Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Theoretical Studies on Charge Transport and Optical Properties of Tris(N-saclicylideneanilines)

R. Nithya and K. Senthilkumar

Department of Physics, Bharathiar University, Coimbatore, India-641 046.

Table S1 The effective charge transfer integral (J_{eff} in eV) for hole and electron transport of Tris(N-saclicylideneanilines).

Stacking angle	TSAN1		TSAN2		TSAN3		TSAN4		TSAN5		TSAN6	
	Hole	Electron	Hole	Electron	Hole	Electron	Hole	Electron	Hole	Electron	Hole	Electron
15	0.16	0.25	0.17	0.25	0.19	0.24	0.18	0.25	0.16	0.26	0.18	0.27
30	0.11	0.11	0.09	0.13	0.10	0.12	0.09	0.13	0.15	0.14	0.11	0.12
45	0.05	0.05	0.02	0.09	0.07	0.08	0.05	0.09	0.05	0.09	0.06	0.08
60	0.04	0.03	0.04	0.09	0.05	0.10	0.01	0.08	0.03	0.09	0.03	0.11
75	0.02	0.01	0.06	0.09	0.03	0.14	0.01	0.08	0.00	0.20	0.00	0.15
90	0.002	0.07	0.10	0.13	0.01	0.15	0.06	0.12	0.05	0.13	0.04	0.17

Table S2 The site energy (ε in eV) for (a) hole and (b) electron transport of Tris(N-saclicylideneanilines).

(a) Hole Transport

Stacking angle	TSAN1		TSAN2		TSAN3		TSAN4		TSAN5		TSAN6	
	ε_1	ε_2	ε_1	ε_2	ε_1	ε_2	ε_1	ε_2	ε_1	ε_2	ε_1	ε_2
15	-5.10	-4.83	-4.45	-4.42	-4.45	-4.40	-4.44	-4.43	-4.65	-4.87	-4.59	-4.81
30	-5.06	-4.88	-4.47	-4.54	-4.47	-4.53	-4.52	-4.50	-4.84	-4.95	-4.73	-4.84
45	-4.77	-4.62	-4.50	-4.57	-4.49	-4.55	-4.56	-4.51	-4.86	-4.92	-4.79	-4.86
60	-4.71	-4.66	-4.54	-4.54	-4.51	-4.51	-4.55	-4.51	-4.86	-4.90	-4.83	-4.91
75	-4.67	-4.64	-4.57	-4.50	-4.53	-4.47	-4.55	-4.52	-4.83	-4.89	-4.89	-5.08
90	-4.69	-4.66	-4.54	-4.46	-4.47	-4.45	-4.54	-4.52	-4.77	-4.87	-4.85	-5.07

(a) Electron Transport

Stacking angle	TSAN1		TSAN2		TSAN3		TSAN4		TSAN5		TSAN6	
	ε_1	ε_2	ε_1	ε_2	ε_1	ε_2	ε_1	ε_2	ε_1	ε_2	ε_1	ε_2
15	-2.20	-2.17	-2.43	-2.38	-2.45	-2.42	-2.39	-2.41	-2.65	-2.77	-2.58	-2.75
30	-2.16	-2.14	-2.43	-2.44	-2.46	-2.49	-2.42	-2.47	-2.76	-2.80	-2.66	-2.76
45	-2.30	-2.24	-2.44	-2.47	-2.46	-2.51	-2.45	-2.47	-2.77	-2.80	-2.70	-2.76
60	-2.28	-2.26	-2.46	-2.46	-2.47	-2.48	-2.45	-2.44	-2.75	-2.78	-2.73	-2.73
75	-2.24	-2.23	-2.47	-2.45	-2.48	-2.46	-2.48	-2.45	-2.72	-2.79	-2.80	-2.90
90	-2.20	-2.21	-2.44	-2.44	-2.46	-2.45	-2.50	-2.45	-2.67	-2.79	-2.78	-2.87

Table S3 Computed absorption wavelength (in nm), oscillator strength (in a.u) and orbital transitions of Tris(N-saclicylideneanilines) calculated at B3LYP/6-311G(d,p) and PBE0/6-311G(d,p) level of theories in gas phase.

Molecule	B3LYP/ 6-311G(d,p)				PBE0/ 6-311G(d,p)			
	Orbital Transitions[(A)]	λ_{abs}		*f*	Orbital Transitions[(A)]	λ_{abs}		*f*
		nm	eV			nm	eV	
TSAN2	H-1→L	420	2.96	0.68	H→L	400	3.10	0.82
	H→L	420	2.96	0.68	H-1→L	400	3.10	0.82
	H-1→L+1	352	3.52	0.74	H-1→L+1	336	3.69	0.66
	H-1→L+2				H→L+1			
	H-1→L+1	352	3.52	0.74	H-1→L+1	336	3.69	0.66
	H→L+1				H→L+1			
TSAN3	H→L	427	2.91	0.62	H→L	408	3.04	0.74
	H-1→L	419	2.96	0.57	H-1→L	398	3.12	0.71
	H→L+1	374	3.32	0.21	H→L+1	355	3.49	0.23
	H-2→L	367	3.38	0.11	H-2→L	346	3.58	0.13
	H-1→L+1	350	3.54	0.60	H-1→L+1	335	3.70	0.51
	H-1→L+2	342	3.63	0.53	H-1→L+2	326	3.80	0.47
	H→L+2	323	3.84	0.04	H→L+2	311	3.98	0.47
TSAN4	H→L	419	2.96	0.65	H→L	399	3.10	0.79
	H-1→L	418	2.97	0.63	H-1→L	398	3.11	0.76
	H-1→L+1	351	3.53	0.71	H-1→L+1	335	3.70	0.64
	H→L+1	350	3.54	0.68	H→L+1	334	3.71	0.62
TSAN5	H→L	414	2.99	0.65	H→L	395	3.14	0.788
	H-1→L	414	2.99	0.65	H-1→L	394	3.14	0.785
	H-1→L+1	347	3.58	0.70	H-1→L+1	331	3.75	0.639
	H→L+2				H→L+2			
	H-1→L+2	346	3.59	0.70	H-1→L+2	331	3.75	0.638
	H→L+1				H→L+1			
TSAN6	H→L	418	2.97	0.58	H→L	399	3.11	0.70
	H-1→L	411	3.01	0.59	H-1→L	391	3.17	0.72
	H→L+1	367	3.38	0.21	H→L+1	349	3.56	0.22
	H-2→L	360	3.44	0.10	H-2→L	340	3.64	0.07
	H-1→L+1	344	3.60	0.56	H-6→L	338	3.67	0.08
	H-1→L+2	336	3.69	0.52	H-1→L+1	329	3.78	0.46
					H-1→L+2	321	3.87	0.46

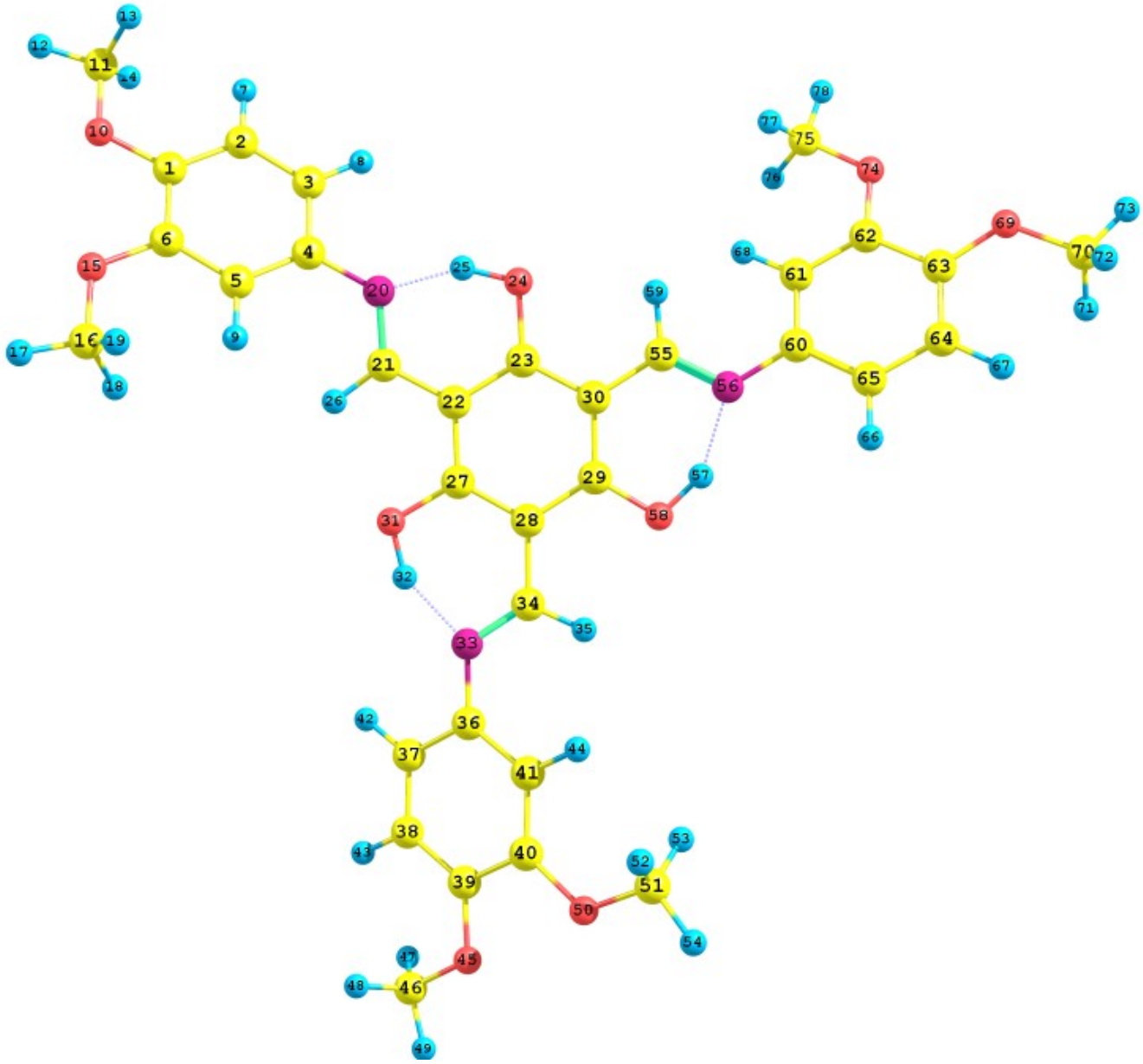
A: H and L represent HOMO and LUMO, respectively. The transitions with oscillator strength higher than 0.01 a.u. are given.

Table S4 The selected geometrical parameters (bond length in Å, angle in degrees) of Tris(N-saclicylideneanilines) at TD-B3LYP/6-311G(d,p) level of theory in gas phase (For labeling of atoms see Figure S1)

Parameters	TSAN2	TSAN3	TSAN4	TSAN5	TSAN6
R_1(N20-H25)	1.030	1.030	1.033	1.036	1.036
R_2(O24-H25)	1.790	1.781	1.756	1.720	1.726
R_3(O24-C23)	1.261	1.284	1.262	1.254	1.252
R_4(N20-C21)	1.348	1.349	1.343	1.385	1.383
R_5(C21-C22)	1.410	1.410	1.40	1.349	1.346
R_6(N20-C4)	1.389	1.388	1.393	1.359	1.358
R_7(C30-C29)	1.431	1.446	1.427	1.456	1.454
R_8(C22-C27)	1.432	1.433	1.436	1.50	1.508
R_9(C21-H26)	1.080	1.079	1.081	1.082	1.083
R_{10}(C1-O10)	1.367	1.367	1.360	1.333	1.331
θ_1(C21-N20-H25)	111.9	111.7	111.4	110.7	110.8
θ_2(N20-H25-O24)	137.6	137.7	138.5	138.9	138.4
θ_3(C21-N20-C4)	128.5	128.6	128.3	127.2	127.2
θ_4(C1-O10-C11)	117.8	117.8	118.2	114.6	114.6
θ_5(C55-N56-H57)	113.6	118.9	113.5	111.6	111.8
Φ_1 (C3-C4-N20-H25)	0.0	0.0	0.0	-1.84	-0.06
Φ_2 (C2-C1-O10-C11)	0.0	0.0	0.0	-86.5	-95.2
Φ_3 (C30-C55-N56-H57)	0.0	0.0	0.0	-0.08	0.23

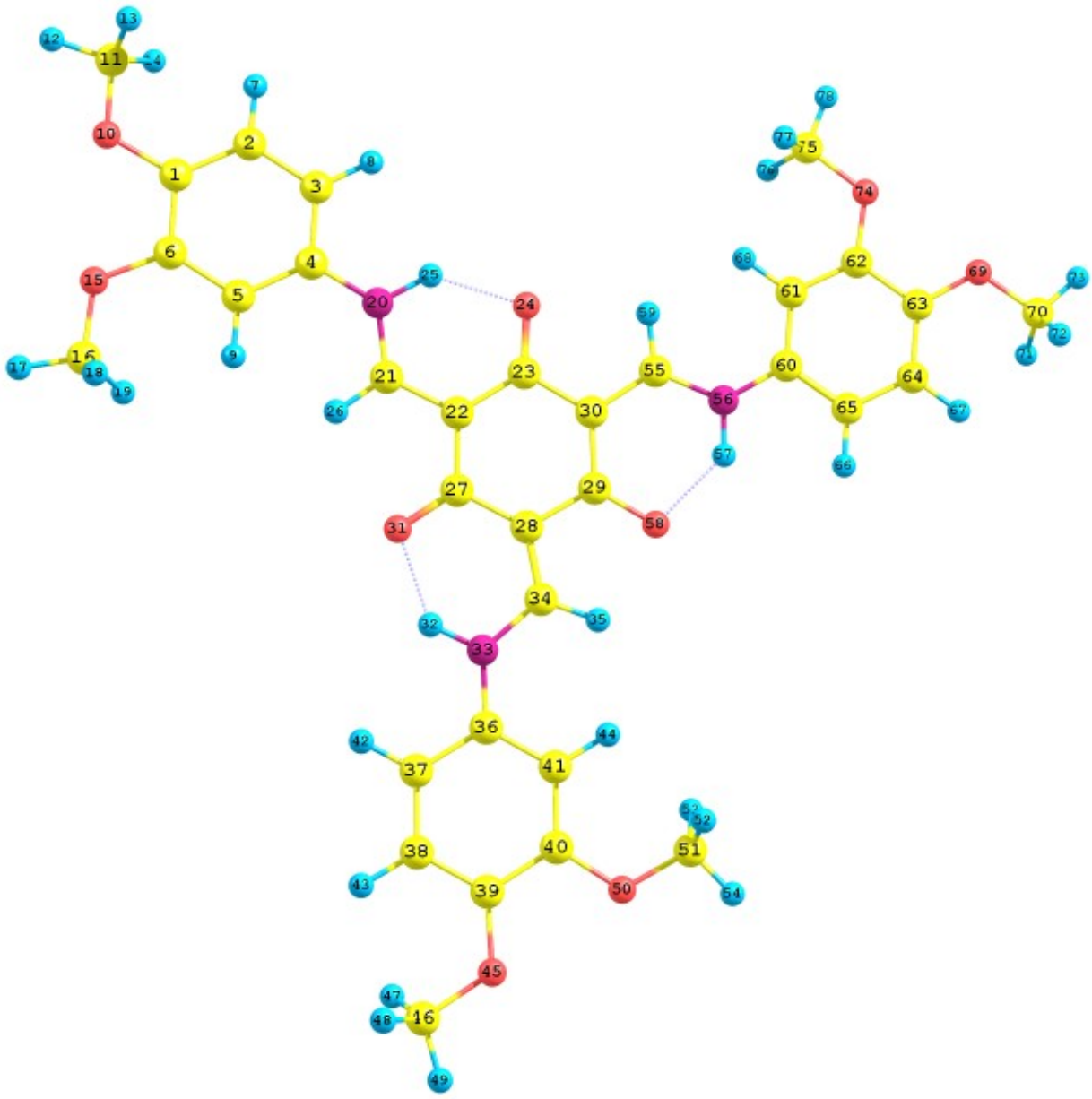
Table S5 Computed emission wavelength (in nm) and oscillator strength (in a.u) corresponding to the electronic transition between HOMO and LUMO energy levels of Tris(N-saclicylideneanilines) calculated at B3LYP/6-311G(d,p) and PBE0/6-311G(d,p) level of theories in gas phase.

Molecule	B3LYP/ 6-311G(d,p)			PBE0/ 6-311G(d,p)		
	λ_{emis}		f	λ_{emis}		f
	nm	eV		nm	eV	
TSAN2	509	2.44	0.39	477	2.60	0.48
TSAN3	541	2.29	0.25	503	2.47	0.30
TSAN4	511	2.43	0.36	478	2.59	0.45
TSAN5	434	2.85	0.79	415	2.99	0.90
TSAN6	606	2.05	0.20	557	2.23	0.24



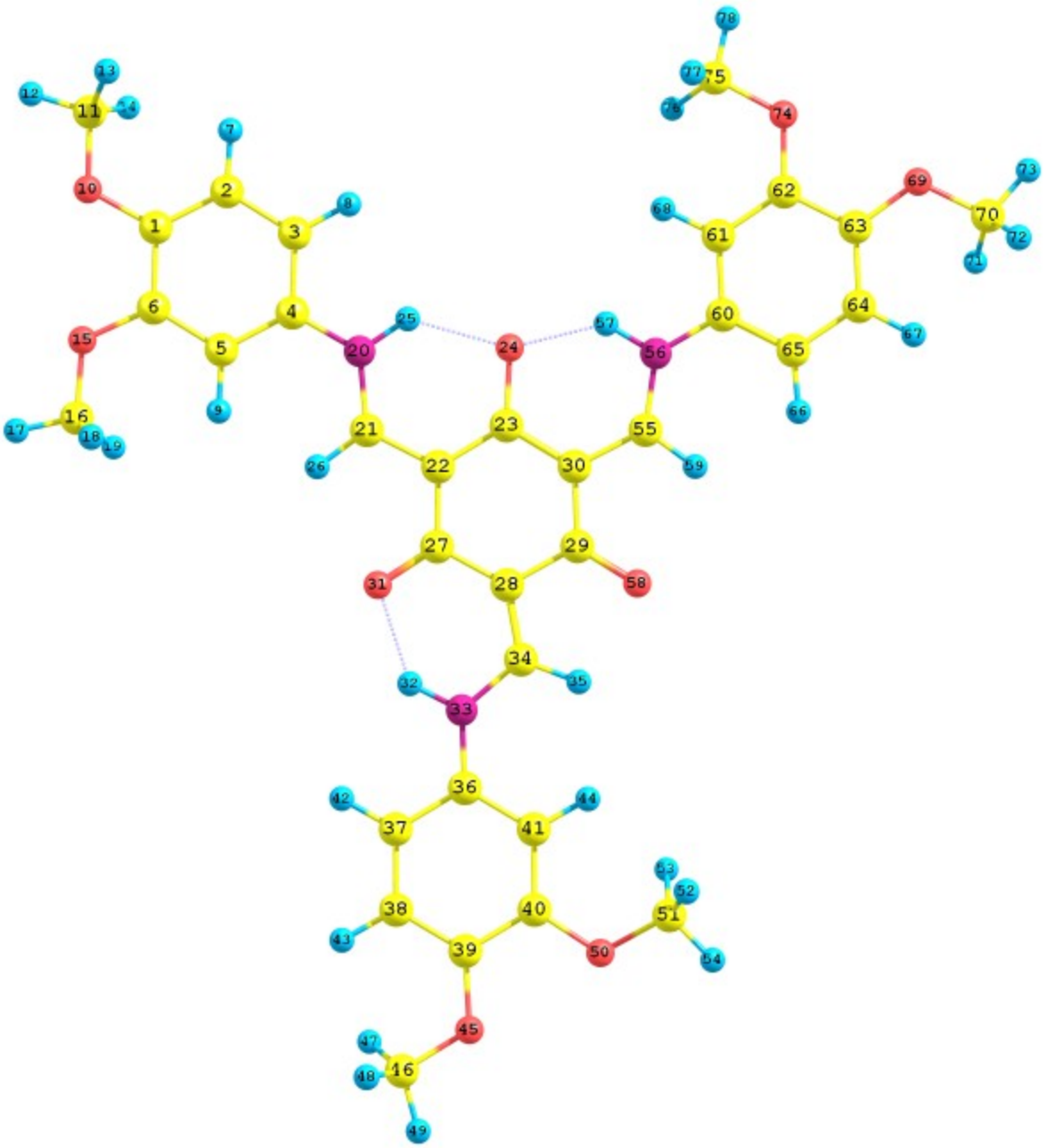
(a)

TSAN1



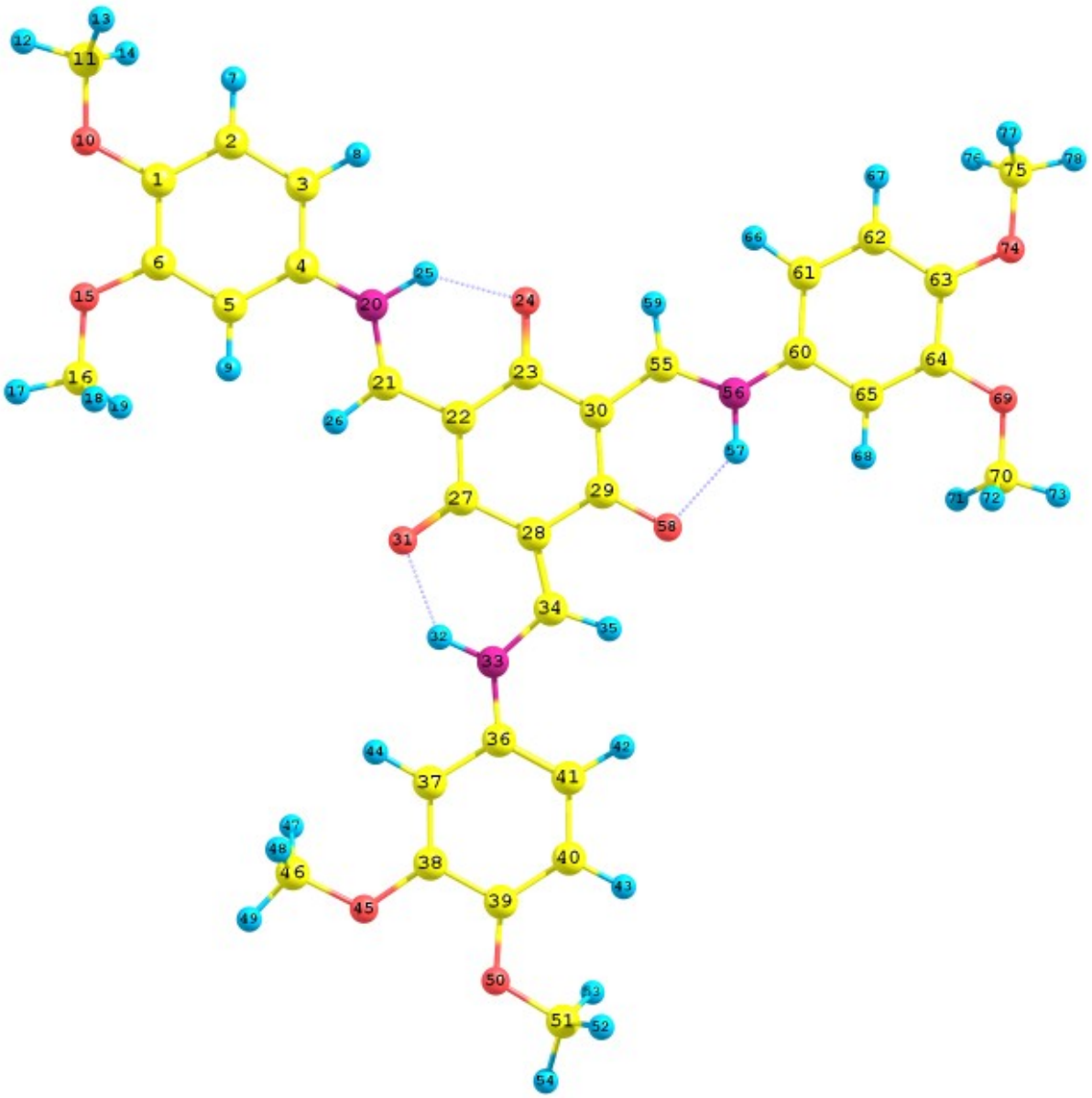
(b)

TSAN2



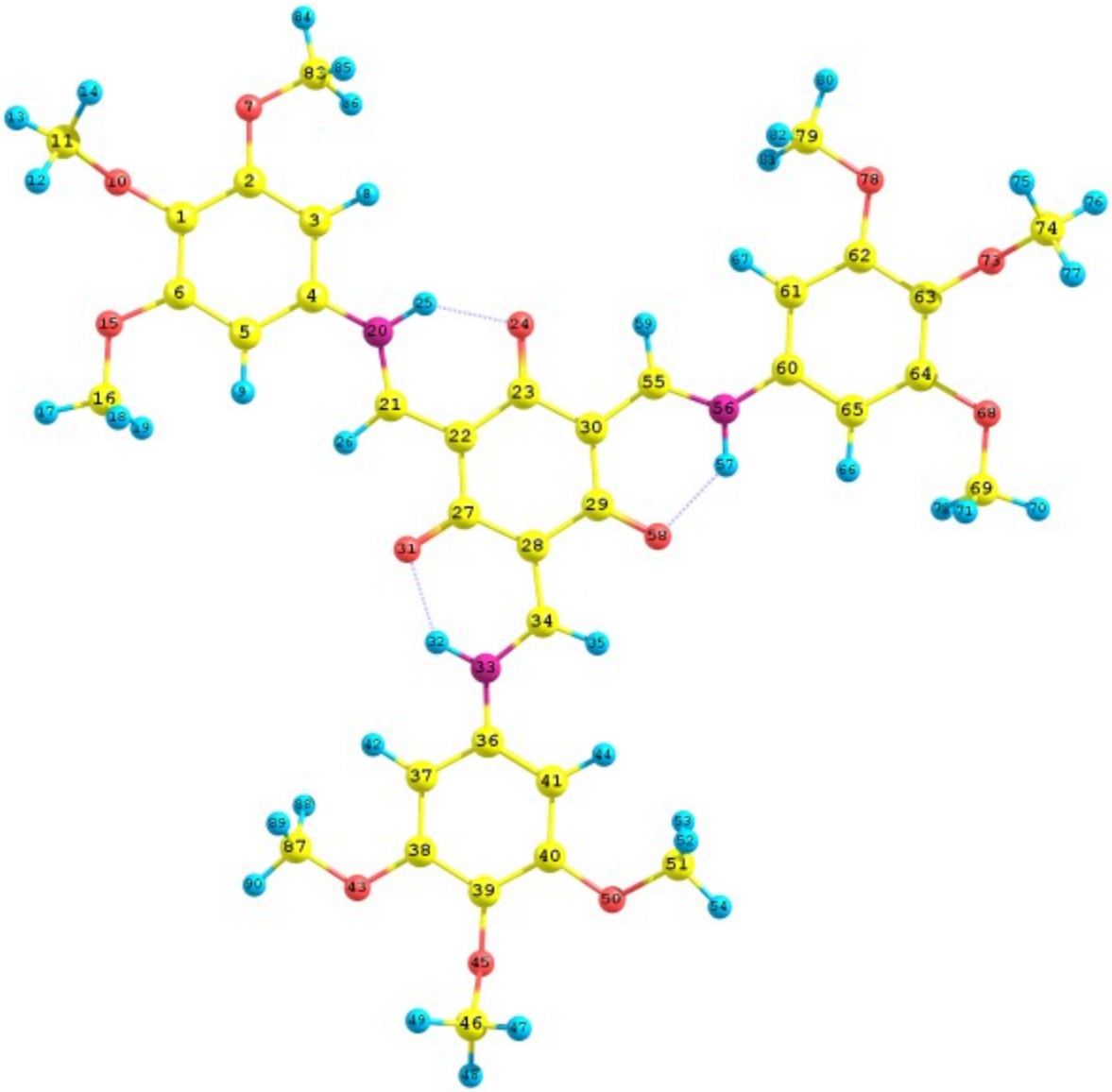
(c)

TSAN3



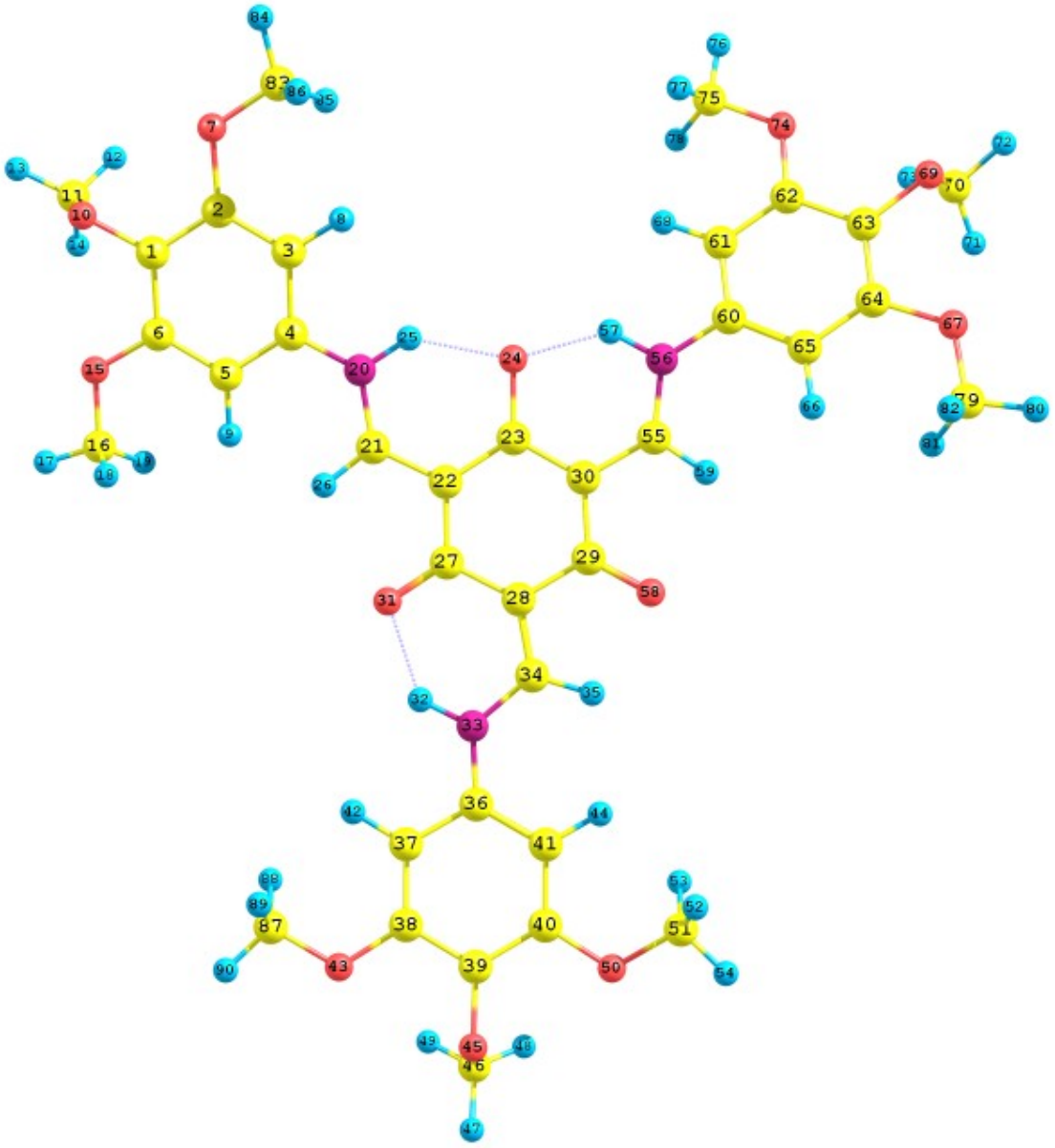
(d)

TSAN4



(e)

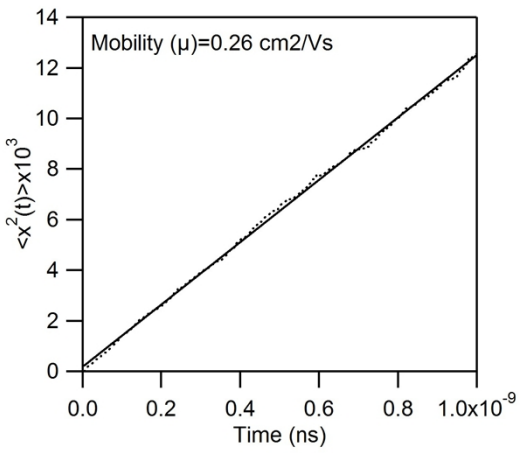
TSAN5



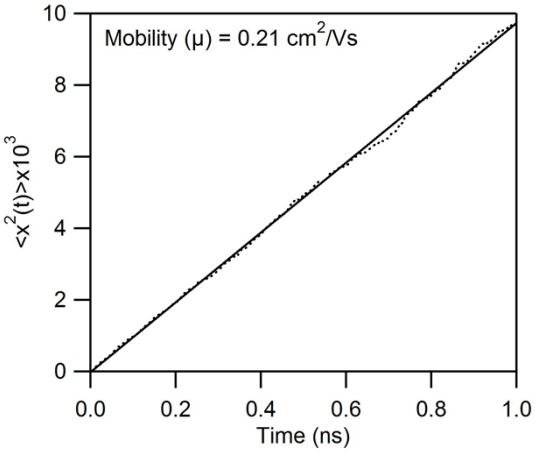
(f)

TSAN6

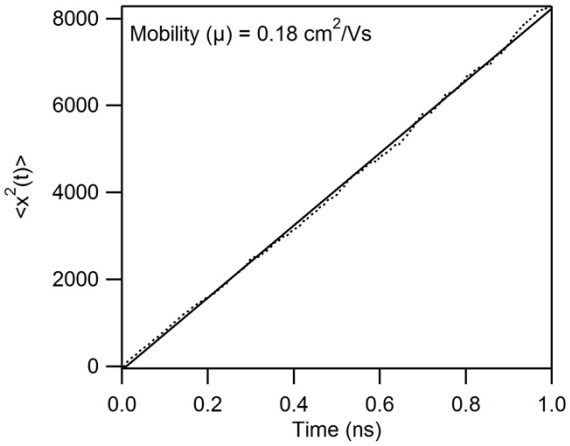
Figure S1 The optimized geometries of Tris(N-saclicylideneanilines) at B3LYP/6-311G(d,p) level of theory



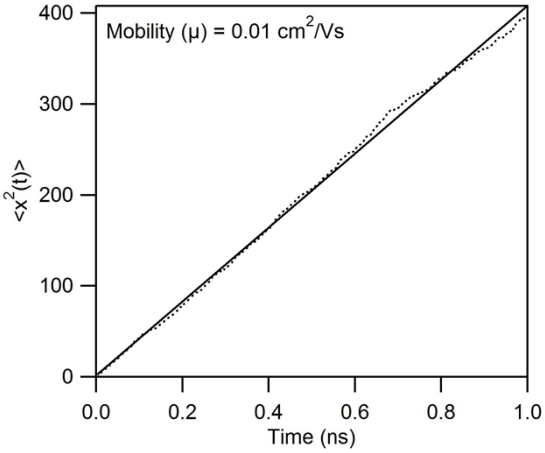
TSAN1



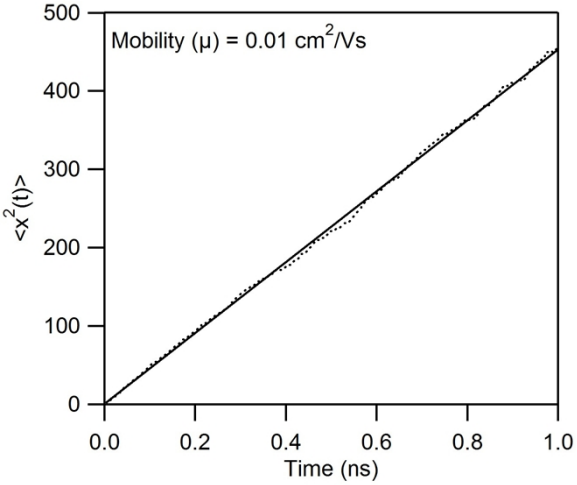
TSAN2



TSAN4



TSAN5



TSAN6

Figure S2 The plot of mean-squared displacement of hole in the studied Tris(N-saclicylideneanilines) as a function of time.

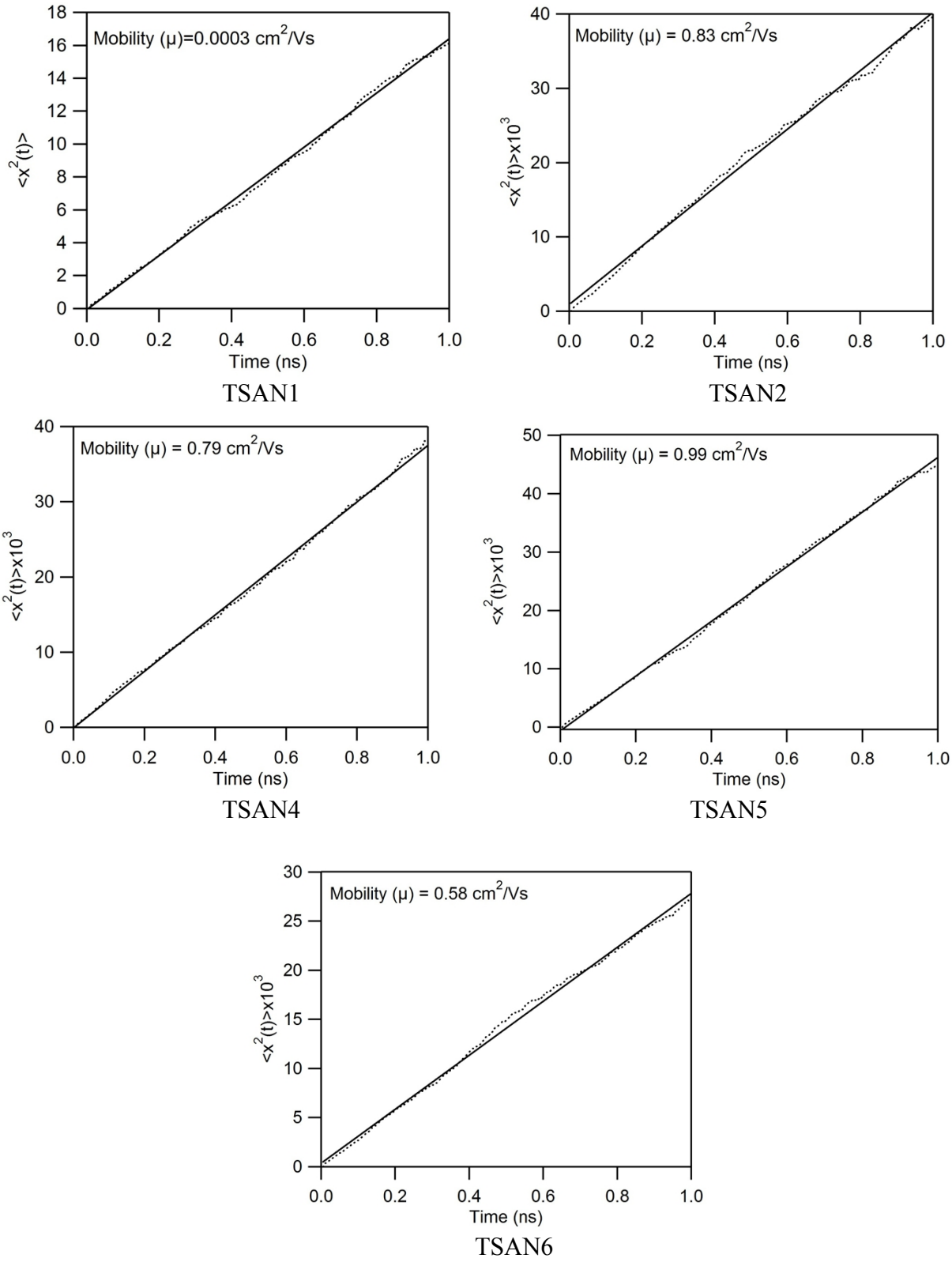


Figure S3 The plot of mean-squared displacement of hole in the studied Tris(N-saclicylideneanilines) as a function of time.