Impact of Electron Acceptor on Three-Photon Absorption Cross-Section of Fluorene Derivatives

Junhui Liu, Guofeng Li, and Yuanxu Wang*

Institute for Computational Materials Science, Department of Physics, Henan University, Kaifeng 475001, Peoples Republic of China.

* wangyx@henu.edu.cn

Table Selected important geometrical features (bond lengths (Å) and angles (°)) of calculated molecular of FATT and TSATL in ground states at B3LYP/6-311+g level.

FATT				TSATL			
	Bond lengths (Å)		Bond angles (°)		Bond lengths (Å)		Bond angles (°)
C9-O	1.247	O-C9-C10	127.1	C9-S	1.690	S-C9-C10	127.1
C9-C10	1.491	O-C9-C13	127.1	C9-C10	1.476	S-C9-C13	127.1
C9-C13	1.491	C13-C9-C10	105.74	C9-C13	1.476	C13-C9-C10	105.8
C10-C11	1.417	C9-C10-C11	108.6	C10-C11	1.422	C9-C10-C11	109.1
C11-C12	1.480	C10-C11-C12	108.5	C11-C12	1.474	C10-C11-C12	108.0
C12-C13	1.417	C11-C12-C13	108.5	C12-C13	1.423	C11-C12-C13	108.0
C8-C13	1.383	C9-C13-C12	108.6	C8-C13	1.387	C9-C13-C12	109.0
C10-C1	1.383	C11-C10-C1	122.0	C10-C1	1.387	C11-C10-C1	121.3
C1-C2	1.419	C10-C1-C2	118.8	C1-C2	1.417	C10-C1-C2	119.1
C2-C3	1.414	C1-C2-C3	118.9	C2-C3	1.414	C1-C2-C3	119.1
C3-C4	1.402	C2-C3-C4	121.7	C3-C4	1.402	C2-C3-C4	121.6
C4-C11	1.391	C3-C4-C11	118.8	C4-C11	1.390	C3-C4-C11	118.9
C2-C14	1.424	C4-C11-C10	119.7	C2-C14	1.425	C4-C11-C10	119.9
C14-C15	1.216	C1-C2-C14	120.4	C14-C15	1.216	C1-C2-C14	120.3
C15-C21	1.425	C15-C21-C16	120.9	C15-C21	1.425	C15-C21-C16	120.9
C21-C16	1.409	C18-O-C22	119.3	C21-C16	1.409	C18-O-C22	119.3
C16-C17	1.396			C16-C17	1.396		
C17-C18	1.400			C17-C18	1.400		
C18-O	1.391			C18-O	1.393		
C22-O	1.461			C22-O	1.461		