

Supporting Information

Electronic Structure of Twisted and Planar Rubrene Molecule: A Density Functional Study

Table S1: Excitation energy, corresponding transition and oscillator strength (f) for the different carbon excitation centres (as mentioned in the figure 4 and 5) by considering them as an excitation center. Highlight in colours are done to show the origin of the different experimentally observed peaks only. Experimentally unobserved transitions are not highlighted. Peaks highlighted with a particular colour indicates similarity in energy of transition.

Excitation Centre (carbon atom number)	Excitation energy (eV)	$f \geq 10^{-3}$	Transition levels	Ionization potential (eV)
TC1	284.20	14.7	1s → LUMO+1	290.57
	287.30	1.45	1s → Rydberg states	
	287.35	1.78	1s → Rydberg states	
	288.12	2.06	1s → Rydberg states	
	291.18	3.02	1s → Rydberg states	
TC23	283.70	3.83	1s → LUMO	290.23
	285.06	9.40	1s → LUMO+1	
	290.29	1.11	1s → Rydberg states	
	291.37	1.38	1s → Rydberg states	
TC24	284.19	1.73	1s → LUMO	290.70

	285.64	8.78	1s→LUMO+1	
	286.12	1.95	1s→LUMO+3	
	287.00	1.23	1s→LUMO+11	
	289.65	1.21	1s→Rydberg states	
	289.85	1.52	1s→Rydberg states	
	289.89	1.29	1s→Rydberg states	
TC25	283.84	3.73	1s→LUMO	290.32
	285.33	8.63	1s→LUMO+1	
	286.62	1.60	1s→LUMO+11	
	286.88	2.23	1s→Rydberg states	
	286.95	1.41	1s→Rydberg states	
TC26	283.44	7.71	1s→LUMO	290.20
	285.33	2.44	1s→LUMO+1	
	286.49	2.88	1s→LUMO+11	
	286.78	2.58	1s→Rydberg states	
	287.11	1.01	1s→Rydberg states	
	290.91	1.74	1s→Rydberg states	
TC33	283.59	3.97	1s→LUMO	290.22
	285.05	9.20	1s→LUMO+1	
	289.28	1.08	1s→Rydberg states	
	290.30	1.03	1s→Rydberg states	
TC34	284.19	1.64	1s→LUMO	290.70
	285.65	8.98	1s→LUMO+1	
	286.11	1.95	1s→LUMO+3	
	286.99	1.23	1s→LUMO+11	
	289.69	1.18	1s→Rydberg states	
	289.77	2.18	1s→Rydberg states	

	289.67	1.30	1s→Rydberg states	
	290.86	1.19	1s→Rydberg states	
	291.00	1.03	1s→Rydberg states	
TC35	283.82	3.66	1s→LUMO	290.33
	285.28	8.75	1s→LUMO+1	
	286.10	1.02	1s→LUMO+4	
	286.60	1.61	1s→LUMO+11	
	286.86	2.21	1s→Rydberg states	
	286.93	1.44	1s→Rydberg states	
TC36	283.42	7.80	1s→LUMO	290.19
	285.31	1.36	1s→LUMO+1	
	285.33	1.15	1s→LUMO+2	
	286.47	2.99	1s→LUMO+11	
	286.76	2.55	1s→Rydberg states	
	291.31	1.51	1s→Rydberg states	
TC27	285.51	15.00	1s→LUMO+1	290.89
	289.53	1.48	1s→Rydberg states	
TC28	285.27	14.28	1s→LUMO+2	290.52
	287.33	1.10	1s→LUMO+14	
	289.20	1.71	1s→Rydberg states	
	289.35	1.61	1s→Rydberg states	
TC29	284.22	1.21	1s→LUMO+1	290.47
	285.23	13.66	1s→LUMO+2	
TC30	285.41	15.05	1s→LUMO+1	290.72
	286.97	1.51	1s→LUMO+8	
TC31	285.39	14.63	1s→LUMO+3	290.71
	286.90	1.14	1s→LUMO+9	

	289.37	1.07	1s → Rydberg states	
TC32	284.37	1.53	1s → LUMO+2	290.58
	285.26	12.38	1s → LUMO+3	
	289.30	1.02	1s → Rydberg states	
TC37	285.51	14.92	1s → LUMO+1	290.89
	289.52	1.54	1s → Rydberg states	
TC38	284.22	1.27	1s → LUMO	290.46
	285.24	13.59	1s → LUMO+2	
TC39	285.27	14.20	1s → LUMO+1	290.51
	287.31	1.08	1s → Rydberg states	
	289.20	1.74	1s → Rydberg states	
	289.35	1.42	1s → Rydberg states	
TC40	285.39	14.62	1s → LUMO+1	290.70
	286.90	1.05	1s → LUMO+8	
	287.45	1.09	1s → Rydberg states	
TC41	285.42	15.04	1s → LUMO+1	290.71
TC42	284.35	1.59	1s → LUMO+1	290.57
	285.26	12.23	1s → LUMO+2	
	286.74	1.42	1s → LUMO+9	

Table S2: Excitation energy, corresponding transition between molecular orbitals and oscillator strength (f) for the different carbon sites (as shown in the figure 7) by considering them as an excitation center. Highlight in colours are done to show the origin of the different experimentally observed peaks only. Experimentally unobserved transitions are not highlighted. Peaks highlighted with a particular colour indicates similarity in energy of transition.

Excitation Centre (carbon atom number)	Excitation energy (eV)	$f \geq 10^{-3}$	Transition levels	Ionization potential (eV)
FC8	285.71	11.98	1s→LUMO+5	290.86
	288.91	1.33	1s→ Rydberg states	
	288.95	1.94	1s→ Rydberg states	
FC9	284.46	7.11	1s→LUMO+1	290.36
	286.06	2.27	1s→LUMO+5	
	287.10	1.41	1s→ Rydberg states	
	287.28	1.91	1s→ Rydberg states	
FC10	285.05	1.48	1s→LUMO+1	290.73
	286.34	8.82	1s→LUMO+5	
	287.20	1.08	1s→LUMO+10	
	287.29	1.00	1s→LUMO+11	
	287.69	1.15	1s→ Rydberg states	
	290.68	1.37	1s→Rydberg states	
	290.89	2.34	1s→Rydberg states	
FC11	284.43	4.36	1s→LUMO+1	290.33
	285.78	7.01	1s→LUMO+4	
	286.83	1.04	1s→ Rydberg states	
	290.62	1.84	1s→Rydberg states	
FC12	284.57	4.24	1s→LUMO	290.36
	285.87	7.22	1s→LUMO+2	
	287.40	1.64	1s→ Rydberg states	
	287.51	1.70	1s→ Rydberg states	
	289.18	1.33	1s→ Rydberg states	
FC24	285.21	1.57	1s→LUMO+3	290.92
	289.15	1.52	1s→ Rydberg states	
	289.18	1.61	1s→ Rydberg states	
FC25	285.10	14.54	1s→LUMO+3	290.60
	287.87	1.02	1s→ Rydberg states	
	289.94	2.11	1s→ Rydberg states	
	289.06	1.16	1s→ Rydberg states	
FC26	285.41	14.36	1s→LUMO+5	290.80
	286.92	1.58	1s→ Rydberg states	
	287.68	1.06	1s→ Rydberg states	
	289.52	1.63	1s→ Rydberg states	
FC27	284.70	1.58	1s→LUMO+3	290.71
	285.07	10.42	1s→LUMO+4	
	286.52	1.22	1s→ Rydberg states	
	288.98	1.76	1s→ Rydberg states	

FC28	284.98	9.15	1s → LUMO+4	290.79
	285.06	5.83	1s → LUMO+5	
	286.65	1.15	1s → Rydberg states	
	287.07	1.16	1s → Rydberg states	
	288.95	1.69	1s → Rydberg states	
FC29	284.95	14.46	1s → LUMO+3	290.58
	288.86	1.53	1s → Rydberg states	
	288.89	1.78	1s → Rydberg states	