STRUCTURAL
CHEMISTRY

Volume 74 (2018)

Supporting information for article:

The [4 + 4] thermocyclization of 9-anthraldehyde: synthesis, crystal structure, experimental and theoretical UV spectra, natural bonding orbital analysis and prediction of third-order nonlinear optical properties

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Table 1S

Selected bond lengths (Å), bond and torsion angles (°) of the dimer compound.

Bond lengths			
C(1)-C(8)	1.602(3)	C(16)-C(23)	1.602(3)
C(1)-C(15)	1.529(3)	C(16)-C(30)	1.531(3)
C(1)-C(2)	1.528(3)	C(16)-C(17)	1.535(3)
C(2)-C(3)	1.395(3)	C(17)-C(18)	1.397(3)
C(4)-C(5)	1.393(3)	C(19)-C(20)	1.381(3)
C(2)-C(7)	1.402(3)	C(17)-C(22)	1.404(3)
Bond angles			
C(1)-C(15)-O(1)	125.5(2)	C(16)-C(30)-O(2)	125.5(2)
C(15)-C(1)-C(8)	110.76(15)	C(30)-C(16)-C(23)	110.87(16)
C(15)-C(1)-C(2)	108.81(16)	C(30)-C(16)-C(17)	106.86(15)
C(15)-C(1)-C(14)	107.06(16)	C(30)-C(16)-C(29)	108.11(15)
C(1)-C(2)-C(7)	116.81(17)	C(16)-C(17)-C(22)	117.31(16)
C(7)-C(2)-C(3)	119.77(18)	C(22)-C(17)-C(18)	119.18(18)
C(1)-C(2)-C(3)	123.39(17)	C(16)-C(17)-C(18)	123.51(17)
Torsion angles			
O(1)-C(15)-C(1)-C(8)	7.1(3)	O(2)-C(30)-C(16)-C(23)	7.2(3)
O(1)-C(15)-C(1)-C(2)	130.3(2)	O(2)-C(30)-C(16)-C(29)	129.5(2)
O(1)-C(15)-C(1)-C(14)	-114.3(2)	O(2)-C(30)-C(16)-C(17)	-115.7(2)

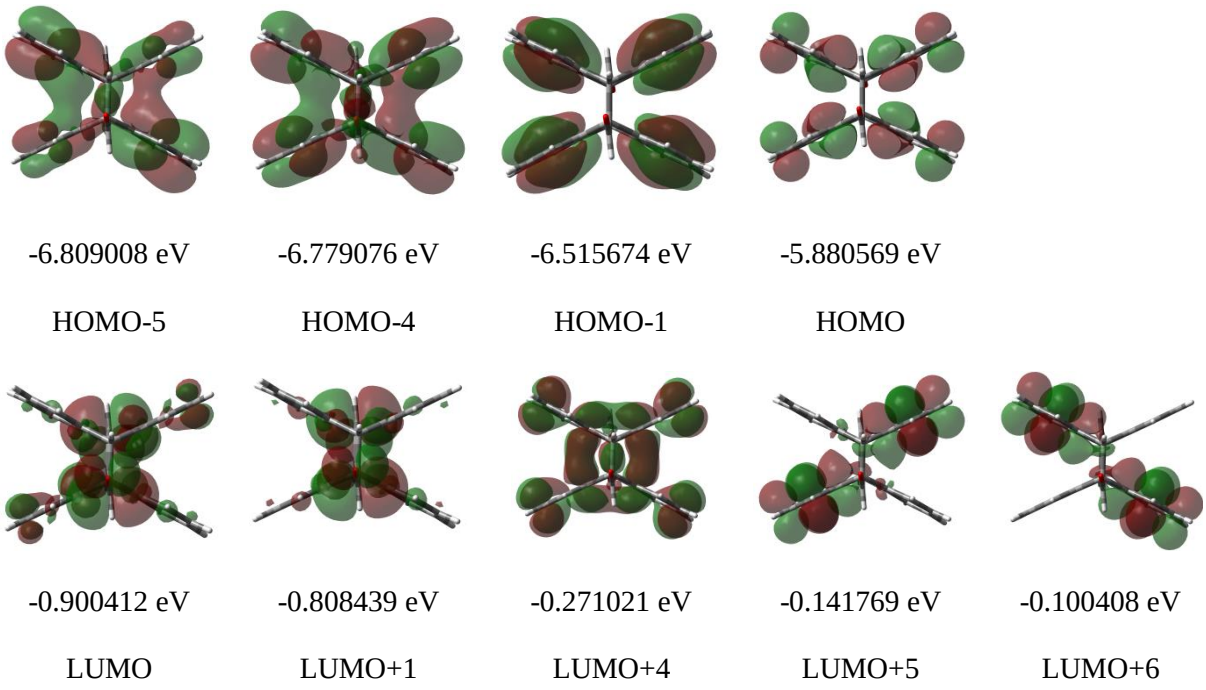

Figure 1S

Molecular orbital diagram of the compound involved in the dominant electron transitions along with their molecular orbital energies.

Table 2S

The selected hyperconjugative interactions of the compound along with their stabilization energies (kcal mol^{-1}) calculated by DFT/RB3LYP/6-31G(d,p).

Donor NBO	Acceptor NBO	Interaction	$E^{(2)}$
C17–C18	C17–C22	σ→σ*	4.60
C17–C18	C16–C23	π→σ*	3.79
C17–C18	C19–C20	π→π*	19.54
C17–C18	C21–C22	π→π*	20..03
C17–C22	C17–C18	σ→σ*	3.92
C17–C22	C21–C22	σ→σ*	3.70
C18–H18	C17–C22	σ→σ*	4.19
C18–H18	C19–C20	σ→σ*	3.17
C18–C19	C16–C17	σ→σ*	4.45
C18–C19	C17–C18	σ→σ*	3.48

C19–H19	C17–C18	σ→σ*	3.76
C19–H19	C20–C21	σ→σ*	3.69
C19–C20	C17–C18	π→π*	19.48
C19–C20	C21-C22	π→π*	18.78
C20–H20	C18–C19	σ→σ*	3.77
C20–H20	C21–C22	σ→σ*	3.61
C20–C21	C21–C22	σ→σ*	3.19
C20–C21	C22–C23	σ→σ*	4.08
C21–H21	C17–C22	σ→σ*	4.53
C21–H21	C19-C20	σ→σ*	3.23
C21–C22	C16-C17	σ→σ*	3.18
C21–C22	C17-C22	σ→σ*	4.48
C21–C22	C17–C18	π→π*	19.98
C21–C22	C19–C20	π→π*	20.54
C23–H23	C17–C22	σ→σ*	3.44
C23–C24	C24–C29	σ→σ*	3.51
C23–C24	C28–C29	σ→σ*	3.01
LP(2)O2	C16–C30	n→σ*	22.47
LP(2)O2	C30–H30	n→σ*	17.05