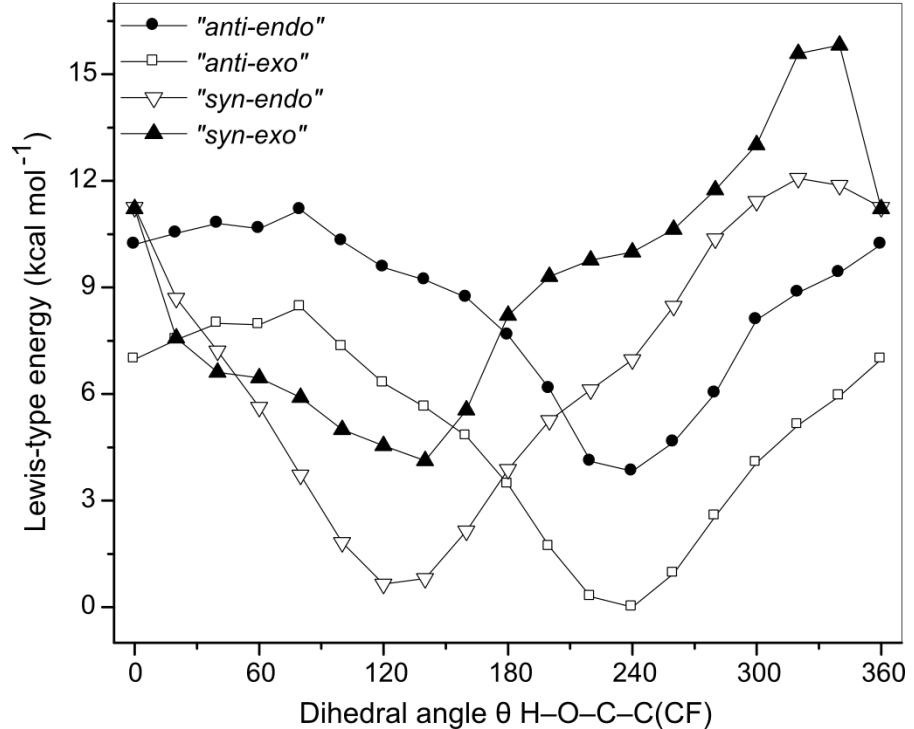
**Figure S3:** Angular dependence of  $J_{F,H(O)}$  and its components FC (*Fermi Contact*), SD (*Spin Dipolar*), PSO (*Paramagnetic Spin-Orbit*) and DSO (*Diamagnetic Spin-Orbit*) in 7.



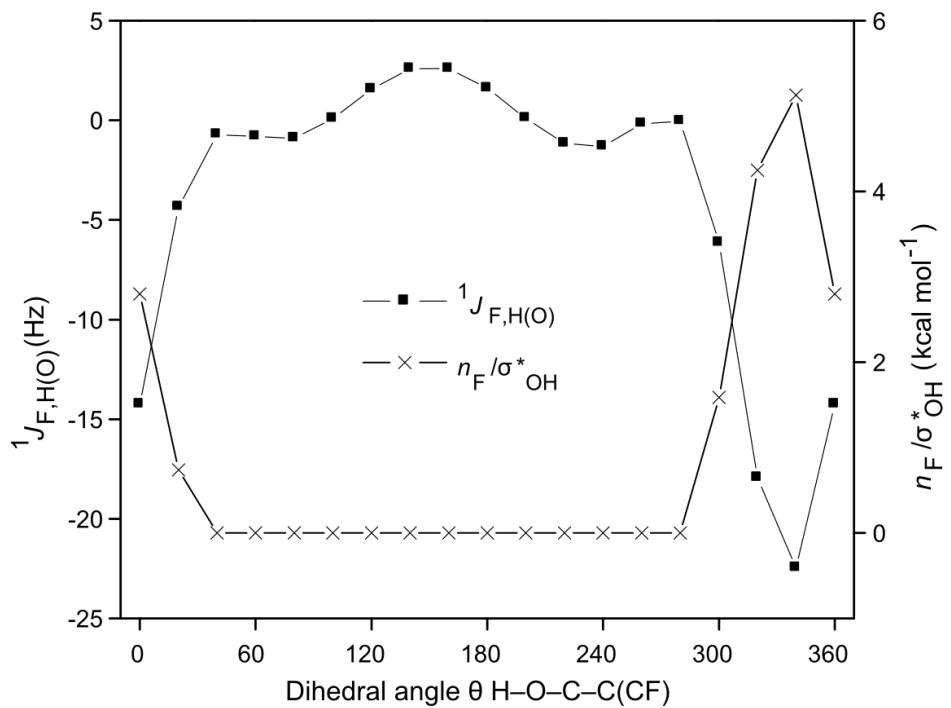
**Figure S4:** Angular dependence of  $J_{F,H(O)}$  and its components FC (*Fermi Contact*), SD (*Spin Dipolar*), PSO (*Paramagnetic Spin-Orbit*) and DSO (*Diamagnetic Spin-Orbit*) in 8.



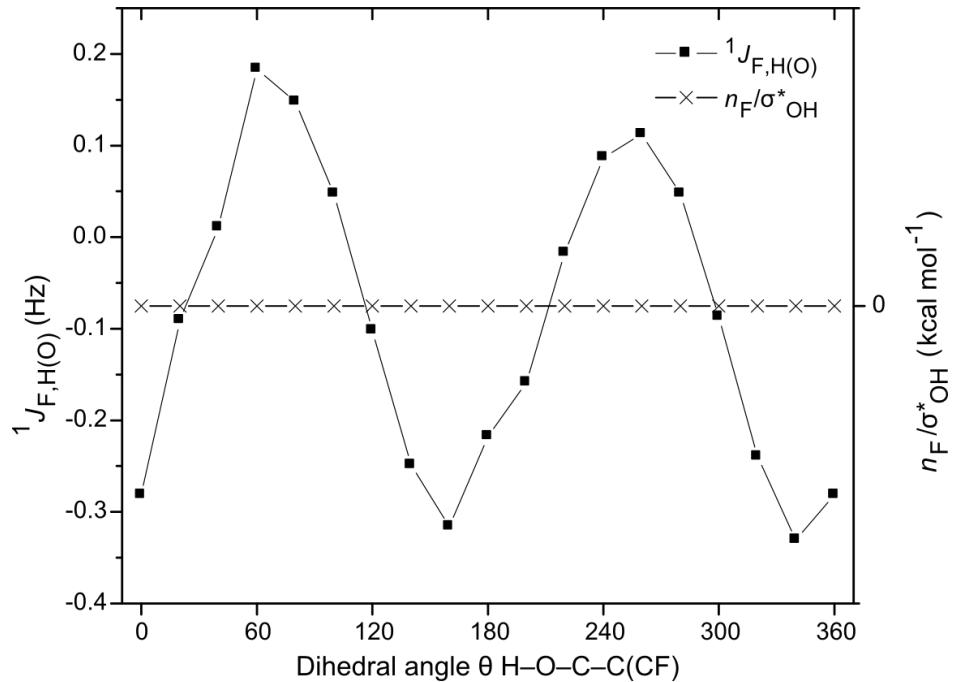
**Figure S5:** Angular dependence of total hyperconjugation in **5–8**.



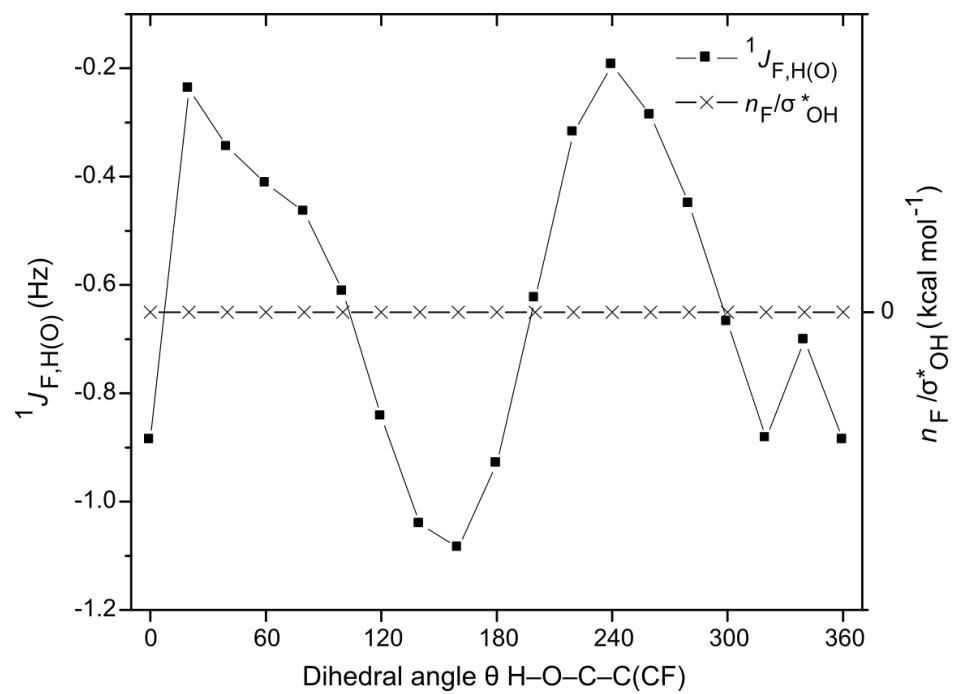
**Figure S6:** Angular dependence of Lewis-type energies in **5–8**.



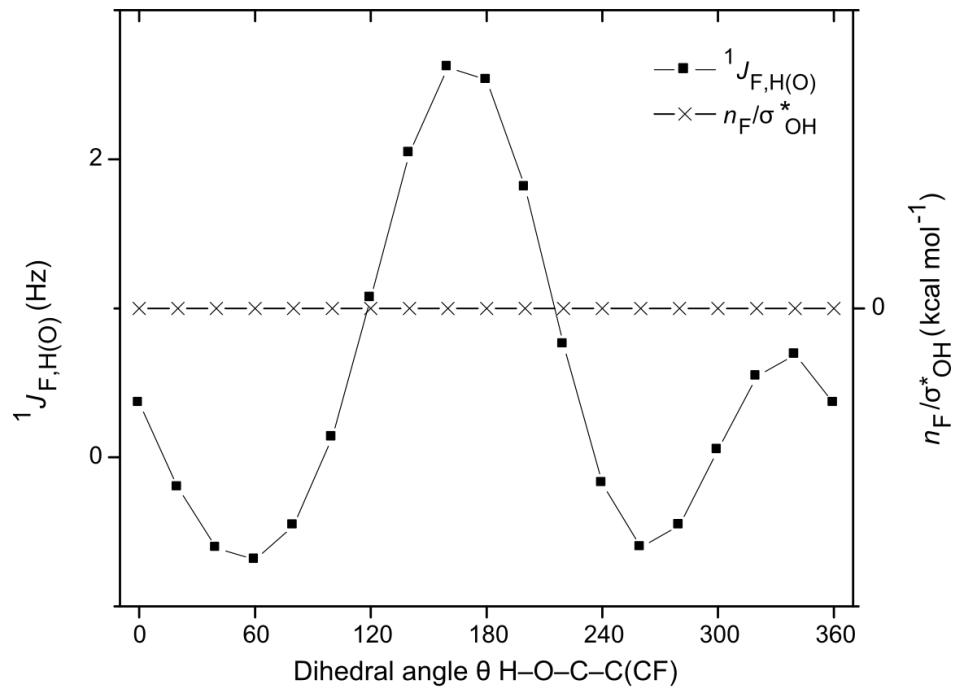
**Figure S7:** Angular dependence of  $^1J_{F,H(O)}$  and  $n_F \rightarrow \sigma^*_{OH}$  in **5**.



**Figure S8:** Angular dependence of  $^1J_{F,H(O)}$  and  $n_F \rightarrow \sigma^*_{OH}$  in **6**.



**Figure S9:** Angular dependence of  $^1J_{F,H(O)}$  and  $n_F \rightarrow \sigma^*_{OH}$  in **7**.



**Figure S10:** Angular dependence of  $^1J_{F,H(O)}$  and  $n_F \rightarrow \sigma^*_{OH}$  in **8**.