Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material

Theoretical investigation on functional group modulation of UV-Vis absorption profiles of triphenylamine derivatives

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TPA-Pyc

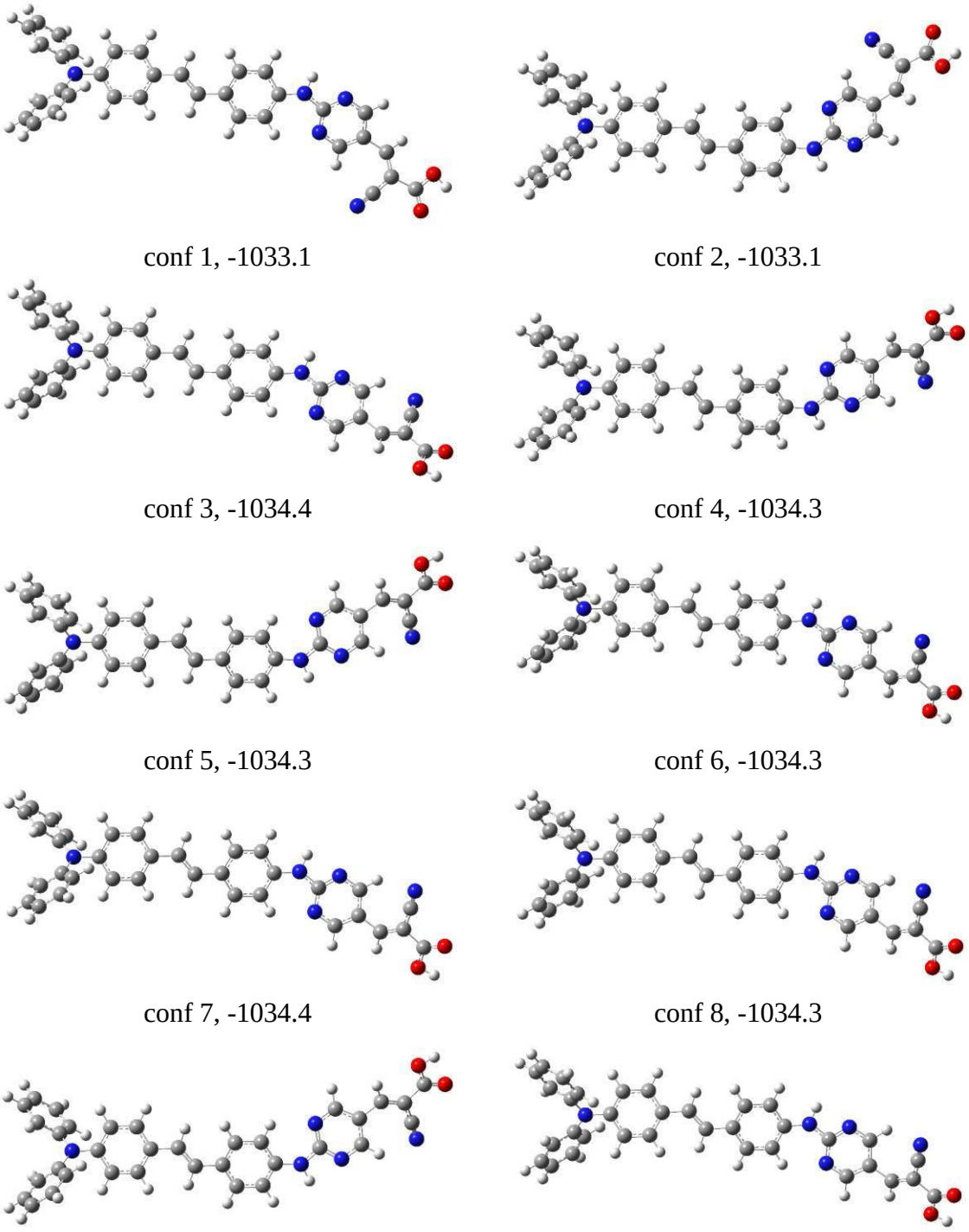
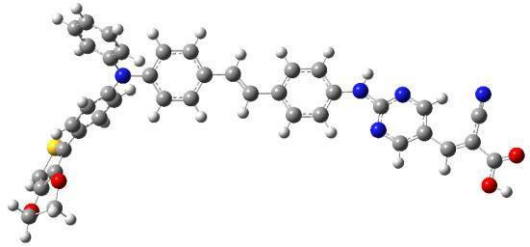


Fig S1. The 10 lowest conformers and their potential energy (in kJ mol^{-1}) of TPA-Pyc obtained by simulated annealing process.

TE-Pyc



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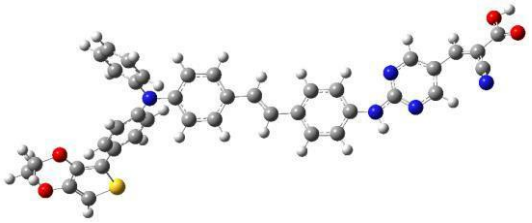

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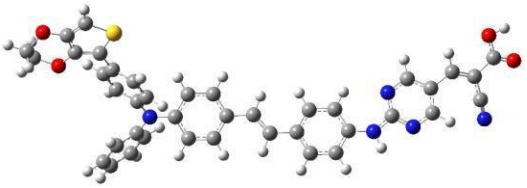

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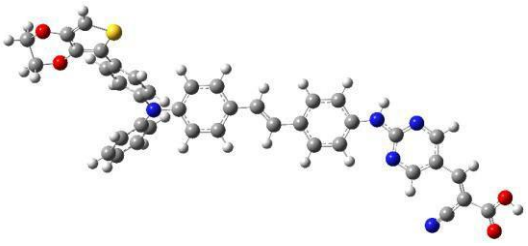

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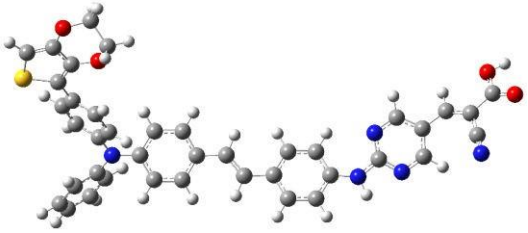

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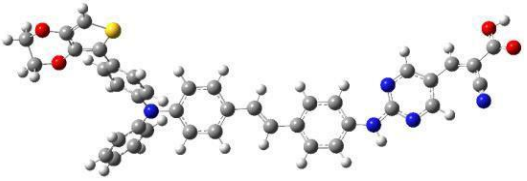

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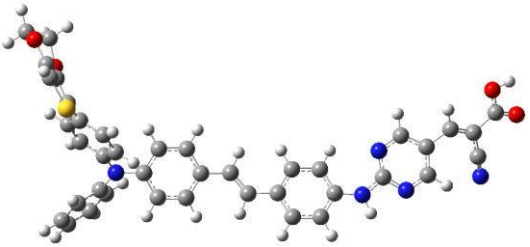

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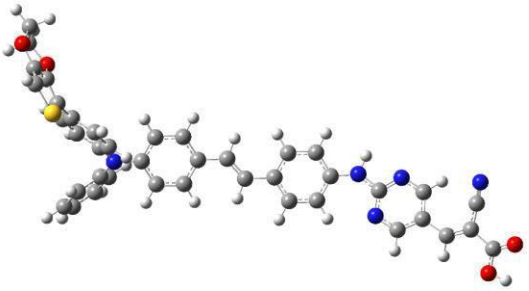

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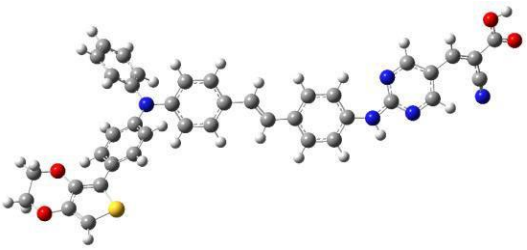

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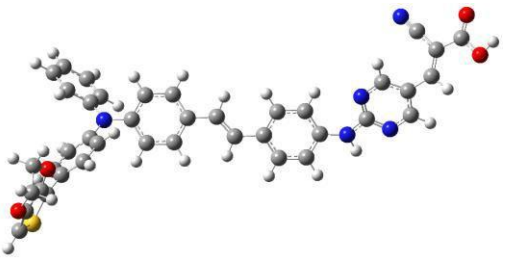

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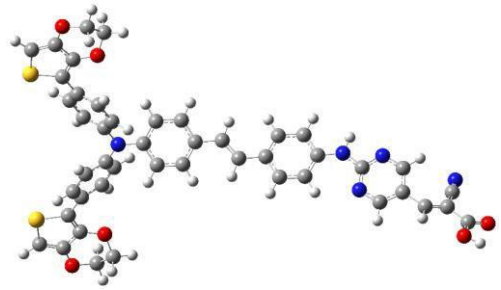
Fig S2. The 10 lowest conformers and their potential energy (in kJ mol^{-1}) of TE-Pyc obtained by simulated annealing process.

ETE-Pyc



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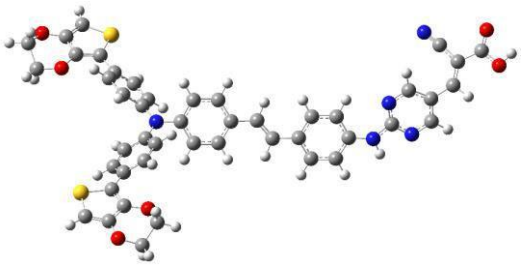

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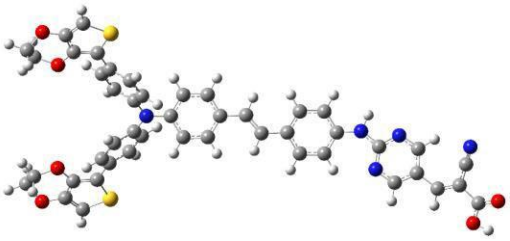

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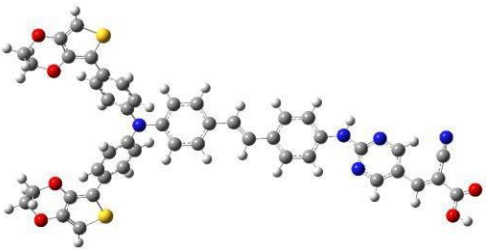

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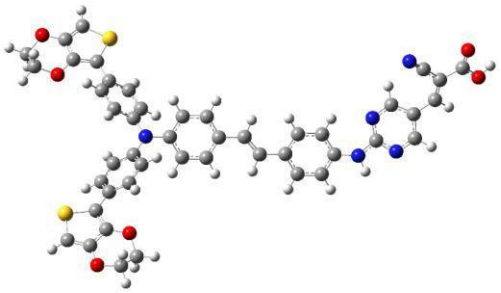

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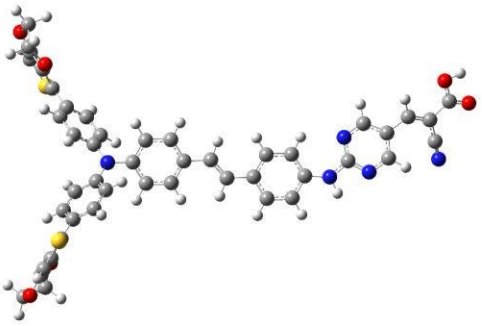

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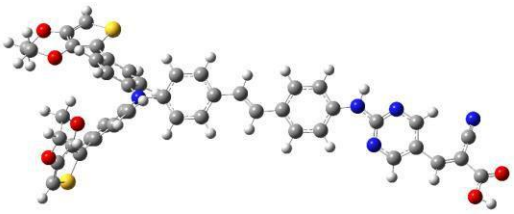

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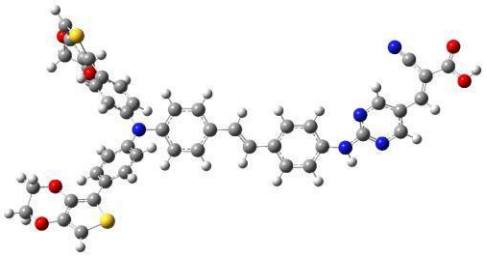

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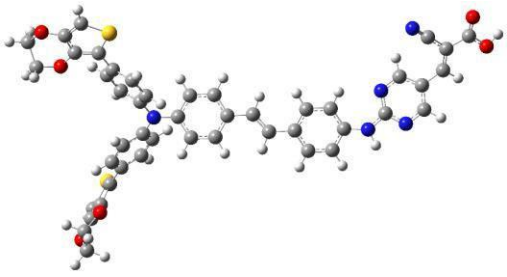

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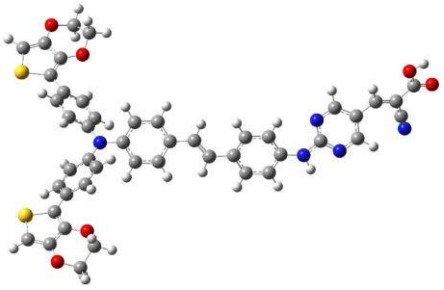

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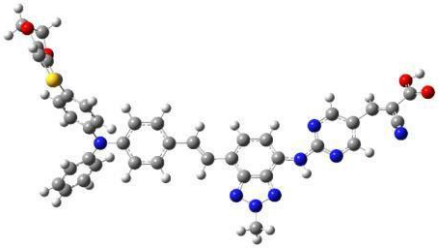
Fig S3. The 10 lowest conformers and their potential energy (in kJ mol^{-1}) of ETE-Pyc obtained by simulated annealing process.

TEBT-Pyc



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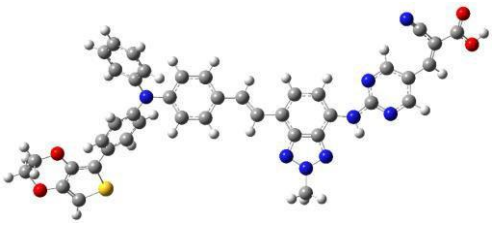

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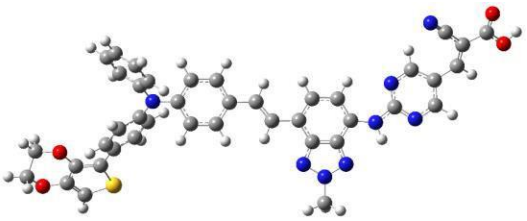

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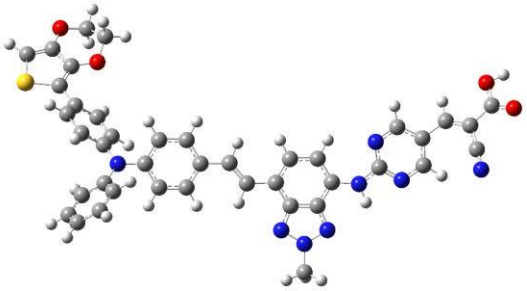

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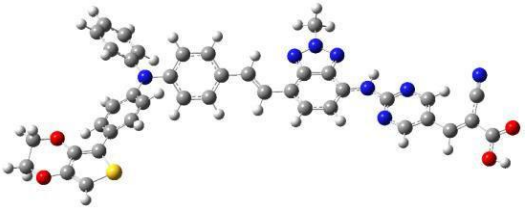

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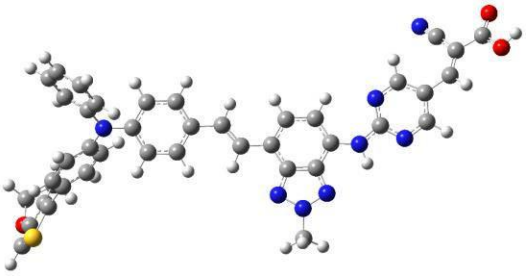

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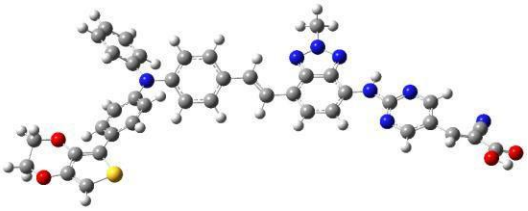

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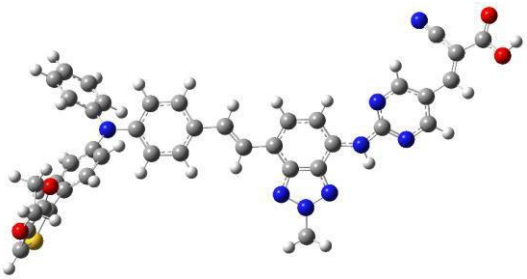

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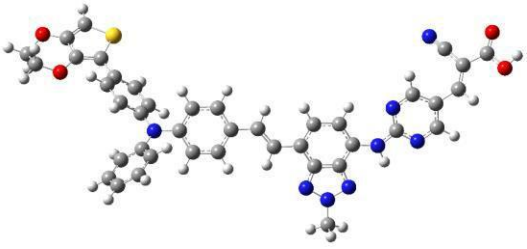

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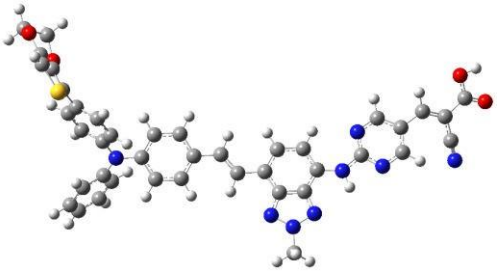

conf 10, -1052.7

Fig S4. The 10 lowest conformers and their potential energy (in kJ mol^{-1}) of TEBT-Pyc obtained by simulated annealing process.

	TPA-Pyc	
	toluene	dichloromethane
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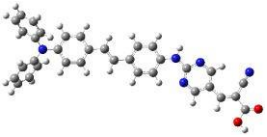
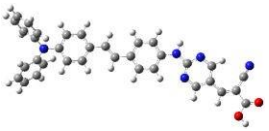
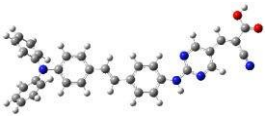
	38.1%	39.5%
conf 2		
	22.2%	24.7%
conf 3		
	14.8%	11.8%
conf 4		
	25.0%	23.9%

Fig S5. The B3LYP/6-311G(d,p) optimized geometries of the shortlisted conformations obtained from simulated annealing process of TPA-Pyc in toluene and dichloromethane.

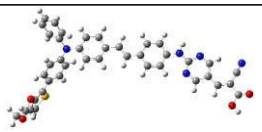
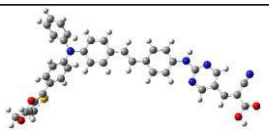
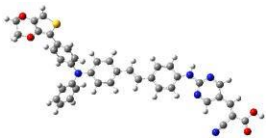
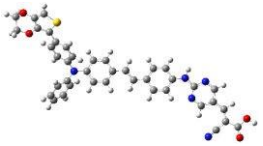
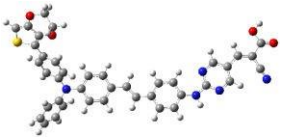
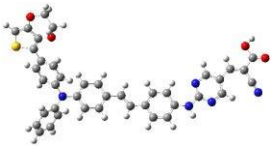
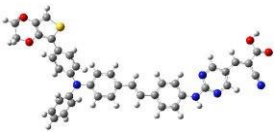
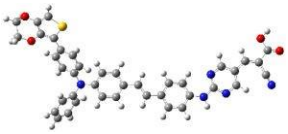
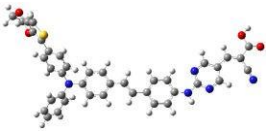
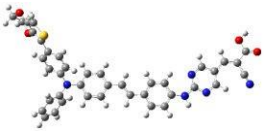
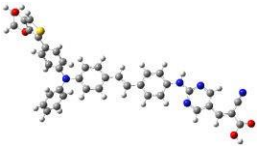
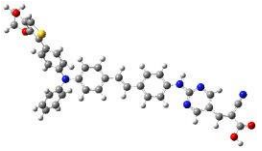
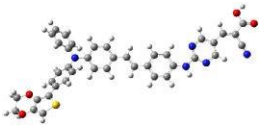
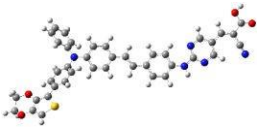
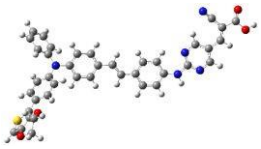
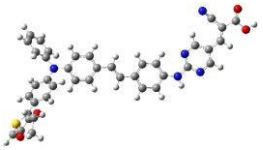
TE-Pyc		
	toluene	dichloromethane
conf 1	 12.5%	 7.1%
conf 4	 6.3%	 3.1%
conf 5	 10.8%	 49.3%
conf 6	 16.7%	 9.6%
conf 7	 10.1%	 5.5%
conf 8	 14.3%	 11.6%
conf 9	 18.9%	 8.5%
conf 10	 10.3%	 5.3%

Fig S6. The B3LYP/6-311G(d,p) optimized geometries of shortlisted conformations obtained from simulated annealing process of TE-Pyc in toluene and dichloromethane.

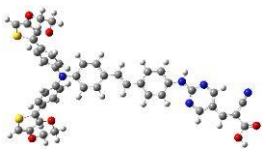
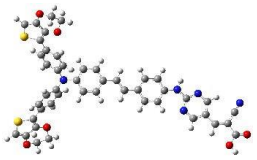
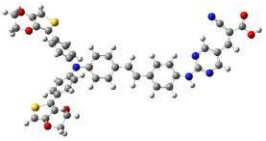
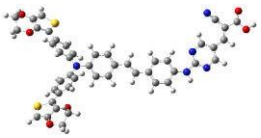
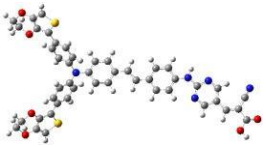
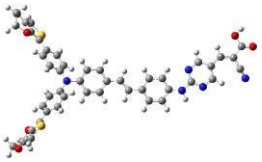
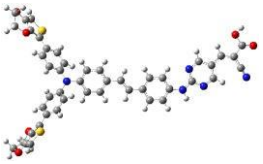
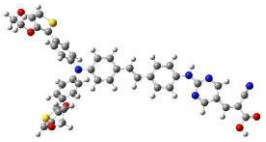
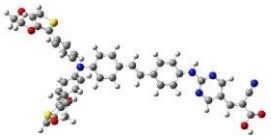
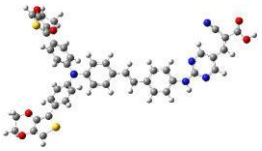
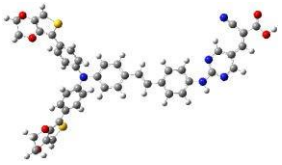
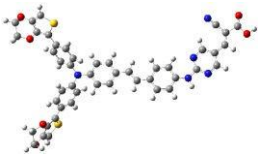
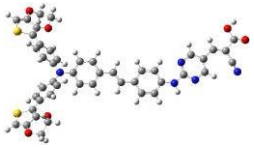
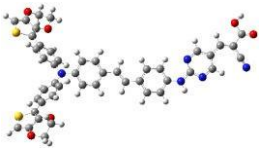
ETE-Pyc		
	toluene	dichloromethane
conf 1	 3.7%	 2.8%
conf 2	 3.9%	 4.8%
conf 3	 3.0%	 3.9%
conf 6	 62.7%	 67.8%
conf 7	 3.5%	 3.0%
conf 8	 7.0%	 5.4%
conf 9	 6.7%	 2.2%
conf 10	 9.4%	 10.2%

Fig S7. The B3LYP/6-311G(d,p) optimized geometries of shortlisted conformations obtained from simulated annealing process of ETE-Pyc in toluene and dichloromethane.

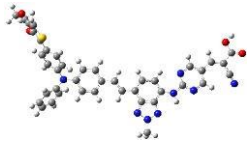
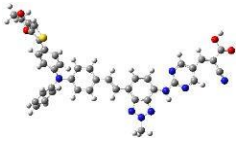
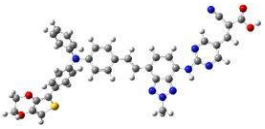
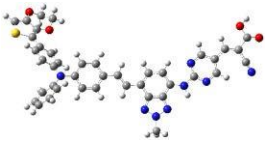
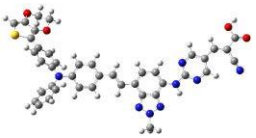
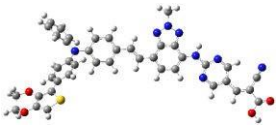
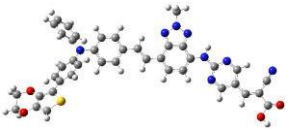
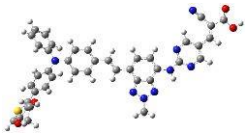
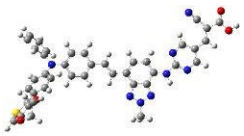
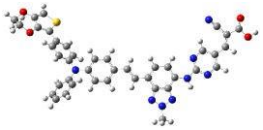
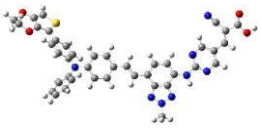
TEBT-Pyc		
	toluene	dichloromethane
conf 1		
	9.9%	9.5%
conf 3		
	9.7%	11.0%
conf 4		
	6.3%	7.6%
conf 5		
	54.0%	60.0%
conf 8		
	7.1%	3.8%
conf 9		
	13.1%	8.1%

Fig S8. The B3LYP/6-311G(d,p) optimized geometries of shortlisted conformations obtained from simulated annealing process of TEBT-Pyc in toluene and dichloromethane.

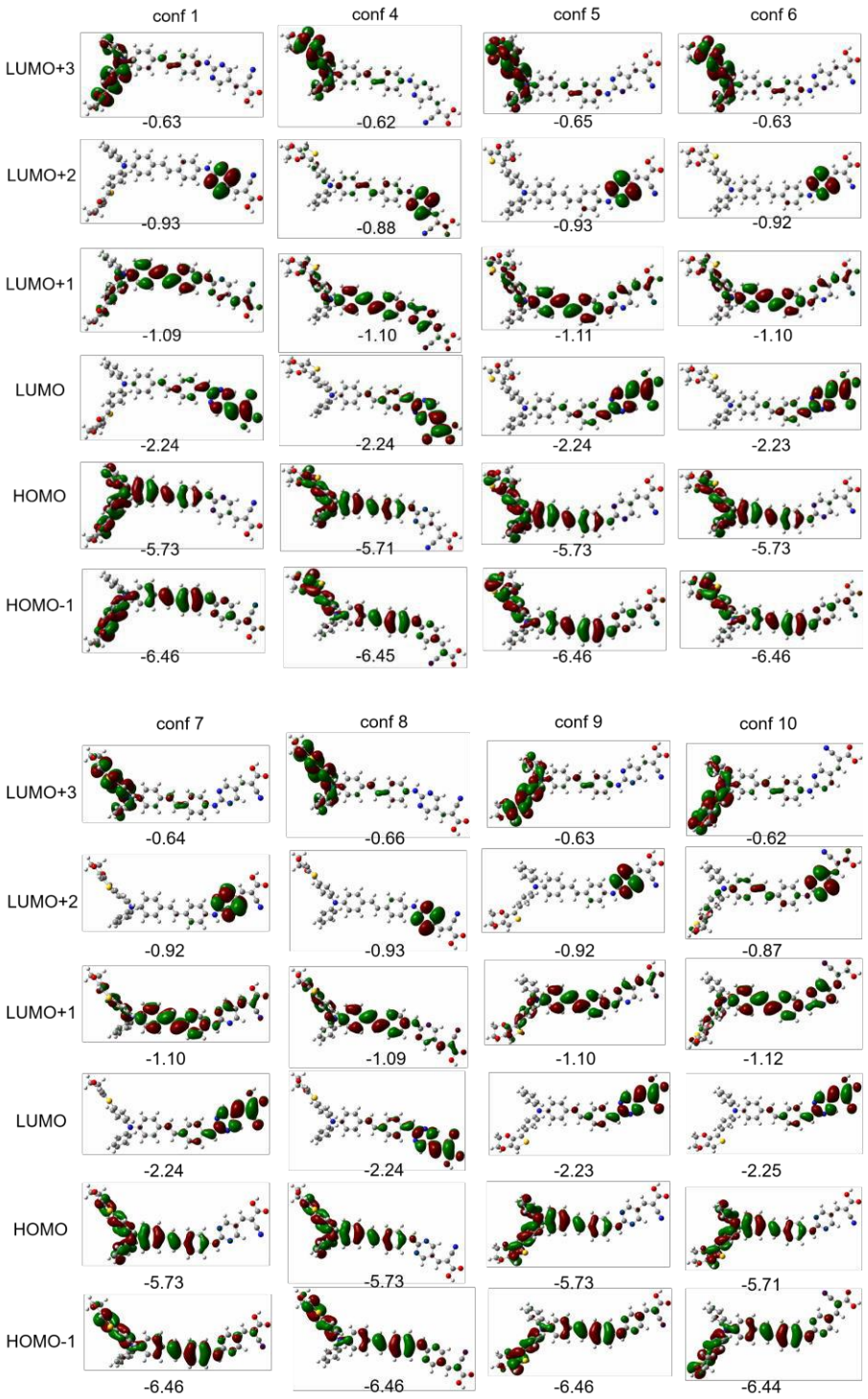


Fig S9. The isosurfaces (isovalue=±0.02 a.u.) and corresponding energy levels (in eV) of HOMO-1 to LUMO+3 of low-lying conformations of TE-Pyc in toluene using MN15.

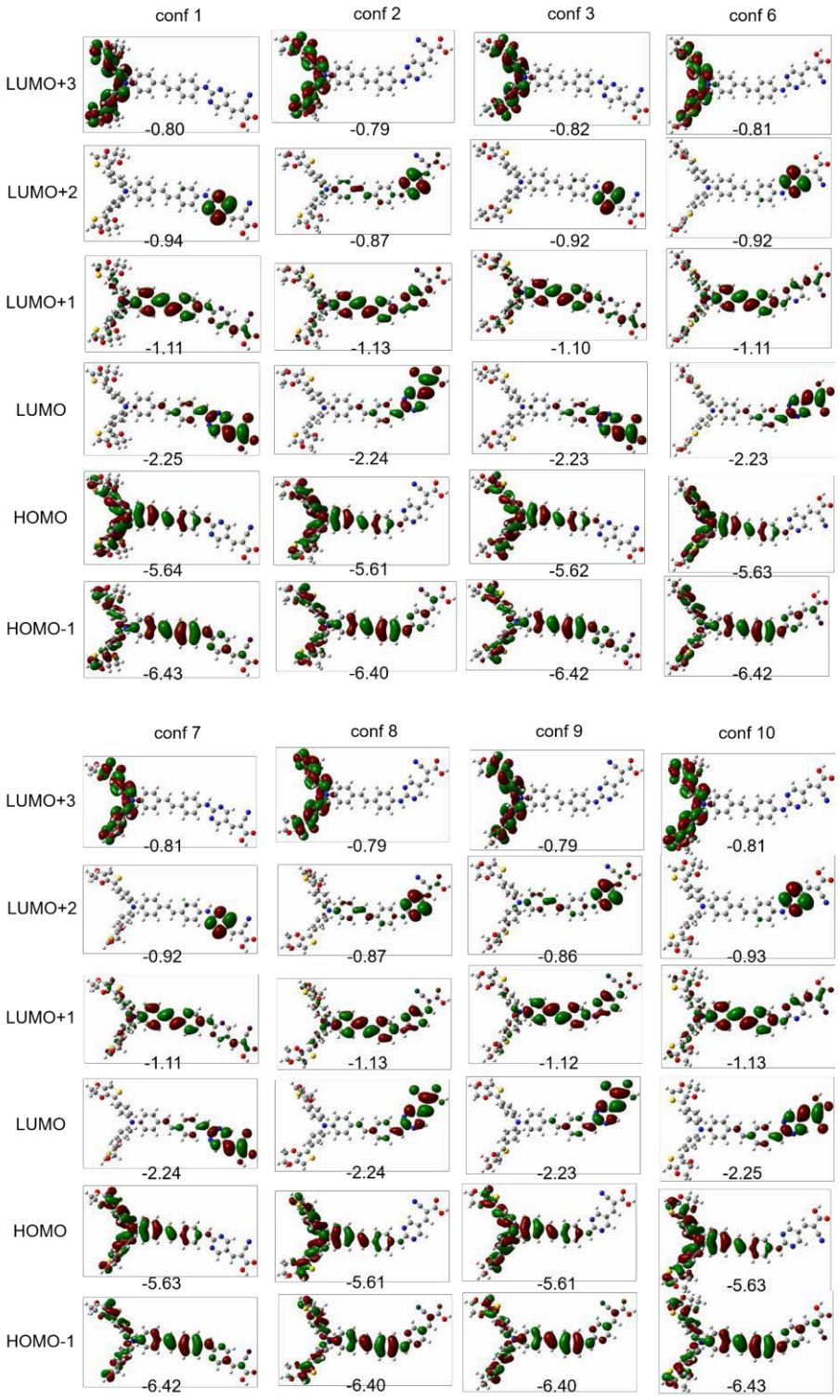


Fig S10. The isosurfaces (isovalue=±0.02 a.u.) and corresponding energy levels (in eV) of HOMO-1 to LUMO+3 of low-lying conformations of ETE-Pyc in toluene using MN15.

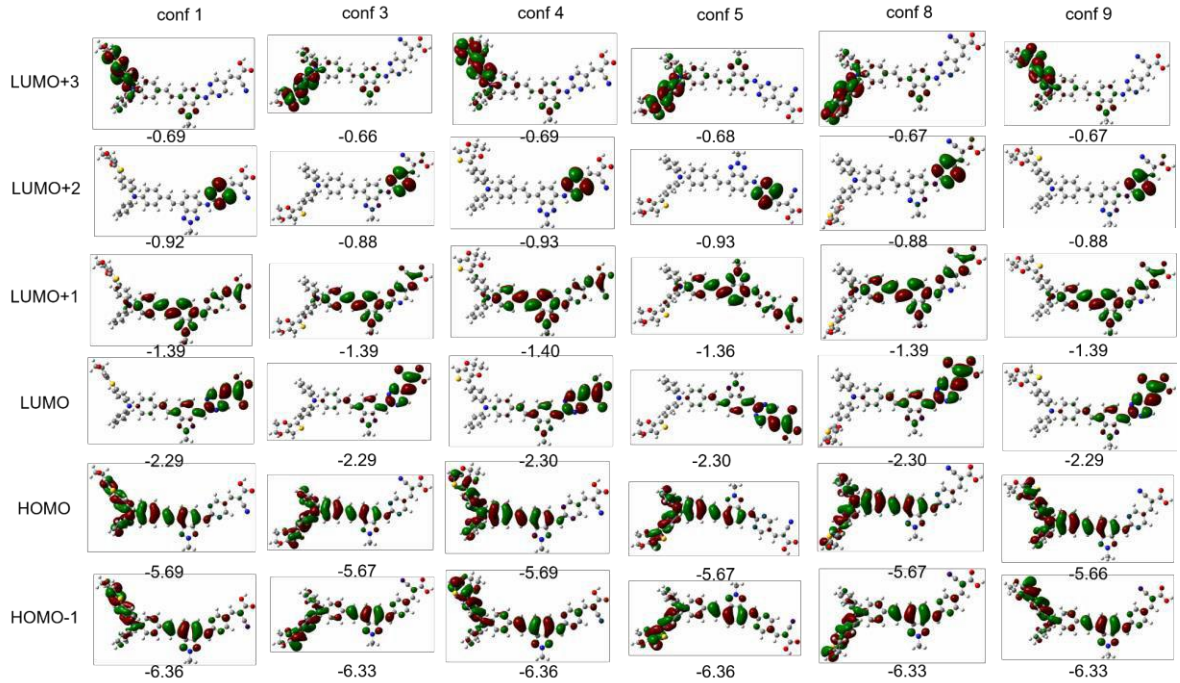


Fig S11. The isosurfaces (isovalue=±0.02 a.u.) and corresponding energy levels (in eV) of HOMO-1 to LUMO+3 of low-lying conformers of TEBT-Pyc in toluene using MN15.

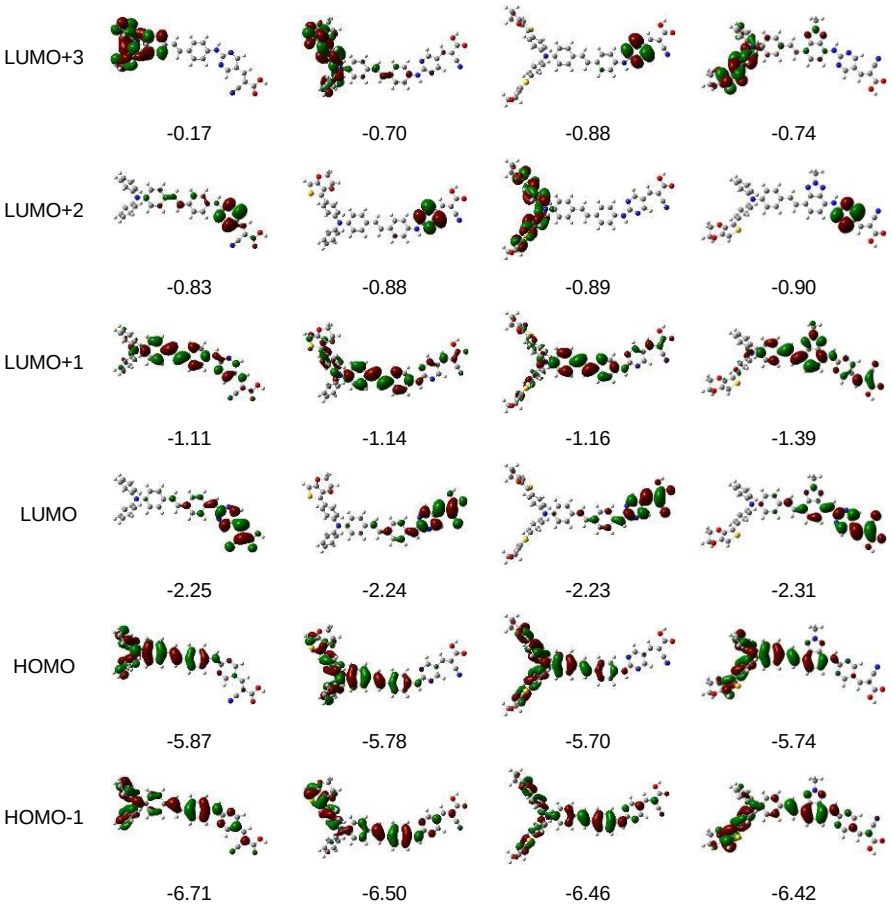


Fig S12. The isosurfaces (isovalue=±0.02 a.u.) and corresponding energy levels (in eV) of HOMO-1 to LUMO+3 for TPA-Pyc (conf 1), TE-Pyc (conf 5), ETE-Pyc (conf 6), and TEBT-Pyc (conf 5) in dichloromethane using MN15.

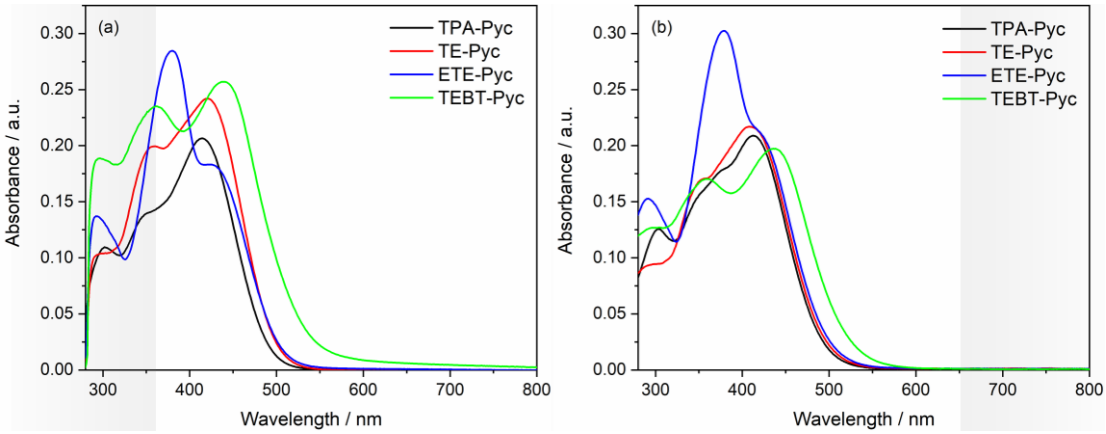


Fig S13. The experimental UV-Vis spectra of the four dyes in toluene (a, data taken from Ref[S1]) and dichloromethane (b). Concentration: 5×10^{-6} mol/L.

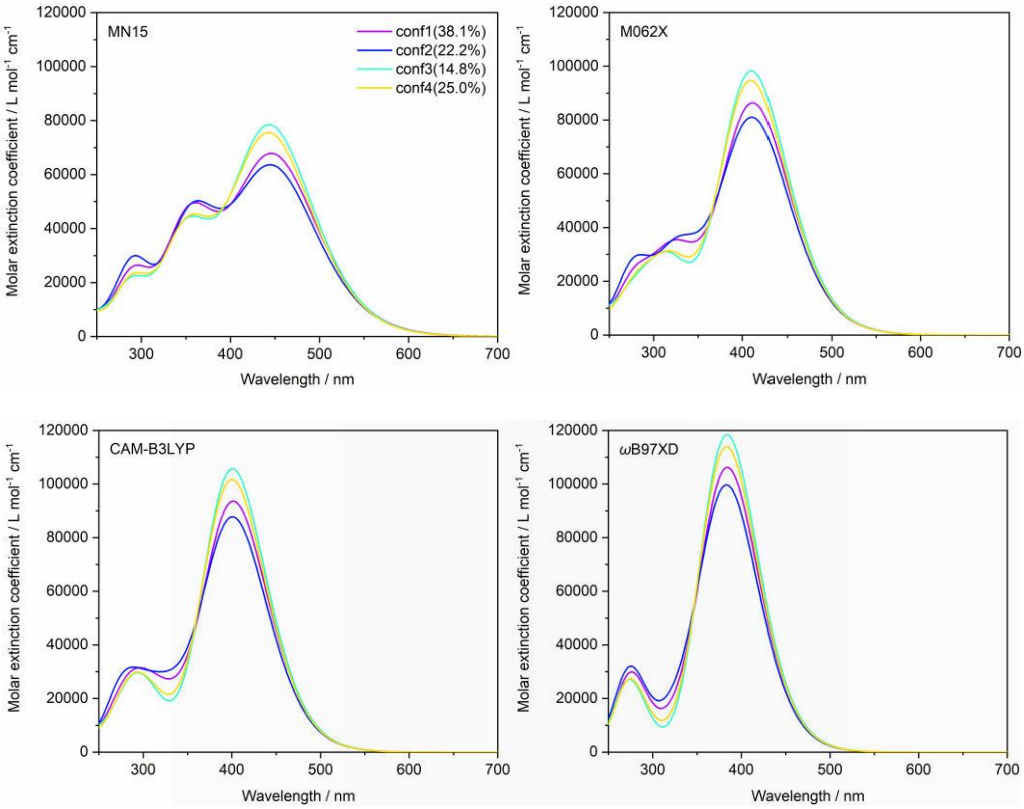


Fig S14. The UV-Vis spectra of various conformations of TPA-Pyc in toluene using MN15, M062X, CAM-B3LYP, and ωB97XD.

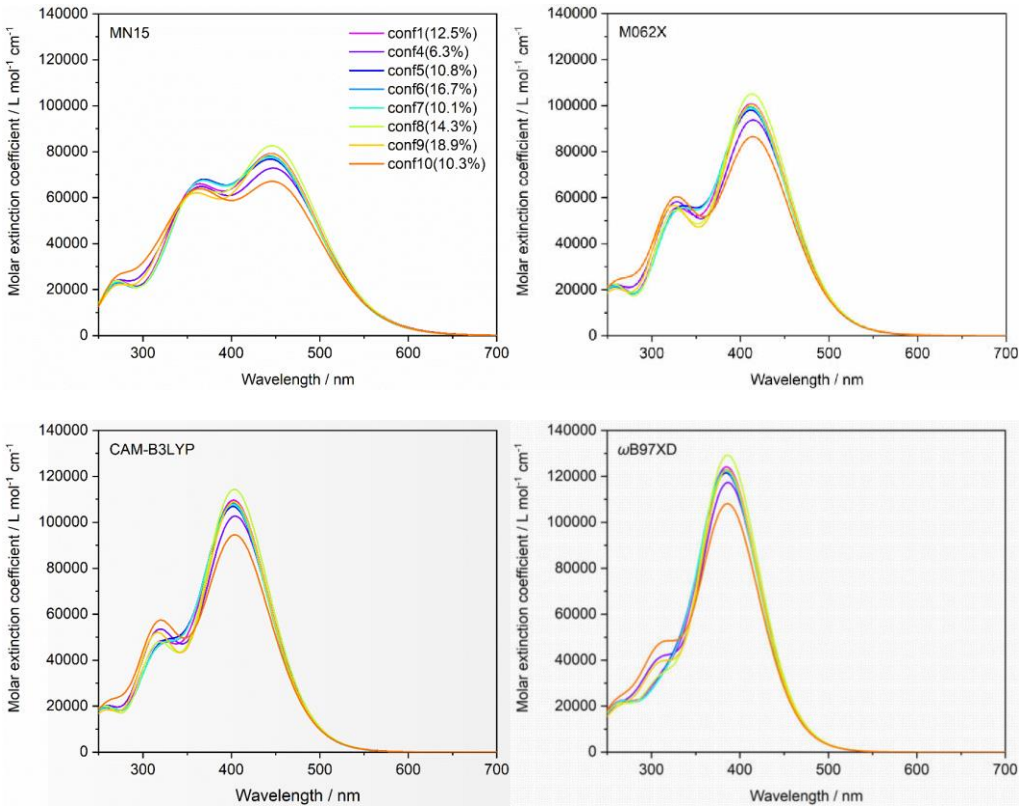


Fig S15. The UV-Vis spectra of various conformations of TE-Pyc in toluene using MN15, M062X, CAM-B3LYP, and ωB97XD.

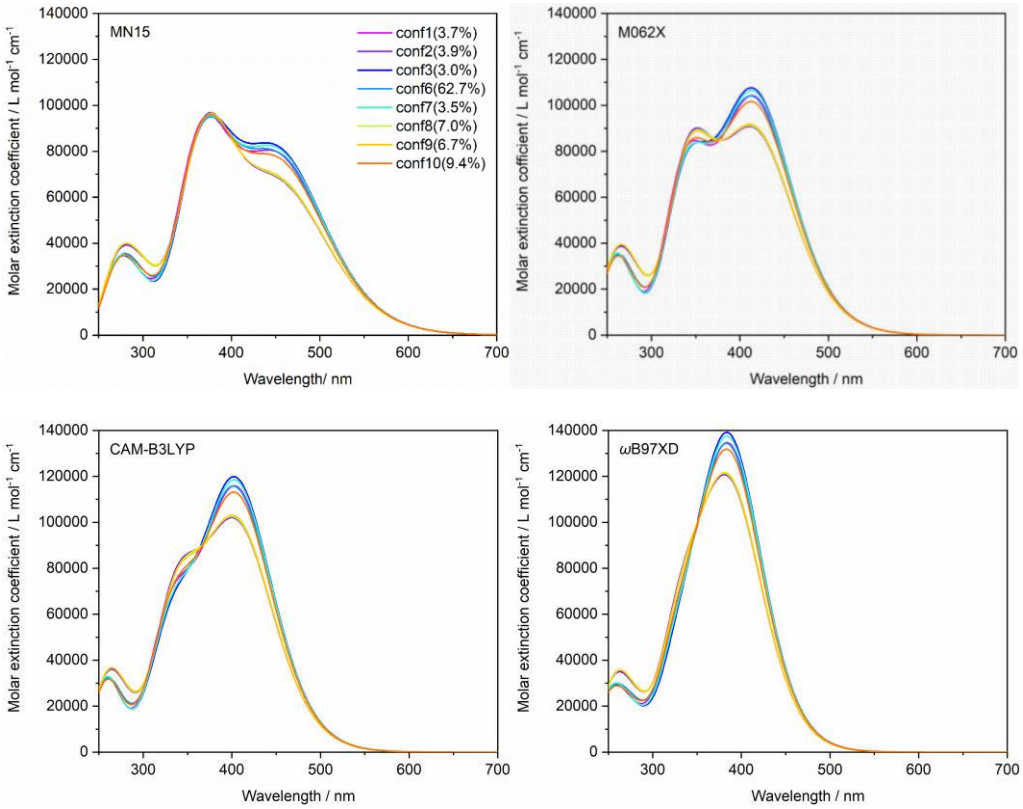


Fig S16. The UV-Vis spectra of various conformations of ETE-Pyc in toluene using MN15, M062X, CAM-B3LYP, and ωB97XD.

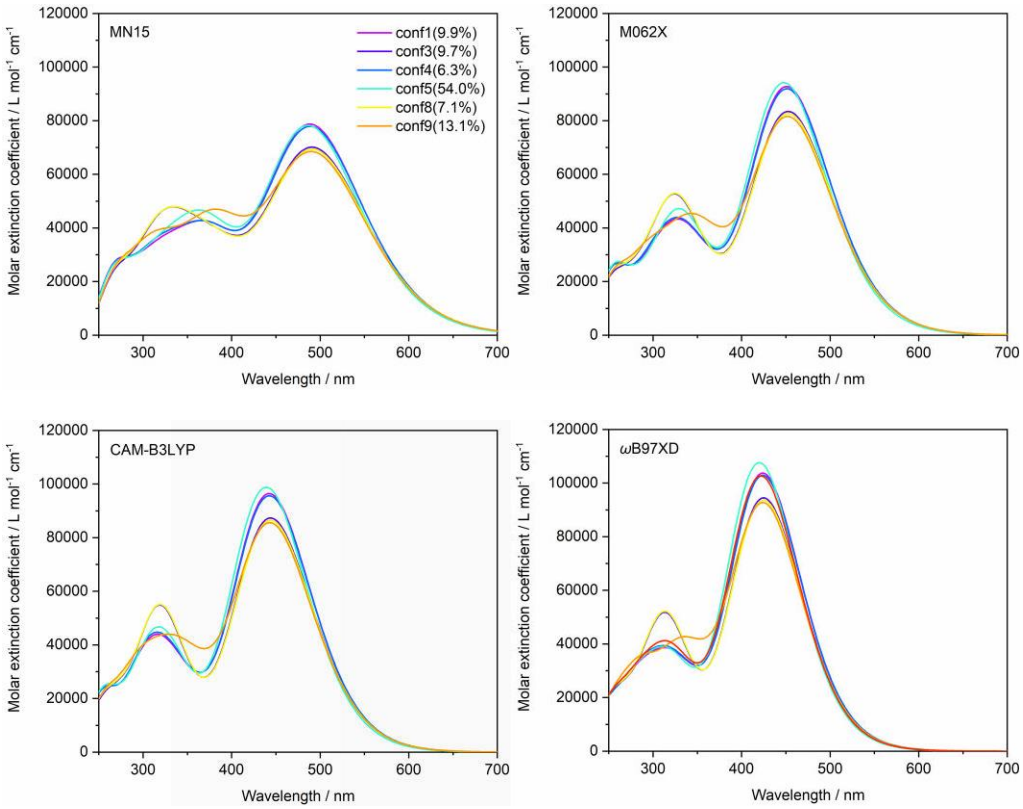


Fig S17. The UV-Vis spectra of various conformations of TEBT-Pyc in toluene using MN15, M062X, CAM-B3LYP, and ωB97XD.

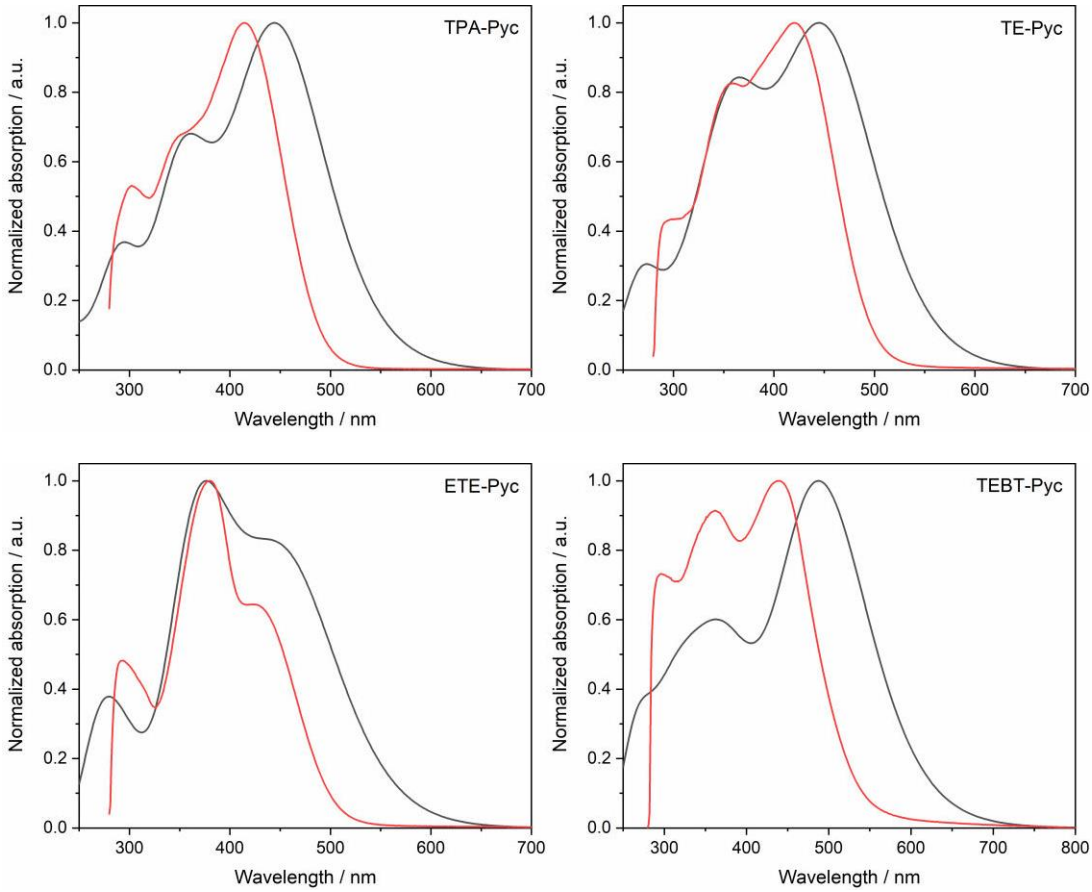


Fig S18. The one-to-one normalized experimental and MN15 computational conformation-weighted absorption spectra of TPA-Pyc, TE-Pyc, ETE-Pyc, and TEBT-Pyc.

Table S1. Gibbs free energies (*G*) and populations of various conformations of TPA-Pyc in toluene and dichloromethane.

		G^a/a.u.	$G_{rel}{}^b$/kJ mol^{-1}	Pop.[c]
Tol	conf1	-1734.872515	0.000	38.1%
	conf2	-1734.872004	1.342	22.2%
	conf3	-1734.871621	2.347	14.8%
	conf4	-1734.872117	1.045	25.0%
DCM	conf1	-1734.882126	0.000	39.5%
	conf2	-1734.881682	1.166	24.7%
	conf3	-1734.880986	2.993	11.8%
	conf4	-1734.881651	1.247	23.9%

[a] The Gibbs free energy is calculated at B3LYP/6-311G(d,p) level; [b] G_{rel} is given relative to the lowest value of the corresponding configuration; [c] Population is calculated by $\mathrm{Pop} = e^{-\frac{G_{rel}(i)}{RT}} \Big/ \sum_j e^{-\frac{G_{rel}(j)}{RT}}$, where R=8.314 J mol^{-1} K^{-1} and T=298.15 K. Both here and after.

Table S2. Gibbs free energies (*G*) and populations of various conformations of TE-Pyc in toluene and dichloromethane.

		G/a.u.	G_{rel}/kJ mol^{-1}	Pop.
Tol	conf1	-2514.562002	1.027	12.5%
	conf4	-2514.561356	2.723	6.3%
	conf5	-2514.561862	1.394	10.8%
	conf6	-2514.562276	0.307	16.7%
	conf7	-2514.561801	1.554	10.1%
	conf8	-2514.562127	0.698	14.3%
	conf9	-2514.562393	0.000	18.9%
	conf10	-2514.561816	1.515	10.3%
DCM	conf1	-2514.573257	4.818	7.1%
	conf4	-2514.572493	6.824	3.1%
	conf5	-2514.575092	0.000	49.3%
	conf6	-2514.573545	4.062	9.6%
	conf7	-2514.573017	5.448	5.5%
	conf8	-2514.573727	3.584	11.6%
	conf9	-2514.573427	4.371	8.5%
	conf10	-2514.572991	5.516	5.3%

Table S3. Gibbs free energies (*G*) and populations of various conformations of ETE-Pyc in toluene and dichloromethane.

		G/a.u.	G_{rel}/kJ mol^{-1}	Pop.
Tol	conf1	-3294.251896	6.989	3.7%
	conf2	-3294.251946	6.858	3.9%
	conf3	-3294.251694	7.519	3.0%
	conf6	-3294.254558	0.000	62.7%
	conf7	-3294.251846	7.120	3.5%
	conf8	-3294.252495	5.416	7.0%
	conf9	-3294.252446	5.545	6.7%
	conf10	-3294.252762	4.715	9.4%
DCM	conf1	-3294.265014	7.898	2.8%
	conf2	-3294.265512	6.590	4.8%
	conf3	-3294.265325	7.081	3.9%
	conf6	-3294.268022	0.000	67.8%
	conf7	-3294.265085	7.711	3.0%
	conf8	-3294.265630	6.280	5.4%
	conf9	-3294.264778	8.517	2.2%
	conf10	-3294.266230	4.705	10.2%

Table S4. Gibbs free energies (*G*) and populations of various conformations of TEBT-Pyc in toluene and dichloromethane.

		G/a.u.	G_{rel}/kJ mol^{-1}	Pop.
Tol	conf1	-2717.519272	4.206051	9.9%
	conf3	-2717.519250	4.263812	9.7%
	conf4	-2717.518842	5.335016	6.3%
	conf5	-2717.520874	0.000000	54.0%
	conf8	-2717.518954	5.040960	7.1%
	conf9	-2717.519533	3.520795	13.1%
DCM	conf1	-2717.531443	4.570996	9.5%
	conf3	-2717.531581	4.208676	11.0%
	conf4	-2717.531233	5.122350	7.6%
	conf5	-2717.533184	0.000000	60.0%
	conf8	-2717.530588	6.815798	3.8%
	conf9	-2717.531298	4.951693	8.1%

Table S5. The selected dihedrals (in degree) of various conformations of TPA-Pyc in toluene and dichloromethane obtained from B3LYP/6-311G(d,p) calculations.[a]

		toluene	dichloromethane
conf1	β	3.2	2.7
	γ	0.8	0.4
	δ	0.0	0.3
	θ	0.1	0.1
conf2	β	0.5	0.7
	γ	1.1	0.7
	δ	0.2	0.6
	θ	0.2	0.3
conf3	β	2.0	1.4
	γ	0.4	0.8
	δ	0.7	0.9
	θ	0.2	0.2
conf4	β	2.6	2.4
	γ	1.5	1.4
	δ	0.4	0.5
	θ	0.2	0.3

[a] The values of the dihedrals were transformed into 0-90° for clarity. Both here and after.

Table S6. The selected dihedrals (in degree) of various conformations of TE-Pyc in toluene and dichloromethane obtained from B3LYP/6-311G(d,p) calculations.

		toluene	dichloromethane
conf1	α_1	21.7	21.8
	β	2.2	2.4
	γ	0.7	1.4
	δ	0.2	0.2
	θ	0.5	0.4
conf4	α_1	21.9	21.9
	β	2.2	1.8
	γ	0.0	0.3
	δ	0.4	1.1
	θ	0.0	0.1
conf5	α_1	18.9	20.0
	β	2.6	2.6
	γ	1.2	1.4
	δ	0.2	0.6
	θ	0.2	0.4
conf6	α_1	21.9	22.1
	β	4.2	4.2
	γ	3.3	3.3
	δ	0.6	0.4
	θ	0.3	0.6
conf7	α_1	20.9	21.1
	β	3.4	3.4
	γ	2.0	2.0
	δ	0.5	0.1
	θ	0.1	0.4
conf8	α_1	15.9	16.4
	β	3.4	1.7
	γ	1.6	1.5
	δ	0.8	0.5
	θ	0.3	0.2
conf9	α_1	22.1	22.3
	β	5.7	4.1
	γ	4.1	2.6
	δ	0.0	0.8
	θ	0.4	0.9
conf10	α_1	21.0	21.3
	β	1.5	1.3
	γ	0.3	0.5
	δ	0.8	1.0
	θ	0.4	0.5

Table S7. The selected dihedrals (in degree) of various conformations of ETE-Pyc in toluene and dichloromethane obtained from B3LYP/6-311G(d,p) calculations.

		toluene	dichloromethane
conf1	α_1	21.9	22.3
	α_2	21.8	22.1
	β	1.9	2.1
	γ	0.4	0.8
	δ	1.7	2.0
	θ	0.9	1.1
conf2	α_1	21.9	22.2
	α_2	18.3	18.9
	β	0.2	0.6
	γ	1.7	1.2
	δ	0.9	1.1
	θ	0.1	0.0
conf3	α_1	18.6	19.2
	α_2	18.0	19.1
	β	3.7	3.6
	γ	2.3	2.3
	δ	0.1	0.3
	θ	0.2	0.1
conf6	α_1	15.2	15.2
	α_2	21.3	20.8
	β	1.5	3.2
	γ	0.6	2.6
	δ	0.4	1.1
	θ	0.0	0.1
conf7	α_1	18.8	19.2
	α_2	20.4	20.3
	β	2.3	2.2
	γ	0.6	0.6
	δ	1.8	1.8
	θ	0.7	0.8
conf8	α_1	15.1	15.9
	α_2	22.8	23.0
	β	2.8	1.4
	γ	1.6	0.2

	δ	0.9	0.5
	θ	0.3	0.6
conf9	α_1	21.5	22.1
	α_2	16.8	17.7
	β	4.1	4.3
	γ	3.2	3.4
	δ	1.6	2.3
	θ	0.0	0.1
conf10	α_1	21.7	21.8
	α_2	18.7	19.1
	β	2.3	2.1
	γ	0.6	0.3
	δ	0.1	0.3
	θ	0.0	0.0

Table S8. The selected dihedrals (in degree) of various conformations of TEBT-Pyc in toluene and dichloromethane obtained from B3LYP/6-311G(d,p) calculations.

		toluene	dichloromethane
conf1	α_1	21.8	22.1
	β	1.9	1.3
	γ	0.2	0.6
	δ	0.1	0.5
	θ	0.2	0.3
conf3	α_1	22.2	22.5
	β	1.4	2.2
	γ	0.3	1.4
	δ	0.0	0.2
	θ	0.2	0.8
conf4	α_1	22.0	22.1
	β	1.4	1.6
	γ	0.0	0.7
	δ	0.2	0.3
	θ	0.5	0.6
conf5	α_1	21.5	22.1
	β	1.5	2.4
	γ	0.0	0.5
	δ	0.3	0.3
	θ	0.5	0.3
conf8	α_1	21.0	20.9
	β	2.7	2.9
	γ	2.3	2.5
	δ	0.1	0.2
	θ	0.5	0.8
conf9	α_1	19.5	22.3
	β	1.6	4.1
	γ	0.2	2.6
	δ	0.2	0.8
	θ	0.2	0.9

Table S9. The first vertical excitation energy (E_{vert}, in eV) and oscillator strength (f) of various conformations of TPA-Pyc in toluene using different functionals.

Functional		conf1	conf2	conf3	conf4
B3LYP	E_{vert}	2.00	2.00	2.04	2.04
	f	0.58	0.54	0.68	0.65
PBE0	E_{vert}	2.22	2.22	2.25	2.25
	f	0.74	0.68	0.87	0.83
MN15	E_{vert}	2.76	2.76	2.78	2.79
	f	1.57	1.46	1.83	1.76
M062X	E_{vert}	3.00	3.01	3.02	3.02
	f	2.02	1.88	2.32	2.23
CAM-B3LYP	E_{vert}	3.08	3.08	3.09	3.09
	f	2.19	2.04	2.50	2.40
ωB97XD	E_{vert}	3.22	3.22	3.23	3.23
	f	2.48	2.30	2.80	2.69

Table S10. The first vertical excitation energy (E_{vert}, in eV) and oscillator strength (f) of various conformations of TE-Pyc in toluene using different functionals.

Functional		conf1	conf4	conf5	conf6	conf7	conf8	conf9	conf10
B3LYP	E_{vert}	1.94	1.91	1.93	1.94	1.94	1.94	1.94	1.90
	f	0.55	0.50	0.52	0.53	0.53	0.57	0.54	0.45
PBE0	E_{vert}	2.17	2.14	2.16	2.17	2.17	2.17	2.17	2.13
	f	0.72	0.65	0.68	0.70	0.69	0.74	0.71	0.59
MN15	E_{vert}	2.75	2.73	2.74	2.75	2.75	2.75	2.75	2.72
	f	1.78	1.63	1.70	1.74	1.73	1.87	1.78	1.48
M062X	E_{vert}	2.99	2.98	2.99	3.00	2.99	2.99	3.00	2.98
	f	2.34	2.18	2.26	2.29	2.28	2.46	2.35	2.00
CAM-B3LYP	E_{vert}	3.07	3.06	3.07	3.07	3.07	3.07	3.07	3.05
	f	2.55	2.39	2.46	2.49	2.48	2.69	2.56	2.19
ωB97XD	E_{vert}	3.21	3.20	3.21	3.21	3.21	3.21	3.21	3.20
	f	2.87	2.74	2.77	2.81	2.80	3.04	2.89	2.50

Table S11. The first vertical excitation energy (E_{vert}, in eV) and oscillator strength (f) of various conformations of ETE-Pyc in toluene using different functionals.

Functional		conf1	conf2	conf3	conf6	conf7	conf8	conf9	conf10
B3LYP	E_{vert}	1.85	1.82	1.85	1.86	1.85	1.82	1.83	1.84
	f	0.47	0.38	0.48	0.47	0.48	0.39	0.39	0.45
PBE0	E_{vert}	2.08	2.05	2.09	2.09	2.09	2.06	2.06	2.08
	f	0.61	0.50	0.63	0.61	0.62	0.50	0.51	0.59
MN15	E_{vert}	2.70	2.69	2.71	2.71	2.71	2.69	2.69	2.70
	f	1.71	1.40	1.76	1.69	1.75	1.40	1.42	1.64
M062X	E_{vert}	2.96	2.95	2.96	2.97	2.97	2.95	2.95	2.96
	f	2.36	1.98	2.42	2.33	2.40	1.98	2.00	2.28
CAM-B3LYP	E_{vert}	3.04	3.03	3.04	3.04	3.04	3.03	3.03	3.04
	f	2.60	2.20	2.67	2.57	2.65	2.21	2.23	2.52
ωB97XD	E_{vert}	3.19	3.18	3.19	3.19	3.19	3.18	3.18	3.04
	f	2.97	2.54	3.05	2.93	3.02	2.54	2.57	2.52

Table S12. The first vertical excitation energy (E_{vert}, in eV) and oscillator strength (f) of various conformations of TEBT-Pyc in toluene using different functionals.

Functional		conf1	conf3	conf4	conf5	conf8	conf9
B3LYP	E_{vert}	1.86	1.83	1.86	1.84	1.83	1.82
	f	0.78	0.67	0.76	0.74	0.66	0.64
PBE0	E_{vert}	2.06	2.03	2.05	2.05	2.03	2.03
	f	0.99	0.85	0.97	0.95	0.84	0.82
MN15	E_{vert}	2.53	2.51	2.53	2.54	2.51	2.51
	f	1.84	1.63	1.82	1.83	1.61	1.58
M062X	E_{vert}	2.74	2.73	2.74	2.76	2.73	2.73
	f	2.19	1.96	2.17	2.22	1.95	1.90
CAM-B3LYP	E_{vert}	2.80	2.79	2.80	2.82	2.79	2.79
	f	2.27	2.06	2.26	2.33	2.04	2.00
ωB97XD	E_{vert}	2.92	2.91	2.92	2.95	2.91	2.91
	f	2.45	2.23	2.43	2.54	2.21	2.17

Table S13. Electronic excitation properties of various conformations of TPA-Pyc in toluene using MN15.

TPA-Pyc (conf1)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.76	449	1.57	H→L 74.0%, H-1→L 13.1%, H→L+1 8.0%
S_2	3.44	360	0.64	H→L+1 77.2%, H→L 6.6%, H→L+2 5.8%
S_3	3.51	353	0.47	H-1→L 63.6%, H→L 18.6%, H-2→L 12.5%
S_4	3.95	314	0.04	H→L+2 56.9%, H-1→L+2 18.4%, H-1→L+1 10.4%
S_5	4.04	307	0.04	H→L+3 82.0%, H-1→L+3 6.9%
S_6	4.07	305	0.00	H-9→L 83.9%, H-9→L+2 7.0%
S_7	4.19	296	0.28	H→L+4 84.0%, H-1→L+4 12.4%
S_8	4.26	291	0.16	H-2→L 57.0%, H-8→L 10.6%, H-1→L+1 10.4%, H-1→L 9.8%
S_9	4.36	284	0.06	H-1→L+1 48.5%, H→L+5 13.0%, H-1→L 8.1%, H-2→L 8.0%, H-1→L+2 6.8%
S_{10}	4.46	278	0.00	H-9→L+2 67.2%, H-9→L+1 17.5%, H-9→L 9.0%
S_{11}	4.51	275	0.05	H→L+5 21.8%, H-5→L 18.5%, H→L+6 14.3%, H-1→L+5 11.4%, H-1→L+1 10.9%, H-5→L+1 6.9%, H-1→L+6 5.0%
S_{12}	4.60	270	0.03	H→L+7 41.7%, H→L+8 24.0%, H-1→L+3 6.1%
S_{13}	4.67	266	0.00	H-11→L 77.0%, H-11→L+10 9.1%
S_{14}	4.69	264	0.02	H-1→L+2 29.0%, H→L+2 19.7%, H-2→L+2 9.9%, H→L+6 6.3%, H-2→L+1 5.9%, H-1→L+1 5.1%
S_{15}	4.75	261	0.01	H→L+8 40.6%, H→L+7 24.9%, H-1→L+8 6.6%, H-1→L+2 5.1%
S_{16}	4.85	256	0.02	H→L+5 29.4%, H→L+6 23.5%, H→L+9 9.8%, H-5→L 8.1%, H-1→L+2 6.5%
S_{17}	4.96	250	0.08	H-5→L 61.9%, H→L+6 17.7%
S_{18}	5.08	244	0.01	H-3→L 31.3%, H-8→L 20.9%, H-4→L 9.6%, H-2→L+1 5.8%, H-2→L 5.6%, H-3→L+1 5.2%
S_{19}	5.11	243	0.04	H-3→L 38.3%, H-8→L 22.8%, H-4→L 6.8%, H-2→L 6.3%
S_{20}	5.27	235	0.01	H-4→L 64.4%, H-2→L+1 11.2%, H-8→L 6.8%
S_{21}	5.36	231	0.01	H→L+9 17.0%, H-8→L 14.1%, H-2→L+1 13.8%, H-1→L+3 10.1%, H-1→L+6 7.2%, H-1→L+5 6.5%, H-4→L 5.6%
S_{22}	5.37	231	0.00	H-1→L+3 39.1%, H-3→L 8.6%, H-2→L+3 6.0%
S_{23}	5.41	229	0.03	H-2→L+2 16.8%, H-2→L+1 15.8%, H-1→L+2 14.2%, H-8→L+2 8.0%, H-8→L 7.4%, H→L+9 6.5%
S_{24}	5.47	227	0.07	H-6→L 31.0%, H-3→L 12.3%, H-1→L+3 10.0%, H-3→L+1 7.3%, H→L+9 6.4%
S_{25}	5.51	225	0.01	H-2→L+2 26.5%, H-2→L+1 23.9%, H→L+9 13.3%, H-8→L+1 5.4%

TPA-Pyc (conf2)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.76	449	1.46	H→L 74.2%, H-1→L 13.1%, H→L+1 7.7%
S_2	3.42	363	0.70	H→L+1 77.1%, H→L 7.5%, H→L+2 6.2%
S_3	3.51	354	0.42	H-1→L 65.1%, H→L 17.4%, H-2→L 12.6%
S_4	3.95	314	0.03	H→L+2 55.7%, H-1→L+2 15.4%, H-1→L+1 14.5%
S_5	4.04	307	0.05	H→L+3 82.4%, H-1→L+3 6.9%
S_6	4.07	305	0.00	H-9→L 83.7%, H-9→L+2 6.8%
S_7	4.20	296	0.28	H→L+4 84.0%, H-1→L+4 12.4%
S_8	4.26	291	0.26	H-2→L 60.5%, H-1→L+1 10.9%, H-8→L 10.8%, H-1→L+1 7.0%
S_9	4.35	285	0.05	H-1→L+1 48.9%, H-1→L+2 12.1%, H→L+5 7.9%, H-1→L 6.6%
S_{10}	4.46	278	0.00	H-9→L+2 64.5%, H-9→L+1 20.0%, H-9→L 9.1%
S_{11}	4.51	275	0.05	H→L+5 38.0%, H-5→L 17.4%, H-1→L+5 15.9%, H-1→L+1 11.2%, H-5→L+1 6.8%
S_{12}	4.60	270	0.03	H→L+7 59.8%, H-1→L+3 6.1%, H→L+8 5.9%
S_{13}	4.67	266	0.00	H-11→L 77.2%, H-11→L+10 9.0%
S_{14}	4.68	265	0.03	H-1→L+2 26.5%, H→L+2 16.9%, H→L+6 11.1%, H-2→L+2 8.0%, H→L+1 7.0%, H-2→L+1 6.2%
S_{15}	4.75	261	0.01	H→L+8 59.6%, H-1→L+8 10.2%, H→L+7 6.8%
S_{16}	4.86	255	0.02	H→L+6 50.9%, H-1→L+2 10.3%, H→L+9 9.7%, H→L+2 7.7%
S_{17}	4.95	250	0.07	H-5→L 65.7%, H→L+5 17.6%
S_{18}	5.08	244	0.03	H-3→L 41.9%, H-8→L 16.2%, H-4→L 5.7%, H-3→L+1 5.6%, H-2→L 5.3%
S_{19}	5.10	243	0.01	H-8→L 27.8%, H-3→L 27.5%, H-4→L 12.6%, H-2→L 8.0%
S_{20}	5.27	235	0.00	H-4→L 63.9%, H-2→L+1 12.7%, H-8→L 7.9%
S_{21}	5.36	232	0.01	H-1→L+3 21.5%, H-2→L+1 16.1%, H-8→L 11.5%, H→L+9 10.5%, H-1→L+6 8.5%, H-4→L 5.5%
S_{22}	5.37	231	0.00	H-1→L+3 24.5%, H-3→L 12.1%, H→L+7 6.8%
S_{23}	5.40	230	0.06	H-2→L+1 18.9%, H-2→L+2 14.0%, H-1→L+2 13.6%, H-8→L 8.0%, H-8→L+2 7.1%, H→L+9 5.6%
S_{24}	5.46	227	0.05	H-6→L 21.0%, H-1→L+3 12.6%, H-3→L 11.8%, H-7→L 8.8%, H-3→L+1 7.9%
S_{25}	5.50	226	0.01	H→L+9 22.7%, H-2→L+2 21.3%, H-2→L+1 12.7%, H→L+12 6.7%, H-8→L+1 5.7%

TPA-Pyc (conf3)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.78	445	1.83	H→L 73.0%, H-1→L 12.7%, H→L+1 10.9%
S_2	3.47	357	0.43	H→L+1 81.0%, H→L 7.1%
S_3	3.54	350	0.56	H-1→L 62.7%, H→L 19.1%, H-2→L 12.2%
S_4	3.94	315	0.01	H→L+2 62.3%, H-1→L+2 28.9%, H-2→L+2 5.6%
S_5	4.04	307	0.04	H→L+3 83.6%, H-1→L+3 7.0%
S_6	4.13	300	0.00	H-9→L 91.6%
S_7	4.20	295	0.28	H→L+4 84.1%, H-1→L+4 12.4%
S_8	4.28	290	0.07	H-2→L 54.6%, H-1→L+1 18.0%, H-8→L 9.3%, H-1→L 7.9%
S_9	4.38	283	0.06	H-1→L+1 51.4%, H→L+5 12.9%, H-2→L 11.0%, H-1→L 9.8%
S_{10}	4.40	282	0.00	H-9→L+2 93.5%
S_{11}	4.51	275	0.07	H→L+5 25.1%, H-5→L 16.1%, H→L+6 13.3%, H-1→L+5 13.2%, H-1→L+1 11.9%, H-5→L+1 7.3%
S_{12}	4.60	269	0.03	H→L+7 54.4%, H→L+8 11.3%, H-1→L+3 6.0%, H-6→L+1 5.0%,
S_{13}	4.67	265	0.00	H-11→L 77.0%, H-11→L+10 9.3%
S_{14}	4.70	264	0.02	H-1→L+2 40.5%, H→L+2 35.2%, H-2→L+2 17.2%
S_{15}	4.74	261	0.01	H→L+8 55.8%, H→L+7 12.6%, H-1→L+8 9.2%
S_{16}	4.84	256	0.02	H→L+6 38.4%, H→L+5 21.9%, H→L+9 11.4%, H-1→L+1 7.9%
S_{17}	5.00	248	0.07	H-5→L 67.8%, H→L+6 10.8%, H→L+5 10.4%
S_{18}	5.10	243	0.04	H-3→L 43.7%, H-8→L 12.8%, H-3→L+1 9.3%, H-4→L 5.1%
S_{19}	5.13	242	0.03	H-8→L 31.7%, H-3→L 22.1%, H-4→L 12.5%, H-2→L 7.8%, H-2→L+1 6.4%
S_{20}	5.30	234	0.01	H-4→L 61.6%, H-2→L+1 11.2%, H-8→L 7.2%
S_{21}	5.37	231	0.01	H-1→L+3 33.4%, H-8→L 10.9%, H→L+9 10.2%, H-4→L 7.1%, H-2→L+1 5.7%
S_{22}	5.37	231	0.00	H-1→L+3 16.0%, H-3→L 10.3%, H→L+9 8.3%, H→L+6 6.2%, H-2→L+1 5.2%
S_{23}	5.41	229	0.04	H-2→L+2 38.6%, H-1→L+2 20.5%, H-8→L+2 14.5%
S_{24}	5.48	226	0.07	H-6→L 27.3%, H-3→L 16.0%, H-1→L+3 9.8%, H-3→L+1 9.0%, H-6→L+1 6.1%, H-2→L+1 5.8%, H-7→L 5.5%
S_{25}	5.50	226	0.00	H-2→L+1 42.5%, H→L+9 22.0%, H-8→L 7.0%, H→L+12 6.4%

TPA-Pyc (conf4)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.79	445	1.76	H→L 73.1%, H-1→L 12.7%, H→L+1 10.5%
S_2	3.46	359	0.49	H→L+1 80.3%, H→L 8.2%
S_3	3.54	351	0.50	H-1→L 64.2%, H→L 17.9%, H-2→L 12.4%
S_4	3.93	315	0.02	H→L+2 61.5%, H-1→L+2 27.0%, H-2→L+2 5.3%
S_5	4.04	307	0.04	H→L+3 83.6%, H-1→L+3 7.0%
S_6	4.14	300	0.00	H-9→L 91.5%
S_7	4.20	295	0.28	H→L+4 84.0%, H-1→L+4 12.4%
S_8	4.28	290	0.09	H-2→L 49.9%, H-1→L+1 22.5%, H-8→L 8.2%, H-1→L 6.5%
S_9	4.36	284	0.08	H-1→L+1 42.3%, H-2→L 16.2%, H→L+5 11.3%, H-1→L 10.9%
S_{10}	4.40	282	0.00	H-9→L+2 90.1%
S_{11}	4.52	274	0.04	H→L+5 33.1%, H-5→L 16.3%, H-1→L+1 15.3%, H-1→L+5 15.0%, H-5→L+1 7.2%
S_{12}	4.60	269	0.03	H→L+7 54.6%, H→L+8 11.6%, H-1→L+3 6.1%
S_{13}	4.67	265	0.00	H-11→L 77.0%, H-11→L+10 9.3%
S_{14}	4.69	264	0.02	H-1→L+2 36.7%, H→L+2 31.5%, H-2→L+2 15.1%
S_{15}	4.74	261	0.01	H→L+8 54.7%, H→L+7 12.5%, H-1→L+8 9.1%
S_{16}	4.84	256	0.02	H→L+6 48.8%, H→L+9 10.5%, H→L+5 9.6%, H-1→L+1 5.7%
S_{17}	5.00	248	0.04	H-5→L 65.0%, H→L+5 14.0%, H→L+6 9.9%
S_{18}	5.10	243	0.01	H-3→L 46.5%, H-8→L 9.8%, H-3→L+1 9.5%, H-4→L 5.4%
S_{19}	5.13	242	0.08	H-8→L 34.4%, H-3→L 18.9%, H-4→L 13.5%, H-2→L 9.3%, H-2→L+1 6.8%
S_{20}	5.30	234	0.03	H-4→L 60.9%, H-2→L+1 12.9%, H-8→L 8.0%
S_{21}	5.36	231	0.01	H-1→L+3 38.5%, H-8→L 9.1%, H→L+9 6.5%, H-4→L 6.3%, H-2→L+1 5.5%, H-1→L+7 5.2%
S_{22}	5.38	231	0.00	H-3→L 12.0%, H→L+9 11.3%, H-1→L+3 10.2%, H-1→L+6 9.8%, H-2→L+1 8.3%, H→L+6 5.9%, H-8→L 5.6%
S_{23}	5.40	230	0.05	H-2→L+2 37.4%, H-1→L+2 21.9%, H-8→L+2 15.2%, H-2→L+1 5.3%
S_{24}	5.47	227	0.07	H-6→L 16.8%, H-2→L+1 15.3%, H-3→L 13.7%, H-1→L+3 10.5%, H-3→L+1 8.6%, H-7→L 5.8%, H-7→L 5.5%
S_{25}	5.49	226	0.02	H→L+9 26.2%, H-2→L+1 23.5%, H-6→L 6.4%, H→L+12 6.1%, H-1→L+6 5.3%

Table S14. Electronic excitation properties of various conformations of TE-Pyc in toluene using MN15.

TE-Pyc (conf1)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.75	451	1.78	H→L 68.7%, H-1→L 13.7%, H→L+1 11.6%
S_2	3.36	369	0.69	H→L+1 73.9%, H→L 12.4%
S_3	3.40	364	0.50	H-1→L 57.3%, H→L 18.3%, H-2→L 11.7%, H-4→L 6.5%
S_4	3.71	334	0.51	H→L+3 76.7%, H-1→L+3 5.2%
S_5	3.92	316	0.01	H→L+2 55.3%, H-1→L+2 28.4%, H-2→L+2 7.9%
S_6	3.96	313	0.03	H→L+4 85.7%
S_7	4.07	305	0.16	H-2→L 37.1%, H-4→L 27.5%, H-1→L 24.0%
S_8	4.13	300	0.00	H-11→L 91.6%
S_9	4.24	292	0.03	H-1→L+1 70.1%, H→L+5 8.6%, H-2→L+1 5.1%
S_{10}	4.40	282	0.00	H-11→L+2 93.7%
S_{11}	4.48	277	0.13	H→L+9 12.4%, H→L+7 9.6%, H→L+6 8.6%, H→L+5 7.7%, H-2→L 6.8%, H-4→L 5.6%
S_{12}	4.48	277	0.00	H-2→L 26.2%, H-4→L 19.7%, H-3→L 9.0%, H→L+5 7.2%, H-7→L 5.2%
S_{13}	4.50	276	0.00	H→L+7 25.8%, H→L+9 13.9%, H-7→L 6.4%, H→L+6 6.4%
S_{14}	4.50	275	0.02	H-3→L 78.9%, H-4→L 6.2%
S_{15}	4.57	272	0.13	H-1→L+3 23.7%, H-2→L+3 14.0%, H-2→L 9.4%, H-2→L+1 7.2%, H-4→L 6.6%, H→L+5 5.6%
S_{16}	4.58	271	0.06	H→L+2 37.9%, H-1→L+2 28.7%, H-2→L+2 10.5%, H-4→L+2 8.9%
S_{17}	4.62	269	0.01	H→L+8 31.3%, H→L+5 19.1%, H→L+6 17.4%
S_{18}	4.65	267	0.01	H→L+8 31.5%, H→L+6 9.5%, H-1→L+3 8.0%, H→L+5 7.7%
S_{19}	4.67	265	0.00	H-13→L 76.9%, H-13→L+11 6.0%, H-13→L+10 5.0%
S_{20}	4.70	264	0.14	H-3→L+3 66.3%, H-3→L+1 17.8%
S_{21}	4.99	249	0.06	H-7→L 66.6%, H→L+6 13.4%, H→L+5 6.3%
S_{22}	5.02	247	0.02	H-2→L+1 53.5%, H-1→L+3 13.6%
S_{23}	5.10	243	0.03	H-6→L 44.4%, H-6→L+1 11.6%, H-5→L 6.7%
S_{24}	5.13	242	0.01	H→L+9 21.6%, H→L+7 15.0%, H→L+10 13.0%, H-1→L+3 6.7%, H-9→L 5.0%
S_{25}	5.16	240	0.01	H-9→L 16.4%, H-5→L 12.5%, H→L+7 11.9%, H-4→L 7.2%, H-4→L+1 6.4%, H-1→L+4 6.3%

TE-Pyc (conf4)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.73	455	1.63	H→L 69.5%, H-1→L 14.4%, H→L+1 9.0%
S_2	3.34	372	0.83	H→L+1 71.1%, H→L 10.5%, H→L+2 5.3%
S_3	3.38	367	0.34	H-1→L 56.4%, H→L 19.2%, H-2→L 11.3%, H-4→L 6.7%
S_4	3.70	335	0.54	H→L+3 74.5%, H-1→L+3 5.4%, H-1→L+1 5.2%
S_5	3.94	315	0.07	H→L+2 38.4%, H→L+4 20.6%, H-1→L+2 15.9%, H-1→L+1 6.2%
S_6	3.96	313	0.04	H→L+4 66.2%, H→L+2 11.4%, H-1→L+2 5.3%
S_7	4.06	306	0.21	H-2→L 32.7%, H-4→L 29.7%, H-1→L 24.2%
S_8	4.07	305	0.00	H-11→L 83.8%, H-11→L+2 7.4%
S_9	4.23	293	0.06	H-1→L+1 59.0%, H→L+5 8.7%, H-1→L+2 7.1%
S_{10}	4.46	278	0.00	H-11→L+2 62.4%, H-11→L+1 11.7%, H-11→L 7.8%
S_{11}	4.46	278	0.02	H-2→L 28.1%, H-4→L 20.4%, H-11→L+2 8.7%, H→L+8 6.0%
S_{12}	4.47	277	0.03	H→L+8 24.1%, H→L+5 8.2%, H-1→L+1 6.9%, H-2→L 6.7%, H→L+6 5.0%
S_{13}	4.49	276	0.02	H-7→L 14.1%, H→L+8 13.7%, H→L+6 11.8%, H-1→L+6 9.5%, H→L+5 9.0%, H-1→L+5 6.4%
S_{14}	4.51	275	0.01	H-3→L 80.5%
S_{15}	4.55	273	0.13	H-1→L+3 15.9%, H-2→L+3 13.0%, H→L+5 7.9%, H→L+7 6.6%, H-2→L+1 6.4%, H-4→L 6.2%, H-1→L+2 6.2%, H→L+2 5.4%, H-2→L 5.1%
S_{16}	4.60	270	0.05	H→L+2 16.8%, H-1→L+2 15.7%, H-1→L+3 11.6%, H-2→L+2 10.9%, H→L+6 5.5%, H→L+9 5.1%
S_{17}	4.64	267	0.04	H→L+7 20.5%, H→L+8 13.4%, H→L+9 9.7%, H-1→L+3 7.5%, H→L+5 5.5%
S_{18}	4.66	266	0.03	H→L+9 19.3%, H→L+5 19.2%, H→L+2 11.2%, H→L+6 11.0%, H-1→L+2 9.2%
S_{19}	4.67	266	0.00	H-13→L 77.0%, H-13→L+11 6.0%
S_{20}	4.70	264	0.14	H-3→L+3 61.6%, H-3→L+1 14.7%
S_{21}	4.95	251	0.08	H-7→L 66.6%, H→L+6 14.6%
S_{22}	5.02	247	0.00	H-2→L+1 47.1%, H-1→L+3 11.5%, H-3→L+1 6.3%
S_{23}	5.07	244	0.02	H-6→L 35.4%, H-5→L 10.6%, H-6→L+1 6.0%, H-9→L 5.3%
S_{24}	5.12	242	0.00	H→L+7 15.7%, H→L+9 12.0%, H→L+10 10.3%, H-9→L 8.6%, H-1→L+3 8.3%
S_{25}	5.17	240	0.02	H-1→L+4 22.4%, H-5→L 18.2%, H→L+9 9.5%, H→L+8 8.1%, H-9→L 7.7%, H-2→L+1 6.3%

TE-Pyc (conf5)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.74	452	1.70	H→L 68.9%, H-1→L 13.7%, H→L+1 11.3%
S_2	3.34	371	0.79	H→L+1 71.7%, H→L 13.7%
S_3	3.39	365	0.47	H-1→L 57.8%, H→L 16.7%, H-2→L 11.1%, H-4→L 6.3%
S_4	3.69	336	0.46	H→L+3 76.4%
S_5	3.92	317	0.01	H→L+2 54.4%, H-1→L+2 27.4%, H-2→L+2 6.7%
S_6	3.96	313	0.05	H→L+4 87.1%
S_7	4.07	305	0.17	H-2→L 34.4%, H-4→L 27.3%, H-1→L 23.7%, H-3→L 5.5%
S_8	4.14	300	0.00	H-11→L 91.5%
S_9	4.22	294	0.04	H-1→L+1 64.7%, H→L+5 10.7%
S_{10}	4.40	282	0.00	H-11→L+2 91.2%
S_{11}	4.44	279	0.04	H→L+7 39.1%, H→L+9 7.4%, H-1→L+3 6.2%, H→L+5 6.0%, H-1→L+4 5.5%
S_{12}	4.48	277	0.02	H-2→L 27.5%, H-3→L 14.4%, H-4→L 12.7%, H-1→L+1 6.8%, H→L+5 6.6%
S_{13}	4.49	276	0.00	H→L+5 16.2%, H-3→L 13.8%, H-7→L 10.6%, H-2→L 9.5%, H-1→L+5 8.6%, H→L+6 8.3%, H-1→L+6 6.8%
S_{14}	4.52	275	0.03	H-3→L 58.5%, H-4→L 16.0%
S_{15}	4.56	272	0.01	H→L+2 27.3%, H-1→L+2 22.5%, H-1→L+3 7.4%, H-2→L+3 6.4%, H-4→L+2 6.4%, H-2→L+2 5.4%
S_{16}	4.58	271	0.20	H-1→L+3 22.3%, H-2→L+3 13.2%, H→L+2 10.1%, H-2→L 6.8%, H-1→L+2 6.7%, H-4→L 6.0%, H-2→L+1 5.5%
S_{17}	4.63	268	0.02	H→L+8 33.7%, H→L+9 16.0%, H→L+6 10.9%, H→L+5 8.7%
S_{18}	4.64	267	0.03	H→L+8 32.4%, H→L+6 16.5%, H→L+5 13.7%
S_{19}	4.67	265	0.00	H-13→L 77.0%, H-13→L+11 5.7%, H-13→L+10 5.3%
S_{20}	4.70	264	0.13	H-3→L+3 63.9%, H-3→L+1 16.4%
S_{21}	4.98	249	0.03	H-7→L 61.8%, H→L+6 12.1%, H→L+5 7.1%
S_{22}	5.02	247	0.05	H-2→L+1 48.6%, H-1→L+3 14.8%, H-3→L+1 8.4%, H-7→L 5.8%
S_{23}	5.08	244	0.01	H-6→L 37.4%, H-6→L+1 9.4%, H→L+7 9.1%, H-5→L 7.2%
S_{24}	5.12	242	0.01	H→L+7 17.1%, H→L+9 12.1%, H→L+10 9.7%, H-9→L 7.8%, H-1→L+3 6.4%, H→L+6 5.4%
S_{25}	5.18	239	0.03	H→L+9 23.8%, H-1→L+4 16.2%, H-5→L 15.8%, H-9→L 8.6%

TE-Pyc (conf6)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.75	451	1.74	H→L 68.7%, H-1→L 13.8%, H→L+1 11.3%
S_2	3.35	370	0.81	H→L+1 72.7%, H→L 13.1%
S_3	3.40	364	0.46	H-1→L 57.5%, H→L 17.4%, H-2→L 11.1%, H-4→L 6.5%
S_4	3.71	334	0.43	H→L+3 76.8%, H-1→L+3 5.3%
S_5	3.92	316	0.01	H→L+2 54.2%, H-1→L+2 27.4%, H-2→L+2 6.7%
S_6	3.96	313	0.04	H→L+4 86.5%
S_7	4.08	304	0.17	H-2→L 34.4%, H-4→L 27.9%, H-1→L 23.9%
S_8	4.13	300	0.00	H-11→L 91.5%
S_9	4.23	293	0.04	H-1→L+1 65.1%, H→L+5 10.9%
S_{10}	4.40	282	0.00	H-11→L+2 91.2%
S_{11}	4.47	277	0.05	H→L+8 36.4%, H-2→L 7.7%, H-4→L 6.7%, H-1→L+4 6.4%, H→L+5 6.3%
S_{12}	4.48	277	0.04	H-2→L 25.5%, H-4→L 13.8%, H-3→L 9.6%, H-1→L+1 5.7%, H-1→L+3 5.5%, H→L+8 5.3%, H-2→L+3 5.2%
S_{13}	4.50	276	0.00	H→L+5 12.2%, H→L+8 11.4%, H-7→L 11.2%, H→L+6 10.5%, H-1→L+6 9.0%, H-3→L 7.2%, H-1→L+5 6.7%, H-2→L 5.5%
S_{14}	4.52	274	0.02	H-3→L 65.3%, H-4→L 8.9%
S_{15}	4.55	272	0.05	H→L+2 12.9%, H-1→L+3 12.8%, H-1→L+2 9.7%, H-2→L+3 9.6%, H→L+7 7.6%, H→L+5 6.4%, H-2→L 5.1%
S_{16}	4.58	270	0.12	H→L+2 25.0%, H-1→L+2 18.6%, H-1→L+3 8.3%, H-2→L+2 7.7%, H-4→L+2 5.1%
S_{17}	4.64	267	0.06	H→L+5 16.3%, H→L+7 14.3%, H→L+6 14.3%, H-1→L+3 9.1%, H→L+3 6.5%, H-2→L+3 5.7%, H-2→L+1 5.4%
S_{18}	4.65	267	0.01	H→L+9 30.0%, H→L+7 14.7%, H→L+5 10.3%, H→L+6 6.8%, H→L+8 5.9%
S_{19}	4.67	265	0.00	H-13→L 77.0%, H-13→L+11 5.8%, H-13→L+10 5.3%
S_{20}	4.70	264	0.14	H-3→L+3 62.3%, H-3→L+1 16.4%
S_{21}	4.98	249	0.03	H-7→L 64.0%, H→L+6 15.2%
S_{22}	5.03	247	0.04	H-2→L+1 48.9%, H-1→L+3 15.0%, H-3→L+1 7.5%
S_{23}	5.09	244	0.01	H-6→L 37.0%, H-6→L+1 9.8%, H→L+7 9.0%, H-5→L 7.6%
S_{24}	5.14	241	0.00	H→L+9 23.7%, H→L+7 12.7%, H→L+10 11.0%, H-9→L 6.7%
S_{25}	5.18	240	0.01	H-1→L+4 30.3%, H-5→L 11.9%, H→L+8 10.5%, H-9→L 8.8%

TE-Pyc (conf7)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.75	451	1.73	H→L 68.9%, H-1→L 13.7%, H→L+1 11.3%
S_2	3.35	370	0.80	H→L+1 72.5%, H→L 13.1%
S_3	3.40	364	0.46	H-1→L 57.4%, H→L 17.3%, H-2→L 12.1%, H-4→L 6.5%
S_4	3.70	335	0.43	H→L+3 76.8%, H-1→L+3 5.3%
S_5	3.92	316	0.01	H→L+2 54.4%, H-1→L+2 27.1%, H-2→L+2 7.3%
S_6	3.96	313	0.04	H→L+4 86.5%
S_7	4.07	304	0.17	H-2→L 37.1%, H-4→L 27.4%, H-1→L 24.1%
S_8	4.13	300	0.00	H-11→L 91.5%
S_9	4.23	293	0.04	H-1→L+1 65.2%, H→L+5 10.7%
S_{10}	4.40	282	0.00	H-11→L+2 91.1%
S_{11}	4.47	277	0.05	H→L+8 37.0%, H-4→L 7.0%, H→L+5 6.9%, H-1→L+4 6.5%, H-2→L 6.3%
S_{12}	4.48	277	0.04	H-2→L 17.1%, H-4→L 14.5%, H-1→L+3 8.7%, H-1→L+1 6.8%, H-2→L+3 6.5%, H→L+6 5.5%
S_{13}	4.50	276	0.00	H→L+8 14.9%, H→L+5 11.1%, H-2→L 9.4%, H-3→L 9.3%, H-7→L 8.7%, H→L+6 7.0%, H-1→L+6 6.8%, H-1→L+5 5.8%
S_{14}	4.51	275	0.02	H-3→L 77.7%, H-4→L 5.1%
S_{15}	4.55	272	0.07	H-1→L+3 16.3%, H-2→L+3 11.1%, H→L+2 10.1%, H-1→L+2 7.8%, H→L+7 7.5%, H-2→L 7.2%, H→L+5 6.1%, H-2→L+1 5.4%, H-4→L 5.3%
S_{16}	4.58	271	0.12	H→L+2 27.4%, H-1→L+2 20.4%, H-2→L+2 9.0%, H-1→L+3 7.7%, H-4→L+2 5.7%
S_{17}	4.64	267	0.05	H→L+7 16.5%, H→L+6 16.4%, H→L+5 16.1%, H-1→L+3 8.1%, H→L+8 5.3%
S_{18}	4.65	267	0.01	H→L+9 31.4%, H→L+7 14.5%, H→L+5 9.1%, H→L+6 7.4%, H→L+8 5.9%
S_{19}	4.67	265	0.00	H-13→L 77.0%, H-13→L+11 5.7%, H-13→L+10 5.4%
S_{20}	4.70	264	0.14	H-3→L+3 67.2%, H-3→L+1 16.3%
S_{21}	4.98	249	0.03	H-7→L 62.8%, H→L+6 13.8%, H→L+5 5.7%
S_{22}	5.02	247	0.04	H-2→L+1 52.5%, H-1→L+3 14.6%, H-7→L 5.2%
S_{23}	5.08	244	0.01	H-6→L 37.9%, H-6→L+1 9.8%, H→L+7 8.8%, H-5→L 6.6%
S_{24}	5.13	242	0.00	H→L+9 24.4%, H→L+7 13.7%, H→L+10 10.9%, H-9→L 5.7%
S_{25}	5.17	240	0.01	H-1→L+4 27.0%, H-5→L 13.8%, H→L+8 10.3%, H-9→L 10.2%

TE-Pyc (conf8)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.75	451	1.87	H→L 68.4%, H-1→L 14.0%, H→L+1 11.6%
S_2	3.35	370	0.68	H→L+1 73.3%, H→L 11.6%, H→L+3 5.3%
S_3	3.40	365	0.43	H-1→L 56.0%, H→L 19.3%, H-2→L 12.5%, H-4→L 6.4%
S_4	3.69	336	0.53	H→L+3 76.6%
S_5	3.92	316	0.01	H→L+2 54.8%, H-1→L+2 28.6%, H-2→L+2 8.2%
S_6	3.96	313	0.04	H→L+4 86.5%
S_7	4.07	304	0.17	H-2→L 36.9%, H-4→L 28.0%, H-1→L 24.2%
S_8	4.13	300	0.00	H-11→L 91.6%
S_9	4.24	292	0.03	H-1→L+1 68.6%, H→L+5 9.0%
S_{10}	4.40	282	0.00	H-11→L+2 93.8%
S_{11}	4.47	278	0.03	H→L+8 28.6%, H-4→L 10.8%, H-2→L 9.2%, H→L+7 5.8%, H→L+5 5.7%, H-1→L+4 5.5%
S_{12}	4.48	277	0.02	H-1→L+3 12.9%, H-4→L 11.4%, H-2→L 10.4%, H-2→L+3 8.7%, H→L+6 7.6%, H→L+8 6.7%, H-2→L+1 5.3%, H-1→L+1 5.0%
S_{13}	4.49	276	0.00	H→L+8 20.5%, H-7→L 11.7%, H→L+6 9.2%, H→L+5 8.9%, H-1→L+6 8.4%, H-1→L+5 5.9%, H-2→L 5.6%
S_{14}	4.52	274	0.02	H-3→L 89.1%
S_{15}	4.55	272	0.19	H-1→L+3 21.4%, H-2→L 14.5%, H-2→L+3 12.0%, H-4→L 11.4%, H→L+7 7.8%, H→L+5 5.6%, H-2→L+1 5.6%
S_{16}	4.58	271	0.03	H→L+2 40.9%, H-1→L+2 29.6%, H-2→L+2 11.9%, H-4→L+2 9.3%
S_{17}	4.62	268	0.06	H→L+5 19.1%, H→L+6 19.0%, H→L+7 16.9%, H-1→L+3 6.6%, H→L+3 6.5%
S_{18}	4.64	267	0.02	H→L+9 33.7%, H→L+7 13.5%, H→L+5 9.0%, H→L+6 7.2%, H→L+8 5.7%
S_{19}	4.67	265	0.00	H-13→L 76.9%, H-13→L+10 5.5%, H-13→L+11 5.5%
S_{20}	4.69	264	0.14	H-3→L+3 65.9%, H-3→L+1 17.3%, H-3→L 5.0%
S_{21}	4.99	249	0.08	H-7→L 65.5%, H→L+6 13.6%, H→L+5 5.8%
S_{22}	5.02	247	0.01	H-2→L+1 56.8%, H-1→L+3 14.7%
S_{23}	5.08	244	0.04	H-6→L 38.4%, H-6→L+1 9.9%, H-5→L 6.8%, H→L+7 5.7%
S_{24}	5.13	242	0.01	H→L+9 18.5%, H→L+7 15.6%, H→L+10 11.7%, H-9→L 7.5%, H-1→L+3 5.9%
S_{25}	5.17	240	0.00	H-1→L+4 30.6%, H-5→L 11.7%, H→L+8 11.7%, H-9→L 7.9%

TE-Pyc (conf9)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.75	451	1.78	H→L 68.7%, H-1→L 13.9%, H→L+1 11.3%
S_2	3.35	370	0.66	H→L+1 73.1%, H→L 12.6%
S_3	3.40	364	0.38	H-1→L 57.0%, H→L 18.0%, H-2→L 11.1%, H-4→L 6.4%
S_4	3.71	334	0.62	H→L+3 76.3%, H-1→L+3 5.0%
S_5	3.92	316	0.02	H→L+2 54.1%, H-1→L+2 27.4%, H-2→L+2 6.7%
S_6	3.96	313	0.04	H→L+4 85.6%
S_7	4.08	304	0.19	H-2→L 33.6%, H-4→L 28.1%, H-1→L 24.0%, H-3→L 5.4%
S_8	4.13	300	0.00	H-11→L 91.5%
S_9	4.23	293	0.04	H-1→L+1 66.1%, H→L+5 10.9%
S_{10}	4.40	282	0.00	H-11→L+2 91.2%
S_{11}	4.48	277	0.09	H→L+9 13.1%, H-2→L 11.1%, H→L+7 9.5%, H-4→L 7.6%, H→L+5 5.9%, H→L+6 5.6%
S_{12}	4.49	276	0.01	H-2→L 26.0%, H-4→L 14.7%, H→L+7 14.0%, H-3→L 8.8%, H→L+5 5.0%
S_{13}	4.50	276	0.01	H→L+7 18.0%, H→L+5 10.5%, H-7→L 9.2%, H→L+6 8.1%, H-1→L+6 7.6%, H→L+9 7.1%, H-1→L+5 5.3%
S_{14}	4.52	274	0.01	H-3→L 69.7%, H-4→L 8.0%
S_{15}	4.56	272	0.05	H→L+2 17.2%, H-1→L+2 12.8%, H-1→L+3 10.7%, H-2→L+3 7.8%, H→L+5 6.9%
S_{16}	4.59	270	0.11	H→L+2 17.2%, H-1→L+2 12.2%, H-1→L+3 11.4%, H→L+8 8.9%, H-4→L 6.2%, H-2→L+3 6.2%, H-2→L+2 5.8%, H-2→L 5.5%
S_{17}	4.62	269	0.02	H→L+8 28.5%, H→L+5 18.3%, H→L+6 11.2%, H→L+2 6.5%, H-1→L+2 5.7%
S_{18}	4.65	267	0.03	H→L+8 26.5%, H-1→L+3 8.9%, H→L+6 8.4%, H→L+5 8.0%, H→L+7 6.1%, H-2→L+3 6.1%, H-2→L+1 5.0%
S_{19}	4.67	265	0.00	H-13→L 77.0%, H-13→L+11 5.6%, H-13→L+10 5.5%
S_{20}	4.71	264	0.14	H-3→L+3 59.4%, H-3→L+1 17.1%
S_{21}	4.98	249	0.03	H-7→L 62.9%, H→L+6 14.8%
S_{22}	5.02	247	0.01	H-2→L+1 45.3%, H-1→L+3 15.0%, H-3→L+1 7.8%, H-7→L 6.0%
S_{23}	5.10	243	0.05	H-6→L 44.2%, H-6→L+1 11.6%, H-5→L 8.5%
S_{24}	5.13	242	0.01	H→L+9 24.1%, H→L+7 17.3%, H→L+10 12.5%
S_{25}	5.17	240	0.02	H-9→L 18.0%, H-5→L 13.6%, H→L+7 9.6%, H-1→L+4 9.4%, H-4→L 8.5%, H-10→L 6.2%, H-4→L+1 5.9%

TE-Pyc (conf10)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.72	455	1.48	H→L 70.1%, H-1→L 14.2%, H→L+1 8.5%
S_2	3.32	374	0.82	H→L+1 69.2%, H→L 12.2%, H→L+2 6.7%
S_3	3.37	368	0.28	H-1→L 57.6%, H→L 17.0%, H-2→L 12.0%, H-4→L 6.5%
S_4	3.68	337	0.61	H→L+3 73.2%, H-1→L+3 5.3%, H-1→L+1 5.2%
S_5	3.93	316	0.03	H→L+2 41.8%, H-1→L+2 15.1%, H-1→L+1 11.2%, H→L+4 10.0%
S_6	3.98	312	0.10	H→L+4 75.6%
S_7	4.04	307	0.25	H-2→L 36.0%, H-4→L 28.2%, H-1→L 24.6%
S_8	4.07	305	0.00	H-11→L 83.6%, H-11→L+2 7.1%
S_9	4.23	293	0.11	H-1→L+1 56.8%, H-1→L+2 11.2%, H→L+5 6.6%, H→L+2 6.6%
S_{10}	4.45	279	0.01	H-2→L 16.6%, H-4→L 14.7%, H→L+8 12.6%, H-1→L+3 8.2%, H→L+7 7.9%, H→L+9 5.2%, H-2→L+3 5.1%
S_{11}	4.46	278	0.00	H-11→L+2 67.0%, H-11→L+1 16.7%, H-11→L 9.1%
S_{12}	4.47	277	0.07	H-2→L 14.0%, H→L+6 11.1%, H→L+5 10.8%, H-4→L 7.7%, H→L+8 7.2%, H-7→L 7.1%, H-1→L+6 7.0%
S_{13}	4.48	277	0.02	H-3→L 20.5%, H→L+5 14.8%, H-2→L 10.4%, H→L+8 6.1%, H-7→L 5.5%, H-1→L+1 5.0%
S_{14}	4.50	276	0.03	H-3→L 68.8%, H-4→L 10.1%
S_{15}	4.54	273	0.07	H→L+8 19.1%, H-1→L+2 11.7%, H→L+2 8.9%, H-2→L+3 7.3%, H-1→L+3 6.6%, H→L+6 6.1%
S_{16}	4.59	270	0.12	H-1→L+3 24.1%, H-2→L+3 10.6%, H→L+7 7.4%, H-2→L+2 6.6%, H→L+6 5.7%, H→L+9 5.6%, H-2→L+1 5.0%
S_{17}	4.63	268	0.03	H→L+7 20.2%, H→L+9 16.0%, H→L+2 11.9%, H-1→L+2 11.3%
S_{18}	4.67	266	0.03	H→L+9 23.7%, H→L+5 20.0%, H→L+6 9.4%, H-1→L+2 6.7%, H→L+2 6.5%, H→L+3 6.1%
S_{19}	4.67	266	0.00	H-13→L 77.2%, H-13→L+10 5.9%
S_{20}	4.70	264	0.14	H-3→L+3 66.1%, H-3→L+1 13.7%, H-3→L+2 6.4%
S_{21}	4.94	251	0.05	H-7→L 64.0%, H→L+6 14.5%
S_{22}	4.99	248	0.00	H-2→L+1 47.0%, H-1→L+3 12.2%, H-7→L 5.5%
S_{23}	5.09	244	0.02	H-6→L 42.8%, H-5→L 12.8%, H-6→L+1 7.2%
S_{24}	5.11	243	0.00	H→L+7 17.6%, H→L+9 11.6%, H-9→L 7.7%, H→L+10 7.6%, H-1→L+3 6.8%, H-1→L+4 6.2%
S_{25}	5.15	241	0.02	H-5→L 16.5%, H-9→L 14.8%, H-4→L 7.4%, H→L+8 6.8%, H→L+7 6.7%, H→L+9 6.1%, H-2→L+1 5.7%

Table S15. Electronic excitation properties of various conformations of ETE-Pyc in toluene using MN15.

ETE-Pyc (conf1)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.70	459	1.71	H→L 68.9%, H-1→L 14.4%, H→L+1 11.8%
S_2	3.29	377	1.04	H→L+1 47.6%, H→L 27.9%, H-1→L 12.6%
S_3	3.33	372	0.09	H-1→L 51.1%, H→L+1 27.8%, H-5→L 9.7%
S_4	3.41	363	1.07	H→L+3 87.6%, H-1→L+3 5.2%
S_5	3.89	319	0.05	H→L+5 82.9%
S_6	3.91	317	0.01	H→L+2 53.7%, H-1→L+2 31.9%, H-5→L+2 7.4%
S_7	4.00	310	0.01	H-2→L 96.9%
S_8	4.07	305	0.01	H→L+4 41.5%, H-1→L+1 29.8%, H-2→L+3 7.0%, H-5→L 6.5%
S_9	4.09	303	0.19	H-5→L 39.1%, H-6→L 22.2%, H-1→L 18.8%, H→L+4 6.5%
S_{10}	4.13	300	0.00	H-12→L 91.4%
S_{11}	4.27	291	0.14	H-1→L+1 53.3%, H→L+4 23.8%, H→L+1 5.1%
S_{12}	4.40	282	0.00	H-12→L+2 93.6%
S_{13}	4.42	280	0.14	H→L+9 39.1%, H-1→L+3 9.7%, H-2→L+1 8.0%, H-2→L+4 5.7%, H-1→L+5 5.1%
S_{14}	4.47	278	0.07	H→L+8 55.4%, H-2→L+5 8.7%, H-3→L 6.0%
S_{15}	4.47	277	0.01	H-4→L 16.8%, H-3→L 15.4%, H→L+6 15.2%, H-1→L+6 12.5%, H-2→L+3 7.5%, H-9→L 6.5%
S_{16}	4.48	277	0.00	H-4→L 24.0%, H-3→L 17.0%, H-1→L+2 11.6%, H→L+2 11.5%, H→L+6 5.9%, H→L+8 5.3%
S_{17}	4.48	277	0.01	H→L+2 30.6%, H-1→L+2 22.6%, H-4→L 11.1%, H-5→L+2 7.3%
S_{18}	4.50	276	0.00	H-3→L 49.4%, H-4→L 42.0%
S_{19}	4.51	275	0.10	H-2→L+1 16.1%, H→L+9 15.4%, H-1→L+3 12.1%, H-2→L+4 8.8%, H-2→L+3 7.2%
S_{20}	4.52	274	0.07	H-2→L+3 36.7%, H→L+4 10.9%, H→L+9 6.0%
S_{21}	4.67	265	0.00	H-15→L 76.9%, H-15→L+10 5.9%, H-15→L+12 5.5%
S_{22}	4.69	265	0.18	H-3→L+3 52.2%, H-4→L+4 23.3%, H-4→L+1 10.1%
S_{23}	4.69	264	0.13	H-4→L+3 44.8%, H-3→L+4 17.6%, H-6→L 8.2%, H-3→L+1 7.5%, H-5→L 5.8%
S_{24}	4.70	264	0.02	H-6→L 30.7%, H-5→L 28.0%, H-11→L 11.2%, H-4→L+3 10.6%
S_{25}	4.80	258	0.01	H-2→L+1 53.8%, H-1→L+3 36.0%

ETE-Pyc (conf2)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.69	462	1.34	H→L 70.2%, H-1→L 15.0%, H→L+1 9.0%
S_2	3.25	382	1.04	H→L+1 50.4%, H→L 24.5%, H-1→L 9.2%
S_3	3.30	376	0.16	H-1→L 54.9%, H→L+1 21.2%, H-5→L 9.7%
S_4	3.40	365	1.06	H→L+3 87.3%
S_5	3.86	321	0.03	H→L+5 46.0%, H→L+4 26.5%, H→L+2 7.8%, H-1→L+1 5.7%
S_6	3.89	319	0.01	H→L+2 35.6%, H→L+5 21.7%, H-1→L+1 15.8%, H-1→L+2 13.1%
S_7	3.98	311	0.00	H-2→L 97.8%
S_8	4.06	306	0.26	H-5→L 44.0%, H-6→L 26.3%, H-1→L 18.2%
S_9	4.07	305	0.00	H-12→L 83.4%, H-12→L+2 7.3%
S_{10}	4.11	302	0.09	H→L+4 24.9%, H-1→L+1 21.3%, H-1→L+2 15.5%, H→L+5 11.5%, H→L+2 10.5%, H-2→L+3 5.7%
S_{11}	4.22	294	0.17	H-1→L+1 40.5%, H→L+4 23.8%, H→L+1 9.0%, H→L+5 6.7%, H-2→L+3 5.0%
S_{12}	4.42	280	0.14	H→L+9 38.5%, H-1→L+3 8.4%, H-2→L+1 8.0%, H-2→L+4 5.2%
S_{13}	4.44	279	0.03	H→L+8 50.6%, H-2→L+3 8.2%, H-2→L+5 6.4%
S_{14}	4.46	278	0.01	H-3→L 92.2%
S_{15}	4.46	278	0.00	H-12→L+2 67.5%, H-12→L+1 14.3%, H-12→L 8.8%
S_{16}	4.48	277	0.04	H→L+6 18.5%, H-1→L+6 17.5%, H-9→L 10.6%, H→L+8 10.2%
S_{17}	4.49	276	0.01	H-4→L 76.8%
S_{18}	4.50	276	0.07	H→L+9 19.2%, H-4→L 18.1%, H-2→L+1 13.5%, H-1→L+3 11.5%, H-2→L+4 7.0%
S_{19}	4.51	275	0.03	H-1→L+2 34.5%, H→L+2 29.6%, H-5→L+2 6.9%, H→L+4 6.1%
S_{20}	4.52	274	0.12	H-2→L+3 41.2%, H→L+4 8.2%, H→L+6 7.6%, H-1→L+6 7.1%, H-9→L 5.6%
S_{21}	4.67	266	0.00	H-15→L 77.1%, H-15→L+10 6.4%
S_{22}	4.68	265	0.06	H-6→L 32.8%, H-5→L 28.7%, H-11→L 12.7%, H-4→L+3 5.6%
S_{23}	4.69	264	0.14	H-3→L+3 47.9%, H-3→L+4 22.7%, H-3→L+1 8.1%
S_{24}	4.69	264	0.13	H-4→L+3 50.3%, H-4→L+4 18.2%, H-4→L+1 8.4%
S_{25}	4.78	259	0.01	H-2→L+1 50.0%, H-1→L+3 37.5%

ETE-Pyc (conf3)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.71	458	1.76	H→L 68.4%, H-1→L 14.7%, H→L+1 12.0%
S_2	3.29	377	1.05	H→L+1 51.0%, H→L 27.4%, H-1→L 10.0%
S_3	3.33	372	0.12	H-1→L 53.7%, H→L+1 24.4%, H-5→L 9.8%
S_4	3.39	366	1.00	H→L+3 87.5%
S_5	3.88	320	0.03	H→L+5 84.3%
S_6	3.91	317	0.01	H→L+2 53.8%, H-1→L+2 33.0%, H-5→L+2 7.3%
S_7	4.01	309	0.01	H-2→L 96.8%
S_8	4.05	306	0.01	H→L+4 48.2%, H-1→L+1 29.5%, H-2→L+3 7.8%
S_9	4.09	303	0.19	H-5→L 42.5%, H-6→L 24.7%, H-1→L 18.1%
S_{10}	4.13	300	0.00	H-12→L 91.5%
S_{11}	4.25	292	0.16	H-1→L+1 54.0%, H→L+4 20.9%
S_{12}	4.40	280	0.09	H→L+8 38.3%, H-2→L+3 8.3%, H→L+9 7.0%, H-2→L+1 5.4%
S_{13}	4.43	280	0.03	H→L+8 50.6%, H-2→L+3 8.2%, H-2→L+5 6.4%
S_{14}	4.45	278	0.13	H→L+9 25.0%, H→L+8 10.0%, H-2→L+1 8.3%, H-1→L+3 8.2%, H→L+7 7.5%, H-2→L+4 5.7%
S_{15}	4.48	277	0.05	H→L+6 10.8%, H→L+9 10.3%, H-2→L+1 9.6%, H-1→L+3 8.5%, H-1→L+6 8.3%, H-2→L+4 5.8%
S_{16}	4.48	277	0.01	H→L+2 36.6%, H-1→L+2 27.6%, H-5→L+2 9.1%, H-2→L+3 5.6%
S_{17}	4.49	276	0.03	H→L+9 14.5%, H→L+8 9.3%, H-1→L+6 7.6%, H→L+6 6.7%, H-2→L+1 6.5%, H-1→L+3 6.5%, H-2→L+3 5.9%
S_{18}	4.50	276	0.01	H-3→L 28.6%, H-4→L 27.9%, H-2→L+3 8.8%, H→L+6 6.7%, H-1→L+6 6.4%
S_{19}	4.51	275	0.05	H-4→L 34.7%, H-2→L+3 25.7%, H→L+6 5.5%
S_{20}	4.52	274	0.03	H-3→L 56.7%, H-4→L 31.1%
S_{21}	4.67	265	0.00	H-15→L 76.9%, H-15→L+11 5.9%
S_{22}	4.69	265	0.06	H-3→L+3 35.8%, H-4→L+4 22.2%, H-4→L+3 15.3%, H-4→L+1 11.3%
S_{23}	4.69	264	0.15	H-4→L+3 37.8%, H-3→L+4 20.8%, H-3→L+3 15.1%, H-3→L+1 9.5%
S_{24}	4.72	263	0.11	H-6→L 37.2%, H-5→L 33.3%, H-11→L 13.7%
S_{25}	4.80	259	0.01	H-2→L+1 51.0%, H-1→L+3 39.9%

ETE-Pyc (conf6)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.71	458	1.69	H→L 68.6%, H-1→L 14.7%, H→L+1 11.6%
S_2	3.28	378	1.00	H→L+1 55.4%, H→L 25.7%, H-1→L 6.9%
S_3	3.33	372	0.18	H-1→L 56.9%, H→L+1 19.1%, H-5→L 10.5%, H→L 5.3%
S_4	3.40	365	0.98	H→L+3 87.3%
S_5	3.89	319	0.03	H→L+5 79.0%, H→L+4 5.7%
S_6	3.90	318	0.01	H→L+2 50.4%, H-1→L+2 28.7%, H-5→L+2 6.5%
S_7	4.01	310	0.01	H-2→L 96.9%
S_8	4.05	306	0.03	H→L+4 46.1%, H-1→L+1 27.9%, H-2→L+3 7.3%
S_9	4.09	303	0.21	H-5→L 44.5%, H-6→L 25.0%, H-1→L 18.0%
S_{10}	4.13	300	0.00	H-12→L 91.5%
S_{11}	4.24	292	0.16	H-1→L+1 51.5%, H→L+4 22.2%, H→L+1 5.0%
S_{12}	4.40	282	0.00	H-12→L+2 91.7%
S_{13}	4.43	280	0.09	H→L+8 35.2%, H-2→L+3 9.5%, H→L+9 8.8%
S_{14}	4.45	279	0.18	H-1→L+3 14.7%, H-2→L+1 14.7%, H-2→L+3 12.2%, H-2→L+4 9.2%, H→L+9 8.3%, H-5→L+3 6.5%
S_{15}	4.48	277	0.01	H→L+9 33.8%, H→L+8 6.1%, H→L+7 5.2%, H-2→L+3 5.0%
S_{16}	4.48	276	0.02	H→L+2 24.6%, H-1→L+2 22.0%, H→L+8 13.7%, H-5→L+2 8.5%
S_{17}	4.49	276	0.03	H→L+2 13.3%, H-1→L+2 9.6%, H→L+9 8.4%, H-1→L+6 7.6%, H-2→L+3 6.4%, H→L+6 6.1%, H→L+8 5.6%, H-9→L 5.5%
S_{18}	4.51	275	0.01	H-4→L 36.6%, H-3→L 23.2%, H→L+6 7.8%, H-2→L+3 7.1%, H-1→L+6 6.6%
S_{19}	4.51	275	0.01	H-4→L 54.5%, H-3→L 30.7%
S_{20}	4.52	275	0.05	H-3→L 39.2%, H-2→L+3 20.0%, H→L+6 7.6%, H-1→L+6 6.3%
S_{21}	4.67	265	0.00	H-15→L 77.0%, H-15→L+10 5.2%
S_{22}	4.68	265	0.13	H-4→L+3 49.0%, H-4→L+4 21.1%, H-4→L+1 10.3%, H-3→L+3 6.4%
S_{23}	4.69	264	0.11	H-3→L+3 45.2%, H-3→L+4 24.8%, H-3→L+1 9.6%, H-4→L+3 6.5%
S_{24}	4.71	263	0.07	H-6→L 39.5%, H-5→L 33.5%, H-11→L 14.6%
S_{25}	4.79	259	0.01	H-2→L+1 52.0%, H-1→L+3 38.4%

ETE-Pyc (conf7)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.71	458	1.75	H→L 68.4%, H-1→L 14.7%, H→L+1 11.9%
S_2	3.29	377	1.06	H→L+1 48.5%, H→L 28.1%, H-1→L 11.6%
S_3	3.33	372	0.09	H-1→L 52.0%, H→L+1 26.8%, H-5→L 9.7%
S_4	3.40	364	1.03	H→L+3 87.4%
S_5	3.87	321	0.03	H→L+5 64.6%, H→L+4 23.2%
S_6	3.91	317	0.01	H→L+2 53.9%, H-1→L+2 33.0%, H-5→L+2 7.5%
S_7	4.01	309	0.01	H-2→L 97.2%
S_8	4.07	304	0.02	H-1→L+1 29.7%, H→L+4 24.7%, H→L+5 13.4%, H-5→L 11.1%, H-6→L 7.5%, H-2→L+3 5.5%
S_9	4.09	303	0.18	H-5→L 34.7%, H-6→L 19.3%, H-1→L 18.2%, H→L+4 8.1%, H-1→L+1 5.1%
S_{10}	4.13	300	0.00	H-12→L 91.4%
S_{11}	4.26	291	0.15	H-1→L+1 49.3%, H→L+4 22.2%, H→L+5 5.2%, H→L+1 5.1%
S_{12}	4.40	282	0.00	H-12→L+2 93.7%
S_{13}	4.43	280	0.16	H→L+9 41.7%, H-2→L+1 8.5%, H-1→L+3 8.4%, H-2→L+4 5.4%
S_{14}	4.44	279	0.03	H→L+8 51.8%, H-2→L+3 8.5%, H-2→L+5 6.0%
S_{15}	4.48	277	0.05	H→L+6 17.3%, H-1→L+6 14.7%, H→L+8 8.9%, H-9→L 7.6%, H-1→L+2 6.3%, H-2→L+3 5.3%
S_{16}	4.48	277	0.01	H→L+2 38.1%, H-1→L+2 28.4%, H-5→L+2 9.4%
S_{17}	4.50	276	0.08	H→L+9 22.5%, H-2→L+1 14.9%, H-1→L+3 11.9%, H-2→L+4 7.8%
S_{18}	4.50	276	0.01	H-4→L 88.3%
S_{19}	4.51	275	0.01	H-3→L 42.3%, H-2→L+3 18.2%, H-4→L 6.7%
S_{20}	4.51	275	0.06	H-3→L 45.9%, H-2→L+3 24.6%
S_{21}	4.67	265	0.00	H-15→L 76.9%, H-15→L+10 5.3%
S_{22}	4.69	265	0.10	H-3→L+3 49.5%, H-3→L+4 22.7%, H-3→L+1 10.7%
S_{23}	4.69	264	0.13	H-4→L+3 51.9%, H-4→L+4 24.0%, H-4→L+1 10.6%
S_{24}	4.71	263	0.10	H-6→L 37.3%, H-5→L 33.1%, H-11→L 13.6%
S_{25}	4.80	258	0.01	H-2→L+1 52.0%, H-1→L+3 38.4%

ETE-Pyc (conf8)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.69	462	1.40	H→L 70.1%, H-1→L 15.0%, H→L+1 9.0%
S_2	3.25	382	1.03	H→L+1 52.7%, H→L 23.7%, H-1→L 7.6%
S_3	3.30	376	0.22	H-1→L 56.2%, H→L+1 19.0%, H-5→L 10.0%, H→L 5.7%
S_4	3.40	365	1.00	H→L+3 87.2%
S_5	3.87	320	0.01	H→L+2 30.0%, H→L+5 21.8%, H-1→L+1 16.0%, H-1→L+2 9.3%, H→L+4 8.8%
S_6	3.90	318	0.03	H→L+5 65.6%, H→L+2 12.0%, H-1→L+1 5.8%
S_7	3.98	311	0.00	H-2→L 95.8%
S_8	4.06	306	0.23	H-5→L 41.4%, H-6→L 24.7%, H-1→L 18.0%
S_9	4.07	305	0.00	H-12→L 83.5%, H-12→L+2 7.3%
S_{10}	4.08	304	0.09	H→L+4 41.0%, H-1→L+2 15.2%, H-1→L+1 12.4%, H→L+2 10.6%, H-2→L+3 6.4%
S_{11}	4.22	294	0.19	H-1→L+1 48.9%, H→L+4 21.7%, H→L+1 8.7%
S_{12}	4.43	280	0.16	H→L+8 22.9%, H→L+9 13.8%, H-2→L+1 12.3%, H-1→L+3 11.7%, H-2→L+4 9.3%, H-5→L+3 5.8%
S_{13}	4.45	279	0.12	H→L+8 21.7%, H-2→L+3 20.3%, H-1→L+3 5.2%
S_{14}	4.46	278	0.00	H-12→L+2 69.5%, H-12→L+1 14.5%, H-12→L 9.0%
S_{15}	4.47	277	0.01	H→L+9 25.4%, H→L+8 13.5%, H-2→L+3 10.3%, H→L+6 9.4%, H-1→L+6 6.0%
S_{16}	4.48	277	0.00	H-4→L 88.8%, H-3→L 6.1%
S_{17}	4.48	277	0.00	H-3→L 85.6%, H-4→L 7.0%
S_{18}	4.49	276	0.03	H-1→L+6 11.5%, H→L+6 10.8%, H→L+9 9.8%, H-9→L 6.9%, H-2→L+1 5.7%, H-1→L+2 5.6%, H-1→L+3 5.1%
S_{19}	4.52	274	0.05	H-1→L+2 31.6%, H→L+2 28.3%, H-5→L+2 7.1%
S_{20}	4.52	274	0.06	H-2→L+3 31.9%, H→L+4 9.6%, H→L+8 6.9%, H-2→L+1 6.2%
S_{21}	4.67	266	0.00	H-15→L 77.0%
S_{22}	4.68	265	0.12	H-4→L+3 32.6%, H-6→L 16.7%, H-5→L 14.4%, H-4→L+4 10.8%, H-11→L 6.4%, H-4→L+1 5.1%
S_{23}	4.68	265	0.08	H-4→L+3 23.5%, H-6→L 20.7%, H-5→L 19.0%, H-4→L+4 9.6%, H-11→L 8.1%
S_{24}	4.70	264	0.14	H-3→L+3 47.2%, H-3→L+4 24.5%, H-3→L+1 9.3%
S_{25}	4.78	259	0.01	H-2→L+1 49.5%, H-1→L+3 38.2%

ETE-Pyc (conf9)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.69	461	1.42	H→L 70.1%, H-1→L 15.0%, H→L+1 8.9%
S_2	3.25	381	1.06	H→L+1 53.9%, H→L 23.2%, H-1→L 6.9%
S_3	3.31	375	0.16	H-1→L 56.7%, H→L+1 17.9%, H-5→L 10.2%, H→L 6.2%
S_4	3.40	365	1.02	H→L+3 87.0%
S_5	3.88	320	0.02	H→L+5 35.2%, H→L+2 21.6%, H-1→L+1 11.9%, H→L+4 11.6%, H-1→L+2 6.3%
S_6	3.89	319	0.02	H→L+5 49.1%, H→L+2 21.2%, H-1→L+1 9.2%, H-1→L+2 7.5%
S_7	3.99	311	0.01	H-2→L 97.9%
S_8	4.06	306	0.24	H-5→L 42.4%, H-6→L 25.1%, H-1→L 18.7%
S_9	4.07	305	0.00	H-12→L 83.1%, H-12→L+2 7.2%
S_{10}	4.09	303	0.08	H→L+4 40.6%, H-1→L+2 14.9%, H-1→L+1 12.8%, H→L+2 9.9%, H-2→L+3 6.7%
S_{11}	4.22	294	0.19	H-1→L+1 48.6%, H→L+4 20.5%, H→L+1 8.3%
S_{12}	4.43	280	0.10	H→L+8 27.1%, H-2→L+3 11.6%, H→L+9 7.1%, H-2→L+1 6.9%, H-1→L+3 6.5%
S_{13}	4.45	278	0.16	H→L+9 16.5%, H→L+8 11.8%, H-1→L+3 9.1%, H-2→L+1 8.6%, H→L+7 7.9%, H-2→L+4 6.8%
S_{14}	4.46	278	0.01	H-12→L+2 68.9%, H-12→L+1 14.6%, H-12→L 8.9%
S_{15}	4.47	277	0.01	H-3→L 89.3%
S_{16}	4.48	277	0.02	H→L+9 18.2%, H→L+6 12.6%, H-1→L+6 9.2%, H-9→L 6.3%, H-2→L+1 6.2%, H-1→L+3 5.6%
S_{17}	4.48	277	0.01	H→L+8 17.3%, H→L+9 15.8%, H-1→L+6 7.1%, H-2→L+3 6.0%, H→L+6 5.3%
S_{18}	4.51	275	0.05	H-4→L 35.6%, H-2→L+3 24.0%, H→L+4 7.5%, H→L+6 5.9%, H-1→L+6 5.0%
S_{19}	4.51	275	0.03	H-4→L 57.4%, H-2→L+3 15.5%, H→L+4 5.2%
S_{20}	4.53	274	0.06	H-1→L+2 30.8%, H→L+2 27.2%, H-5→L+2 7.7%
S_{21}	4.67	266	0.00	H-15→L 77.1%
S_{22}	4.68	265	0.05	H-6→L 34.1%, H-5→L 30.0%, H-11→L 13.2%
S_{23}	4.69	265	0.09	H-4→L+3 36.4%, H-4→L+4 18.5%, H-3→L+3 16.2%, H-4→L+1 8.7%
S_{24}	4.69	264	0.19	H-3→L+3 31.7%, H-3→L+4 18.0%, H-4→L+3 15.7%, H-3→L+1 6.8%, H-5→L 5.0%
S_{25}	4.79	259	0.01	H-2→L+1 50.3%, H-1→L+3 38.0%

ETE-Pyc (conf10)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.70	459	1.64	H→L 69.2%, H-1→L 14.3%, H→L+1 11.5%
S_2	3.27	379	1.00	H→L+1 51.8%, H→L 26.5%, H-1→L 9.4%
S_3	3.33	373	0.13	H-1→L 54.7%, H→L+1 22.7%, H-5→L 10.1%
S_4	3.40	364	1.07	H→L+3 87.7%
S_5	3.89	319	0.05	H→L+5 80.0%
S_6	3.90	318	0.00	H→L+2 51.0%, H-1→L+2 28.2%, H-5→L+2 6.5%
S_7	4.00	310	0.01	H-2→L 97.2%
S_8	4.05	306	0.03	H→L+4 44.3%, H-1→L+1 29.2%, H-2→L+3 7.2%
S_9	4.08	304	0.21	H-5→L 44.3%, H-6→L 24.6%, H-1→L 18.4%
S_{10}	4.14	300	0.00	H-12→L 91.5%
S_{11}	4.25	292	0.14	H-1→L+1 51.5%, H→L+4 24.5%, H→L+1 5.9%
S_{12}	4.40	282	0.00	H-12→L+2 91.5%
S_{13}	4.42	281	0.15	H→L+9 36.7%, H-1→L+3 11.3%, H-2→L+1 9.3%, H-2→L+4 6.3%, H-5→L+3 5.2%
S_{14}	4.46	278	0.09	H→L+8 50.8%, H-2→L+3 11.5%, H-2→L+5 7.7%
S_{15}	4.47	278	0.01	H→L+2 19.2%, H-1→L+2 18.1%, H→L+8 9.7%, H-5→L+2 7.9%, H→L+6 7.1%, H-2→L+3 7.0%, H-1→L+6 5.0%
S_{16}	4.48	277	0.00	H→L+2 20.6%, H-1→L+2 16.1%, H-2→L+3 10.5%, H→L+6 8.8%, H-1→L+6 8.4%, H-9→L 5.9%
S_{17}	4.48	277	0.00	H-3→L 66.1%, H-4→L 23.9%
S_{18}	4.49	276	0.00	H-4→L 72.1%, H-3→L 21.9%
S_{19}	4.50	275	0.08	H→L+9 23.6%, H-2→L+1 19.0%, H-1→L+3 14.2%, H-2→L+4 10.5%, H-5→L+3 5.5%
S_{20}	4.52	274	0.06	H-2→L+3 32.3%, H→L+6 14.1%, H-1→L+6 12.2%, H→L+4 9.3%, H-9→L 7.9%
S_{21}	4.67	265	0.00	H-15→L 77.0%, H-15→L+10 6.2%
S_{22}	4.68	265	0.17	H-3→L+3 44.9%, H-4→L+4 23.2%, H-4→L+1 10.1%, H-4→L+3 8.8%
S_{23}	4.69	264	0.11	H-4→L+3 43.4%, H-3→L+4 21.3%, H-3→L+1 8.8%, H-3→L+3 7.9%
S_{24}	4.70	264	0.03	H-6→L 37.3%, H-5→L 31.5%, H-11→L 13.6%
S_{25}	4.79	259	0.01	H-2→L+1 53.0%, H-1→L+3 36.2%

Table S16. Electronic excitation properties of various conformations of TEBT-Pyc in toluene using MN15.

TEBT-Pyc (conf1)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.53	490	1.84	H→L 68.8%, H-1→L 13.6%, H→L+1 12.4%
S_2	3.21	386	0.45	H→L+1 71.9%, H→L 9.4%
S_3	3.28	378	0.30	H-1→L 61.0%, H→L 20.3%, H-2→L 6.8%, H-1→L+1 5.3%
S_4	3.64	341	0.48	H→L+3 72.2%, H-1→L+3 9.2%, H-1→L+1 6.6%
S_5	3.81	325	0.01	H→L+2 62.1%, H-1→L+2 27.6%
S_6	3.92	316	0.08	H→L+4 35.1%, H-1→L+1 28.5%, H→L+5 15.9%
S_7	3.97	312	0.05	H→L+5 61.0%, H-1→L+1 20.2%
S_8	3.99	310	0.26	H-2→L 39.6%, H-4→L 32.1%, H-1→L 13.6%
S_9	4.11	302	0.00	H-11→L 90.4%
S_{10}	4.13	300	0.10	H→L+4 42.5%, H-1→L+1 21.4%, H-1→L+4 7.0%, H→L+5 6.8%, H→L+1 6.3%, H→L+3 5.7%
S_{11}	4.33	286	0.13	H-2→L 39.5%, H-4→L 29.3%, H-8→L 11.3%
S_{12}	4.41	281	0.00	H-11→L+2 94.3%
S_{13}	4.44	279	0.00	H-3→L 94.2%
S_{14}	4.45	279	0.03	H→L+8 24.7%, H→L+6 15.3%, H→L+9 10.4%, H→L+7 6.5%, H-1→L+5 6.1%, H-1→L+3 5.3%
S_{15}	4.50	275	0.06	H-1→L+3 30.6%, H-2→L+3 21.6%, H→L+8 12.4%, H→L+6 5.4%
S_{16}	4.55	272	0.14	H-7→L 40.9%, H-7→L+1 15.3%, H→L+10 5.6%
S_{17}	4.59	270	0.03	H-1→L+2 41.8%, H→L+2 35.1%, H-4→L+2 8.6%, H-2→L+2 7.8%
S_{18}	4.63	268	0.02	H→L+9 30.1%, H→L+8 26.3%, H→L+6 5.8%, H-1→L+8 5.3%
S_{19}	4.66	266	0.00	H-14→L 72.9%, H-14→L+11 9.5%, H-14→L+1 8.0%, H-14→L+7 5.3%
S_{20}	4.69	264	0.08	H-3→L+3 47.1%, H→L+6 8.3%, H-1→L+4 7.2%, H-7→L 5.9%, H-3→L+1 5.0%
S_{21}	4.70	264	0.10	H-3→L+3 29.7%, H→L+6 16.2%, H-1→L+4 13.6%, H-7→L 9.5%
S_{22}	4.76	260	0.08	H-2→L+1 41.2%, H-4→L+1 13.9%, H-8→L 9.1%, H-4→L 6.3%
S_{23}	4.90	253	0.01	H-1→L+3 19.3%, H→L+6 16.1%, H-2→L+1 12.3%, H-8→L 6.9%, H-1→L+4 5.2%
S_{24}	4.94	251	0.01	H-6→L 30.7%, H-1→L+4 13.2%, H-4→L 8.0%, H-8→L 7.4%, H-2→L+1 7.4%, H-6→L+1 6.7%
S_{25}	5.03	246	0.06	H-5→L 18.0%, H-6→L 15.8%, H-8→L 14.2%, H→L+9 8.9%, H-6→L+1 5.7%

TEBT-Pyc (conf3)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.51	494	1.63	H→L 69.1%, H-1→L 14.3%, H→L+1 11.2%
S_2	3.16	392	0.47	H→L+1 73.1%, H→L 9.2%
S_3	3.26	381	0.20	H-1→L 62.1%, H→L 20.0%, H-2→L 6.6%
S_4	3.63	342	0.64	H→L+3 67.8%, H-1→L+1 9.1%, H-1→L+3 8.6%
S_5	3.82	324	0.10	H→L+2 40.8%, H-1→L+2 17.1%, H-1→L+1 12.6%, H→L+4 10.1%, H→L+3 5.2%
S_6	3.92	316	0.02	H→L+4 24.4%, H-1→L+1 18.8%, H→L+5 16.4%, H→L+2 15.5%, H-1→L+2 7.9%
S_7	3.96	313	0.05	H→L+5 52.0%, H-1→L+1 14.1%, H-2→L 6.0%
S_8	3.98	312	0.32	H-4→L 31.2%, H-2→L 31.2%, H-1→L 9.2%, H-1→L+1 5.8%, H→L+5 5.3%
S_9	4.06	306	0.00	H-11→L 84.1%, H-11→L+2 6.6%
S_{10}	4.11	302	0.17	H→L+4 44.0%, H-1→L+1 18.1%, H→L+5 9.0%, H-1→L+4 6.3%, H→L+1 6.3%, H→L+3 5.7%
S_{11}	4.32	287	0.09	H-2→L 43.0%, H-4→L 27.5%, H-8→L 12.2%
S_{12}	4.43	280	0.00	H-3→L 92.9%
S_{13}	4.45	278	0.00	H-11→L+2 81.2%, H-11→L 7.8%, H-11→L+1 5.2%
S_{14}	4.47	277	0.03	H→L+9 24.9%, H→L+6 21.0%, H→L+7 8.0%, H-1→L+5 6.2%
S_{15}	4.49	276	0.16	H-1→L+3 27.3%, H→L+9 15.6%, H-2→L+3 13.9%
S_{16}	4.54	273	0.02	H-7→L 34.2%, H-7→L+1 12.9%, H-2→L+3 8.5%, H→L+8 6.9%, H→L+10 5.1%, H-1→L+4 5.0%
S_{17}	4.60	270	0.03	H→L+8 20.7%, H-1→L+2 18.7%, H→L+2 15.4%, H-7→L 8.3%
S_{18}	4.62	268	0.01	H→L+8 28.3%, H-1→L+2 18.9%, H→L+2 16.2%, H→L+9 5.2%
S_{19}	4.66	266	0.00	H-14→L 73.6%, H-14→L+11 9.4%, H-14→L+1 6.2%, H-14→L+7 5.1%
S_{20}	4.69	264	0.06	H-3→L+3 32.9%, H→L+6 14.3%, H-1→L+4 7.8%, H-2→L+3 7.5%, H-7→L 6.5%
S_{21}	4.71	263	0.13	H-3→L+3 39.3%, H→L+6 12.2%, H-1→L+4 9.0%, H-3→L+1 7.1%, H-7→L 5.0%
S_{22}	4.74	261	0.04	H-2→L+1 36.3%, H-4→L+1 13.5%, H-8→L 7.6%, H-4→L 5.8%
S_{23}	4.88	254	0.01	H-1→L+3 17.5%, H→L+6 16.6%, H-2→L+1 10.9%, H-8→L 8.4%, H-1→L+4 5.3%
S_{24}	4.95	250	0.00	H-6→L 25.1%, H-1→L+4 11.0%, H-4→L 8.9%, H-8→L 8.1%, H→L+9 6.4%, H-6→L+1 5.0%
S_{25}	4.99	248	0.04	H-6→L 24.5%, H-5→L 13.6%, H-8→L 11.4%, H-1→L+4 8.1%, H-6→L+1 7.5%

TEBT-Pyc (conf4)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.53	491	1.82	H→L 68.6%, H-1→L 13.8%, H→L+1 12.4%
S_2	3.21	387	0.44	H→L+1 71.6%, H→L 9.5%
S_3	3.27	379	0.31	H-1→L 61.2%, H→L 20.4%, H-2→L 6.3%， H-1→L+1 5.3%
S_4	3.64	341	0.49	H→L+3 72.1%, H-1→L+3 8.6%, H-1→L+1 7.0%
S_5	3.81	325	0.01	H→L+2 61.7%, H-1→L+2 28.0%
S_6	3.92	316	0.11	H-1→L+1 35.3%, H→L+4 32.7%, H→L+5 9.4%, H-2→L+1 5.6%
S_7	3.96	313	0.04	H→L+5 68.6%, H-1→L+1 14.3%
S_8	3.99	311	0.26	H-2→L 37.5%, H-4→L 31.7%, H-1→L 13.2%
S_9	4.11	301	0.00	H-11→L 90.4%
S_{10}	4.13	300	0.11	H→L+4 44.5%, H-1→L+1 20.3%, H-1→L+4 7.0%, H→L+1 6.4%, H→L+3 5.8%, H→L+5 5.5%
S_{11}	4.33	287	0.12	H-2→L 40.1%, H-4→L 28.5%, H-8→L 10.9%
S_{12}	4.41	281	0.00	H-11→L+2 94.2%
S_{13}	4.41	281	0.02	H→L+6 32.0%, H→L+9 10.8%, H-1→L+3 8.6%, H→L+7 5.5%, H-3→L 5.3%
S_{14}	4.43	280	0.02	H-3→L 86.7%
S_{15}	4.54	273	0.07	H-1→L+3 29.1%, H-2→L+3 21.8%, H→L+9 11.6%, H-2→L+1 5.4%
S_{16}	4.55	272	0.12	H-7→L 40.7%, H-7→L+1 15.2%, H→L+10 5.1%
S_{17}	4.58	271	0.03	H-1→L+2 41.4%, H→L+2 34.7%, H-4→L+2 8.2%, H-2→L+2 7.1%
S_{18}	4.63	268	0.03	H→L+8 52.7%, H→L+9 14.6%, H-1→L+8 5.5%
S_{19}	4.66	266	0.00	H-14→L 72.8%, H-14→L+11 9.5%, H-14→L+1 8.0%, H-14→L+7 5.3%
S_{20}	4.69	264	0.10	H-3→L+3 52.8%, H-2→L+3 6.9%, H-3→L+1 5.7%
S_{21}	4.71	263	0.07	H-3→L+3 20.9%, H-1→L+4 17.9%, H→L+6 14.6%, H-7→L 11.0%
S_{22}	4.76	261	0.09	H-2→L+1 38.5%, H-4→L+1 14.3%, H-8→L 9.1%, H-4→L 6.5%
S_{23}	4.90	253	0.01	H-1→L+3 20.1%, H→L+6 17.6%, H-2→L+1 10.2%, H-1→L+4 6.2%
S_{24}	4.93	252	0.01	H-6→L 30.3%, H-1→L+4 11.5%, H-8→L 9.4%, H-2→L+1 8.9%, H-4→L 8.8%, H-6→L+1 6.2%
S_{25}	5.03	246	0.05	H-5→L 17.5%, H-6→L 16.1%, H-8→L 13.8%, H→L+9 9.4%, H-6→L+1 5.8%

TEBT-Pyc (conf5)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.54	488	1.83	H→L 70.1%, H-1→L 13.5%, H→L+1 11.1%
S_2	3.24	383	0.44	H→L+1 71.9%, H→L 10.2%, H→L+3 5.2%
S_3	3.27	379	0.34	H-1→L 63.2%, H→L 18.4%, H-2→L 6.9%
S_4	3.63	341	0.53	H→L+3 72.8%, H-1→L+3 7.8%, H-1→L+1 6.1%
S_5	3.82	324	0.01	H→L+2 62.1%, H-1→L+2 27.1%
S_6	3.92	317	0.07	H→L+4 42.6%, H→L+5 22.8%, H-1→L+1 18.7%
S_7	3.97	312	0.01	H→L+5 44.1%, H-1→L+1 14.4%, H-2→L 10.6%, H-1→L 7.4%
S_8	3.98	311	0.31	H-4→L 28.1%, H-2→L 28.0%, H→L+5 12.0%, H-1→L 8.8%, H-1→L+1 6.2%
S_9	4.11	301	0.00	H-11→L 90.7%
S_{10}	4.15	299	0.12	H-1→L+1 33.9%, H→L+4 32.7%, H→L+1 7.6%, H→L+3 5.7%, H→L+5 5.3%
S_{11}	4.34	286	0.13	H-2→L 42.4%, H-4→L 28.6%, H-8→L 7.3%, H-7→L 5.0%
S_{12}	4.41	281	0.00	H-11→L+2 94.5%
S_{13}	4.42	281	0.00	H-3→L 92.7%
S_{14}	4.47	277	0.03	H→L+9 31.9%, H→L+7 17.7%, H→L+6 12.0%, H-1→L+5 8.1%
S_{15}	4.50	276	0.09	H-1→L+3 39.0%, H-2→L+3 22.1%, H→L+9 8.5%, H→L+6 5.8%, H-2→L+1 5.7%
S_{16}	4.57	271	0.02	H-1→L+2 34.4%, H→L+2 31.3%, H-7→L 8.0%, H-4→L+2 7.2%, H-2→L+2 6.3%
S_{17}	4.59	270	0.09	H-7→L 30.0%, H-7→L+1 11.3%, H-8→L 10.2%, H-1→L+2 8.0%, H→L+8 5.4%, H→L+10 5.2%, H→L+2 5.2%
S_{18}	4.61	269	0.03	H→L+8 50.5%, H→L+7 7.7%
S_{19}	4.66	266	0.00	H-14→L 73.1%, H-14→L+11 8.6%, H-14→L+1 7.9%
S_{20}	4.69	264	0.06	H-3→L+3 55.1%, H-2→L+3 8.5%, H→L+6 7.4%, H-3→L+1 6.0%
S_{21}	4.73	262	0.14	H→L+6 23.0%, H-1→L+4 20.1%, H-3→L+3 19.7%, H→L+9 5.3%
S_{22}	4.78	260	0.05	H-2→L+1 33.3%, H-4→L+1 15.5%, H-8→L 8.5%, H-4→L 7.4%
S_{23}	4.90	253	0.02	H-1→L+3 19.3%, H-2→L+1 16.4%, H→L+6 13.0%, H-1→L+4 5.7%
S_{24}	4.96	250	0.02	H-6→L 21.8%, H-5→L 9.9%, H→L+9 8.3%, H-1→L+4 7.8%, H-4→L 7.3%
S_{25}	5.00	248	0.02	H-5→L 30.8%, H-8→L 11.6%, H-1→L+4 8.3%, H-2→L+1 8.1%, H-7→L 6.4%

TEBT-Pyc (conf8)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.51	494	1.61	H→L 69.2%, H-1→L 14.2%, H→L+1 11.2%
S_2	3.16	392	0.46	H→L+1 73.1%, H→L 9.4%
S_3	3.25	381	0.21	H-1→L 62.2%, H→L 19.8%, H-2→L 7.0%
S_4	3.62	342	0.65	H→L+3 68.8%, H-1→L+3 8.9%, H-1→L+1 8.3%
S_5	3.82	325	0.08	H→L+2 40.0%, H-1→L+2 16.4%, H-1→L+1 13.7%, H→L+4 10.9%
S_6	3.92	317	0.02	H→L+4 24.4%, H-1→L+1 21.3%, H→L+2 17.9%, H→L+5 10.0%, H-1→L+2 9.2%
S_7	3.97	313	0.33	H-2→L 30.6%, H-4→L 21.0%, H→L+5 18.4%, H-1→L 12.3%
S_8	3.98	312	0.06	H→L+5 42.4%, H-1→L+1 16.3%, H-4→L 11.2%, H-2→L 8.4%
S_9	4.06	306	0.00	H-11→L 84.1%, H-11→L+2 6.6%
S_{10}	4.11	302	0.19	H→L+4 42.9%, H-1→L+1 17.6%, H→L+5 11.4%, H-1→L+4 6.5%, H→L+1 6.2%, H→L+3 5.0%
S_{11}	4.31	287	0.09	H-2→L 40.5%, H-4→L 28.3%, H-8→L 12.5%
S_{12}	4.42	280	0.01	H-3→L 94.0%
S_{13}	4.45	279	0.10	H→L+8 21.6%, H-1→L+3 18.2%, H→L+9 13.6%, H-2→L+3 9.2%, H-1→L+5 5.3%, H→L+6 5.1%
S_{14}	4.45	278	0.00	H-11→L+2 81.1%, H-11→L 7.7%, H-11→L+1 5.2%
S_{15}	4.50	276	0.06	H→L+6 15.0%, H→L+8 13.6%, H-1→L+3 11.7%, H→L+9 8.6%, H-1→L+4 5.8%, H-7→L 5.5%, H-2→L+3 5.1%
S_{16}	4.54	273	0.02	H-7→L 31.6%, H-7→L+1 11.8%, H-2→L+3 10.2%, H-1→L+3 7.8%, H→L+10 5.4%
S_{17}	4.60	269	0.04	H-1→L+2 24.4%, H→L+2 20.7%, H→L+8 7.6%, H-7→L 7.1%, H→L+9 6.1%, H-2→L+2 5.6%
S_{18}	4.62	269	0.05	H→L+9 24.2%, H→L+8 13.4%, H-1→L+2 13.1%, H→L+2 10.9%, H→L+6 6.1%
S_{19}	4.66	266	0.00	H-14→L 73.6%, H-14→L+11 9.4%, H-14→L+1 6.2%, H-14→L+7 5.4%
S_{20}	4.69	264	0.10	H-3→L+3 54.4%, H→L+6 5.9%, H-3→L+1 5.7%
S_{21}	4.70	264	0.10	H-3→L+3 21.7%, H→L+6 16.9%, H-1→L+4 12.8%, H-7→L 8.2%, H→L+9 6.6%
S_{22}	4.74	262	0.04	H-2→L+1 40.3%, H-4→L+1 12.8%, H-8→L 6.7%, H-4→L 5.4%
S_{23}	4.88	254	0.01	H-1→L+3 16.9%, H→L+6 16.7%, H-2→L+1 10.7%, H-8→L 8.6%, H-1→L+4 5.6%
S_{24}	4.95	251	0.01	H-6→L 25.4%, H-1→L+4 10.3%, H-4→L 9.1%, H-8→L 7.9%, H→L+9 6.6%
S_{25}	4.99	249	0.04	H-6→L 22.7%, H-5→L 14.7%, H-8→L 11.6%, H-1→L+4 8.9%, H-6→L+1 7.1%

TEBT-Pyc (conf9)

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.51	494	1.58	H→L 69.0%, H-1→L 14.3%, H→L+1 11.2%
S_2	3.16	392	0.62	H→L+1 72.9%, H→L 9.8%
S_3	3.25	382	0.28	H-1→L 62.9%, H→L 19.5%, H-2→L 6.7%
S_4	3.61	343	0.46	H→L+3 68.5%, H-1→L+1 8.9%, H-1→L+3 8.7%
S_5	3.82	324	0.02	H→L+2 40.9%, H-1→L+2 17.3%, H-1→L+1 13.0%, H→L+4 9.5%, H→L+3 5.2%
S_6	3.92	317	0.05	H→L+4 22.2%, H-1→L+1 18.1%, H→L+5 15.0%, H→L+2 14.9%, H-1→L+2 7.5%, H-1→L 5.1%
S_7	3.95	314	0.02	H→L+5 58.9%, H-1→L+1 14.9%
S_8	3.97	312	0.38	H-2→L 34.0%, H-4→L 30.4%, H-1→L 9.2%, H-1→L+1 5.9%
S_9	4.06	305	0.00	H-11→L 84.1%, H-11→L+2 6.7%
S_{10}	4.11	302	0.14	H→L+4 44.9%, H-1→L+1 17.4%, H→L+5 8.7%, H-1→L+4 6.8%, H→L+1 6.4%, H→L+3 5.5%
S_{11}	4.31	288	0.17	H-2→L 41.6%, H-4→L 28.0%, H-8→L 12.1%
S_{12}	4.41	281	0.00	H-3→L 94.3%
S_{13}	4.44	279	0.02	H→L+8 23.8%, H→L+6 16.9%, H→L+9 9.9%, H-1→L+3 6.9%, H-1→L+5 5.3%
S_{14}	4.45	278	0.00	H-11→L+2 81.1%, H-11→L 7.8%, H-11→L+1 5.2%
S_{15}	4.49	276	0.03	H-1→L+3 27.0%, H-2→L+3 18.0%, H→L+8 15.7%
S_{16}	4.54	273	0.16	H-7→L 40.9%, H-7→L+1 15.0%, H→L+10 5.5%
S_{17}	4.60	270	0.04	H-1→L+2 33.4%, H→L+2 27.4%, H-2→L+2 6.4%, H-4→L+2 6.0%
S_{18}	4.62	268	0.02	H→L+9 24.5%, H→L+8 22.8%, H→L+6 5.6%
S_{19}	4.66	266	0.00	H-14→L 73.6%, H-14→L+11 9.4%, H-14→L+1 6.3%, H-14→L+7 5.3%
S_{20}	4.69	265	0.04	H-3→L+3 31.4%, H→L+6 12.7%, H-1→L+4 9.1%, H-7→L 7.6%, H-2→L+3 5.8%
S_{21}	4.70	264	0.11	H-3→L+3 42.0%, H→L+6 11.8%, H-1→L+4 9.0%, H-3→L+1 7.2%, H-7→L 5.9%
S_{22}	4.74	262	0.04	H-2→L+1 38.0%, H-4→L+1 14.2%, H-8→L 7.6%, H-4→L 6.2%
S_{23}	4.89	254	0.01	H-1→L+3 17.6%, H→L+6 15.5%, H-2→L+1 11.9%, H-8→L 9.5%, H→L+9 5.2%
S_{24}	4.92	252	0.03	H-6→L 27.8%, H-1→L+4 15.4%, H-4→L 8.3%, H-8→L 7.1%, H-6→L+1 5.6%, H-2→L+1 5.3%
S_{25}	5.02	247	0.03	H-5→L 18.9%, H-6→L 17.3%, H-8→L 10.9%, H→L+9 9.8%, H-6→L+1 5.6%

Table S17. Electronic excitation properties of TPA-Pyc (conf1) in dichloromethane using MN15.

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.79	445	1.63	H→L 73.0%, H-1→L 13.5%, H→L+1 9.2%
S_2	3.46	358	0.57	H→L+1 79.7%, H→L 5.8%
S_3	3.54	350	0.48	H-1→L 61.4%, H→L 20.3%, H-2→L 12.3%
S_4	4.01	309	0.05	H→L+2 50.4%, H-1→L+2 18.6%, H→L+3 11.3%, H-1→L+1 8.2%
S_5	4.04	307	0.03	H→L+3 71.8%, H→L+2 7.7%, H-1→L+3 6.5%
S_6	4.05	306	0.00	H-9→L 85.6%, H-9→L+2 6.3%
S_7	4.20	295	0.27	H→L+4 83.4%, H-1→L+4 13.0%
S_8	4.28	290	0.15	H-2→L 54.9%, H-1→L+1 14.3%, H-8→L 9.5%, H-1→L 8.4%
S_9	4.38	283	0.06	H-1→L+1 47.2%, H→L+5 12.7%, H-2→L 11.3%, H-1→L 9.4%
S_{10}	4.48	277	0.00	H-9→L+2 75.7%, H-9→L+1 10.8%, H-9→L 7.3%
S_{11}	4.52	274	0.04	H→L+5 20.6%, H-5→L 18.3%, H→L+6 15.2%, H-1→L+1 11.7%, H-1→L+5 10.6%, H-5→L+1 7.4%, H-1→L+6 5.2%
S_{12}	4.60	269	0.03	H→L+7 57.2%, H→L+8 8.8%, H-1→L+3 6.1%
S_{13}	4.72	262	0.00	H-11→L 77.0%, H-11→L+10 9.2%
S_{14}	4.74	262	0.01	H→L+8 37.3%, H-1→L+2 7.6%, H→L+2 6.5%, H-1→L+8 6.4%, H→L+7 6.4%, H→L+6 5.9%
S_{15}	4.77	260	0.01	H→L+8 24.0%, H-1→L+2 20.2%, H→L+2 14.8%, H-2→L+2 7.8%
S_{16}	4.87	255	0.02	H→L+5 28.5%, H→L+6 18.5%, H-1→L+2 10.3%, H-5→L 9.5%, H→L+2 9.0%, H→L+9 6.9%
S_{17}	4.99	248	0.08	H-5→L 61.3%, H→L+6 18.6%
S_{18}	5.11	243	0.01	H-8→L 29.0%, H-3→L 18.5%, H-4→L 10.6%, H-2→L+1 9.5%, H-2→L 6.9%
S_{19}	5.14	241	0.05	H-3→L 46.8%, H-8→L 15.0%, H-3→L+1 8.4%, H→L+7 5.2%
S_{20}	5.31	234	0.00	H-4→L 58.4%, H-2→L+1 15.3%
S_{21}	5.36	231	0.01	H-1→L+3 48.4%, H-4→L 7.0%, H-2→L+3 6.3%, H-1→L+7 6.2%, H→L+3 6.0%
S_{22}	5.38	230	0.01	H→L+9 13.9%, H-8→L 12.8%, H-2→L+1 12.1%, H-3→L 8.6%, H-1→L+5 7.4%, H-1→L+6 6.5%, H-4→L 5.8%, H→L+6 5.0%
S_{23}	5.45	227	0.03	H-2→L+1 23.9%, H-8→L 10.6%, H→L+9 10.5%, H-1→L+2 9.8%, H-2→L+2 7.4%
S_{24}	5.49	226	0.08	H-6→L 22.6%, H-3→L 17.6%, H-3→L+1 11.5%, H→L+9 7.9%, H-6→L+1 6.4%
S_{25}	5.53	224	0.02	H-2→L+2 29.1%, H-2→L+1 14.6%, H→L+9 8.0%, H-1→L+2 6.7%, H-5→L+1 5.4%, H-8→L+2 5.1%, H-8→L+1 5.1%

Table S18. Electronic excitation properties of TE-Pyc (conf5) in dichloromethane using MN15.

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.74	452	1.70	H→L 68.9%, H-1→L 13.7%, H→L+1 11.3%
S_2	3.34	371	0.79	H→L+1 71.7%, H→L 13.7%
S_3	3.39	365	0.47	H-1→L 57.8%, H→L 16.7%, H-2→L 11.1%, H-4→L 6.3%
S_4	3.69	336	0.46	H→L+3 76.4%
S_5	3.92	317	0.01	H→L+2 54.4%, H-1→L+2 27.4%, H-2→L+2 6.7%
S_6	3.96	313	0.05	H→L+4 87.1%
S_7	4.07	305	0.17	H-2→L 34.4%, H-4→L 27.3%, H-1→L 23.7%, H-3→L 5.5%
S_8	4.14	300	0.00	H-11→L 91.5%
S_9	4.22	294	0.04	H-1→L+1 64.7%, H→L+5 10.7%
S_{10}	4.40	282	0.00	H-11→L+2 91.2%
S_{11}	4.44	279	0.04	H→L+7 39.1%, H→L+9 7.4%, H-1→L+3 6.2%, H→L+5 6.0%, H-1→L+4 5.5%
S_{12}	4.48	277	0.02	H-2→L 27.5%, H-3→L 14.4%, H-4→L 12.7%, H-1→L+1 6.8%, H→L+5 6.6%
S_{13}	4.49	276	0.00	H→L+5 16.2%, H-3→L 13.8%, H-7→L 10.6%, H-2→L 9.5%, H-1→L+5 8.6%, H→L+6 8.3%, H-1→L+6 6.8%
S_{14}	4.52	275	0.03	H-3→L 58.5%, H-4→L 16.0%
S_{15}	4.56	272	0.01	H→L+2 27.3%, H-1→L+2 22.5%, H-1→L+3 7.4%, H-2→L+3 6.4%, H-4→L+2 6.4%, H-2→L+2 5.4%
S_{16}	4.58	271	0.20	H-1→L+3 22.3%, H-2→L+3 13.2%, H→L+2 10.1%, H-2→L 6.8%, H-1→L+2 6.7%, H-4→L 6.0%, H-2→L+1 5.5%
S_{17}	4.63	268	0.02	H→L+8 33.7%, H→L+9 16.0%, H→L+6 10.9%, H→L+5 8.7%
S_{18}	4.64	267	0.03	H→L+8 32.4%, H→L+6 16.5%, H→L+5 13.7%
S_{19}	4.67	265	0.00	H-13→L 77.0%, H-13→L+11 5.7%, H-13→L+10 5.3%
S_{20}	4.70	264	0.13	H-3→L+3 63.9%, H-3→L+1 16.4%
S_{21}	4.98	249	0.03	H-7→L 61.8%, H→L+6 12.1%, H→L+5 7.1%
S_{22}	5.02	247	0.05	H-2→L+1 48.6%, H-1→L+3 14.8%, H-3→L+1 8.4%, H-7→L 5.8%
S_{23}	5.08	244	0.01	H-6→L 37.4%, H-6→L+1 9.4%, H→L+7 9.1%, H-5→L 7.2%
S_{24}	5.12	242	0.01	H→L+7 17.1%, H→L+9 12.1%, H→L+10 9.7%, H-9→L 7.8%, H-1→L+3 6.4%, H→L+6 5.4%
S_{25}	5.18	239	0.03	H→L+9 23.8%, H-1→L+4 16.2%, H-5→L 15.8%, H-9→L 8.6%

Table S19. Electronic excitation properties of ETE-Pyc (conf6) in dichloromethane using MN15.

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.75	451	1.82	H→L 65.8%, H-1→L 15.9%, H→L+1 12.9%
S_2	3.22	374	0.77	H→L+1 67.4%, H→L 21.2%
S_3	3.36	369	0.30	H-1→L 62.0%, H→L 12.4%, H-5→L 11.2%, H→L+1 7.0%
S_4	3.40	365	0.96	H→L+2 86.7%
S_5	3.88	319	0.03	H→L+5 83.4%, H→L+4 5.0%
S_6	3.96	313	0.01	H→L+3 48.2%, H-1→L+3 31.6%, H-5→L+3 7.2%
S_7	4.06	305	0.03	H→L+4 44.2%, H-1→L+1 28.8%, H-2→L+2 6.9%
S_8	4.07	305	0.01	H-2→L 95.7%
S_9	4.12	301	0.01	H-12→L 88.9%
S_{10}	4.12	301	0.18	H-5→L 43.7%, H-6→L 24.2%, H-1→L 16.7%
S_{11}	4.25	292	0.15	H-1→L+1 50.5%, H→L+4 22.8%
S_{12}	4.42	280	0.00	H-12→L+3 92.9%
S_{13}	4.43	280	0.09	H→L+8 37.7%, H-2→L+2 8.1%, H→L+9 7.6%
S_{14}	4.44	279	0.19	H-1→L+2 16.9%, H-2→L+1 14.4%, H-2→L+2 11.1%, H-2→L+4 10.0%, H-5→L+2 7.4%, H→L+9 6.7%, H→L+7 5.8%, H→L+4 5.0%
S_{15}	4.47	277	0.00	H→L+9 31.5%, H-2→L+2 11.7%, H→L+7 10.7%, H→L+8 6.2%
S_{16}	4.49	276	0.04	H-2→L+2 20.0%, H→L+8 13.7%, H→L+9 8.5%, H-1→L+2 6.3%, H-2→L+1 5.8%, H-2→L+4 5.3%
S_{17}	4.52	274	0.04	H→L+6 24.5%, H-1→L+6 21.9%, H-9→L 15.6%, H-2→L+2 14.1%, H-9→L+1 6.2%
S_{18}	4.55	272	0.02	H-4→L 74.9%, H-3→L 12.8%
S_{19}	4.56	272	0.02	H-3→L 75.1%, H-4→L 13.4%
S_{20}	4.57	271	0.02	H→L+3 46.3%, H-1→L+3 32.2%, H-5→L+3 11.6%
S_{21}	4.67	266	0.12	H-4→L+2 45.0%, H-4→L+4 18.9%, H-4→L 9.7%, H-4→L+1 9.2%, H-3→L+2 7.6%
S_{22}	4.68	265	0.11	H-3→L+2 41.4%, H-3→L+4 21.9%, H-3→L 9.1%, H-3→L+1 8.7%, H-4→L+2 8.0%
S_{23}	4.73	262	0.00	H-15→L 76.8%, H-15→L+11 7.6%
S_{24}	4.75	261	0.06	H-6→L 42.6%, H-5→L 31.6%, H-11→L 14.4%
S_{25}	4.79	259	0.00	H-2→L+1 52.7%, H-1→L+2 39.3%

Table S20. Electronic excitation properties of TEBT-Pyc (conf5) in dichloromethane using MN15.

Excited state	E_{vert}/eV	λ_{cal}/nm	f	assignment
S_1	2.58	481	1.89	H→L 69.5%, H-1→L 13.6%, H→L+1 11.7%
S_2	3.27	379	0.38	H→L+1 69.6%, H-1→L 7.1%, H→L 6.7%, H→L+3 6.0%
S_3	3.31	374	0.40	H-1→L 57.8%, H→L 22.5%, H-2→L 6.0%, H-1→L+1 5.5%
S_4	3.65	340	0.50	H→L+3 72.0%, H-1→L+3 7.9%, H-1→L+1 6.1%
S_5	3.89	319	0.01	H→L+2 60.4%, H-1→L+2 27.6%
S_6	3.93	316	0.04	H→L+5 41.7%, H→L+4 33.3%, H-1→L+1 9.7%
S_7	3.98	311	0.07	H→L+5 36.1%, H-1→L+1 29.4%, H→L+4 13.3%
S_8	4.01	309	0.24	H-2→L 35.1%, H-4→L 34.4%, H-1→L 14.2%
S_9	4.10	302	0.00	H-11→L 90.8%
S_{10}	4.17	297	0.11	H-1→L+1 33.5%, H→L+4 33.0%, H→L+1 6.9%, H→L+3 5.8%, H→L+5 5.3%
S_{11}	4.37	284	0.12	H-2→L 41.8%, H-4→L 28.1%, H-8→L 8.2%
S_{12}	4.44	279	0.00	H-11→L+2 94.8%
S_{13}	4.45	279	0.00	H-3→L 90.0%
S_{14}	4.47	277	0.04	H→L+7 23.1%, H→L+6 16.2%, H→L+9 15.2%, H→L+8 8.9%, H-1→L+5 8.4%
S_{15}	4.51	275	0.08	H-1→L+3 39.1%, H-2→L+3 22.4%, H→L+6 7.1%, H-2→L+1 5.2%
S_{16}	4.59	270	0.09	H-7→L 45.6%, H-7→L+1 16.6%, H-8→L 8.5%, H→L+10 6.0%, H-1→L+1 5.0%
S_{17}	4.62	269	0.03	H→L+8 34.3%, H→L+7 29.8%
S_{18}	4.66	266	0.02	H-1→L+2 40.1%, H→L+2 36.2%, H-4→L+2 9.7%, H-2→L+2 7.5%
S_{19}	4.69	264	0.08	H-3→L+3 63.4%, H-2→L+3 7.6%, H-3→L+1 7.4%
S_{20}	4.71	263	0.00	H-14→L 72.7%, H-14→L+11 9.0%, H-14→L+1 8.2%
S_{21}	4.73	262	0.10	H→L+6 28.2%, H-1→L+4 22.0%, H-3→L+3 9.2%
S_{22}	4.80	258	0.05	H-2→L+1 33.5%, H-4→L+1 15.5%, H-8→L 9.7%, H-4→L 6.8%
S_{23}	4.91	252	0.01	H-1→L+3 20.9%, H→L+6 14.2%, H-2→L+1 14.0%, H-1→L+4 7.6%, H-2→L+3 5.6%
S_{24}	4.99	248	0.02	H-6→L 30.3%, H-4→L 7.1%, H-1→L+4 6.9%, H-2→L+1 6.8%, H-8→L 6.6%, H→L+9 6.1%, H-6→L+1 5.3%
S_{25}	5.03	246	0.02	H-5→L 23.6%, H-8→L 12.4%, H-6→L 9.4%, H-1→L+4 8.8%, H-2→L+1 6.9%, H→L+8 5.9%

Table S21. Vibrational frequencies (in cm^{-1}) of TPA-Pyc in toluene and dichloromethane obtained from B3LYP/6-311G(d,p) calculations.

in toluene

Freq. #	conf1	conf2	conf3	conf4
1	4.5	5.1	5.9	6.5
2	12.7	13.1	15.5	11.0
3	15.3	15.6	16.0	16.0
4	20.3	23.6	20.6	20.1
5	24.4	28.6	30.8	27.2
6	30.4	29.4	31.2	30.4
7	35.2	35.5	36.6	34.8
8	41.8	42.1	41.5	41.0
9	44.3	42.8	46.1	44.6
10	52.1	52.8	58.4	56.3
11	63.1	63.8	64.6	65.5
12	66.8	67.2	66.3	66.0
13	68.3	68.6	69.8	69.6
14	78.1	79.0	79.3	78.8
15	82.1	81.4	82.7	81.7
16	94.8	92.1	97.1	95.2
17	109.4	103.0	99.6	96.3
18	120.4	137.8	124.4	142.9
19	150.1	149.3	150.3	150.6
20	155.1	161.5	159.6	153.7
21	180.7	176.1	182.0	180.8
22	191.4	179.5	190.5	190.2
23	210.0	209.2	210.2	208.0
24	218.1	219.9	214.1	211.8
25	243.9	242.3	235.3	233.1
26	245.3	253.5	246.3	244.9
27	264.9	261.5	276.2	276.2
28	277.4	278.2	282.6	280.6
29	310.7	307.7	296.9	300.7
30	318.8	318.1	328.0	327.0
31	335.3	334.8	332.3	334.0
32	341.1	340.9	344.7	349.1
33	360.8	359.9	375.0	361.2
34	388.0	390.5	386.4	385.8
35	396.9	397.2	398.1	403.9
36	412.6	414.0	404.2	405.9
37	416.8	417.8	417.9	417.1
38	420.1	419.9	420.1	420.1
39	420.4	420.6	420.6	420.6
40	425.2	425.1	425.3	425.3
41	427.1	426.8	426.7	428.0
42	441.0	442.1	444.0	443.6

43	450.3	449.2	450.1	450.3
44	485.9	485.2	486.2	485.2
45	503.5	504.3	506.0	504.6
46	510.9	511.7	511.8	511.4
47	513.6	513.8	512.8	513.2
48	520.3	520.5	521.0	520.1
49	524.5	524.3	524.8	524.6
50	546.3	549.3	549.3	546.4
51	551.0	551.9	552.2	551.4
52	586.1	586.2	582.2	582.4
53	628.8	629.5	629.7	629.8
54	630.6	631.3	631.6	631.1
55	631.3	631.6	631.7	631.7
56	632.0	631.8	633.3	633.6
57	636.1	635.9	636.2	636.0
58	645.6	644.2	646.4	645.9
59	651.3	652.9	653.7	654.2
60	657.5	656.6	658.2	658.0
61	666.9	671.5	673.9	672.5
62	679.1	677.5	674.4	672.8
63	701.8	701.9	710.5	710.8
64	711.3	711.2	711.2	711.3
65	712.2	712.0	712.8	712.5
66	722.6	721.4	724.2	722.1
67	725.6	726.2	726.2	726.1
68	747.0	747.5	747.2	747.3
69	771.8	771.6	771.8	771.8
70	774.0	773.7	774.0	773.8
71	783.9	784.2	781.9	783.6
72	797.9	797.6	784.1	784.0
73	816.8	816.3	816.5	816.4
74	817.3	819.4	823.3	820.3
75	819.3	821.4	825.6	825.5
76	829.3	830.3	830.5	831.0
77	833.0	838.0	833.2	837.9
78	845.8	845.9	845.6	846.1
79	846.8	847.2	848.1	848.4
80	848.7	848.4	849.2	850.2
81	857.0	855.6	857.0	854.8
82	868.6	868.8	866.8	866.8
83	887.6	883.7	887.4	884.5
84	894.3	890.4	894.5	890.6
85	910.4	910.1	910.3	910.2
86	916.0	915.7	916.0	915.8
87	936.2	935.9	936.2	936.2
88	939.8	939.4	939.8	939.7
89	946.2	945.8	946.1	946.0

90	947.9	953.1	954.3	954.2
91	960.5	963.4	956.4	961.1
92	963.8	963.7	964.2	964.1
93	973.5	973.0	973.5	973.5
94	981.1	980.8	981.0	981.0
95	981.8	981.6	981.8	981.8
96	986.4	986.4	985.9	985.4
97	995.0	995.7	995.3	995.4
98	995.7	996.8	996.7	996.8
99	998.2	997.9	998.2	998.2
100	998.5	998.4	998.6	998.5
101	1005.5	1004.2	1007.0	1005.0
102	1013.6	1013.4	1013.5	1013.5
103	1014.2	1014.1	1014.2	1014.1
104	1025.3	1025.1	1025.4	1025.4
105	1028.4	1027.9	1029.1	1028.9
106	1041.9	1041.9	1041.8	1041.4
107	1047.1	1046.9	1046.9	1046.8
108	1048.8	1048.5	1048.5	1048.5
109	1076.4	1076.6	1075.7	1075.5
110	1102.8	1102.6	1102.7	1102.5
111	1104.8	1104.6	1104.6	1104.5
112	1142.1	1141.1	1141.8	1142.0
113	1145.9	1147.3	1146.2	1147.7
114	1173.3	1173.8	1172.9	1172.8
115	1177.9	1177.2	1177.7	1177.2
116	1179.2	1178.8	1179.0	1178.7
117	1189.2	1188.8	1188.9	1189.0
118	1195.7	1195.4	1195.4	1195.5
119	1197.6	1196.8	1197.3	1197.1
120	1203.3	1202.1	1203.7	1202.7
121	1213.2	1212.8	1213.0	1213.1
122	1215.3	1216.0	1220.1	1220.9
123	1222.2	1220.6	1224.1	1223.6
124	1245.4	1252.1	1250.0	1253.2
125	1263.6	1258.9	1267.4	1266.1
126	1281.5	1281.2	1273.0	1272.4
127	1289.2	1289.5	1289.2	1289.4
128	1294.0	1294.2	1294.1	1294.4
129	1302.0	1301.0	1301.8	1301.8
130	1305.2	1305.1	1305.6	1305.3
131	1326.2	1325.8	1325.8	1324.9
132	1332.6	1332.5	1332.3	1332.2
133	1337.5	1337.4	1337.4	1337.4
134	1343.7	1343.4	1343.6	1343.5
135	1352.0	1351.0	1351.2	1350.3
136	1355.1	1354.8	1354.8	1354.9

137	1358.7	1357.6	1358.8	1359.3
138	1360.3	1360.1	1360.1	1360.1
139	1370.7	1370.9	1371.0	1370.8
140	1372.4	1371.9	1372.8	1373.0
141	1405.3	1405.1	1407.5	1407.7
142	1418.9	1418.4	1410.4	1409.1
143	1434.8	1435.5	1430.6	1430.4
144	1446.8	1447.8	1449.7	1450.4
145	1454.9	1454.2	1457.2	1457.2
146	1464.4	1463.2	1480.6	1479.5
147	1481.2	1480.9	1481.3	1480.9
148	1488.2	1488.0	1488.1	1487.9
149	1520.9	1520.6	1520.7	1520.6
150	1522.9	1522.6	1522.7	1522.4
151	1535.8	1533.2	1535.2	1531.8
152	1543.7	1542.6	1536.8	1539.9
153	1548.0	1550.4	1544.2	1543.3
154	1577.6	1577.9	1579.8	1580.8
155	1590.0	1589.8	1590.4	1589.9
156	1609.3	1609.3	1613.6	1613.4
157	1617.2	1616.9	1617.2	1617.0
158	1622.3	1622.1	1622.3	1622.1
159	1628.2	1625.9	1627.9	1625.3
160	1631.1	1631.4	1630.4	1631.3
161	1631.6	1631.9	1631.5	1631.4
162	1641.3	1641.0	1640.3	1639.9
163	1646.6	1646.5	1645.0	1645.0
164	1653.2	1652.7	1652.9	1652.5
165	1679.9	1680.8	1680.0	1680.9
166	1783.6	1783.0	1783.3	1783.6
167	2326.0	2326.0	2326.4	2326.2
168	3134.2	3134.3	3134.0	3135.1
169	3137.9	3137.1	3136.5	3138.3
170	3144.2	3143.0	3143.1	3144.2
171	3155.8	3155.8	3158.4	3155.8
172	3160.6	3161.3	3160.9	3160.9
173	3163.7	3163.7	3163.7	3163.6
174	3163.9	3163.8	3163.9	3163.8
175	3166.6	3171.1	3165.2	3171.0
176	3171.13	13171.	3170.8	3171.1
177	3171.2	1	3171.0	3173.7
178	3173.6	3174.2	3171.2	3174.7
179	3175.6	3174.3	3175.5	3175.4
180	3184.5	3175.1	3184.5	3182.1
181	3184.6	3182.7	3184.6	3184.4
182	3188.3	3184.5	3188.5	3184.6
183	3190.9	3184.7	3190.8	3190.8
		3191.0		

184	3191.1	3191.1	3191.0	3191.0
185	3192.9	3192.7	3192.9	3192.9
186	3194.4	3193.8	3194.3	3194.2
187	3194.9	3195.0	3194.9	3194.9
188	3195.0	3195.1	3195.0	3195.0
189	3196.1	3196.6	3195.2	3195.2
190	3245.3	3244.4	3245.5	3244.5
191	3591.2	3589.5	3591.4	3588.8
192	3767.1	3768.2	3768.4	3768.2

in dichloromethane

Freq. #	conf1	conf2	conf3	conf4
1	4.9	5.0	6.2	7.2
2	12.4	12.5	15.4	10.0
3	14.3	15.5	16.1	15.8
4	19.6	23.3	21.0	19.9
5	24.5	27.4	29.4	27.0
6	29.0	28.6	30.9	29.5
7	35.1	34.2	37.3	33.9
8	41.3	41.9	41.5	40.7
9	43.3	42.2	45.9	44.2
10	50.1	49.4	58.0	54.6
11	62.7	64.0	64.3	65.1
12	65.1	66.9	66.2	66.0
13	67.1	68.7	69.3	69.8
14	78.5	78.7	79.3	78.3
15	81.4	80.8	82.3	81.0
16	96.6	93.5	98.7	94.9
17	108.4	102.8	99.7	97.2
18	120.1	137.5	124.2	142.4
19	150.4	149.4	151.3	150.8
20	156.3	162.4	160.6	154.4
21	181.6	176.2	183.5	181.4
22	190.9	180.2	190.6	190.1
23	210.1	209.3	210.4	207.9
24	217.8	219.8	214.1	212.1
25	243.6	242.2	235.3	233.0
26	245.3	253.0	246.0	244.8
27	264.5	261.3	276.8	276.4
28	277.8	278.5	282.7	280.5
29	310.2	307.3	296.4	300.3
30	318.1	317.9	327.6	326.5
31	335.5	334.8	332.3	334.3
32	340.7	340.7	344.83	8349.0
33	360.6	359.7	374.9	360.7
34	388.6	390.6	387.1	385.8

35	396.4	396.4	397.6	403.7
36	412.1	413.6	404.9	405.8
37	417.3	417.9	418.5	417.5
38	420.1	419.9	420.1	420.2
39	420.3	420.6	420.7	420.7
40	424.9	424.8	425.2	425.2
41	427.1	426.2	427.6	428.2
42	441.1	442.6	444.5	444.4
43	450.1	449.2	449.8	450.2
44	485.7	485.2	486.2	485.1
45	505.1	506.0	507.4	506.4
46	511.3	511.7	512.2	511.6
47	513.6	514.0	512.9	513.3
48	519.8	520.2	520.6	519.9
49	524.3	524.1	524.5	524.4
50	541.0	545.3	543.5	542.5
51	550.9	551.1	551.6	551.1
52	585.3	585.4	581.5	581.8
53	628.1	628.9	629.2	629.3
54	629.7	630.6	630.8	630.4
55	630.6	630.8	631.1	631.2
56	631.4	631.3	632.7	633.0
57	635.5	635.3	635.6	635.5
58	645.1	643.7	645.9	645.3
59	650.7	652.2	653.1	653.5
60	656.7	655.9	657.5	657.2
61	667.7	672.8	671.4	670.8
62	678.5	676.9	674.1	672.3
63	701.6	702.1	710.3	710.6
64	710.9	710.8	710.8	711.0
65	711.4	711.3	712.4	712.1
66	722.0	720.8	723.8	721.7
67	725.9	726.1	726.5	726.0
68	747.1	747.3	747.3	747.1
69	771.7	771.5	771.6	771.7
70	774.1	773.8	774.0	773.9
71	783.0	783.3	781.5	782.8
72	797.1	796.7	783.4	783.1
73	816.3	815.9	816.0	815.9
74	817.0	820.7	822.8	823.3
75	823.7	822.8	827.7	825.2
76	830.2	831.1	831.5	831.8
77	833.4	838.6	834.0	838.7
78	846.2	846.2	846.1	846.6
79	846.3	846.7	847.4	847.7
80	847.9	847.7	848.8	849.8
81	856.5	854.8	856.8	854.6

82	869.0	869.2	867.5	867.3
83	886.7	883.1	886.6	883.9
84	895.5	892.4	896.0	892.7
85	910.5	910.3	910.5	910.5
86	916.1	915.9	916.1	916.1
87	935.2	935.0	935.5	935.4
88	939.6	939.3	939.6	939.6
89	946.2	945.8	946.1	946.1
90	955.5	958.4	959.7	959.4
91	964.4	965.4	962.9	964.8
92	965.4	965.6	966.0	966.2
93	975.9	975.5	976.0	976.1
94	983.4	983.2	983.3	983.4
95	983.9	983.7	983.9	983.9
96	986.9	987.0	987.1	986.7
97	995.4	995.4	996.2	995.2
98	996.1	996.9	996.8	997.8
99	1000.9	1000.7	1000.9	1000.9
100	1001.3	1001.1	1001.3	1001.3
101	1006.4	1005.5	1009.1	1006.5
102	1012.8	1012.7	1012.7	1012.7
103	1013.3	1013.1	1013.2	1013.2
104	1024.5	1024.2	1024.5	1024.4
105	1027.8	1027.3	1028.5	1028.2
106	1041.2	1041.1	1041.3	1040.6
107	1045.9	1045.7	1045.7	1045.7
108	1047.5	1047.4	1047.4	1047.4
109	1080.1	1080.5	1079.7	1079.4
110	1101.4	1101.4	1101.3	1101.3
111	1103.2	1103.2	1103.1	1103.2
112	1140.9	1139.9	1140.8	1141.2
113	1144.7	1145.9	1145.0	1147.0
114	1168.4	1169.3	1168.7	1168.1
115	1175.2	1175.0	1174.9	1174.9
116	1176.4	1176.3	1176.3	1176.3
117	1187.7	1187.5	1187.5	1187.7
118	1193.2	1193.1	1192.9	1193.2
119	1195.6	1195.0	1195.3	1195.3
120	1202.5	1201.2	1202.9	1202.0
121	1211.8	1211.4	1211.6	1211.8
122	1215.1	1215.9	1219.5	1219.6
123	1221.1	1219.1	1223.5	1223.6
124	1245.4	1252.8	1249.8	1253.7
125	1263.5	1258.6	1266.7	1264.9
126	1280.8	1280.7	1272.7	1272.1
127	1287.1	1287.4	1287.2	1287.3
128	1292.8	1292.9	1292.9	1293.0

129	1300.0	1299.1	1299.8	1299.8
130	1304.5	1304.1	1304.7	1304.3
131	1325.9	1325.6	1326.3	1325.1
132	1332.4	1332.2	1331.8	1331.8
133	1335.8	1335.7	1335.7	1335.7
134	1342.8	1342.5	1342.6	1342.7
135	1351.4	1350.8	1351.2	1350.2
136	1354.2	1354.0	1354.0	1354.1
137	1358.4	1357.8	1358.6	1358.8
138	1359.1	1359.1	1359.5	1360.2
139	1370.7	1371.2	1371.6	1371.1
140	1372.3	1372.3	1373.2	1373.7
141	1404.3	1404.4	1407.6	1407.2
142	1418.8	1418.5	1411.4	1410.2
143	1434.4	1435.0	1430.0	1429.3
144	1444.4	1445.7	1447.7	1448.2
145	1453.5	1453.0	1455.7	1456.0
146	1462.7	1462.0	1479.7	1479.2
147	1479.9	1479.7	1480.6	1479.8
148	1486.8	1486.8	1486.8	1486.7
149	1518.9	1518.7	1518.8	1518.8
150	1521.3	1521.1	1521.1	1520.9
151	1534.6	1532.0	1529.8	1529.1
152	1542.1	1541.5	1534.5	1535.5
153	1543.4	1545.3	1543.1	1542.1
154	1575.6	1575.7	1578.1	1578.9
155	1588.6	1588.5	1589.1	1588.7
156	1603.5	1603.7	1607.4	1607.4
157	1615.8	1615.6	1615.7	1615.6
158	1620.8	1620.5	1620.7	1620.4
159	1626.1	1623.9	1625.8	1623.4
160	1629.1	1629.0	1628.9	1629.0
161	1629.4	1630.3	1629.1	1629.9
162	1639.7	1639.4	1638.9	1638.5
163	1644.7	1644.6	1643.1	1643.0
164	1651.2	1650.7	1650.9	1650.5
165	1678.2	1679.2	1678.3	1679.3
166	1764.5	1764.1	1764.3	1764.6
167	2321.2	2321.4	2321.5	2321.3
168	3136.1	3135.3	3135.3	3136.0
169	3143.7	3143.2	3143.8	3144.3
170	3145.1	3143.8	3144.0	3144.8
171	3161.2	3160.3	3162.4	3159.6
172	3162.3	3162.6	3163.0	3162.4
173	3165.0	3164.9	3165.0	3165.0
174	3165.2	3165.1	3165.2	3165.2
175	3167.0	3171.9	3166.5	3172.0

176	3172.0	3172.0	3171.9	3172.1
177	3172.1	3176.0	3172.2	3175.9
178	3176.0	3176.6	3174.7	3176.2
179	3176.2	3177.0	3176.3	3176.6
180	3184.7	3182.7	3184.7	3182.6
181	3184.8	3184.7	3184.8	3184.7
182	3189.2	3184.9	3189.2	3184.9
183	3190.7	3190.7	3190.7	3190.7
184	3190.8	3190.9	3190.8	3190.9
185	3193.0	3192.6	3192.8	3193.0
186	3194.6	3194.1	3194.4	3194.4
187	3195.1	3195.1	3195.1	3195.0
188	3195.2	3195.2	3195.1	3195.1
189	3196.2	3196.4	3195.3	3195.3
190	3245.0	3244.1	3245.0	3244.1
191	3586.6	3585.3	3588.4	3585.3
192	3760.5	3761.8	3761.9	3762.0

Table S22. Vibrational frequencies (in cm^{-1}) of TE-Pyc in toluene and dichloromethane obtained from B3LYP/6-311G(d,p) calculations.

in toluene

Freq. #	conf1	conf4	conf5	conf6	conf7	conf8	conf9	conf10
1	5.9	5.7	5.3	6.1	6.3	4.5	4.7	5.6
2	8.2	9.7	9.2	8.2	8.7	7.3	6.6	8.5
3	11.0	12.3	11.5	9.5	10.7	10.4	8.5	12.5
4	14.5	16.5	12.3	13.6	15.5	13.6	13.3	14.6
5	18.8	19.2	18.1	19.8	20.0	18.3	19.6	19.4
6	25.1	23.7	24.3	24.7	25.3	23.6	22.9	22.2
7	29.0	29.8	29.8	28.8	27.1	30.2	29.9	25.3
8	32.5	32.1	30.6	29.8	30.5	31.8	34.2	32.0
9	35.6	37.7	37.3	36.7	37.4	36.3	37.8	37.3
10	38.3	41.7	40.3	39.7	40.6	41.8	38.5	40.0
11	49.3	49.6	47.4	49.4	47.9	47.8	51.9	48.0
12	58.2	55.2	56.8	56.0	55.2	57.1	58.5	53.8
13	61.3	57.5	59.7	59.7	59.8	60.7	61.7	58.2
14	66.1	67.8	66.4	66.2	65.9	66.2	66.5	67.5
15	68.9	69.8	72.1	67.8	70.5	69.6	68.5	70.7
16	75.0	73.3	72.7	73.0	75.8	75.8	74.2	70.9
17	82.2	80.0	81.7	79.2	79.2	82.3	79.7	81.9
18	84.6	84.9	85.4	84.5	84.4	84.3	85.3	87.6
19	94.1	93.0	91.8	93.3	93.7	95.2	97.8	93.4
20	97.6	110.8	98.0	98.0	98.6	99.9	99.7	99.8
21	113.7	114.4	111.1	112.5	114.3	110.9	111.0	113.7
22	119.3	116.8	133.5	137.9	132.5	120.5	138.2	131.2

23	150.4	147.3	144.9	144.8	148.2	144.0	145.2	147.9
24	155.2	149.8	150.1	149.3	149.4	150.4	151.7	150.0
25	155.9	155.4	155.9	156.0	157.1	159.8	156.2	158.0
26	172.1	172.9	178.5	171.6	174.4	174.6	169.9	176.1
27	188.7	189.2	185.4	190.2	189.9	190.8	191.8	182.6
28	196.3	202.7	192.9	194.8	199.1	199.0	194.0	191.5
29	210.4	210.3	211.2	209.8	210.1	209.8	213.1	210.9
30	216.7	218.8	219.5	218.9	219.3	225.3	215.5	221.5
31	220.6	237.2	233.8	227.0	222.4	231.2	226.9	225.6
32	249.1	245.1	245.8	245.0	239.4	235.8	246.2	257.6
33	275.4	269.9	271.7	276.2	276.2	271.6	271.2	270.5
34	276.9	277.8	276.3	278.8	279.4	276.0	276.8	278.0
35	294.2	288.1	282.7	284.2	284.0	287.0	298.3	286.0
36	306.7	301.0	301.5	301.3	306.7	305.5	308.8	305.6
37	321.9	324.3	327.5	330.1	327.3	321.1	319.1	323.7
38	329.1	331.4	332.1	332.8	332.8	332.1	330.6	330.6
39	338.3	338.1	335.5	337.5	338.4	338.2	337.6	335.8
40	347.0	350.1	351.6	350.8	347.9	347.6	352.9	337.6
41	362.9	360.4	368.5	362.1	357.3	368.6	363.9	358.6
42	380.0	373.2	370.2	370.9	380.8	377.8	371.5	378.8
43	385.1	383.9	383.0	385.5	384.8	384.2	376.7	386.0
44	387.9	394.0	395.7	393.4	391.4	390.4	391.3	395.4
45	404.0	399.5	406.1	405.0	404.7	404.3	406.2	399.3
46	411.8	417.3	407.5	410.3	409.7	407.0	417.1	416.3
47	418.2	418.6	417.8	417.6	417.3	417.9	418.9	418.5
48	419.9	420.3	419.3	420.2	419.8	419.2	420.3	420.0
49	420.4	420.9	421.5	421.5	421.2	421.2	421.9	421.8
50	424.9	425.4	425.6	425.5	425.3	425.1	426.1	425.0
51	429.6	427.7	427.0	426.2	426.0	428.1	429.4	427.2
52	438.6	438.5	438.5	438.3	438.7	439.3	438.2	437.9
53	443.5	442.8	443.9	443.7	443.7	444.1	444.4	442.2
54	446.1	450.4	447.6	450.4	446.6	445.1	450.6	444.6
55	466.0	459.3	460.3	460.1	465.5	465.1	460.2	466.9
56	487.3	486.0	485.6	484.9	486.4	485.7	484.5	486.7
57	501.7	503.0	503.0	502.9	501.3	501.1	503.0	501.4
58	506.0	506.2	506.3	506.0	505.9	505.9	506.3	506.2
59	513.5	513.5	513.6	513.8	513.4	513.3	514.6	513.4
60	520.1	520.7	521.0	520.4	520.0	520.0	520.6	520.6
61	523.1	523.5	523.4	523.1	522.7	523.0	523.8	522.8
62	535.7	535.7	535.4	535.4	535.3	535.9	535.2	535.4
63	545.6	545.7	546.6	545.7	545.5	545.3	545.4	544.7
64	547.9	549.1	549.1	550.0	547.7	546.4	550.9	551.1
65	552.5	553.2	552.5	553.1	552.3	552.6	553.4	553.2
66	570.2	569.8	569.1	569.8	570.2	569.2	569.5	569.4
67	583.7	587.2	583.8	583.8	583.6	583.2	583.9	588.2
68	631.1	629.5	631.0	631.0	631.2	631.0	631.0	630.2
69	631.6	631.3	631.6	631.8	631.3	631.1	632.2	631.8

70	632.3	632.0	633.1	633.2	633.5	633.1	632.6	631.9
71	643.4	640.5	642.3	642.5	642.8	641.9	641.2	639.8
72	647.7	648.5	648.0	647.9	647.9	649.5	648.8	647.1
73	651.9	651.9	652.2	651.8	651.9	652.3	651.7	652.1
74	655.4	653.6	655.9	655.8	655.7	655.7	657.5	655.3
75	660.9	659.4	660.8	660.8	660.7	659.5	658.8	659.3
76	668.0	672.7	673.3	672.9	670.4	671.4	673.6	672.8
77	675.7	679.4	674.5	673.0	673.3	675.3	676.8	678.0
78	684.9	685.6	685.8	685.0	684.7	685.3	684.7	685.0
79	708.2	702.7	707.4	708.5	708.4	707.5	708.4	702.0
80	711.0	709.6	711.3	711.0	711.1	711.1	711.3	709.1
81	712.6	711.7	712.9	712.7	712.4	712.7	712.5	711.6
82	714.9	712.7	713.9	713.2	713.1	714.7	713.3	712.3
83	726.0	725.3	725.4	725.3	725.4	725.7	726.0	725.4
84	732.3	732.3	732.0	731.7	731.7	732.7	731.5	731.3
85	745.1	745.7	745.6	745.7	745.0	745.2	745.8	745.0
86	748.3	748.9	749.0	749.0	748.8	748.7	748.4	748.3
87	773.2	773.2	773.4	773.3	773.4	773.4	773.6	773.5
88	782.8	784.0	783.7	783.8	783.7	782.2	783.7	784.2
89	784.4	798.3	784.3	784.0	783.9	783.9	784.6	798.0
90	816.7	816.6	816.7	816.5	816.6	816.7	816.5	816.6
91	822.7	817.3	821.7	821.1	820.7	822.6	821.5	818.7
92	824.4	822.2	825.0	824.7	824.9	824.2	824.9	820.8
93	829.3	828.9	830.6	830.2	830.7	829.7	830.6	829.9
94	832.0	832.7	832.9	834.1	835.7	832.3	834.1	834.5
95	835.7	834.2	838.0	837.1	835.9	835.2	837.0	835.6
96	837.7	837.9	839.3	839.4	839.3	837.3	840.1	839.4
97	845.6	845.0	847.2	845.9	846.2	845.8	846.0	846.2
98	848.9	847.4	849.4	849.2	849.8	848.8	849.2	847.8
99	850.9	850.3	851.2	851.1	851.1	851.9	851.0	850.8
100	856.6	857.0	854.5	854.0	854.8	855.8	854.5	854.9
101	857.5	858.8	857.5	858.6	857.2	856.3	858.5	857.1
102	867.2	869.2	867.0	866.9	866.9	866.9	866.9	868.7
103	887.8	887.5	884.4	884.7	884.5	887.7	884.8	883.8
104	894.3	894.4	890.8	890.1	890.2	894.7	891.0	889.6
105	912.0	912.1	912.4	911.9	912.0	912.0	911.8	912.0
106	914.0	913.7	914.0	913.5	914.0	914.2	913.8	913.6
107	930.5	931.4	931.2	931.3	930.6	930.3	931.2	930.9
108	936.4	936.2	935.6	936.5	936.5	935.8	936.0	935.8
109	936.7	936.8	936.3	936.6	936.8	936.7	936.4	935.8
110	943.7	943.0	944.2	943.3	943.6	943.7	943.7	944.0
111	952.8	950.2	955.6	955.1	954.7	952.6	955.5	952.6
112	963.3	961.4	959.9	957.3	956.0	960.9	964.8	962.7
113	965.3	963.7	963.9	963.8	964.1	964.0	966.9	963.3
114	968.7	968.6	967.7	968.8	968.7	967.7	968.7	967.9
115	973.5	973.6	973.4	973.5	973.8	974.0	974.3	973.5
116	980.5	980.1	981.5	980.7	980.6	981.4	980.3	981.0

117	981.8	981.6	981.9	981.7	981.8	981.4	981.9	981.6
118	982.0	982.3	982.3	982.3	982.0	982.5	982.2	982.1
119	985.8	986.5	985.2	984.4	985.2	984.8	985.4	985.7
120	994.9	995.2	995.7	995.8	995.8	995.3	995.6	995.2
121	996.4	996.0	996.5	996.5	996.5	995.9	996.3	996.4
122	998.3	998.3	998.7	998.3	998.5	998.4	998.5	998.6
123	1006.4	1005.4	1005.6	1005.8	1005.1	1004.4	1006.1	1005.0
124	1013.8	1013.7	1013.8	1013.8	1013.8	1013.7	1014.0	1013.9
125	1025.3	1025.1	1025.0	1025.1	1025.1	1024.9	1025.2	1025.2
126	1029.0	1028.2	1028.7	1029.2	1029.1	1027.9	1028.4	1028.4
127	1029.4	1029.6	1029.4	1029.5	1029.6	1029.5	1029.4	1029.5
128	1042.1	1042.7	1041.7	1041.8	1041.7	1041.8	1041.6	1042.0
129	1044.8	1044.8	1044.1	1044.9	1044.9	1044.3	1044.7	1044.8
130	1047.7	1047.8	1047.6	1047.6	1047.7	1047.7	1047.7	1047.8
131	1076.2	1077.0	1075.6	1075.9	1075.7	1075.6	1075.8	1076.6
132	1082.2	1082.2	1083.6	1082.3	1082.4	1083.3	1082.0	1082.1
133	1103.4	1103.7	1103.4	1103.5	1103.6	1103.7	1103.5	1103.4
134	1117.9	1117.2	1118.1	1117.4	1117.6	1118.1	1117.2	1117.7
135	1141.5	1141.1	1141.7	1141.8	1141.9	1140.8	1142.1	1141.7
136	1146.1	1145.4	1147.4	1147.7	1147.7	1144.9	1146.8	1147.1
137	1148.1	1148.3	1148.4	1148.6	1148.9	1149.4	1148.1	1148.9
138	1159.9	1160.0	1159.6	1159.9	1160.2	1159.6	1159.7	1159.8
139	1174.5	1175.2	1173.4	1173.8	1173.4	1173.1	1173.2	1174.4
140	1177.7	1178.1	1177.9	1177.9	1178.4	1178.1	1178.1	1178.1
141	1187.7	1188.1	1188.1	1188.2	1187.9	1188.1	1187.7	1188.0
142	1190.7	1191.3	1191.9	1191.5	1191.1	1191.5	1190.6	1191.0
143	1196.0	1196.2	1196.0	1196.0	1196.2	1196.1	1196.0	1196.0
144	1203.4	1202.6	1201.8	1202.4	1202.4	1202.1	1202.0	1202.0
145	1205.0	1204.9	1204.8	1205.0	1205.1	1204.9	1205.1	1205.3
146	1220.0	1215.8	1220.8	1220.8	1221.0	1219.9	1220.4	1216.0
147	1220.4	1220.8	1221.0	1221.1	1221.2	1221.5	1220.9	1220.4
148	1224.0	1221.8	1223.7	1223.8	1223.7	1223.6	1223.5	1220.9
149	1249.8	1245.2	1251.5	1251.7	1251.8	1249.0	1251.6	1251.1
150	1267.5	1263.2	1265.3	1265.3	1265.4	1266.6	1265.6	1258.6
151	1269.9	1269.8	1268.9	1270.0	1269.9	1268.5	1269.3	1270.3
152	1273.3	1281.8	1272.7	1272.5	1272.4	1272.8	1272.9	1281.7
153	1286.9	1287.0	1286.1	1287.3	1286.8	1285.7	1287.2	1287.0
154	1290.6	1290.6	1291.0	1290.8	1290.7	1290.4	1290.9	1291.3
155	1292.8	1293.3	1292.0	1293.0	1292.9	1292.5	1292.7	1292.0
156	1296.8	1296.9	1297.2	1297.1	1297.2	1296.5	1296.4	1297.1
157	1301.4	1301.9	1302.3	1302.2	1302.2	1302.2	1301.4	1301.3
158	1304.5	1303.5	1303.5	1303.5	1303.6	1303.6	1304.2	1304.1
159	1324.7	1325.5	1324.3	1324.6	1324.7	1325.6	1324.0	1324.0
160	1326.8	1327.1	1326.0	1326.5	1326.6	1326.4	1326.3	1327.2
161	1332.9	1332.8	1332.2	1331.9	1332.1	1332.0	1332.3	1332.7
162	1342.0	1341.8	1341.7	1341.7	1341.8	1341.7	1342.1	1342.1
163	1349.0	1349.5	1349.0	1349.2	1349.3	1349.4	1348.4	1349.2

164	1352.3	1352.5	1351.5	1351.8	1351.9	1352.1	1351.6	1352.0
165	1357.6	1356.1	1356.5	1356.6	1356.8	1354.9	1357.2	1356.9
166	1358.6	1358.5	1358.7	1358.8	1359.0	1358.3	1358.3	1358.3
167	1371.8	1371.5	1371.7	1371.7	1371.6	1370.5	1371.4	1371.3
168	1372.9	1372.6	1372.7	1372.8	1372.8	1371.8	1372.4	1372.1
169	1390.9	1390.9	1391.6	1391.2	1391.0	1391.0	1390.7	1391.0
170	1394.5	1395.1	1394.5	1394.1	1394.7	1394.2	1393.8	1394.4
171	1409.3	1407.1	1408.5	1408.3	1408.2	1408.3	1408.2	1404.7
172	1410.6	1419.4	1409.9	1409.9	1409.7	1409.7	1409.1	1418.1
173	1431.1	1437.8	1430.9	1430.9	1430.8	1430.6	1430.8	1434.7
174	1443.5	1443.9	1443.5	1443.8	1443.9	1444.0	1443.6	1443.7
175	1450.2	1446.8	1450.9	1450.8	1450.9	1449.8	1450.9	1447.8
176	1455.9	1454.6	1456.1	1455.9	1456.0	1455.6	1456.1	1454.8
177	1459.9	1458.8	1459.7	1459.9	1460.0	1459.4	1460.0	1458.6
178	1481.3	1465.3	1480.1	1480.2	1480.1	1480.5	1479.6	1463.7
179	1484.4	1484.9	1484.3	1484.6	1484.8	1484.8	1484.6	1484.3
180	1490.2	1489.9	1489.7	1490.0	1490.3	1490.2	1489.4	1490.3
181	1493.3	1492.7	1492.4	1492.7	1492.9	1492.9	1492.3	1493.1
182	1518.4	1518.0	1517.7	1518.0	1518.3	1517.9	1517.9	1518.4
183	1521.2	1521.5	1521.4	1521.3	1521.4	1521.4	1521.2	1521.5
184	1534.5	1534.7	1531.3	1531.6	1531.5	1534.1	1531.2	1532.8
185	1536.7	1542.1	1539.7	1539.8	1539.8	1536.5	1539.7	1541.2
186	1542.9	1546.1	1541.7	1542.0	1542.1	1542.2	1541.8	1546.3
187	1546.5	1547.9	1546.2	1546.3	1546.5	1546.3	1546.2	1550.4
188	1579.3	1577.2	1580.8	1580.9	1580.7	1579.0	1580.2	1577.7
189	1585.3	1585.0	1584.9	1585.0	1585.1	1585.2	1584.7	1584.4
190	1595.7	1595.0	1595.1	1595.2	1595.2	1595.2	1595.4	1595.6
191	1613.5	1609.1	1613.5	1613.4	1613.3	1613.3	1613.5	1609.3
192	1619.8	1620.0	1619.9	1620.0	1620.1	1620.0	1619.9	1619.9
193	1626.1	1625.9	1624.4	1624.6	1624.6	1625.5	1624.9	1625.0
194	1627.7	1628.2	1625.8	1626.0	1626.1	1627.6	1625.9	1626.3
195	1630.1	1631.0	1631.2	1631.3	1631.2	1629.8	1631.0	1631.6
196	1635.1	1635.0	1635.0	1635.1	1635.2	1634.9	1635.1	1635.4
197	1641.7	1643.1	1641.3	1641.3	1641.4	1641.4	1641.3	1642.8
198	1646.5	1647.5	1646.3	1646.3	1646.4	1646.5	1646.3	1647.3
199	1653.0	1653.2	1652.5	1652.5	1652.5	1652.8	1652.5	1652.7
200	1679.7	1679.7	1680.6	1680.5	1680.6	1679.5	1680.4	1680.5
201	1783.5	1783.3	1783.5	1783.2	1783.2	1783.7	1783.4	1783.3
202	2326.1	2326.0	2326.0	2326.2	2326.1	2326.2	2326.3	2325.9
203	3023.5	3022.5	3022.4	3022.7	3022.5	3022.4	3022.6	3023.2
204	3035.0	3034.2	3033.7	3034.4	3034.2	3033.7	3034.4	3034.7
205	3119.3	3119.0	3118.8	3118.8	3119.5	3118.5	3118.7	3119.1
206	3122.0	3121.8	3120.7	3121.5	3121.9	3120.6	3121.5	3121.9
207	3134.2	3134.5	3133.9	3133.2	3133.9	3133.4	3133.9	3134.5
208	3141.2	3137.5	3139.9	3139.4	3138.8	3138.6	3139.1	3137.2
209	3143.7	3143.9	3143.0	3142.2	3142.9	3142.0	3143.0	3143.1
210	3157.9	3155.3	3158.2	3157.5	3156.6	3156.8	3156.6	3154.7

211	3160.5	3160.6	3161.0	3161.3	3161.4	3160.9	3160.9	3161.2
212	3163.8	3163.9	3163.9	3163.8	3163.8	3163.8	3163.8	3163.9
213	3165.4	3166.6	3168.6	3168.8	3169.8	3164.8	3169.1	3169.8
214	3169.7	3169.1	3171.3	3171.2	3171.2	3169.2	3171.3	3171.3
215	3171.2	3171.2	3174.7	3173.8	3173.8	3171.2	3174.1	3173.7
216	3175.6	3173.8	3174.9	3174.8	3174.7	3173.4	3174.7	3173.9
217	3176.0	3175.5	3175.9	3175.4	3175.3	3175.1	3175.2	3174.7
218	3184.6	3184.7	3181.7	3181.2	3181.5	3184.6	3181.7	3182.4
219	3185.2	3185.4	3184.6	3184.6	3184.5	3185.2	3184.5	3184.6
220	3189.2	3188.3	3184.9	3185.2	3185.2	3188.1	3185.3	3185.2
221	3191.1	3191.1	3191.0	3191.0	3191.0	3191.1	3191.1	3191.0
222	3191.7	3191.7	3191.9	3191.6	3191.8	3191.7	3191.8	3192.1
223	3192.7	3193.1	3193.2	3193.1	3193.1	3193.0	3193.0	3192.9
224	3194.3	3194.4	3194.3	3194.3	3194.3	3194.3	3194.3	3194.0
225	3195.1	3195.1	3195.1	3195.0	3195.0	3195.0	3195.0	3195.0
226	3195.3	3196.3	3195.3	3195.6	3195.7	3195.1	3195.0	3196.8
227	3217.4	3217.5	3220.8	3217.7	3217.8	3222.9	3217.4	3217.7
228	3245.7	3245.7	3244.4	3244.0	3243.9	3245.5	3244.2	3244.6
229	3257.3	3257.2	3257.7	3257.8	3257.5	3257.6	3257.0	3257.3
230	3591.7	3590.9	3589.9	3589.6	3588.4	3590.6	3589.7	3590.5
231	3767.7	3768.3	3767.6	3767.8	3768.2	3767.5	3768.0	3768.6

in dichloromethane

Freq. #	conf1	conf4	conf5	conf6	conf7	conf8	conf9	conf10
1	6.4	6.5	1.9	7.2	7.3	5.0	6.2	6.3
2	8.4	9.4	7.1	8.5	8.8	7.4	7.4	9.6
3	11.8	13.1	9.6	10.0	11.1	10.4	10.5	13.1
4	14.8	17.7	10.6	14.2	15.9	12.2	15.4	14.8
5	19.3	19.5	17.2	20.3	20.2	17.5	21.8	19.9
6	25.1	23.6	24.0	24.8	25.2	23.4	23.5	22.3
7	28.2	30.7	28.7	26.9	27.9	28.4	25.8	25.6
8	32.4	33.0	29.5	29.6	30.5	33.1	32.5	31.6
9	35.7	37.0	37.2	36.1	36.9	35.4	37.5	36.8
10	37.9	41.7	39.6	39.6	40.5	41.5	38.0	39.3
11	49.0	49.3	47.2	49.1	47.6	47.4	50.9	47.6
12	57.4	55.0	54.6	53.8	54.8	56.3	56.8	52.5
13	60.8	57.9	59.3	59.6	59.7	59.2	60.1	57.8
14	66.2	68.1	65.5	66.6	65.9	65.4	66.2	67.1
15	69.0	69.4	72.0	67.7	70.3	69.0	67.4	70.4
16	75.0	72.8	72.1	72.7	75.7	76.7	74.1	71.0
17	81.9	79.5	81.1	79.3	78.9	81.1	79.0	80.8
18	84.0	84.3	84.9	83.8	83.7	83.7	85.1	87.5
19	95.6	94.1	91.4	93.9	94.1	94.9	95.6	93.7
20	97.9	110.6	98.4	97.9	99.0	100.5	99.2	99.5
21	112.9	113.1	109.0	112.2	114.0	110.2	111.4	113.8
22	119.1	116.5	133.1	137.5	132.2	119.7	137.6	130.8

23	150.6	146.3	144.5	144.7	148.4	143.9	145.0	147.9
24	154.8	150.4	149.9	148.9	149.3	150.9	150.4	149.8
25	157.0	156.6	156.5	156.9	157.8	160.4	156.4	158.5
26	172.6	173.5	179.0	172.2	175.0	175.1	169.8	175.9
27	189.3	189.2	185.1	190.3	190.2	190.5	190.6	182.7
28	196.3	203.2	192.7	194.7	199.2	199.2	194.1	191.5
29	210.7	210.4	211.7	209.9	210.9	211.7	210.9	211.6
30	216.3	218.9	219.2	218.5	218.9	224.9	215.0	221.0
31	220.3	236.9	232.9	226.9	221.9	230.4	226.8	225.4
32	248.9	245.0	245.6	244.8	239.2	235.9	245.8	257.3
33	275.5	269.5	271.4	276.7	276.9	271.4	270.7	270.3
34	277.1	278.8	276.6	278.8	279.2	276.6	278.0	278.7
35	293.9	287.9	282.3	283.7	283.4	286.7	297.6	285.6
36	306.2	300.3	301.3	300.7	306.4	305.1	308.1	305.2
37	321.8	324.2	327.0	329.9	326.8	320.2	318.5	323.4
38	328.9	330.7	331.2	332.4	332.2	332.0	330.4	330.1
39	337.9	337.6	334.8	337.1	338.1	338.2	337.1	335.4
40	346.7	349.7	351.3	350.4	347.5	347.6	352.3	337.4
41	362.7	360.2	368.6	361.5	356.7	368.3	363.1	358.1
42	380.0	373.1	370.1	370.8	380.4	377.9	371.1	378.6
43	384.8	383.6	382.7	385.4	384.8	382.9	375.8	385.9
44	387.8	393.8	395.2	392.9	390.9	390.9	391.0	394.8
45	403.6	399.6	406.0	404.9	404.7	404.3	405.5	399.1
46	411.5	417.5	406.8	409.8	409.2	406.7	416.7	416.3
47	418.6	418.4	418.1	417.9	418.0	418.4	418.4	418.7
48	419.9	420.3	419.7	420.3	419.9	419.3	420.3	420.0
49	420.5	420.9	421.5	421.5	421.2	421.2	421.7	421.8
50	424.7	425.2	425.7	425.4	425.3	424.9	425.8	424.7
51	428.8	427.6	426.8	425.7	425.7	427.2	429.2	427.0
52	438.3	438.0	438.0	438.1	438.3	439.0	438.0	437.6
53	444.5	443.9	444.3	444.6	444.6	444.0	444.7	442.8
54	445.7	449.9	447.4	450.0	446.3	444.9	450.2	444.7
55	465.7	459.1	460.0	460.0	465.2	463.9	459.5	466.6
56	486.9	486.1	485.5	484.8	486.3	485.9	484.5	486.4
57	501.6	503.0	503.5	503.0	501.3	501.1	502.9	501.5
58	508.6	508.4	508.1	508.1	508.2	507.8	507.8	508.0
59	513.9	513.9	513.8	513.9	513.8	513.9	514.3	513.6
60	519.8	520.3	520.6	519.9	519.7	520.1	520.3	520.4
61	522.9	523.3	523.1	522.8	522.5	523.0	523.6	522.6
62	535.6	535.2	535.1	535.5	535.1	535.7	535.3	535.5
63	543.6	543.1	543.2	543.6	542.5	542.9	544.6	544.0
64	544.8	545.3	546.2	545.3	544.9	544.7	546.9	545.8
65	552.3	553.0	552.1	552.6	552.0	552.5	552.8	552.5
66	569.7	569.3	568.7	569.3	569.8	568.8	569.1	569.1
67	583.0	586.5	583.1	583.0	582.8	582.4	583.0	587.4
68	630.6	629.0	630.4	630.5	630.6	630.4	630.4	629.6
69	630.7	630.5	630.5	630.8	630.7	630.5	631.3	630.8

70	631.7	631.4	632.6	632.6	632.9	632.6	631.9	631.2
71	642.8	640.1	641.7	641.9	642.2	641.4	640.5	639.5
72	647.1	648.1	647.5	647.4	647.4	649.1	648.2	646.7
73	651.3	651.4	651.5	651.1	651.3	651.7	651.1	651.4
74	654.7	652.9	655.2	655.1	654.9	654.9	656.7	654.8
75	660.2	658.7	660.0	660.0	659.9	658.8	658.1	658.6
76	667.4	676.8	671.9	669.6	670.5	674.9	667.4	674.9
77	675.6	679.1	673.0	672.7	673.1	677.4	673.4	677.4
78	684.5	685.1	685.3	684.6	684.2	685.3	684.0	684.8
79	707.8	703.0	707.0	708.2	708.1	707.2	708.0	702.2
80	710.7	709.0	710.9	710.7	710.7	710.6	711.0	708.7
81	712.2	711.2	712.7	712.5	712.1	712.4	712.2	711.2
82	714.8	712.5	713.6	713.1	713.0	714.5	713.1	712.1
83	726.2	725.6	725.5	725.4	725.5	725.8	725.9	725.6
84	731.7	731.7	731.4	731.2	731.2	732.3	730.8	730.7
85	744.6	745.4	745.5	745.4	744.6	744.8	745.3	744.7
86	748.1	748.6	748.9	748.6	748.5	748.6	748.2	748.1
87	773.5	773.4	773.6	773.6	773.5	773.4	773.8	773.7
88	782.2	783.3	782.9	782.9	782.9	781.6	782.9	783.2
89	783.4	797.6	783.4	783.2	783.1	783.2	783.6	797.2
90	816.3	816.2	816.2	816.1	816.1	816.1	816.0	816.4
91	822.7	816.9	824.2	823.4	823.3	822.3	822.6	820.2
92	826.6	826.2	824.7	824.3	824.8	826.6	824.6	823.2
93	830.7	829.7	831.1	830.6	831.5	831.0	830.5	830.6
94	832.7	832.5	832.2	832.4	833.4	833.5	832.6	833.1
95	833.3	833.4	836.8	836.5	835.5	834.2	836.3	834.6
96	837.1	836.8	839.5	839.2	839.6	835.7	839.7	839.3
97	845.4	844.2	846.4	845.3	845.8	845.6	845.3	845.5
98	848.5	847.1	848.9	848.3	849.1	848.3	848.4	847.5
99	849.4	848.9	850.2	850.3	849.8	850.3	850.2	849.4
100	855.6	856.3	854.2	853.9	854.6	854.0	854.3	854.2
101	856.6	856.8	856.0	856.7	855.3	856.8	856.6	855.2
102	868.0	869.6	867.5	867.4	867.3	867.4	867.3	869.0
103	887.0	886.8	883.7	884.0	883.9	886.7	883.6	883.3
104	895.9	895.7	893.1	892.1	892.4	896.2	892.4	891.8
105	912.5	912.5	912.7	912.6	912.5	912.5	912.4	912.6
106	914.3	914.0	914.1	914.0	914.3	914.5	914.2	913.9
107	927.8	928.5	928.3	928.5	927.9	927.6	928.3	928.1
108	935.6	935.5	935.2	935.5	935.5	935.2	935.0	934.9
109	936.0	936.2	935.4	935.9	936.0	936.1	935.7	935.2
110	943.8	943.2	944.3	943.6	943.8	943.5	943.9	944.2
111	958.6	957.2	960.4	959.0	958.0	958.3	958.8	958.7
112	965.3	964.2	963.4	959.7	959.8	961.3	966.0	965.2
113	966.0	965.4	966.1	965.7	966.1	965.8	968.9	965.7
114	969.3	969.2	968.8	969.4	969.5	968.7	969.1	968.5
115	976.1	975.9	976.1	975.9	976.4	976.5	976.4	975.8
116	981.1	980.6	980.8	981.0	981.0	980.4	980.8	980.9

117	981.5	981.5	982.9	981.7	981.7	982.7	981.6	981.6
118	984.0	983.8	984.2	983.8	983.9	983.9	984.2	984.1
119	987.2	987.1	986.4	985.9	986.5	986.8	986.6	986.2
120	995.7	995.9	995.1	995.8	996.0	995.3	996.2	995.5
121	996.4	996.4	997.4	996.8	997.2	996.8	996.8	996.7
122	1001.4	1001.3	1001.6	1001.5	1001.5	1001.4	1001.7	1001.6
123	1007.5	1006.3	1007.2	1006.5	1006.1	1006.9	1006.5	1005.8
124	1013.1	1013.0	1013.0	1013.1	1013.0	1012.9	1013.3	1013.2
125	1024.5	1024.3	1024.4	1024.4	1024.4	1024.3	1024.5	1024.2
126	1027.9	1027.8	1027.9	1027.8	1027.9	1027.4	1027.5	1027.8
127	1028.3	1028.0	1028.2	1028.6	1028.4	1027.9	1027.8	1028.0
128	1040.9	1040.8	1040.2	1040.9	1040.9	1040.2	1040.8	1041.0
129	1041.9	1042.1	1041.1	1041.1	1040.9	1041.1	1041.0	1041.4
130	1046.6	1046.6	1046.5	1046.5	1046.4	1046.6	1046.6	1046.7
131	1076.7	1076.7	1078.2	1077.0	1077.1	1077.8	1076.7	1076.8
132	1080.3	1080.9	1079.5	1079.7	1079.6	1079.5	1079.6	1080.3
133	1102.2	1102.4	1102.2	1102.3	1102.2	1102.4	1102.2	1102.1
134	1116.4	1115.5	1116.2	1116.0	1115.9	1116.6	1116.2	1116.4
135	1140.2	1140.2	1140.5	1140.8	1141.1	1139.5	1140.8	1140.5
136	1145.1	1144.4	1146.4	1146.6	1146.6	1143.5	1145.7	1146.3
137	1146.6	1146.8	1147.2	1147.3	1147.4	1147.6	1147.0	1147.3
138	1158.0	1158.2	1157.9	1158.1	1158.4	1157.9	1158.0	1158.1
139	1170.3	1170.6	1168.7	1169.1	1168.9	1168.5	1168.2	1169.4
140	1175.6	1175.8	1175.8	1175.9	1176.1	1175.8	1175.9	1175.8
141	1186.3	1186.6	1186.6	1186.9	1186.5	1186.6	1186.2	1186.4
142	1189.4	1189.7	1189.8	1190.2	1189.6	1189.9	1189.2	1189.5
143	1194.1	1194.2	1194.1	1194.2	1194.2	1194.1	1194.0	1194.0
144	1202.4	1202.0	1201.3	1201.7	1201.6	1201.2	1200.7	1201.4
145	1203.7	1203.6	1203.8	1204.0	1204.0	1203.5	1203.9	1203.9
146	1218.7	1215.8	1219.1	1219.2	1219.4	1219.3	1218.9	1216.0
147	1219.7	1219.1	1219.7	1219.9	1219.8	1219.8	1219.2	1219.1
148	1223.6	1220.9	1223.4	1223.6	1223.6	1222.6	1223.4	1219.3
149	1249.6	1245.5	1252.0	1252.1	1252.3	1249.2	1251.3	1251.4
150	1266.7	1263.4	1264.2	1264.2	1264.3	1266.1	1264.4	1258.6
151	1268.9	1268.5	1268.2	1269.1	1268.9	1268.0	1269.2	1269.4
152	1272.8	1281.3	1272.3	1271.9	1271.8	1272.3	1272.3	1281.2
153	1285.8	1286.0	1285.3	1286.3	1285.8	1284.8	1286.2	1285.9
154	1289.4	1289.3	1289.3	1289.2	1289.1	1289.2	1289.7	1289.7
155	1291.0	1291.5	1290.5	1291.4	1291.3	1290.9	1291.0	1290.6
156	1296.2	1296.1	1296.7	1296.5	1296.5	1296.2	1296.1	1296.6
157	1299.9	1300.0	1300.4	1300.5	1300.2	1300.0	1300.1	1299.8
158	1303.5	1303.0	1302.4	1302.8	1302.8	1303.1	1302.9	1302.7
159	1323.8	1324.5	1323.6	1324.2	1324.2	1324.6	1323.3	1323.1
160	1327.0	1326.5	1325.5	1325.7	1325.8	1326.3	1326.1	1326.7
161	1332.5	1332.8	1331.8	1331.6	1331.8	1331.5	1331.9	1332.2
162	1340.7	1340.6	1340.6	1340.5	1340.6	1340.5	1340.8	1340.8
163	1348.4	1348.8	1348.4	1348.6	1348.6	1348.9	1347.8	1348.5

164	1352.4	1352.4	1351.2	1351.4	1351.4	1351.6	1351.3	1351.6
165	1356.7	1356.2	1356.2	1356.0	1356.1	1355.5	1356.3	1356.7
166	1358.2	1358.0	1358.5	1358.6	1358.8	1357.7	1357.3	1357.7
167	1372.0	1372.0	1372.2	1371.7	1371.7	1371.0	1371.4	1371.2
168	1373.5	1372.9	1373.1	1372.9	1373.1	1372.2	1372.1	1372.6
169	1388.6	1388.6	1389.0	1389.0	1388.7	1388.8	1389.0	1389.0
170	1394.9	1394.9	1394.8	1394.8	1395.1	1394.7	1394.6	1394.9
171	1409.5	1406.4	1408.0	1407.8	1407.6	1407.4	1407.4	1403.7
172	1412.3	1420.1	1410.6	1410.2	1410.1	1410.6	1409.5	1418.2
173	1431.1	1437.2	1429.9	1429.8	1429.7	1429.6	1429.9	1434.3
174	1441.9	1442.2	1442.0	1442.3	1442.1	1442.3	1442.1	1442.0
175	1448.2	1444.6	1448.7	1448.6	1448.7	1447.8	1448.5	1445.6
176	1454.1	1453.0	1454.3	1454.1	1454.2	1453.8	1454.2	1453.0
177	1458.3	1457.3	1458.3	1458.5	1458.5	1457.9	1458.5	1456.9
178	1481.7	1464.3	1479.9	1479.7	1479.6	1480.1	1479.3	1462.4
179	1483.2	1483.6	1483.1	1483.4	1483.5	1483.6	1483.3	1483.1
180	1488.4	1487.7	1487.5	1488.0	1488.0	1488.3	1487.8	1488.3
181	1490.9	1490.4	1489.7	1490.4	1490.7	1490.9	1490.5	1490.8
182	1516.5	1516.0	1515.9	1516.1	1516.4	1516.1	1516.1	1516.5
183	1519.6	1519.9	1519.9	1519.8	1519.8	1519.9	1519.7	1520.0
184	1529.9	1533.3	1528.9	1529.0	1528.9	1529.4	1528.5	1531.6
185	1533.6	1540.9	1535.0	1535.1	1535.1	1533.2	1535.2	1540.2
186	1541.9	1542.8	1540.4	1540.6	1540.6	1541.0	1540.2	1544.8
187	1545.1	1544.8	1544.7	1544.8	1544.9	1544.8	1544.6	1545.4
188	1578.0	1575.5	1579.1	1579.0	1578.8	1577.3	1578.4	1575.8
189	1584.0	1583.7	1583.6	1583.7	1583.8	1584.0	1583.4	1583.1
190	1594.5	1593.7	1594.0	1593.9	1594.0	1594.0	1594.2	1594.4
191	1607.4	1603.6	1607.3	1607.2	1607.1	1607.1	1607.3	1603.7
192	1618.5	1618.7	1618.7	1618.7	1618.8	1618.7	1618.6	1618.5
193	1624.1	1623.8	1622.3	1622.5	1622.6	1623.6	1622.9	1623.1
194	1625.8	1626.3	1623.9	1623.9	1624.1	1625.7	1623.8	1624.4
195	1628.8	1629.6	1629.6	1629.6	1629.5	1628.4	1629.4	1629.9
196	1633.0	1632.8	1633.1	1633.1	1633.2	1632.7	1633.1	1633.4
197	1640.3	1641.5	1639.9	1639.8	1639.8	1639.8	1639.7	1641.2
198	1644.7	1645.6	1644.5	1644.4	1644.4	1644.5	1644.4	1645.4
199	1651.1	1651.3	1650.6	1650.6	1650.6	1650.8	1650.5	1650.8
200	1678.1	1678.1	1679.0	1678.8	1678.9	1678.1	1678.7	1678.9
201	1764.5	1764.4	1764.5	1764.3	1764.2	1764.3	1764.2	1764.3
202	2321.4	2321.4	2321.1	2321.5	2321.4	2321.3	2321.2	2321.2
203	3030.0	3029.0	3029.0	3029.6	3029.0	3029.1	3029.1	3029.7
204	3040.6	3039.8	3039.4	3040.3	3039.7	3039.9	3040.2	3040.3
205	3126.0	3125.9	3125.4	3125.6	3125.9	3125.4	3125.5	3126.1
206	3128.7	3128.6	3127.6	3128.5	3128.7	3127.9	3128.2	3129.0
207	3135.7	3136.0	3135.1	3134.4	3135.0	3134.6	3135.3	3135.4
208	3144.6	3143.7	3143.9	3143.0	3143.7	3143.3	3143.9	3143.1
209	3146.8	3144.6	3146.3	3145.2	3144.7	3144.1	3145.2	3143.8
210	3162.3	3161.5	3162.2	3161.3	3160.4	3161.9	3160.3	3159.2

211	3163.1	3162.5	3162.7	3162.9	3163.1	3162.5	3162.4	3162.7
212	3165.3	3165.4	3165.4	3165.4	3165.2	3165.3	3165.4	3165.3
213	3166.6	3167.0	3169.0	3169.2	3170.3	3166.3	3169.7	3170.4
214	3170.2	3169.9	3172.4	3172.4	3172.2	3169.6	3172.4	3172.3
215	3172.3	3172.3	3176.1	3176.0	3176.0	3172.3	3175.6	3175.5
216	3176.3	3176.4	3177.5	3176.3	3176.3	3175.6	3176.6	3176.0
217	3178.0	3176.8	3178.0	3177.2	3176.9	3176.2	3176.7	3176.2
218	3184.9	3184.9	3182.4	3182.0	3182.2	3184.9	3182.1	3182.2
219	3185.7	3185.9	3184.9	3184.8	3184.7	3185.7	3184.8	3184.8
220	3190.3	3189.7	3185.6	3185.7	3185.5	3189.0	3185.9	3186.0
221	3190.8	3190.9	3190.8	3190.8	3190.7	3191.0	3190.9	3190.8
222	3192.3	3192.2	3192.3	3192.2	3192.2	3192.2	3192.3	3192.4
223	3192.7	3193.0	3193.1	3193.1	3193.1	3192.8	3193.0	3192.9
224	3194.3	3194.6	3194.3	3194.5	3194.5	3194.3	3194.3	3194.0
225	3195.3	3195.3	3195.1	3195.3	3195.2	3195.4	3195.3	3195.3
226	3195.3	3196.2	3195.3	3195.3	3195.5	3195.4	3195.4	3196.9
227	3216.5	3216.7	3218.9	3216.4	3216.8	3221.6	3216.0	3216.6
228	3245.7	3245.6	3244.0	3243.7	3243.7	3245.1	3243.8	3244.5
229	3255.8	3255.7	3255.9	3256.2	3256.0	3256.2	3255.6	3255.9
230	3588.3	3587.3	3586.6	3585.8	3584.8	3587.7	3585.5	3586.5
231	3761.4	3761.7	3761.1	3761.4	3761.8	3761.3	3761.3	3762.3

Table S23. Vibrational frequencies (in cm^{-1}) of ETE-Pyc in toluene and dichloromethane obtained from B3LYP/6-311G(d,p) calculations.

in toluene

Freq. #	conf1	conf2	conf3	conf6	conf7	conf8	conf9	conf10
1	5.0	4.4	5.5	0.6	5.0	3.6	4.6	3.9
2	9.0	7.5	7.4	6.1	7.7	7.3	6.0	7.1
3	9.6	9.3	9.3	7.7	9.2	8.6	7.1	9.0
4	11.0	9.6	10.3	8.9	11.0	9.9	8.7	9.8
5	12.0	13.4	12.5	11.6	11.6	13.1	12.2	10.9
6	16.3	14.1	13.6	14.3	14.7	14.3	13.3	14.5
7	16.9	17.2	15.3	15.3	16.5	16.0	18.5	15.7
8	24.0	22.4	24.7	22.4	24.1	21.6	22.0	23.9
9	29.4	28.1	29.9	30.8	31.7	27.9	29.8	25.3
10	33.7	33.7	33.6	33.3	34.4	32.6	33.1	32.2
11	38.3	39.2	40.4	35.1	37.4	35.6	39.7	40.0
12	48.4	44.4	42.3	44.7	43.2	45.2	42.7	45.3
13	54.3	52.7	54.6	54.5	55.0	50.9	52.0	53.5
14	59.4	53.4	57.4	57.2	57.8	51.8	53.6	54.4
15	61.5	57.5	61.8	59.8	63.1	58.8	60.1	60.7
16	64.8	62.6	62.8	60.6	63.5	63.4	61.1	63.2
17	67.8	65.4	66.4	66.1	66.8	65.9	67.5	66.9
18	73.6	73.9	70.6	71.0	71.9	70.2	72.9	73.3

19	74.5	76.7	73.3	75.6	75.0	77.3	75.9	75.8
20	81.2	84.2	84.3	84.3	84.1	84.9	85.0	80.7
21	89.0	87.9	87.4	87.8	86.3	89.0	89.8	87.6
22	90.2	93.4	96.6	93.6	94.0	94.6	95.2	90.1
23	98.0	96.8	101.5	99.3	100.0	98.3	97.5	96.5
24	112.1	111.4	110.6	111.3	110.4	111.1	110.3	110.6
25	112.7	113.3	110.8	112.4	112.6	112.6	112.4	112.4
26	115.7	126.2	116.1	124.5	115.6	124.3	126.1	126.7
27	140.3	139.5	136.9	134.7	139.7	139.0	143.3	139.9
28	148.7	148.1	146.5	149.7	144.9	145.2	146.0	146.0
29	152.6	149.8	149.5	151.9	150.4	149.9	150.6	148.8
30	157.5	154.0	156.9	154.1	156.8	153.5	153.2	156.6
31	175.5	173.4	168.1	173.0	171.2	170.5	172.6	175.2
32	177.6	178.5	173.5	175.6	181.0	180.2	178.4	177.8
33	192.0	187.1	194.6	193.6	191.8	189.9	183.8	192.6
34	200.9	208.6	209.6	210.0	210.0	211.1	209.7	203.5
35	211.6	214.0	220.8	213.1	216.7	218.8	221.7	211.8
36	224.7	225.6	223.0	223.8	223.3	225.2	230.4	220.5
37	241.8	239.7	240.0	230.1	230.7	238.4	233.8	241.8
38	251.5	257.1	250.6	251.4	251.5	248.8	258.3	248.1
39	267.7	268.1	273.4	270.6	274.8	266.6	265.8	264.3
40	276.6	276.9	277.2	275.1	276.8	277.2	276.3	276.0
41	282.2	284.7	277.7	278.7	280.5	284.6	280.2	283.4
42	298.2	289.4	284.9	291.0	289.6	288.5	288.4	299.9
43	303.3	303.5	302.6	303.9	305.1	302.6	301.2	304.9
44	316.9	308.2	311.7	313.8	310.2	311.6	310.8	316.3
45	329.5	327.6	333.5	333.6	331.4	329.7	326.9	330.8
46	331.1	333.5	334.6	334.3	335.1	334.2	333.7	334.3
47	339.2	336.4	337.1	343.3	338.7	337.1	337.9	335.5
48	343.2	340.8	346.2	349.0	342.4	345.3	343.6	342.2
49	358.7	360.2	360.5	356.5	363.8	351.6	359.3	360.1
50	368.4	366.7	372.6	360.8	372.1	369.5	371.3	365.5
51	380.7	382.8	377.7	374.0	374.3	377.0	374.0	374.8
52	384.0	384.4	386.2	384.7	384.1	385.6	388.4	383.9
53	394.9	396.2	392.0	400.1	398.7	395.7	395.6	393.4
54	403.5	400.6	400.9	404.1	402.7	402.1	396.7	405.5
55	406.2	404.8	407.1	406.6	407.4	404.6	406.3	409.9
56	416.9	417.8	414.0	416.4	410.1	418.2	418.3	416.7
57	418.4	419.7	418.1	418.0	418.3	418.5	419.2	417.1
58	419.9	419.9	419.0	419.0	418.9	421.0	420.7	419.7
59	422.5	421.5	421.1	420.8	421.4	424.1	424.0	421.3
60	426.1	425.1	425.0	424.4	424.9	425.8	425.2	425.1
61	431.2	427.4	427.1	427.0	428.5	426.9	426.4	426.0
62	438.5	438.8	437.0	437.3	437.5	437.3	437.6	438.4
63	438.9	440.3	440.9	440.2	440.6	440.3	440.4	439.8
64	444.0	442.7	444.2	443.3	443.9	441.7	442.9	444.2
65	449.5	449.9	446.5	443.8	447.0	444.7	444.4	449.6

66	451.5	453.2	455.1	451.6	451.1	452.9	453.9	450.6
67	467.2	464.8	466.2	472.8	470.7	470.3	470.5	466.7
68	486.2	487.2	486.2	489.3	487.5	487.3	486.9	486.6
69	500.9	501.8	501.0	501.6	502.3	501.4	502.3	501.5
70	505.8	506.0	505.2	505.8	506.0	505.9	506.5	506.3
71	510.5	509.9	509.6	506.1	508.1	508.1	507.1	510.0
72	515.7	515.9	516.1	514.9	515.3	515.7	515.8	515.5
73	524.0	522.6	523.2	521.9	523.6	522.6	522.6	522.0
74	532.9	533.5	533.8	533.3	533.4	533.6	533.4	533.3
75	535.3	534.3	534.7	535.8	534.7	534.4	534.1	534.9
76	543.4	548.2	547.0	544.0	547.0	547.0	547.5	545.0
77	549.2	548.5	548.6	547.2	548.4	548.6	548.7	548.4
78	551.6	548.8	549.9	549.6	550.2	551.2	550.3	551.0
79	554.4	553.2	553.3	553.1	553.7	553.7	553.3	553.2
80	568.9	569.0	568.6	568.3	569.6	569.3	569.4	569.2
81	572.0	570.5	571.1	571.9	569.9	570.3	570.1	570.9
82	584.5	589.2	584.3	585.0	585.0	589.2	589.1	585.2
83	631.9	631.1	631.4	631.2	631.8	631.2	631.3	631.3
84	633.9	631.7	633.9	635.1	634.2	631.8	631.5	634.5
85	644.3	642.7	644.6	645.0	644.5	643.2	643.3	644.1
86	645.9	645.5	646.4	646.5	646.8	645.9	646.1	645.7
87	651.5	650.4	652.0	651.7	651.8	650.7	650.5	651.5
88	653.6	654.1	653.9	653.9	653.7	654.0	654.2	653.9
89	657.0	656.7	657.1	658.0	656.9	656.7	656.9	658.0
90	666.3	666.8	666.7	665.6	667.1	667.1	666.2	666.5
91	668.1	676.8	675.9	674.3	674.1	669.8	672.0	673.8
92	675.9	678.4	676.6	681.1	675.7	678.2	678.6	674.3
93	684.6	684.8	685.4	684.9	684.6	684.5	684.9	685.5
94	687.0	686.1	685.8	685.3	686.2	685.8	685.8	685.9
95	706.1	701.8	705.4	706.2	705.8	701.7	701.9	706.0
96	712.5	706.7	712.0	711.7	712.2	706.8	706.5	712.3
97	712.8	712.3	712.7	712.3	712.4	711.8	712.0	712.4
98	714.3	712.8	714.5	712.5	714.3	712.7	713.0	712.9
99	714.5	715.6	715.9	716.0	715.4	715.2	716.0	715.3
100	726.3	726.2	726.5	726.3	726.4	726.2	726.4	726.0
101	737.0	735.9	736.6	735.5	736.7	735.9	735.5	736.2
102	743.6	743.4	743.3	742.9	743.1	743.0	743.3	743.4
103	749.4	749.5	749.2	748.8	749.0	749.1	749.0	749.3
104	749.8	749.7	749.9	749.3	749.8	749.5	749.9	749.7
105	781.9	784.3	782.6	783.1	781.7	784.1	783.9	783.3
106	784.7	797.6	783.9	784.2	784.2	798.0	797.8	783.8
107	816.7	816.2	817.0	816.4	816.6	816.5	816.5	816.4
108	822.2	819.0	822.0	821.5	822.4	820.6	819.3	820.0
109	823.4	821.5	824.7	824.6	824.3	821.2	821.0	824.9
110	829.1	829.6	828.5	830.3	829.0	829.6	829.3	830.6
111	830.5	832.0	831.0	833.6	831.7	832.6	833.8	831.1
112	833.8	834.3	834.1	835.7	833.9	834.4	834.8	835.3

113	835.3	837.2	835.8	836.1	835.4	836.9	836.7	837.3
114	837.5	838.9	837.8	837.3	836.7	838.3	838.3	839.0
115	839.1	839.7	839.1	840.2	838.8	840.1	840.1	839.5
116	846.2	846.2	847.4	849.0	847.0	846.1	846.4	847.1
117	849.5	849.7	849.1	849.2	850.4	849.6	849.1	850.0
118	850.6	850.4	852.0	851.9	851.5	850.9	851.3	850.9
119	856.1	855.7	856.0	854.4	855.8	855.2	855.3	854.2
120	858.3	857.4	857.1	855.7	856.9	855.8	856.2	857.3
121	859.3	858.8	858.2	857.5	858.1	859.0	858.6	858.8
122	866.9	868.8	866.9	866.8	866.9	868.9	869.0	866.6
123	887.8	884.2	887.9	884.5	887.9	884.5	884.9	884.5
124	894.6	890.7	894.5	890.6	894.7	890.8	890.7	890.0
125	912.6	912.5	913.2	912.5	912.1	912.3	912.5	912.4
126	913.1	913.1	913.4	913.3	913.4	913.3	913.0	913.0
127	931.3	930.7	930.4	929.9	930.4	930.3	930.0	930.9
128	931.5	931.3	931.4	931.0	931.0	931.3	931.6	931.4
129	935.5	936.0	935.8	936.3	936.1	936.2	935.8	935.7
130	935.8	936.2	936.3	936.8	936.5	936.5	936.3	936.3
131	937.8	937.8	938.1	937.5	937.7	937.4	937.7	938.1
132	952.3	953.1	953.3	955.9	953.4	954.5	953.5	954.1
133	963.1	963.8	954.5	959.4	959.7	962.3	960.3	955.6
134	967.5	965.8	963.6	963.7	963.4	963.9	964.0	964.1
135	968.3	967.5	967.3	967.1	967.2	966.6	967.7	967.8
136	968.9	968.6	968.2	968.7	968.5	968.9	968.9	968.8
137	973.4	974.0	974.1	974.2	973.7	974.1	974.4	973.9
138	980.4	980.5	980.9	980.7	980.8	980.6	980.3	980.5
139	981.2	981.5	981.4	981.3	981.4	981.4	981.3	981.5
140	982.2	981.8	982.1	981.9	981.8	982.0	982.2	981.7
141	982.3	982.5	982.3	982.3	982.1	982.5	982.7	982.2
142	985.5	986.8	985.5	984.6	985.5	986.4	986.6	984.4
143	995.1	995.4	994.6	995.3	995.1	995.4	995.4	995.4
144	995.9	996.9	995.8	996.4	996.0	996.8	997.0	996.2
145	1005.6	1005.4	1005.9	1004.7	1005.7	1005.4	1004.4	1005.2
146	1025.2	1025.6	1025.2	1025.3	1025.3	1025.0	1025.1	1025.3
147	1028.4	1029.0	1028.9	1029.1	1028.9	1028.8	1027.9	1029.0
148	1029.1	1029.2	1029.3	1029.3	1029.1	1029.0	1029.2	1029.5
149	1029.8	1029.5	1029.6	1029.6	1029.7	1029.6	1029.6	1029.8
150	1041.7	1041.8	1042.3	1040.9	1041.6	1042.5	1042.0	1040.6
151	1044.4	1044.1	1044.3	1044.2	1044.2	1044.2	1044.2	1044.3
152	1045.1	1044.9	1044.8	1044.9	1044.8	1044.7	1044.9	1045.0
153	1075.5	1076.5	1075.5	1075.3	1075.5	1076.5	1076.5	1075.3
154	1082.1	1082.2	1083.4	1082.3	1082.5	1082.2	1082.3	1082.3
155	1082.4	1083.7	1084.0	1083.4	1083.7	1083.5	1083.6	1083.5
156	1117.1	1117.4	1117.9	1117.4	1117.3	1117.0	1117.1	1117.0
157	1117.1	1117.7	1118.1	1118.2	1118.0	1118.0	1117.8	1117.8
158	1140.9	1142.1	1141.3	1141.9	1141.2	1141.7	1142.0	1142.2
159	1145.0	1147.7	1145.8	1148.1	1145.7	1147.8	1147.3	1147.3

160	1147.2	1148.8	1148.2	1148.8	1147.8	1148.9	1148.3	1148.6
161	1148.7	1149.2	1149.1	1149.6	1149.0	1149.5	1149.5	1149.0
162	1159.4	1159.2	1159.4	1159.5	1159.4	1159.3	1159.1	1159.2
163	1160.3	1160.1	1160.0	1160.2	1160.1	1160.2	1159.8	1160.0
164	1172.4	1173.5	1172.6	1172.9	1172.4	1174.2	1173.5	1172.3
165	1187.6	1187.7	1187.9	1187.6	1187.6	1187.7	1187.8	1187.8
166	1190.5	1190.6	1190.8	1190.3	1190.7	1191.0	1190.7	1190.8
167	1192.2	1192.2	1192.5	1192.0	1192.3	1192.4	1192.3	1192.4
168	1201.9	1202.3	1202.2	1201.9	1202.4	1201.9	1201.0	1202.1
169	1203.6	1204.7	1204.1	1204.2	1204.0	1204.5	1204.0	1204.5
170	1208.5	1209.2	1209.3	1209.6	1209.0	1209.2	1209.5	1208.9
171	1219.9	1216.2	1219.9	1220.9	1219.9	1216.3	1216.0	1221.0
172	1222.7	1220.9	1223.8	1223.7	1223.4	1221.0	1220.7	1223.7
173	1226.0	1226.5	1226.7	1226.9	1226.4	1226.5	1226.6	1226.2
174	1250.4	1253.3	1249.9	1253.7	1250.5	1252.2	1252.1	1253.5
175	1267.7	1259.6	1267.1	1266.3	1267.9	1259.2	1259.0	1266.5
176	1269.2	1269.5	1269.3	1269.4	1269.1	1269.0	1268.8	1269.2
177	1269.8	1269.5	1269.8	1269.7	1269.3	1269.4	1269.5	1269.2
178	1272.6	1281.5	1273.2	1272.6	1272.7	1281.8	1281.5	1272.6
179	1286.0	1285.5	1284.7	1285.0	1285.3	1285.3	1285.1	1285.5
180	1288.0	1287.4	1286.9	1287.4	1287.3	1287.4	1287.5	1287.5
181	1290.5	1290.4	1290.1	1290.3	1290.1	1290.4	1290.2	1290.3
182	1293.6	1294.5	1295.2	1294.7	1293.8	1294.5	1294.4	1293.9
183	1295.6	1295.3	1296.3	1295.5	1295.6	1295.3	1295.0	1295.3
184	1297.9	1298.2	1298.5	1297.8	1297.8	1298.2	1297.5	1297.9
185	1302.4	1301.3	1301.3	1301.4	1301.4	1300.7	1301.0	1302.3
186	1303.6	1303.2	1303.6	1303.6	1303.6	1303.3	1303.2	1303.6
187	1321.3	1321.2	1321.2	1321.5	1321.3	1321.2	1321.3	1321.0
188	1325.8	1325.7	1325.9	1324.7	1325.8	1325.6	1325.5	1324.8
189	1330.7	1331.5	1330.8	1331.1	1330.8	1331.4	1331.4	1331.0
190	1333.3	1333.7	1333.5	1333.4	1333.4	1333.5	1333.5	1333.5
191	1348.8	1349.1	1348.9	1348.6	1348.9	1348.9	1349.2	1348.4
192	1351.9	1352.4	1352.0	1352.2	1352.1	1352.4	1352.3	1351.9
193	1352.2	1352.8	1352.5	1352.7	1352.3	1352.9	1352.5	1352.2
194	1358.5	1360.3	1357.5	1360.9	1358.8	1358.7	1358.2	1360.8
195	1370.6	1370.9	1370.8	1371.1	1370.6	1371.3	1371.0	1370.0
196	1372.5	1373.7	1372.2	1373.8	1372.6	1373.1	1372.6	1373.9
197	1390.6	1390.9	1391.0	1390.9	1391.1	1390.9	1390.7	1390.7
198	1390.9	1391.8	1392.0	1391.6	1391.5	1391.5	1392.0	1391.1
199	1394.1	1394.3	1395.1	1394.5	1393.5	1393.7	1393.5	1393.5
200	1395.1	1394.6	1395.3	1394.9	1395.2	1394.8	1393.7	1394.6
201	1407.8	1405.3	1407.7	1406.9	1407.4	1405.6	1405.4	1405.7
202	1408.9	1418.9	1410.3	1409.9	1409.7	1419.2	1418.5	1409.8
203	1430.4	1435.5	1431.0	1430.0	1430.4	1436.3	1435.8	1429.6
204	1440.7	1441.0	1440.7	1440.8	1440.8	1440.9	1440.7	1440.9
205	1446.6	1447.3	1448.1	1447.9	1447.2	1447.2	1447.7	1446.6
206	1450.4	1448.0	1450.1	1450.9	1450.2	1448.1	1447.9	1451.5

207	1455.7	1454.8	1455.3	1455.5	1455.7	1455.0	1454.4	1455.6
208	1458.5	1458.1	1458.2	1458.2	1458.1	1458.0	1458.1	1458.4
209	1460.5	1458.7	1460.3	1460.5	1460.4	1458.8	1458.5	1460.9
210	1480.0	1464.5	1480.8	1479.6	1480.3	1464.6	1464.0	1479.4
211	1489.1	1489.4	1489.6	1489.9	1489.5	1489.1	1489.5	1489.5
212	1489.5	1489.9	1489.9	1490.3	1489.8	1490.0	1489.7	1489.6
213	1492.2	1492.1	1492.3	1492.4	1492.1	1492.4	1492.1	1492.2
214	1492.6	1492.7	1492.8	1492.9	1492.3	1492.6	1492.6	1492.5
215	1517.1	1517.4	1517.2	1517.5	1517.4	1517.5	1517.4	1516.9
216	1518.5	1517.9	1518.0	1518.5	1518.2	1518.0	1518.3	1518.4
217	1533.3	1532.9	1533.9	1531.3	1533.7	1532.6	1532.5	1531.0
218	1536.4	1541.6	1536.5	1539.6	1536.4	1541.6	1541.1	1539.5
219	1541.9	1542.5	1542.1	1542.2	1542.4	1542.5	1542.2	1542.1
220	1542.6	1548.0	1542.5	1542.3	1542.5	1548.0	1548.1	1542.4
221	1548.3	1550.5	1548.3	1548.5	1548.3	1550.5	1550.5	1548.2
222	1577.9	1577.8	1578.2	1579.4	1578.2	1577.9	1577.5	1579.4
223	1581.6	1580.8	1581.7	1582.1	1581.8	1580.7	1580.6	1582.0
224	1594.3	1594.3	1594.5	1594.7	1594.4	1594.4	1594.6	1594.3
225	1595.8	1595.6	1595.6	1595.5	1595.9	1595.4	1595.2	1595.7
226	1613.1	1609.3	1613.4	1613.5	1613.2	1609.2	1609.1	1613.4
227	1625.5	1625.0	1625.3	1624.8	1625.4	1624.8	1625.1	1624.5
228	1625.6	1625.7	1625.5	1625.3	1625.8	1625.7	1625.6	1625.4
229	1627.9	1626.2	1627.9	1626.1	1628.1	1626.2	1626.0	1626.2
230	1630.4	1633.1	1630.7	1632.2	1630.8	1632.9	1632.5	1632.3
231	1639.2	1639.3	1639.4	1639.6	1639.4	1639.3	1639.4	1639.2
232	1641.4	1643.2	1641.5	1641.3	1641.5	1643.2	1642.9	1641.3
233	1646.9	1647.7	1647.1	1647.1	1647.1	1647.8	1647.7	1646.8
234	1652.8	1652.8	1652.8	1652.5	1652.9	1652.8	1652.6	1652.6
235	1679.6	1680.8	1679.5	1680.8	1679.8	1680.6	1680.4	1680.7
236	1783.4	1783.1	1783.3	1783.4	1783.3	1783.2	1782.9	1783.2
237	2326.1	2325.8	2326.1	2326.0	2326.2	2325.6	2326.0	2326.1
238	3022.4	3022.6	3022.3	3022.6	3022.8	3022.2	3022.6	3022.2
239	3022.6	3022.7	3022.7	3023.3	3023.1	3023.0	3022.7	3022.4
240	3034.1	3033.9	3033.7	3034.4	3034.3	3034.1	3033.9	3033.7
241	3034.2	3034.6	3034.1	3034.6	3034.4	3034.5	3034.2	3033.7
242	3118.2	3118.6	3118.8	3119.1	3118.8	3117.8	3118.3	3119.1
243	3118.8	3119.5	3119.1	3119.5	3119.7	3118.9	3119.0	3119.7
244	3120.9	3121.1	3120.3	3120.8	3120.7	3120.9	3119.9	3120.6
245	3122.0	3121.3	3120.7	3121.3	3121.2	3122.4	3121.6	3121.7
246	3134.2	3134.5	3133.8	3134.1	3134.4	3134.5	3134.8	3134.3
247	3137.6	3135.2	3141.2	3136.5	3136.6	3138.0	3136.5	3137.0
248	3143.6	3143.2	3143.6	3143.0	3143.8	3143.1	3143.5	3143.3
249	3156.0	3156.9	3158.1	3156.7	3156.6	3156.6	3155.1	3157.3
250	3161.1	3161.4	3161.0	3161.0	3161.5	3161.1	3161.8	3161.0
251	3165.8	3168.5	3165.5	3169.0	3165.9	3168.8	3168.8	3168.9
252	3169.3	3169.0	3168.4	3169.6	3168.6	3169.3	3169.0	3169.4
253	3169.5	3171.9	3168.5	3172.2	3169.7	3173.5	3172.7	3173.2

254	3172.4	3174.4	3174.0	3174.5	3171.2	3174.4	3174.2	3174.9
255	3175.6	3175.7	3175.9	3175.7	3175.8	3175.1	3175.0	3175.8
256	3184.9	3183.2	3185.4	3181.9	3185.3	3183.1	3182.9	3181.7
257	3185.1	3185.1	3185.6	3185.3	3185.3	3185.0	3185.3	3184.7
258	3188.5	3185.4	3188.3	3185.5	3188.7	3185.4	3185.6	3185.0
259	3191.9	3191.7	3191.5	3191.7	3191.5	3191.8	3191.6	3192.0
260	3192.0	3192.1	3191.7	3191.9	3192.3	3192.1	3191.9	3192.1
261	3193.2	3192.9	3193.1	3192.9	3193.0	3192.9	3193.1	3193.2
262	3194.5	3194.1	3194.4	3194.2	3194.4	3194.0	3194.2	3194.5
263	3194.9	3196.7	3195.0	3195.0	3194.8	3196.7	3196.8	3195.4
264	3217.2	3217.6	3221.0	3217.7	3218.7	3216.4	3217.9	3217.6
265	3217.5	3221.6	3222.0	3223.6	3221.1	3223.7	3222.4	3221.1
266	3245.6	3244.4	3246.1	3244.6	3245.9	3243.9	3244.2	3244.0
267	3257.4	3257.4	3257.5	3257.3	3257.5	3257.5	3257.5	3257.4
268	3257.5	3257.4	3257.6	3257.6	3257.6	3257.6	3257.7	3257.5
269	3588.2	3591.8	3591.4	3589.6	3589.3	3592.3	3589.5	3589.7
270	3768.0	3768.0	3767.6	3767.8	3767.9	3767.7	3768.5	3767.7

in dichloromethane

Freq. #	conf1	conf2	conf3	conf6	conf7	conf8	conf9	conf10
1	5.6	4.5	5.9	1.7	5.5	4.1	6.3	3.8
2	9.2	7.7	6.8	4.8	8.0	7.2	7.2	7.9
3	9.6	9.2	9.4	6.1	9.2	9.0	8.7	8.9
4	10.9	10.1	10.6	7.6	11.4	10.6	10.9	10.3
5	13.5	13.2	11.9	10.7	12.9	14.1	13.1	11.3
6	16.4	14.2	13.7	13.5	14.5	14.8	13.7	15.4
7	17.9	18.3	15.6	14.2	17.6	17.3	19.2	15.5
8	24.0	22.4	24.4	22.7	24.2	22.1	22.2	23.6
9	30.1	25.7	28.8	29.2	30.7	27.0	30.3	25.8
10	34.3	33.5	33.9	32.4	34.5	32.7	33.7	32.0
11	37.8	39.0	39.8	35.6	36.7	35.2	39.9	39.0
12	48.3	43.3	42.0	44.1	42.5	44.5	43.1	45.0
13	54.2	50.8	54.1	53.7	54.8	50.8	51.9	51.5
14	59.3	52.4	56.8	54.3	57.3	51.2	53.3	53.3
15	61.2	57.4	61.4	59.8	62.4	58.9	60.6	60.1
16	65.3	62.3	62.5	60.8	63.2	63.0	61.0	62.6
17	67.9	65.4	66.6	65.9	67.1	65.1	68.4	67.4
18	73.4	73.4	70.0	70.3	71.8	71.0	73.0	72.9
19	74.1	76.5	72.9	74.9	74.9	77.0	75.7	75.4
20	80.8	83.1	83.6	83.2	83.1	84.0	84.5	80.1
21	88.7	87.4	86.7	87.8	86.2	88.6	89.6	87.1
22	90.1	93.5	97.1	93.8	94.4	94.4	95.1	89.5
23	98.7	96.7	100.8	101.0	100.0	97.8	97.9	96.8
24	111.7	111.0	110.3	110.5	110.1	109.8	110.0	109.8
25	112.1	112.5	110.8	111.0	112.2	113.4	113.3	112.0
26	115.3	125.7	115.5	124.3	115.2	123.7	125.8	126.2

27	139.9	139.0	136.5	134.2	139.3	138.7	143.1	139.3
28	148.7	147.9	146.3	149.7	144.7	144.6	146.3	145.7
29	152.4	150.1	149.3	151.5	149.9	149.0	150.9	148.1
30	158.1	154.7	157.2	155.8	157.3	155.0	154.2	157.4
31	175.4	173.4	168.1	173.9	171.2	171.5	173.0	175.0
32	178.0	178.1	173.6	175.6	181.1	179.0	178.5	177.4
33	191.9	187.1	194.6	193.6	191.6	190.0	184.0	192.6
34	200.5	208.5	210.1	210.6	210.5	210.4	210.5	203.3
35	212.4	213.7	219.9	212.9	216.4	218.5	220.9	211.9
36	224.3	225.4	222.5	223.5	222.8	224.2	229.8	220.1
37	241.2	239.2	239.7	229.7	230.2	237.9	233.5	241.2
38	251.3	256.9	250.3	251.0	251.3	248.8	258.3	247.7
39	267.7	267.4	273.3	270.5	274.6	266.5	265.3	264.1
40	277.1	277.2	276.9	275.0	277.1	277.1	276.5	276.3
41	282.2	284.2	277.9	278.5	280.5	284.1	280.5	282.9
42	297.6	289.3	284.6	290.6	289.0	288.4	288.3	299.5
43	302.4	302.8	302.0	302.7	304.5	302.1	301.1	304.2
44	316.8	307.8	311.4	313.0	309.6	311.1	310.7	315.9
45	328.8	327.1	332.6	332.5	330.7	328.8	326.6	330.2
46	330.3	332.8	333.4	333.2	334.2	333.7	333.1	333.2
47	338.1	335.6	337.0	343.5	337.9	336.2	337.2	334.4
48	343.1	340.1	345.6	348.2	342.6	344.8	343.8	341.7
49	358.4	360.0	360.6	356.2	363.2	350.9	358.8	359.9
50	368.2	366.4	372.4	360.3	372.0	369.1	371.3	365.2
51	380.8	382.8	377.8	373.2	374.4	376.8	374.1	374.4
52	384.0	384.6	386.3	385.5	384.1	385.3	388.6	384.0
53	395.0	395.6	391.6	399.5	398.4	395.2	395.4	393.0
54	403.0	400.2	400.5	403.8	402.4	401.9	396.7	405.4
55	406.6	404.8	407.1	406.5	407.2	405.1	406.2	409.5
56	416.4	418.0	413.4	416.2	409.8	418.3	418.8	416.2
57	418.7	419.3	418.3	418.1	418.4	418.6	419.4	417.3
58	419.8	419.8	418.9	418.7	418.9	420.8	420.8	419.7
59	422.5	421.5	421.2	420.8	421.4	423.9	423.6	421.4
60	426.0	425.0	424.9	424.4	424.7	425.3	425.1	423.8
61	431.3	427.6	426.8	427.2	427.9	426.3	426.6	426.0
62	438.1	438.5	436.5	437.1	437.2	436.8	437.4	438.1
63	438.6	439.9	440.4	439.8	440.1	439.9	439.9	439.3
64	444.6	443.3	444.7	443.0	444.3	442.2	443.5	444.6
65	449.1	449.6	446.0	444.7	446.8	444.2	444.0	449.2
66	450.9	452.8	454.8	451.2	450.7	452.6	453.4	450.2
67	466.8	464.6	465.9	473.0	470.2	469.7	470.3	466.2
68	486.1	487.0	486.2	488.4	487.4	487.8	486.8	486.3
69	500.8	501.7	501.1	501.4	501.9	501.5	502.7	501.2
70	507.8	507.8	507.4	505.2	507.8	508.1	507.1	508.6
71	510.6	509.8	509.7	508.5	508.2	508.8	508.8	509.9
72	515.9	515.7	516.3	515.3	515.4	515.4	516.1	515.2
73	523.9	522.3	523.2	522.3	523.6	521.8	523.0	521.6

74	532.7	533.2	533.8	533.1	533.3	533.6	533.5	533.1
75	535.1	534.2	534.5	535.5	534.6	534.1	534.1	534.8
76	542.6	542.9	543.8	543.2	545.8	542.1	546.4	542.5
77	544.8	547.8	546.4	543.6	546.2	546.3	547.2	544.2
78	550.8	547.9	549.4	549.0	547.8	547.9	548.1	550.4
79	554.0	552.9	553.1	552.8	553.3	553.2	553.0	552.8
80	568.5	568.7	568.2	567.8	569.1	568.7	569.1	568.7
81	571.6	570.1	570.5	571.4	569.5	570.0	569.8	570.4
82	583.9	588.4	583.6	584.1	584.4	588.4	588.4	584.4
83	631.2	630.3	630.5	630.4	631.1	630.0	630.8	630.3
84	633.5	631.0	633.4	634.3	633.7	631.0	630.9	633.9
85	643.8	642.2	644.0	644.4	644.0	642.8	642.9	643.5
86	645.3	644.9	645.8	645.9	646.3	645.3	645.6	645.1
87	651.0	649.9	651.5	651.1	651.3	650.1	649.9	650.9
88	653.0	653.5	653.3	653.3	653.1	653.4	653.5	653.3
89	656.3	656.1	656.4	657.2	656.2	656.1	656.3	657.2
90	665.7	666.1	666.1	664.9	666.5	666.3	665.7	665.8
91	668.3	674.1	675.8	673.9	673.8	674.9	672.3	673.4
92	675.9	677.8	677.4	674.0	675.7	677.8	678.2	673.8
93	684.3	684.7	685.2	684.7	684.4	684.5	685.1	685.2
94	686.6	686.2	685.6	685.3	686.1	685.6	685.9	685.6
95	705.9	702.0	705.1	705.9	705.6	702.0	702.3	705.7
96	712.4	706.4	711.9	711.5	711.9	706.5	706.2	712.1
97	712.7	712.2	712.8	712.0	712.3	711.7	712.3	712.4
98	714.0	712.8	714.4	712.4	714.3	713.0	713.0	712.8
99	714.5	715.2	715.5	715.5	715.0	714.7	715.7	714.8
100	726.6	726.4	726.7	726.7	726.6	726.5	726.6	726.2
101	736.4	735.3	736.0	734.7	736.1	735.3	734.9	735.5
102	743.5	743.2	743.2	742.7	742.9	742.7	743.3	743.2
103	749.2	749.0	749.2	748.3	748.6	748.6	749.0	749.0
104	749.5	749.5	749.5	749.3	749.5	749.4	749.5	749.4
105	781.3	783.4	781.9	782.5	781.1	783.0	783.2	782.4
106	783.8	796.8	783.2	782.9	783.3	797.0	797.0	783.0
107	816.3	815.8	816.6	816.3	816.2	815.9	816.2	815.8
108	822.0	819.9	821.8	822.7	822.0	820.5	820.1	822.1
109	826.0	822.9	827.2	824.0	826.5	822.8	823.8	824.4
110	829.9	830.1	829.3	831.0	830.1	830.1	830.1	830.2
111	830.5	831.3	831.6	833.2	832.2	832.8	832.7	831.6
112	832.8	832.6	832.8	833.6	832.7	832.9	834.1	833.2
113	833.8	835.8	834.7	834.3	833.3	834.3	834.8	836.0
114	836.5	837.1	836.9	835.6	835.8	836.8	836.9	837.5
115	837.6	839.6	837.4	840.2	837.1	840.1	840.3	839.4
116	845.1	845.1	846.3	847.7	845.9	845.1	845.5	846.0
117	847.5	847.9	847.7	848.2	848.7	848.1	847.9	848.2
118	849.6	848.9	850.8	850.5	850.6	849.7	849.9	850.1
119	855.8	854.9	854.4	853.6	854.2	853.3	854.4	854.0
120	856.4	855.6	856.3	854.7	856.1	855.1	854.8	855.4

121	857.6	856.6	856.6	855.3	856.3	857.0	856.8	857.0
122	867.6	869.3	867.5	867.2	867.5	869.2	869.4	867.1
123	887.1	883.7	887.1	884.2	887.1	883.8	884.2	883.8
124	896.0	892.6	895.8	892.8	896.1	892.6	892.9	892.2
125	912.8	912.9	913.4	912.9	912.7	913.0	913.1	913.0
126	913.4	913.5	913.7	913.5	913.6	913.4	913.3	913.4
127	928.3	927.9	927.6	927.1	927.7	927.5	927.3	928.0
128	928.6	928.5	928.5	928.1	928.1	928.5	928.7	928.5
129	935.2	935.3	935.3	935.4	935.6	935.3	935.2	935.3
130	935.5	935.6	935.7	936.0	935.7	935.8	935.7	935.5
131	937.1	937.1	937.4	936.9	937.2	936.8	937.1	937.4
132	958.2	958.2	957.6	959.1	958.4	958.5	959.7	956.2
133	965.0	965.7	959.5	964.0	961.5	963.8	965.1	958.5
134	968.9	968.4	965.5	965.5	965.1	965.7	965.9	966.1
135	969.5	969.0	968.4	968.3	967.8	967.8	968.9	968.6
136	970.7	969.2	969.2	969.4	969.3	969.5	969.7	969.4
137	976.0	976.4	976.6	976.9	976.2	976.5	976.8	976.6
138	980.7	980.7	980.4	980.3	980.7	980.3	980.4	980.6
139	981.3	980.8	981.3	981.0	981.1	980.9	980.9	981.1
140	981.8	981.6	982.0	981.5	981.5	981.7	981.7	982.1
141	982.1	982.4	982.8	982.7	982.5	982.7	983.7	982.5
142	986.5	987.3	986.4	987.1	986.4	987.2	987.2	985.6
143	995.7	995.0	995.3	994.3	995.6	995.4	995.8	995.1
144	996.4	996.9	995.9	997.1	996.2	996.7	997.3	996.8
145	1007.2	1006.4	1006.8	1006.4	1007.2	1006.5	1006.0	1007.2
146	1024.6	1024.7	1024.6	1024.5	1024.6	1024.5	1024.3	1024.7
147	1027.6	1027.5	1027.9	1027.7	1027.7	1027.5	1027.4	1027.6
148	1028.1	1028.0	1028.2	1028.1	1028.2	1027.9	1027.8	1028.2
149	1028.2	1028.4	1028.5	1028.2	1028.3	1028.0	1028.0	1028.7
150	1040.2	1040.0	1040.3	1040.2	1040.2	1040.0	1040.0	1039.8
151	1041.0	1040.8	1040.9	1040.2	1040.9	1040.9	1041.0	1040.1
152	1041.4	1041.3	1041.5	1040.8	1041.2	1041.4	1041.4	1041.1
153	1076.6	1076.9	1077.9	1076.9	1077.1	1076.9	1076.9	1077.1
154	1077.0	1078.3	1078.3	1077.7	1078.2	1078.0	1077.9	1078.0
155	1079.5	1080.5	1079.5	1079.3	1079.5	1080.4	1080.4	1079.3
156	1115.4	1116.0	1116.4	1115.9	1115.9	1115.9	1115.9	1115.7
157	1115.8	1116.4	1116.5	1116.9	1116.8	1116.5	1116.5	1116.3
158	1139.9	1140.7	1140.2	1140.7	1140.0	1140.5	1140.8	1140.9
159	1144.4	1146.3	1144.8	1146.7	1144.8	1146.5	1146.1	1145.9
160	1145.7	1147.4	1146.7	1147.2	1146.5	1147.5	1147.0	1147.3
161	1147.2	1147.8	1147.4	1148.2	1147.5	1148.0	1147.6	1147.6
162	1157.6	1157.6	1157.7	1157.8	1157.6	1157.6	1157.6	1157.5
163	1158.5	1158.5	1158.4	1158.5	1158.5	1158.6	1158.3	1158.4
164	1168.4	1169.0	1168.6	1168.0	1168.4	1169.3	1169.1	1167.8
165	1186.1	1186.4	1186.4	1186.2	1186.2	1186.3	1186.6	1186.5
166	1188.7	1189.2	1188.9	1188.7	1188.8	1189.1	1189.4	1189.2
167	1190.6	1191.0	1190.9	1190.7	1190.8	1190.9	1191.1	1191.0

168	1201.2	1201.4	1201.4	1200.7	1201.5	1201.1	1200.4	1201.2
169	1203.0	1203.6	1203.3	1203.1	1203.3	1203.5	1203.0	1203.5
170	1206.7	1207.5	1207.6	1208.0	1207.3	1207.5	1207.6	1207.3
171	1219.6	1216.1	1219.5	1219.4	1219.7	1216.2	1216.1	1219.4
172	1222.7	1219.4	1223.3	1223.5	1223.1	1219.4	1219.3	1223.6
173	1224.4	1224.8	1224.9	1225.4	1224.9	1224.8	1224.8	1224.6
174	1250.3	1253.8	1249.8	1253.3	1250.4	1253.1	1252.6	1253.7
175	1267.0	1259.4	1266.4	1264.9	1267.1	1259.2	1258.8	1265.3
176	1268.5	1268.7	1268.7	1268.4	1268.5	1268.8	1268.4	1268.5
177	1268.9	1268.9	1269.2	1268.8	1269.0	1268.9	1269.1	1268.7
178	1272.4	1281.0	1272.4	1272.0	1272.3	1281.1	1280.9	1272.0
179	1285.0	1284.7	1284.0	1284.2	1284.5	1284.4	1284.3	1284.5
180	1287.2	1286.6	1286.2	1286.4	1286.4	1286.5	1286.8	1286.6
181	1289.5	1289.5	1289.1	1289.3	1289.2	1289.5	1289.4	1289.4
182	1292.4	1293.4	1293.8	1293.2	1292.9	1293.4	1293.2	1292.6
183	1295.2	1295.1	1295.4	1294.7	1295.2	1295.1	1294.7	1295.1
184	1297.5	1297.7	1297.7	1296.8	1297.4	1297.7	1296.7	1297.6
185	1299.7	1299.1	1299.6	1299.4	1299.3	1298.8	1299.3	1299.8
186	1302.9	1302.4	1302.9	1302.6	1303.0	1302.3	1302.3	1302.6
187	1320.0	1319.8	1319.8	1320.1	1320.0	1319.9	1319.9	1319.7
188	1326.2	1325.3	1326.0	1324.6	1326.1	1325.2	1325.2	1324.8
189	1330.2	1330.8	1330.1	1330.5	1330.2	1330.7	1330.6	1330.4
190	1332.9	1333.0	1333.0	1332.9	1333.0	1333.0	1332.9	1332.9
191	1348.1	1348.3	1348.4	1348.2	1348.4	1348.3	1348.6	1347.8
192	1350.7	1351.1	1350.6	1351.2	1351.0	1351.3	1350.7	1350.9
193	1352.2	1352.2	1352.1	1351.8	1352.2	1352.0	1352.2	1351.4
194	1358.7	1360.9	1358.0	1359.6	1359.0	1359.6	1358.6	1361.0
195	1371.5	1371.1	1371.4	1370.9	1371.4	1371.1	1371.1	1370.3
196	1372.8	1374.1	1372.7	1373.3	1372.9	1373.6	1372.9	1374.1
197	1388.6	1388.7	1388.8	1388.5	1389.1	1388.8	1388.7	1388.7
198	1388.9	1389.5	1389.6	1389.1	1389.3	1389.3	1389.4	1389.1
199	1394.7	1394.9	1395.5	1394.8	1394.5	1394.8	1394.4	1394.2
200	1394.9	1395.2	1395.6	1395.1	1395.5	1395.3	1394.6	1395.0
201	1407.7	1404.5	1407.4	1406.5	1407.2	1404.4	1404.7	1405.2
202	1410.7	1419.0	1411.4	1410.6	1411.2	1419.1	1419.0	1410.4
203	1429.9	1435.0	1430.0	1429.0	1429.7	1434.8	1435.2	1428.5
204	1439.0	1439.3	1439.1	1439.0	1439.2	1439.3	1439.0	1439.2
205	1445.1	1445.7	1446.5	1446.2	1445.7	1445.7	1445.8	1445.2
206	1448.5	1446.0	1448.2	1448.5	1448.2	1446.2	1446.2	1449.2
207	1453.8	1453.0	1453.6	1453.6	1453.8	1453.2	1452.7	1453.8
208	1456.8	1456.4	1456.4	1456.4	1456.4	1456.4	1456.3	1456.7
209	1458.7	1457.0	1458.7	1458.9	1458.8	1457.0	1457.1	1459.2
210	1480.2	1463.1	1480.4	1479.1	1480.2	1462.9	1462.8	1479.1
211	1487.2	1487.6	1487.7	1487.9	1487.6	1487.6	1487.8	1487.6
212	1487.6	1487.8	1487.9	1488.1	1487.9	1488.0	1488.0	1487.8
213	1490.1	1490.2	1490.3	1490.5	1490.1	1490.4	1490.4	1490.0
214	1490.4	1490.3	1490.5	1490.6	1490.3	1490.7	1490.4	1490.3

215	1515.2	1515.7	1515.5	1515.8	1515.7	1515.8	1515.7	1515.1
216	1516.6	1516.0	1516.2	1516.5	1516.2	1516.2	1516.4	1516.6
217	1529.3	1531.6	1529.5	1528.4	1529.4	1531.4	1531.3	1528.5
218	1532.8	1540.5	1533.1	1534.9	1533.1	1540.4	1540.1	1534.9
219	1540.6	1540.6	1540.2	1540.4	1540.6	1540.6	1540.4	1540.5
220	1541.5	1545.3	1541.7	1540.6	1541.8	1545.4	1545.1	1540.7
221	1546.8	1546.7	1546.8	1546.9	1546.8	1546.7	1546.9	1546.7
222	1576.8	1576.1	1577.1	1578.1	1577.0	1576.2	1575.8	1578.2
223	1580.5	1579.5	1580.5	1580.4	1580.6	1579.5	1579.4	1580.5
224	1593.1	1593.1	1593.3	1593.4	1593.1	1593.2	1593.4	1593.0
225	1594.9	1594.6	1594.6	1594.4	1594.9	1594.4	1594.2	1594.7
226	1607.3	1603.8	1607.3	1607.3	1607.3	1603.8	1603.7	1607.4
227	1623.5	1623.1	1623.5	1622.8	1623.4	1622.9	1623.3	1622.6
228	1623.6	1623.7	1623.6	1623.2	1623.7	1623.8	1623.6	1623.5
229	1626.5	1624.4	1626.2	1624.0	1626.5	1624.4	1624.2	1624.2
230	1629.5	1631.8	1629.7	1630.9	1629.8	1631.7	1631.4	1631.2
231	1636.9	1637.0	1637.1	1637.3	1637.2	1637.0	1637.2	1636.9
232	1640.1	1641.6	1640.1	1639.7	1640.1	1641.6	1641.4	1639.8
233	1645.2	1645.9	1645.2	1645.1	1645.3	1645.9	1645.9	1645.0
234	1651.0	1650.9	1651.0	1650.6	1651.0	1650.9	1650.8	1650.6
235	1678.1	1679.3	1678.0	1679.0	1678.3	1679.3	1678.9	1679.3
236	1764.4	1764.3	1764.4	1764.4	1764.4	1764.2	1764.1	1764.3
237	2321.4	2321.2	2321.2	2321.3	2321.4	2321.2	2321.5	2321.4
238	3028.9	3029.5	3029.2	3029.4	3029.4	3029.1	3029.6	3029.0
239	3029.2	3029.6	3029.3	3030.1	3029.9	3029.6	3029.6	3029.2
240	3039.8	3040.1	3039.9	3040.3	3040.1	3039.8	3040.2	3039.6
241	3040.0	3040.4	3039.9	3040.8	3040.7	3040.8	3040.4	3039.7
242	3125.4	3125.9	3125.8	3125.9	3125.7	3125.1	3125.3	3125.8
243	3125.7	3126.3	3125.9	3126.3	3126.6	3125.4	3126.5	3125.9
244	3128.0	3128.2	3127.7	3127.8	3127.9	3128.0	3126.9	3128.2
245	3129.0	3128.6	3127.9	3128.5	3128.7	3128.9	3128.5	3128.7
246	3135.8	3135.6	3135.4	3135.5	3135.7	3135.8	3135.8	3135.5
247	3144.0	3141.6	3144.4	3143.5	3143.2	3143.7	3142.9	3142.6
248	3144.5	3144.1	3147.0	3144.3	3144.4	3144.2	3144.2	3144.2
249	3162.0	3161.0	3162.7	3160.0	3162.2	3160.9	3159.9	3161.2
250	3163.1	3162.9	3162.9	3162.7	3163.3	3162.6	3163.2	3162.9
251	3167.0	3169.4	3166.7	3169.6	3167.0	3169.5	3169.5	3169.4
252	3169.7	3169.6	3169.0	3170.0	3169.3	3170.1	3169.8	3170.0
253	3169.9	3174.3	3169.3	3174.2	3170.2	3175.5	3175.5	3175.3
254	3175.2	3176.6	3176.4	3176.3	3174.1	3176.4	3176.1	3176.7
255	3176.8	3177.1	3177.0	3176.9	3176.9	3176.8	3176.7	3177.1
256	3185.5	3183.3	3185.7	3182.1	3185.7	3183.4	3182.7	3182.3
257	3185.7	3185.7	3185.8	3185.6	3186.0	3185.7	3185.6	3185.5
258	3189.5	3185.8	3189.1	3185.7	3189.6	3185.8	3185.7	3185.8
259	3192.1	3192.2	3192.0	3192.2	3191.9	3192.3	3192.1	3192.2
260	3192.4	3192.4	3192.2	3192.5	3192.5	3192.5	3192.4	3192.2
261	3192.9	3192.6	3192.9	3192.8	3192.8	3192.6	3193.0	3192.9

262	3194.4	3194.1	3194.5	3194.4	3194.4	3194.0	3194.4	3194.4
263	3194.9	3196.7	3194.9	3195.1	3194.8	3196.5	3196.7	3195.2
264	3216.2	3216.4	3219.4	3217.5	3218.1	3215.2	3216.3	3216.8
265	3216.6	3220.1	3220.0	3222.5	3219.6	3222.1	3220.7	3219.9
266	3245.0	3243.9	3245.7	3243.9	3245.5	3243.5	3243.6	3243.6
267	3256.0	3256.0	3255.9	3256.1	3256.0	3256.0	3256.0	3255.9
268	3256.0	3256.0	3256.1	3256.2	3256.2	3256.1	3256.2	3256.0
269	3586.3	3587.7	3588.3	3585.9	3586.9	3588.8	3585.0	3586.6
270	3762.2	3761.8	3761.0	3760.8	3762.1	3761.6	3761.8	3761.0

Table S24. Vibrational frequencies (in cm^{-1}) of TEBT-Pyc in toluene and dichloromethane obtained from B3LYP/6-311G(d,p) calculations.

in toluene

Freq. #	conf1	conf3	conf4	conf5	conf8	conf9
1	4.6	2.7	4.4	4.6	2.9	3.8
2	7.2	8.3	7.6	7.7	8.3	7.0
3	8.4	9.3	10.8	8.9	12.8	8.2
4	14.2	15.3	13.3	13.2	14.7	13.3
5	18.4	16.8	18.7	18.3	17.1	18.2
6	21.6	19.9	20.8	20.6	19.0	19.2
7	23.6	23.5	23.7	24.0	21.6	23.9
8	30.4	31.2	30.8	32.8	31.8	30.5
9	35.6	37.1	38.5	36.9	37.4	33.7
10	41.3	39.1	41.1	37.4	39.6	40.9
11	46.2	47.7	46.2	49.9	45.8	45.0
12	50.1	55.2	56.2	51.3	54.5	52.1
13	54.2	57.5	57.9	56.8	56.1	53.5
14	58.3	58.0	59.4	60.0	57.9	54.1
15	66.2	67.2	66.6	63.7	65.5	65.2
16	68.2	68.3	69.5	66.8	69.5	67.6
17	74.3	72.9	73.2	73.8	71.3	72.9
18	78.4	78.8	81.9	79.3	81.9	79.6
19	83.4	84.3	83.4	85.2	86.1	82.8
20	92.2	93.4	90.2	96.9	94.3	92.5
21	97.0	98.9	97.4	101.9	97.8	98.2
22	112.2	112.7	113.5	112.1	113.1	110.5
23	119.8	119.0	119.5	117.2	115.9	117.4
24	133.6	133.9	134.2	129.4	134.5	133.2
25	134.7	141.2	137.6	139.6	141.0	138.6
26	144.4	147.1	142.7	149.9	147.3	146.1
27	147.2	148.4	147.5	152.3	147.4	150.3
28	164.8	158.6	165.7	161.9	157.7	157.2
29	178.1	165.2	177.2	177.1	167.1	169.3
30	181.3	174.1	181.0	194.7	181.4	173.3

31	195.3	199.2	189.5	198.9	193.8	198.6
32	206.2	205.2	204.5	208.1	206.5	205.8
33	214.4	222.8	213.5	214.7	223.2	224.8
34	219.5	233.7	228.8	225.2	232.9	234.7
35	231.6	242.6	234.3	231.1	239.8	240.9
36	240.1	260.0	246.3	247.9	260.5	258.3
37	278.2	261.1	276.4	278.4	265.9	260.1
38	281.7	279.3	277.9	281.4	279.0	278.8
39	300.4	286.5	299.1	298.8	280.9	284.8
40	302.7	300.1	302.1	301.4	300.9	300.2
41	309.5	302.6	305.4	306.5	307.6	301.9
42	327.6	322.9	332.5	327.7	321.9	318.0
43	338.3	333.3	335.4	334.4	330.8	333.5
44	339.4	343.8	340.3	350.4	340.0	346.4
45	347.3	347.6	347.4	354.6	347.4	350.1
46	358.1	360.6	363.7	359.3	358.1	360.4
47	363.9	374.0	371.9	367.4	381.4	373.2
48	382.7	385.6	376.7	379.5	386.8	376.4
49	391.0	389.5	388.0	395.9	390.5	394.2
50	396.3	397.5	396.2	412.4	396.5	399.2
51	410.9	405.1	411.3	417.6	406.1	405.5
52	419.5	420.0	420.0	420.0	419.9	418.9
53	421.1	420.2	421.3	422.1	420.3	420.9
54	425.1	425.4	425.7	425.7	425.1	424.8
55	426.5	428.8	427.2	428.5	427.2	427.0
56	438.4	438.2	437.2	437.9	433.7	438.8
57	439.8	441.2	441.0	442.6	441.1	441.7
58	445.4	449.4	447.9	446.2	442.6	448.6
59	452.9	452.4	452.4	450.6	457.8	449.7
60	472.9	469.6	469.0	468.0	474.4	468.3
61	499.8	501.4	501.2	501.3	499.9	501.3
62	505.8	505.7	505.0	504.5	505.1	505.1
63	513.0	515.8	513.3	514.4	515.3	514.2
64	521.8	521.4	522.0	522.9	521.5	520.3
65	523.7	522.6	524.2	526.8	522.8	523.7
66	529.4	529.4	529.3	531.4	528.7	529.7
67	536.7	536.5	537.0	536.7	536.8	537.3
68	546.0	547.2	547.1	548.3	546.3	546.5
69	550.9	549.6	551.6	552.0	547.9	547.3
70	569.7	569.4	569.9	569.3	569.3	569.0
71	572.5	571.4	572.3	572.2	571.2	571.1
72	603.8	602.8	603.2	604.8	603.7	602.8
73	604.8	604.0	604.9	606.9	604.1	604.2
74	615.9	614.0	615.8	616.2	613.9	613.8
75	618.9	618.8	619.3	622.3	618.6	618.3
76	631.8	631.5	631.7	631.6	630.8	630.6
77	631.8	631.7	632.2	632.2	631.7	631.7

78	643.7	642.8	642.9	636.4	643.6	643.4
79	651.5	651.3	651.4	647.1	651.8	651.5
80	654.7	655.0	654.7	651.8	655.0	654.7
81	658.1	658.9	658.4	656.3	659.1	658.2
82	681.8	679.4	681.9	662.1	679.5	680.6
83	682.5	681.7	682.4	682.5	681.9	682.0
84	685.5	685.6	685.4	684.5	685.4	686.2
85	692.8	695.4	692.6	692.6	695.1	695.7
86	696.1	696.0	696.9	694.9	695.6	696.2
87	710.2	710.2	710.6	708.6	710.8	709.8
88	712.8	712.2	712.9	711.2	712.5	712.4
89	713.2	713.2	713.3	712.6	713.3	714.4
90	727.1	719.8	727.2	726.4	719.6	719.3
91	735.7	735.4	735.8	741.7	735.5	735.1
92	741.8	741.5	741.7	742.5	741.5	741.8
93	747.3	747.4	747.8	747.3	746.4	747.6
94	773.5	773.6	773.4	773.3	774.0	773.5
95	783.9	784.2	784.0	782.3	783.6	783.3
96	784.6	796.3	784.7	784.2	796.4	795.8
97	812.0	811.5	812.1	809.0	811.7	811.5
98	813.8	813.6	813.8	810.4	813.7	813.6
99	817.2	816.8	817.0	817.1	817.0	816.9
100	830.2	829.7	830.4	829.5	830.1	829.9
101	834.0	830.3	833.0	833.6	831.1	830.3
102	835.6	834.0	834.0	834.0	834.7	834.1
103	836.0	837.2	837.6	836.5	836.0	837.6
104	840.6	841.3	841.1	839.1	841.6	840.8
105	846.9	846.3	847.1	845.7	847.7	847.0
106	850.7	849.8	849.8	849.6	850.8	850.4
107	857.2	858.6	857.8	858.2	857.4	857.5
108	858.1	859.5	858.8	859.1	859.4	858.9
109	862.6	864.2	862.6	860.8	863.9	863.8
110	879.0	878.6	879.2	867.7	879.1	878.8
111	898.1	898.3	898.1	901.8	898.7	898.2
112	902.8	902.5	902.8	906.3	902.4	902.2
113	911.8	912.1	912.5	912.1	912.6	912.1
114	914.1	913.8	914.0	913.7	914.0	914.0
115	930.6	931.4	931.8	931.3	931.0	931.1
116	936.9	936.3	935.9	936.3	936.0	936.9
117	943.7	943.7	944.0	943.2	944.6	943.3
118	954.8	963.9	956.6	960.2	959.2	956.2
119	963.7	965.3	964.0	964.1	964.7	964.5
120	967.9	968.7	967.7	968.1	967.9	968.2
121	969.4	970.2	968.4	969.0	970.1	969.3
122	974.6	974.5	974.4	974.5	974.9	974.8
123	980.4	980.5	981.0	979.9	981.7	980.7
124	982.1	981.8	981.9	981.7	982.0	982.0

125	982.1	982.3	982.6	982.4	982.4	982.1
126	995.4	995.6	994.7	995.8	995.7	995.1
127	998.8	998.6	998.8	998.2	999.1	998.5
128	1001.7	1001.5	1002.1	1005.8	1002.0	1002.0
129	1004.3	1005.2	1004.5	1007.7	1005.7	1004.1
130	1013.9	1014.1	1013.9	1013.9	1014.1	1013.9
131	1024.5	1024.6	1024.5	1025.3	1024.6	1024.6
132	1029.8	1029.4	1029.6	1029.3	1029.5	1029.6
133	1033.4	1033.1	1033.3	1035.6	1033.1	1033.1
134	1041.4	1042.2	1041.4	1042.2	1042.3	1041.3
135	1044.7	1044.8	1045.1	1044.8	1044.8	1044.4
136	1047.9	1047.8	1047.9	1047.7	1047.7	1047.9
137	1069.8	1069.8	1069.7	1076.1	1069.9	1069.9
138	1075.6	1076.3	1075.6	1078.9	1076.2	1076.0
139	1079.8	1079.6	1079.5	1082.3	1079.6	1079.8
140	1082.3	1082.4	1082.3	1098.9	1082.4	1083.6
141	1103.8	1103.4	1103.8	1103.5	1103.2	1103.8
142	1104.4	1105.4	1104.2	1115.3	1105.3	1105.0
143	1116.9	1117.1	1117.5	1117.6	1117.6	1118.2
144	1140.1	1140.8	1140.6	1141.1	1140.8	1140.3
145	1143.1	1142.7	1142.8	1142.9	1142.9	1142.7
146	1147.9	1148.4	1148.4	1148.3	1148.9	1147.9
147	1160.0	1159.9	1160.1	1159.8	1160.1	1159.5
148	1173.8	1173.2	1173.7	1174.3	1172.8	1174.6
149	1178.5	1178.0	1178.6	1178.1	1178.2	1178.5
150	1188.2	1188.4	1188.3	1187.5	1188.3	1188.2
151	1191.3	1191.5	1191.5	1191.3	1191.5	1191.3
152	1196.3	1196.0	1196.2	1195.6	1195.9	1196.3
153	1202.8	1203.8	1203.1	1203.3	1203.9	1203.2
154	1206.7	1207.4	1206.4	1206.6	1207.4	1207.3
155	1220.6	1220.5	1220.8	1220.5	1220.7	1220.7
156	1235.6	1222.3	1235.4	1234.2	1222.3	1222.3
157	1248.6	1247.1	1248.4	1252.9	1247.6	1247.1
158	1269.3	1269.3	1269.9	1261.9	1270.1	1269.3
159	1272.4	1281.3	1272.6	1269.5	1281.4	1280.8
160	1286.8	1286.9	1287.3	1272.9	1286.8	1286.0
161	1289.2	1289.8	1289.8	1287.2	1290.2	1289.2
162	1292.8	1292.7	1292.1	1292.8	1291.6	1292.7
163	1296.9	1296.2	1297.3	1293.4	1297.2	1297.0
164	1300.9	1301.8	1301.5	1298.4	1302.0	1301.1
165	1304.9	1304.2	1304.7	1302.0	1304.5	1304.8
166	1311.4	1312.2	1311.3	1315.8	1312.2	1311.8
167	1319.6	1319.6	1319.5	1321.6	1319.5	1319.3
168	1326.1	1326.0	1326.1	1326.6	1326.0	1325.7
169	1330.9	1329.7	1330.8	1329.6	1329.7	1329.4
170	1332.8	1332.5	1332.8	1342.1	1332.6	1332.4
171	1341.3	1341.7	1341.3	1342.7	1341.8	1341.1

172	1344.4	1344.1	1344.4	1349.3	1344.5	1344.6
173	1350.9	1350.6	1351.0	1351.7	1351.1	1350.9
174	1354.7	1355.5	1355.1	1357.8	1355.8	1354.8
175	1358.9	1358.1	1358.8	1360.4	1357.8	1358.8
176	1365.4	1367.4	1365.6	1370.2	1367.4	1367.3
177	1371.9	1371.1	1371.5	1372.5	1370.8	1371.0
178	1390.5	1390.0	1390.4	1386.1	1390.0	1389.9
179	1390.9	1390.9	1391.1	1390.9	1390.9	1391.8
180	1394.5	1393.9	1394.9	1394.5	1395.5	1394.5
181	1405.1	1401.0	1405.0	1403.3	1401.2	1400.9
182	1407.9	1409.2	1408.0	1408.7	1409.3	1408.1
183	1409.7	1418.2	1409.8	1410.1	1418.0	1417.5
184	1433.4	1440.4	1433.3	1434.0	1440.5	1438.9
185	1443.5	1443.9	1443.3	1443.8	1443.8	1443.8
186	1444.7	1445.1	1444.5	1446.6	1445.3	1445.2
187	1455.0	1454.8	1455.4	1455.1	1454.8	1454.2
188	1458.3	1456.5	1458.1	1459.0	1456.8	1455.9
189	1462.2	1458.5	1462.2	1463.6	1458.6	1458.3
190	1478.3	1462.5	1478.5	1478.9	1462.8	1462.3
191	1479.3	1479.1	1479.5	1479.6	1479.2	1478.9
192	1484.8	1484.4	1484.6	1484.6	1484.2	1484.8
193	1489.4	1489.5	1490.1	1490.1	1490.3	1489.8
194	1492.3	1492.1	1492.9	1492.7	1493.1	1492.6
195	1498.4	1498.9	1498.7	1498.8	1498.8	1498.5
196	1518.2	1518.0	1518.0	1518.0	1518.3	1517.6
197	1521.5	1521.3	1521.6	1521.3	1521.4	1521.6
198	1530.5	1534.1	1530.3	1531.9	1534.0	1533.9
199	1537.6	1544.3	1537.4	1536.7	1544.2	1544.1
200	1545.0	1545.9	1545.0	1544.7	1546.2	1545.9
201	1551.6	1554.4	1551.4	1549.9	1554.4	1554.4
202	1584.1	1583.0	1583.9	1583.2	1582.8	1583.6
203	1590.9	1585.1	1590.7	1589.9	1585.1	1584.8
204	1594.8	1594.8	1594.7	1594.4	1595.1	1594.5
205	1605.0	1604.9	1605.0	1598.7	1604.9	1604.8
206	1618.0	1617.8	1618.1	1617.0	1617.7	1617.9
207	1620.2	1620.1	1620.2	1620.0	1620.1	1620.1
208	1626.1	1625.9	1625.9	1625.7	1626.0	1625.6
209	1630.9	1631.0	1630.9	1631.9	1630.9	1631.0
210	1635.6	1635.8	1635.5	1636.6	1635.9	1635.6
211	1644.0	1644.7	1644.0	1643.7	1644.7	1644.7
212	1644.6	1646.7	1644.5	1645.3	1646.5	1646.2
213	1649.5	1649.8	1649.4	1647.5	1649.8	1649.8
214	1674.3	1674.3	1674.3	1671.9	1674.3	1674.3
215	1783.4	1782.9	1783.5	1783.7	1783.0	1783.4
216	2326.4	2326.0	2326.2	2326.4	2325.9	2326.0
217	3022.6	3022.6	3023.0	3022.7	3022.9	3022.5
218	3034.5	3034.3	3034.5	3034.2	3034.5	3033.8

219	3061.8	3061.8	3062.3	3062.8	3061.8	3061.6
220	3118.2	3119.0	3119.4	3118.6	3119.3	3119.0
221	3122.0	3121.5	3121.8	3121.2	3121.3	3120.9
222	3135.1	3136.9	3136.2	3137.8	3136.5	3134.7
223	3138.3	3139.3	3139.0	3139.1	3137.5	3135.3
224	3142.5	3142.3	3142.7	3142.6	3142.0	3142.1
225	3160.9	3161.5	3161.4	3162.7	3161.2	3161.4
226	3163.0	3162.8	3163.1	3163.6	3162.9	3162.7
227	3164.0	3163.9	3164.0	3168.7	3164.1	3163.8
228	3170.0	3168.9	3169.2	3169.4	3170.1	3168.8
229	3171.4	3171.4	3171.5	3171.0	3171.5	3171.3
230	3173.1	3174.6	3173.8	3173.1	3173.3	3171.5
231	3177.5	3177.0	3177.5	3173.9	3177.4	3177.4
232	3178.5	3178.3	3178.6	3175.3	3177.9	3178.1
233	3182.9	3183.7	3182.7	3178.7	3183.9	3183.2
234	3184.7	3184.5	3184.7	3184.5	3184.6	3184.6
235	3185.2	3185.3	3184.9	3185.2	3185.5	3185.3
236	3191.2	3191.1	3191.1	3191.1	3191.0	3191.2
237	3191.6	3191.9	3191.8	3191.6	3192.2	3191.5
238	3193.7	3193.4	3193.6	3192.3	3193.5	3193.5
239	3195.1	3194.6	3195.1	3193.9	3194.9	3194.8
240	3195.2	3195.1	3195.2	3195.0	3195.1	3195.0
241	3196.0	3197.1	3195.9	3195.7	3197.2	3196.1
242	3217.1	3217.2	3217.4	3217.8	3218.3	3220.6
243	3243.8	3243.9	3244.0	3245.4	3243.8	3242.9
244	3257.5	3257.5	3257.5	3257.3	3257.4	3257.6
245	3571.9	3573.3	3571.8	3570.7	3573.0	3573.5
246	3768.6	3767.6	3768.2	3767.8	3767.7	3767.9

in dichloromethane

Freq. #	conf1	conf3	conf4	conf5	conf8	conf9
1	3.9	2.6	4.3	4.4	4.1	3.7
2	7.6	7.3	7.4	7.2	8.4	8.1
3	9.3	8.7	10.6	8.6	13.0	8.6
4	14.5	15.2	13.1	13.2	14.7	13.6
5	18.2	17.7	18.7	18.1	17.2	17.9
6	20.1	19.6	19.2	19.3	19.1	18.6
7	23.5	23.0	23.2	23.8	21.4	23.8
8	30.2	29.9	30.2	32.1	31.1	30.6
9	34.9	36.5	37.9	36.2	36.9	35.0
10	40.8	38.33	339.8	36.8	38.9	40.7
11	45.8	46.8	45.3	49.0	45.5	45.6
12	48.4	53.3	52.6	50.1	50.2	50.5
13	53.4	54.6	55.1	55.6	54.8	52.1
14	56.7	57.0	56.2	56.9	57.7	53.3
15	64.5	66.8	65.4	63.0	65.4	64.9

16	67.8	67.8	69.1	65.4	69.3	67.3
17	74.0	72.7	72.7	73.0	70.8	73.3
18	78.0	77.9	80.9	78.4	80.9	79.0
19	82.5	83.5	82.9	84.3	85.9	82.8
20	92.3	93.8	89.7	96.7	93.9	93.3
21	97.0	98.4	97.2	101.5	98.3	97.5
22	111.9	111.5	112.6	111.5	112.2	109.9
23	119.4	118.9	119.2	117.0	115.7	117.4
24	133.0	133.7	134.1	129.4	134.4	133.2
25	134.3	140.7	137.3	139.7	140.7	138.8
26	144.4	146.7	142.6	149.5	146.9	146.0
27	147.2	147.5	147.3	150.8	147.7	150.0
28	164.8	159.3	165.6	162.3	159.3	158.8
29	178.2	164.7	177.0	177.4	167.3	169.1
30	181.7	174.3	181.3	194.7	181.4	174.1
31	195.0	199.0	189.2	198.4	193.8	198.4
32	205.9	204.9	204.6	208.7	206.6	205.2
33	213.9	222.0	213.1	214.8	222.6	224.5
34	218.8	233.0	228.4	224.4	232.5	234.2
35	231.1	242.3	233.7	230.0	239.8	240.6
36	240.1	259.3	246.1	247.6	260.0	257.9
37	278.4	260.9	276.3	278.4	265.8	259.6
38	281.2	279.7	278.1	281.4	279.5	279.3
39	301.2	286.5	298.6	298.4	280.5	284.6
40	302.2	299.6	302.9	301.8	301.7	300.0
41	309.4	303.6	305.0	306.1	307.5	303.0
42	327.5	322.4	331.8	327.7	321.7	317.6
43	337.7	332.1	335.0	333.2	330.3	332.6
44	338.9	343.8	339.8	350.5	339.2	346.2
45	346.9	347.0	347.1	354.1	347.2	350.1
46	357.6	360.1	363.6	359.6	358.2	360.2
47	363.7	374.2	371.6	366.6	381.3	373.0
48	382.2	385.2	376.4	379.3	386.5	376.3
49	390.4	388.9	387.5	395.1	390.3	393.4
50	396.1	395.9	395.7	412.0	396.0	398.5
51	410.6	405.2	411.3	417.6	406.1	405.6
52	419.4	420.0	420.1	420.0	420.1	419.1
53	420.9	420.2	421.3	421.6	420.5	420.8
54	424.7	425.1	425.3	424.6	425.1	424.3
55	425.8	427.4	426.7	426.9	427.1	426.4
56	438.1	437.7	437.0	437.5	433.6	438.4
57	440.34	3441.4	441.2	442.8	441.6	442.2
58	445.0		447.6	446.6	442.4	448.2
59	452.7	449.3	452.3	450.0	457.5	449.5
60	472.6	452.1	468.8	467.7	474.1	468.3
61	499.6	469.2	500.9	501.2	499.8	501.5
62	507.5	501.4	507.0	506.8	507.2	506.7

63	512.4	515.1	512.6	513.8	514.7	513.8
64	521.0	520.7	520.9	521.4	521.5	519.9
65	523.4	521.6	523.7	526.4	522.3	523.6
66	528.9	529.1	529.2	531.4	528.5	529.4
67	536.5	536.2	536.8	536.3	536.5	537.1
68	544.4	543.7	544.4	545.8	544.0	542.6
69	545.3	546.6	546.4	547.7	545.7	546.9
70	569.4	569.1	569.5	569.0	568.9	568.6
71	572.5	571.3	572.3	572.0	571.2	571.1
72	603.2	602.2	602.6	604.7	603.0	602.4
73	605.1	604.7	605.0	606.4	604.7	604.5
74	615.1	613.3	615.1	615.3	613.3	613.2
75	619.7	619.6	619.8	622.8	619.5	619.1
76	630.6	630.5	630.9	630.7	630.1	630.1
77	631.2	631.1	631.1	631.1	631.1	631.1
78	643.2	642.3	642.4	636.1	643.1	642.9
79	650.9	650.7	650.8	646.4	651.2	650.8
80	654.4	654.5	654.3	651.1	654.7	654.5
81	657.4	658.2	657.7	656.1	658.5	657.5
82	676.3	677.5	678.3	661.5	678.0	678.0
83	681.9	679.2	681.9	677.0	679.4	680.6
84	685.2	685.6	685.0	684.1	685.4	686.0
85	687.9	688.2	688.6	688.6	688.3	688.3
86	692.4	696.0	692.2	692.9	695.0	695.5
87	709.7	709.8	710.1	708.2	710.4	709.5
88	712.3	712.0	712.4	710.9	712.2	712.1
89	712.9	713.0	712.8	712.5	712.9	714.1
90	726.5	718.6	726.6	725.7	718.6	718.3
91	734.9	734.6	734.9	741.5	734.6	734.4
92	741.4	741.2	741.4	741.6	741.3	741.4
93	746.7	746.7	747.2	746.6	745.9	747.1
94	773.7	773.9	773.7	773.7	774.3	773.9
95	782.9	783.1	783.2	781.8	782.8	782.3
96	783.9	795.7	783.9	783.1	795.7	795.3
97	810.7	810.3	810.8	808.5	810.4	810.1
98	813.8	813.6	813.7	809.3	813.7	813.7
99	816.6	816.4	816.2	816.6	816.7	816.6
100	830.6	829.2	830.5	829.6	829.2	829.1
101	833.0	830.0	831.9	832.2	831.3	830.4
102	833.2	832.3	833.0	833.1	833.3	832.8
103	835.6	836.2	836.4	835.7	834.7	836.6
104	840.5	840.6	840.8	838.6	841.0	840.7
105	846.4	845.6	846.0	845.2	847.2	846.6
106	849.3	848.6	848.8	848.4	849.5	849.3
107	855.1	856.7	856.5	856.4	855.4	855.7
108	857.7	858.2	857.5	858.6	858.1	857.7
109	863.2	864.9	863.3	861.1	864.8	864.5

110	878.3	877.8	878.5	867.9	878.4	878.1
111	899.2	898.9	898.9	902.2	899.4	899.0
112	902.4	901.9	902.3	905.9	902.0	901.9
113	912.2	912.6	913.0	912.5	913.2	912.6
114	914.4	914.2	914.3	914.0	914.4	914.4
115	927.9	928.5	928.8	928.4	928.2	928.2
116	936.0	935.7	935.3	935.7	935.3	936.3
117	943.9	944.1	944.2	943.7	944.9	943.7
118	956.3	963.5	959.5	957.1	962.9	958.1
119	964.8	965.0	965.1	965.1	965.7	965.2
120	968.5	969.0	968.2	968.8	968.5	968.4
121	970.1	969.7	969.2	969.7	969.7	969.6
122	976.8	976.6	976.7	976.7	977.1	977.1
123	981.2	980.9	981.4	980.5	980.9	981.0
124	981.5	981.7	982.1	981.7	982.8	982.5
125	984.3	984.1	984.1	984.1	984.6	984.3
126	995.7	995.3	994.2	995.4	995.9	995.7
127	1001.8	1001.3	1001.8	1001.6	1002.2	1001.9
128	1002.1	1001.9	1002.1	1006.6	1002.3	1002.1
129	1005.4	1005.9	1006.5	1007.3	1006.6	1005.4
130	1013.2	1013.4	1013.2	1013.3	1013.5	1013.2
131	1023.5	1023.6	1023.6	1024.2	1023.6	1023.8
132	1028.3	1027.9	1028.2	1027.7	1028.0	1028.1
133	1034.2	1034.1	1034.2	1036.4	1034.2	1034.2
134	1040.7	1040.8	1041.0	1040.7	1040.7	1040.4
135	1040.9	1042.1	1041.0	1043.0	1042.3	1041.4
136	1046.6	1046.6	1046.5	1046.6	1046.4	1046.6
137	1068.9	1068.7	1068.8	1076.9	1068.8	1068.8
138	1076.7	1076.9	1077.0	1078.5	1077.0	1078.1
139	1079.2	1079.5	1079.3	1080.3	1079.4	1079.5
140	1079.8	1080.2	1079.9	1098.2	1080.2	1079.9
141	1102.4	1102.0	1102.3	1102.2	1101.7	1102.3
142	1103.9	1105.1	1103.8	1114.0	1105.0	1104.6
143	1115.8	1115.7	1116.2	1115.9	1116.2	1116.5
144	1139.5	1139.6	1140.2	1140.3	1140.0	1140.0
145	1142.0	1141.6	1142.3	1141.9	1141.8	1141.7
146	1146.3	1147.2	1147.2	1146.4	1147.4	1146.4
147	1158.1	1158.2	1158.4	1158.0	1158.2	1157.8
148	1169.0	1169.5	1168.7	1170.0	1168.7	1169.8
149	1175.7	1175.8	1176.3	1175.9	1175.8	1175.9
150	1186.6	1186.8	1186.7	1186.1	1186.9	1186.6
151	1189.6	1189.8	1189.6	1189.5	1190.1	1189.7
152	1194.1	1193.9	1194.1	1193.6	1193.8	1194.1
153	1201.5	1202.6	1202.1	1201.9	1202.5	1201.9
154	1205.3	1205.9	1205.3	1205.4	1205.9	1205.8
155	1218.8	1218.9	1219.4	1218.5	1218.9	1219.0
156	1235.2	1222.4	1235.0	1234.0	1222.4	1222.3

157	1248.4	1246.9	1248.2	1252.0	1247.4	1247.0
158	1268.6	1268.5	1269.3	1261.1	1268.9	1268.3
159	1271.4	1280.8	1271.6	1268.3	1281.4	1280.9
160	1285.9	1285.8	1286.4	1272.2	1285.7	1285.2
161	1287.4	1288.7	1287.7	1286.2	1288.6	1287.5
162	1291.3	1290.6	1291.0	1290.8	1289.9	1291.1
163	1296.0	1295.8	1297.0	1292.0	1296.3	1296.0
164	1299.5	1300.6	1299.8	1297.7	1300.6	1299.7
165	1304.2	1303.6	1304.0	1300.4	1303.8	1304.2
166	1310.3	1311.6	1310.2	1314.7	1311.5	1310.9
167	1319.1	1319.2	1319.0	1320.8	1319.0	1318.8
168	1324.9	1324.8	1324.9	1325.7	1324.8	1324.4
169	1330.2	1328.0	1330.2	1329.2	1328.1	1327.9
170	1331.7	1331.6	1331.6	1340.0	1331.8	1331.7
171	1340.1	1340.4	1340.2	1340.8	1340.6	1339.9
172	1343.3	1342.6	1343.3	1348.4	1343.1	1343.5
173	1349.9	1349.7	1350.0	1351.0	1350.0	1349.9
174	1354.3	1354.6	1354.9	1356.4	1355.1	1354.4
175	1357.7	1356.7	1357.9	1358.4	1356.5	1357.7
176	1364.1	1365.9	1364.4	1369.5	1366.0	1365.8
177	1371.7	1371.5	1371.4	1373.0	1371.3	1370.9
178	1388.8	1388.5	1389.0	1385.0	1388.5	1388.9
179	1389.5	1388.9	1389.5	1388.7	1389.0	1389.3
180	1394.6	1394.4	1395.3	1394.3	1395.3	1394.7
181	1404.3	1399.3	1404.3	1402.6	1399.7	1399.3
182	1406.8	1408.8	1407.3	1408.5	1409.2	1407.9
183	1408.9	1417.0	1409.0	1410.3	1417.3	1416.5
184	1431.3	1438.7	1431.4	1433.9	1439.1	1437.7
185	1441.7	1442.4	1441.9	1442.1	1442.1	1442.2
186	1443.1	1443.9	1443.4	1444.8	1444.1	1444.0
187	1453.3	1453.3	1453.8	1453.4	1453.4	1452.9
188	1456.5	1455.1	1456.5	1457.5	1455.8	1454.4
189	1460.7	1456.8	1460.7	1461.6	1457.1	1456.6
190	1474.3	1460.9	1474.8	1475.0	1461.2	1460.8
191	1478.4	1474.5	1478.5	1480.0	1474.9	1475.0
192	1483.4	1483.2	1483.4	1483.3	1482.9	1483.4
193	1487.7	1487.7	1488.2	1488.0	1488.4	1487.4
194	1490.0	1490.1	1490.7	1490.5	1491.0	1490.3
195	1493.6	1494.1	1494.0	1494.2	1494.0	1493.9
196	1516.4	1516.1	1516.1	1516.1	1516.4	1515.8
197	1519.8	1519.8	1519.9	1519.7	1519.8	1519.9
198	1526.4	1532.3	1526.3	1527.1	1532.3	1532.3
199	1534.7	1541.7	1534.5	1534.3	1541.6	1541.7
200	1543.4	1543.7	1543.4	1543.0	1544.1	1543.7
201	1549.9	1551.9	1549.7	1548.2	1551.9	1551.7
202	1582.9	1579.9	1582.8	1581.9	1580.0	1580.2
203	1587.6	1582.6	1587.3	1586.7	1582.6	1582.9

204	1593.4	1593.6	1593.4	1593.2	1593.9	1593.3
205	1603.4	1603.4	1603.4	1597.3	1603.4	1603.4
206	1613.4	1614.1	1613.6	1612.4	1614.0	1614.1
207	1618.9	1618.9	1618.9	1618.8	1618.9	1618.9
208	1624.1	1623.8	1623.8	1623.8	1623.9	1623.7
209	1628.7	1628.7	1628.7	1629.6	1628.7	1628.8
210	1633.4	1633.6	1633.4	1634.3	1633.7	1633.3
211	1642.1	1643.0	1642.2	1641.8	1643.0	1643.0
212	1642.9	1644.9	1642.9	1644.4	1644.9	1644.5
213	1647.9	1648.3	1647.9	1645.8	1648.4	1648.3
214	1672.7	1672.6	1672.8	1670.2	1672.7	1672.8
215	1764.9	1764.7	1764.9	1765.2	1764.7	1764.9
216	2321.8	2321.8	2321.7	2322.0	2321.7	2321.6
217	3029.4	3029.1	3029.7	3029.4	3029.8	3029.2
218	3040.4	3039.8	3040.4	3040.1	3040.4	3039.9
219	3065.0	3065.1	3065.3	3065.8	3065.0	3065.1
220	3124.8	3125.6	3126.2	3124.8	3126.3	3125.4
221	3129.0	3128.7	3128.8	3128.3	3128.3	3127.8
222	3136.9	3138.7	3138.1	3140.7	3138.2	3136.6
223	3144.7	3146.2	3146.0	3144.1	3145.3	3143.2
224	3146.2	3146.3	3146.5	3146.3	3146.1	3146.2
225	3161.1	3161.1	3161.6	3163.5	3161.1	3160.8
226	3163.3	3163.5	3163.7	3165.3	3163.3	3163.6
227	3165.5	3165.5	3165.5	3169.5	3165.6	3165.5
228	3170.8	3169.4	3169.8	3170.9	3170.8	3169.4
229	3172.5	3172.6	3172.5	3172.3	3172.6	3172.5
230	3175.6	3177.0	3176.5	3173.2	3176.4	3175.1
231	3178.1	3177.2	3177.9	3175.3	3177.8	3178.1
232	3180.9	3181.0	3181.1	3176.0	3180.7	3180.8
233	3184.2	3184.1	3183.9	3181.1	3184.4	3184.0
234	3184.9	3184.8	3184.9	3184.8	3184.8	3184.9
235	3185.7	3185.7	3185.6	3185.9	3186.1	3185.9
236	3190.9	3190.8	3190.9	3190.8	3190.8	3190.9
237	3192.2	3192.3	3192.2	3192.3	3192.7	3192.2
238	3193.7	3193.8	3193.7	3192.8	3193.8	3193.8
239	3195.3	3195.0	3195.4	3194.2	3195.2	3195.3
240	3195.4	3195.3	3195.4	3195.2	3195.4	3195.3
241	3196.4	3197.5	3196.4	3196.4	3197.7	3197.2
242	3215.8	3216.1	3216.8	3216.1	3217.7	3219.4
243	3243.9	3244.0	3244.4	3245.8	3244.0	3242.8
244	3255.9	3256.0	3255.8	3255.9	3256.0	3256.1
245	3572.0	3572.1	3571.7	3570.4	3571.9	3572.5
246	3762.1	3760.7	3761.3	3761.3	3761.2	3761.5

Reference

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