RSC Advances

Molecular design of organic small molecules based on indolo[7,6-g]indole-diimide with fused aromatic heterocycles as donors for organic solar cells

Ruifa Jin[a,b,*], Ahmad Irfan[c,d]

aInner Mongolia Key Laboratory of Photoelectric Functional Materials, Chifeng 024000, P. R. China

bCollege of Chemistry and Chemical Engineering, Chifeng University, Chifeng 024000, P. R. China

cResearch Center for Advanced Materials Science, King Khalid University, Abha 61413, P.O. Box 9004, Saudi Arabia

dDepartment of Chemistry, Faculty of Science, King Khalid University, Abha 61413, P.O. Box 9004, Saudi Arabia

Index

Table SI

Calculated the longest wavelength of absorption λ_{max} and corresponding oscillator strength f of molecule **1** by various methods with 6-31G(d,p) basis set, along with available experimental data.

Methods	λ_{max}	f
TD-B3LYP/6-31G(d,p)//B3LYP//6-31G(d,p)	542	0.127
TD-PBE0/6-31G(d,p)//PBE0/6-31G(d,p)	514	0.138
TD-CAM-B3LYP/6-31G(d,p)//CAM-B3LYP/6-31G(d,p)	441	0.167
TD-wB97XD/6-31G(d,p)//wB97XD/6-31G(d,p)	435	0.168
TD-M062X /6-31G(d,p)//M062X /6-31G(d,p)	433	0.178
TD- LCWPBE/6-31G(d,p)//LCWPBE/6-31G(d,p)	388	0.192
Exp[a]	540	

[a] Experimental data for molecule **1** were taken from ref. [13]

Table SII

The λ_{abs} and corresponding oscillator strength f (in parenthesis) and absorption region R of the first fifteen excited states for **1–6** obtained by the TD-B3LYP/6-31G(d,p) level.

Species	1	2	3	4	5	6
S_1	542(0.127)	473(0.084)	559(0.088)	595(0.175)	565(0.188)	708(0.195)
S_2	478(0.049)	430(0.015)	515(0.095)	520(0.077)	480(0.042)	614(0.0)
S_3	445(0.0)	395(0.0)	468(0.0)	497(0.0)	472(0.0)	550(0.0)
S_4	441(0.0)	388(0.00)	429(0.0)	484(0.0)	455(0.0)	535(0.113)
S_5	380(0.0)	384(0.0)	411(0.0)	435(0.0)	393(0.057)	479(0.063)
S_6	372(0.028)	372(0.0)	369(0.018)	423(0.0)	389(0.0)	478(0.0)
S_7	367(0.0)	371(0.210)	366(0.0)	415(0.092)	380(0.0)	430(0.131)
S_8	355(0.083)	352(0.0)	351(0.016)	406(0.090)	375(0.054)	423(0.020)
S_9	339(0.321)	349(0.004)	334(0.0)	375(0.029)	365(0.239)	405(0.0)
S_{10}	334(0.001)	346(0.0)	333(0.00)	367(0.153)	341(0.0)	378(0.0)
S_{11}	333(0.0)	345(0.0)	321(0.211)	356(0.0)	335(0.010)	364(0.067)
S_{12}	318(0.283)	338(0.001)	310(0.0)	353(1.265)	334(0.0)	360(0.0)
S_{13}	315(0.0)	333(0.808)	308(0.550)	346(0.0)	334(1.001)	354(0.0)
S_{14}	308(0.0)	321(0.0)	300(0.229)	335(0.000)	321（0.0）	352(0.123)
S_{15}	306(0.291)	312(0.042)	295(0.0)	334(0.0)	321（0.110）	346(1.251)
R	236	140	259	242	244	362

Table SIII
The calculated total energies and crystal cell parameters of **5** in different space groups.

Space groups	Total energies	a (Å)	b (Å)	c (Å)	α (deg)	β (deg)	γ (deg)
C2	612.79487788	61.80	6.26	59.87	90.0	162.5	90.0
C2/c	633.49840288	42.90	36.68	28.86	90.0	144.8	90.0
Cc	630.51867650	8.68	57.72	18.19	90.0	100.5	90.0
P2$_1$	606.24905143	33.23	25.12	4.81	90.0	114.0	90.0
P2$_1$/c	632.00029706	16.74	18.68	39.16	90.0	117.5	90.0
P2$_1$2$_1$2$_1$	630.90048464	12.27	32.61	31.34	90.0	90.0	90.0
P$\bar{1}$	616.90495361	35.34	6.74	28.36	73.7	87.7	70.9
Pbca	641.49652287	35.95	36.11	25.73	90.0	90.0	90.0
Pbcn	631.56607314	33.20	44.98	20.65	90.0	90.0	90.0
Pna2$_1$	636.22629013	27.86	25.08	18.75	90.0	90.0	90.0

Table SIV
The calculated total energies and crystal cell parameters of **6** in different space groups.

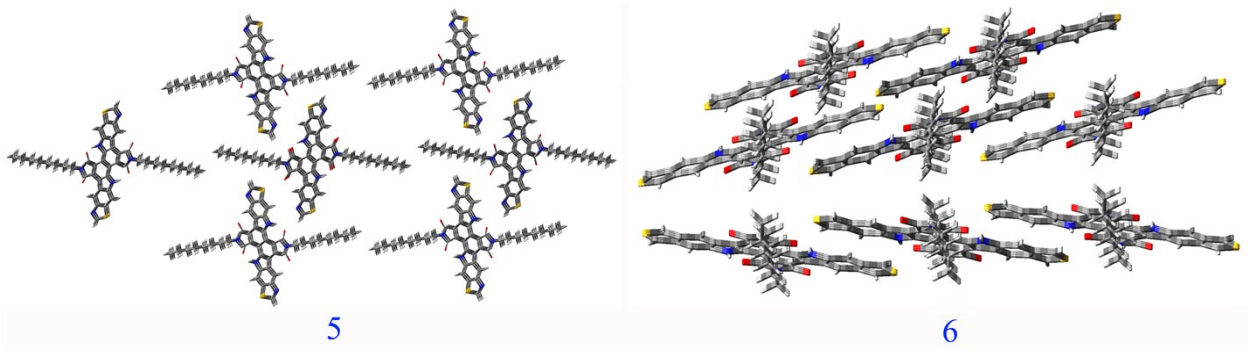| Space groups	Total energies	a (Å)	b (Å)	c (Å)	α (deg)	β (deg)	γ (deg)
$C2$	419.85271579	31.24	23.40	15.04	90.0	89.5	90.0
$C2/c$	416.82590713	70.36	20.16	49.54	90.0	154.2	90.0
Cc	414.68879048	21.37	26.80	17.49	90.0	81.6	90.0
$P2_1$	412.73668316	17.87	24.61	11.06	90.0	69.7	90.0
$P2_1/c$	415.62613857	24.89	34.24	11.03	90.0	101.0	90.0
$P2_12_12_1$	421.00145620	10.94	32.46	28.34	90.0	90.0	90.0
$P\bar{1}$	412.17292067	20.18	20.14	19.18	93.2	117.3	107.6
$Pbca$	422.82068477	12.65	56.31	35.11	90.0	90.0	90.0
$Pbcn$	411.53702602	30.04	23.60	26.16	90.0	90.0	90.0
$Pna2_1$	416.50439053	14.95	20.61	31.35	90.0	90.0	90.0

Figure SI Herringbone Structures of **5** in *P2₁* space group and **6** in *Pbcn* space group.