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SUPPLEMENTARY MATERIAL

Solvent effects on the conformational space of Tryptamine. Structural and Electronic Analysis

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Figure S1. Twelve most stable conformers of TRA. According to IUPAC recommendations the first letter characterizes the orientation of the C_9 atom relative to the central C_3—C_8 bond, the second letter describes the C_3—C_8—C_9—N_{10} angle, and the third letter specifies the orientation of the H_a relative to the central C_9—N_{10}.

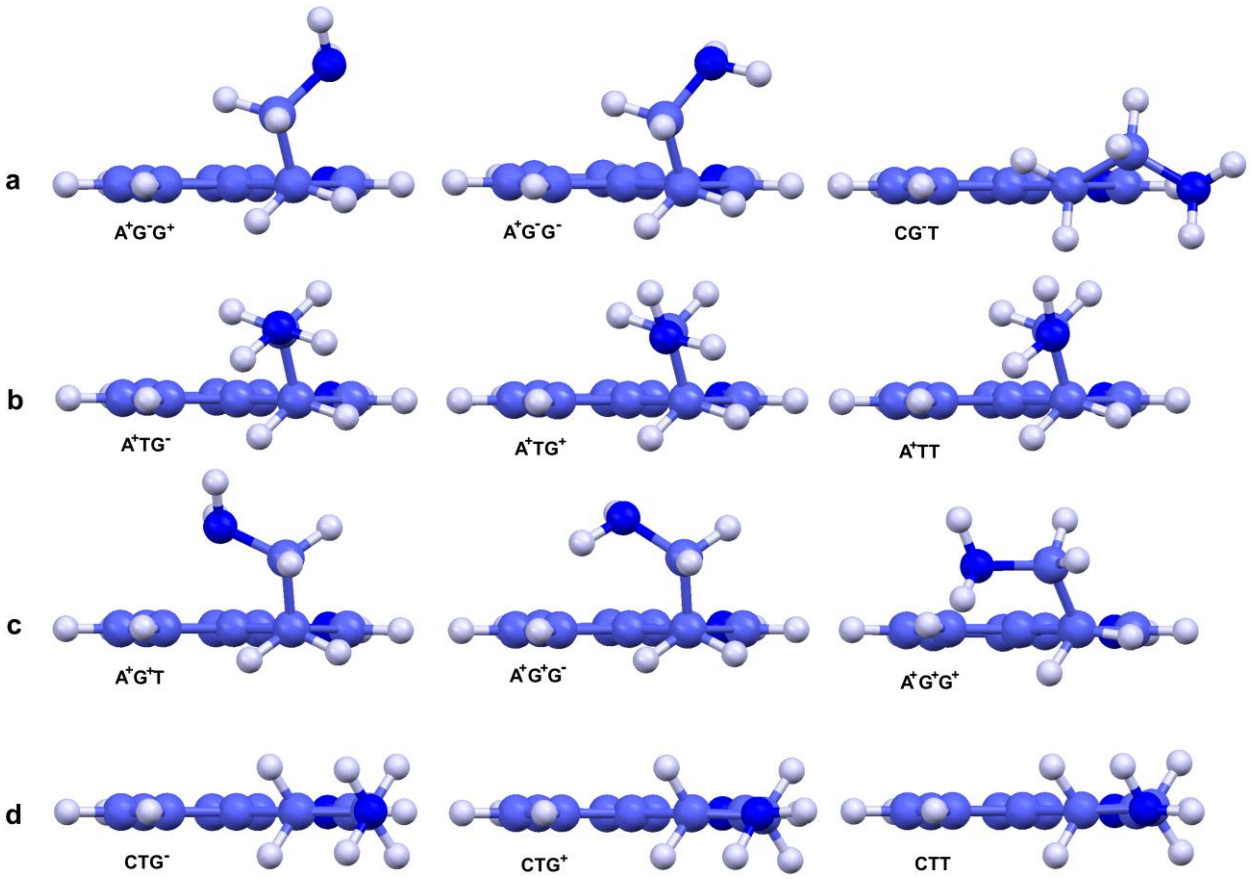

Table S1. Bond lengths and topological properties at bond critical points (BCPs) for $A^{+}TG^{-}$ conformer of TRA in aqueous solution calculated at the B3LYP/6-311++G** level of theory[a]

	Bond	Bond length	ρ_b	$\nabla^2\rho_b$	λ_1	λ_2	λ_3	E	$\lvert\lambda_1\rvert/\lambda_3$	G_b/ρ_b
Ring A	N_1—C_{7a}	1.378	0.303	-0.768	-0.613	-0.544	0.389	0.128	1.577	0.730
	N_1—C_2	1.382	0.298	-0.723	-0.596	-0.521	0.394	0.144	1.512	0.763
	C_2—C_3	1.379	0.317	-0.866	-0.676	-0.506	0.316	0.336	2.138	0.373
	C_3—C_{3a}	1.445	0.279	-0.690	-0.558	-0.475	0.344	0.175	1.623	0.305
	C_{3a}—C_{7a}	1.427	0.296	-0.792	-0.620	-0.518	0.345	0.198	1.795	0.307
	N_1—H	1.023	0.325	-1.652	-1.259	-1.206	0.813	0.044	1.549	0.133
	C_2—H	1.085	0.282	-0.978	-0.777	-0.747	0.545	0.040	1.424	0.119
Ring B	C_{3a}—C_4	1.410	0.297	-0.802	-0.614	-0.519	0.331	0.181	1.853	0.310
	C_4—C_5	1.393	0.308	-0.843	-0.645	-0.523	0.325	0.235	1.985	0.335
	C_5—C_6	1.415	0.296	-0.791	-0.611	-0.514	0.334	0.190	1.830	0.310
	C_6—C_7	1.394	0.307	-0.839	-0.643	-0.520	0.324	0.236	1.983	0.335
	C_7—C_{7a}	1.403	0.302	-0.826	-0.630	-0.522	0.326	0.209	1.936	0.320
	C_4—H	1.089	0.278	-0.948	-0.743	-0.727	0.523	0.022	1.421	0.133
	C_5—H	1.089	0.279	-0.947	-0.743	-0.724	0.520	0.026	1.428	0.136
	C_6—H	1.089	0.279	-0.950	-0.745	-0.728	0.523	0.024	1.425	0.134
	C_7—H	1.089	0.278	-0.945	-0.744	-0.726	0.525	0.024	1.417	0.132
Aminoethyl	C_3—C_8	1.504	0.250	-0.587	-0.478	-0.458	0.349	0.043	1.370	0.239
Moiety	C_8—C_9	1.547	0.236	-0.512	-0.449	-0.430	0.367	0.045	1.224	0.228
	C_9—N_{10}	1.469	0.260	-0.669	-0.510	-0.499	0.341	0.023	1.498	0.404
	C_8—H_a	1.100	0.271	-0.890	-0.698	-0.692	0.499	0.009	1.399	0.156
	C_8—H_b	1.098	0.273	-0.900	-0.703	-0.697	0.501	0.008	1.404	0.154
	C_9—H_a	1.097	0.277	-0.934	-0.735	-0.716	0.517	0.027	1.421	0.141
	C_9—H_b	1.097	0.278	-0.935	-0.736	-0.717	0.517	0.026	1.423	0.142
	N_{10}—H_a	1.023	0.331	-1.450	-1.197	-1.145	0.892	0.045	1.341	0.175
	N_{10}—H_b	1.023	0.331	-1.450	-1.197	-1.145	0.893	0.045	1.341	0.175

[a] ρ_b, $\nabla^2\rho_b$, G_b/ρ_b, λ_1, λ_2, λ_3 are expressed in a.u. and bond lengths in Å

Table S2a. Second-order stabilization energies, $E^{(2)}$, calculated at the B3LYP/6-311++G** level of theory for donation transferences in solution related to the group G^{+} [a,b]

Donor	Acceptor	Group G^+					
		$A^+G^+G^-$	%Δ	A^+G^+T	%Δ	$A^+G^+G^+$	%Δ
LP_{N10}	$\sigma^*_{C8—C9}$	8.49	-6.39	0.74	-28.16	0.70	-55.70
	$\sigma^*_{C8—Hb}$	0.61	-6.15	-	-	-	
	$\sigma^*_{C9—Ha}$	1.36	4.62	1.21	2.54	7.07	4.59
	$\sigma^*_{C9—Hb}$	1.25	-27.33	7.35	-7.55	1.29	-
$\sigma_{C3a—C3}$	$\sigma^*_{C8—Hb}$	0.63	-7.35	0.56	-17.65	0.54	-19.40
$\sigma_{C2—C3}$	$\sigma^*_{C8—Ha}$	0.75	1.35	0.65	16.07	0.66	11.86
$\sigma_{C8—C9}$	$\pi^*_{C2—C3}$	2.61	-7.45	2.46	-3.91	2.27	20.74
$\sigma_{C8—Ha}$	$\sigma^*_{C2—C3}$	4.73	3.73	4.70	16.05	4.74	105.19
	$\pi^*_{C2—C3}$	0.90	-18.18	0.95	-46.93	0.95	-71.22
	$\sigma^*_{C9—Hb}$	2.64	2.33	2.66	-1.85	2.74	11.84
$\sigma_{C8—Hb}$	$\sigma^*_{C3a—C3}$	4.44	-3.90	4.50	-12.96	4.34	-29.08
	$\pi^*_{C2—C3}$	1.41	18.49	1.40	89.19	1.53	-
	$\sigma^*_{C9—N10}$	4.61	3.60	4.05	4.38	4.12	26.77
$\sigma_{C9—Ha}$	$\sigma^*_{N10—Ha}$	3.13	-5.72	-	-	-	-
	$\sigma^*_{N10—Hb}$	-	-	3.06	-5.26	-	-
$\sigma_{C9—Hb}$	$\sigma^*_{N10—Ha}$	-	-	-	-	3.00	-0.66
	$\sigma^*_{N10—Hb}$	3.09	-7.21	-	-	-	-
$\sigma_{N10—Ha}$	$\sigma^*_{C8—C9}$	-	-	3.10	6.53	-	-
	$\sigma^*_{C9—Ha}$	2.34	0.43	-	-	-	-
	$\sigma^*_{C9—Hb}$	-	-	-	-	2.41	8.56
$\sigma_{N10—Hb}$	$\sigma^*_{C8—C9}$	-	-	-	-	3.12	16.85
	$\sigma^*_{C9—Ha}$	-	-	2.24	1.36	-	-
	$\sigma^*_{C9—Hb}$	2.44	2.52	-	-	-	-
Σ		**45.43**		**39.63**		**39.48**	

[a] All values are expressed in Kcal mol^{-1}

[b] %Δ represents the percentage values of changes of $E^{(2)}$ in solution with respect to vacuum

Table S2b. Second-order stabilization energies, $E^{(2)}$, calculated at the B3LYP/6-311++G** level of theory for donation transferences in solution related to the group G^{-} [a,b]

Donor	Acceptor	Group G^-					
		$A^+G^-G^-$	%Δ	$A^+G^-G^+$	%Δ	CG^-T	%Δ
LP_{N10}	σ^*_{C8-C9}	8.39	-6.26	0.80	-11.11	0.80	3.90
	σ^*_{C9-Ha}	1.19	-27.88	7.27	-6.68	1.08	-18.18
	σ^*_{C9-Hb}	1.35	4.65	1.14	-13.64	6.71	-4.28
σ_{C3a-C3}	σ^*_{C3-C8}	1.77	30.15	1.74	1.75	1.69	-1.17
σ_{C2-C3}	σ^*_{C3-C8}	2.16	18.03	2.12	-0.47	2.24	0.90
	σ^*_{C2-H}	1.14	-11.63	1.15	-8.00	1.21	-7.63
	σ^*_{N1-H}	2.94	-9.54	2.94	-7.84	2.92	-9.88
π_{C2-C3}	σ^*_{C8-C9}	3.81	3.81	3.74	1.36	-	-
$\sigma_{C3a-C7a}$	σ^*_{C3-C8}	5.18	2.98	5.20	1.76	5.03	-1.81
σ_{C3-C8}	σ^*_{C3a-C3}	2.31	27.62	2.28	0.88	2.15	1.90
σ_{C8-C9}	π^*_{C2-C3}	2.56	-6.57	2.40	-7.69	-	-
σ_{C9-N10}	σ^*_{C8-Ha}	0.88	0.00	1.13	-5.04	1.08	-3.57
σ_{C8-Ha}	σ^*_{C2-C3}	3.54	0.00	3.44	-4.71	3.23	-33.68
σ_{C8-Hb}	σ^*_{C3a-C3}	5.55	1.28	5.56	2.58	-	-
σ_{C9-Ha}	σ^*_{C8-Hb}	2.72	-3.20	2.78	2.96	2.88	-0.35
	σ^*_{N10-Ha}	3.07	-8.36	-	-	-	-
	σ^*_{N10-Hb}	-	-	-	-	2.90	-8.81
σ_{C9-Hb}	σ^*_{C3-C8}	3.40	3.34	3.46	2.67	3.51	4.46
	σ^*_{N10-Ha}	-	-	3.04	-4.70	-	-
	σ^*_{N10-Hb}	3.13	-6.01	-	-	-	-
σ_{N10-Ha}	σ^*_{C8-C9}	-	-	-	-	3.03	7.83
	σ^*_{C9-Ha}	2.44	4.27	-	-	-	-
	σ^*_{C9-Hb}	-	-	2.23	0.90	-	-
σ_{N10-Hb}	σ^*_{C8-C9}	-	-	3.04	6.67	-	-
	σ^*_{C9-Ha}	-	-	-	-	2.42	6.61
	σ^*_{C9-Hb}	2.33	0.43	-	-	-	-
Σ		**59.86**		**55.46**		**42.88**	

[a] All values are expressed in Kcal mol^{-1}

[b] %Δ represents the percentage values of changes of $E^{(2)}$ in solution with respect to vacuum

Table S2c. Second-order stabilization energies, $E^{(2)}$, calculated at the B3LYP/6-311++G** level of theory for donation transferences in solution related to the group T´[a,b]

Donor	Acceptor	Group T´					
		CTG^-	%Δ	CTG^+	%Δ	CTT	%Δ
LP_{N10}	σ^*_{C3-C8}	0.81	-1.22	-	-	-	-
	σ^*_{C8-C9}	7.71	-6.55	0.89	-22.02	0.85	-18.35
	σ^*_{C9-Ha}	1.27	-13.61	7.07	-5.36	1.06	-7.34
	σ^*_{C9-Hb}	1.27	-13.61	1.02	-7.47	7.06	-8.93
σ_{C3a-C3}	σ^*_{C8-C9}	1.27	-2.31	1.26	-3.08	1.26	-3.08
$\sigma_{C3a-C7a}$	σ^*_{C7-C7a}	2.79	-4.45	2.78	-4.79	2.78	-4.79
	σ^*_{C3-C8}	5.00	0.60	4.98	1.43	4.98	1.43
σ_{C3-C8}	σ^*_{C3a-C3}	2.17	0.46	2.16	0.47	2.16	0.47
	σ^*_{C9-N10}	2.11	-0.47	1.76	0.57	1.75	1.15
σ_{C8-C9}	π^*_{C2-C3}	-	-	0.86	2.38	-	-
	σ^*_{C3-C8}	0.95	0.00	-	-	0.86	2.38
σ_{C9-Ha}	σ^*_{C8-Ha}	2.84	-1.39	2.84	4.80	2.91	-0.34
	σ^*_{N10-Ha}	3.03	-9.01	-	-	-	-
	σ^*_{N10-Hb}	-	-	-	-	2.97	-9.17
σ_{C9-Hb}	σ^*_{C8-Hb}	2.85		2.91	-0.34	2.84	4.80
	σ^*_{N10-Hb}	3.04	-8.71	2.97	-9.17	-	-
σ_{N10-Ha}	σ^*_{C8-C9}	-	-	-	-	2.78	6.51
	σ^*_{C9-Ha}	2.39		-	-	-	-
	σ^*_{C9-Hb}	-	-	2.30	3.60	-	-
σ_{N10-Hb}	σ^*_{C8-C9}	-	-	2.78	6.51	-	-
	σ^*_{C9-Ha}	-	-	-	-	2.31	4.05
	σ^*_{C9-Hb}	2.39	4.37	-	-	-	-
Σ		**41.89**		**36.58**		**36.57**	

[a] All values are expressed in Kcal mol^{-1}

[b] %Δ represents the percentage values of changes of $E^{(2)}$ in solution with respect to vacuum

Table S3. Percentage values of the main changes in solution for bond lengths, electron density at BCPs, electron density at NCPs of hydrogen atom and polarization of C—H and N—H bonds, calculated at B3LYP/6-311++G** level of theory for TRA conformers.

	Bond Lengths											
	Group T			**Group G⁻**			**Group T´**			**Group G⁺**		
Bond	**A⁺TG⁻**	**A⁺TG⁺**	**A⁺TT**	**A⁺G⁻G⁻**	**A⁺G⁻G⁺**	**CG⁻T**	**CTG⁻**	**CTG⁺**	**CTT**	**A⁺G⁺G⁻**	**A⁺G⁺T**	**A⁺G⁺G⁺**
C_8—H_a	0.02	0.15	0.02	0.17	0.09	0.20	0.03	0.15	0.01	0.02	0.05	-0.10
C_8—H_b	-0.01	0.00	0.11	0.22	0.12	-0.05	0.02	0.02	0.16	0.04	0.05	0.06
C_9—H_a	0.08	-0.03	0.07	-0.58	-0.06	0.09	0.05	-0.08	0.03	0.04	0.04	0.05
C_9—H_b	0.08	0.07	-0.02	0.08	0.04	-0.05	0.05	0.04	-0.08	0.03	-0.08	0.18
N_{10}—H_a	0.61	0.59	0.60	0.58	0.43	0.56	0.61	0.58	0.61	0.44	0.63	0.56
N_{10}—H_b	0.61	0.61	0.58	0.54	0.61	0.51	0.61	0.61	0.60	0.58	0.46	0.60
	Electron Density at BCP											
	Group T			**Group G⁻**			**Group T´**			**Group G⁺**		
Bond	**A⁺TG⁻**	**A⁺TG⁺**	**A⁺TT**	**A⁺G⁻G⁻**	**A⁺G⁻G⁺**	**CG⁻T**	**CTG⁻**	**CTG⁺**	**CTT**	**A⁺G⁺G⁻**	**A⁺G⁺T**	**A⁺G⁺G⁺**
C_8—H_a	0.08	-0.53	0.14	-0.06	-0.10	-0.53	0.06	-0.55	0.18	0.25	-0.23	0.49
C_8—H_b	0.26	0.31	-0.35	0.23	-0.37	0.31	0.09	0.15	-0.58	-0.04	0.06	-0.15
C_9—H_a	-0.18	0.14	-0.15	-0.21	0.20	-0.31	-0.03	0.34	0.03	0.06	0.04	0.01
C_9—H_b	-0.23	-0.19	0.05	0.02	0.05	0.29	-0.03	0.03	0.35	-0.05	0.29	-0.44
N_{10}—H_a	-1.34	-1.29	-1.33	-1.27	-1.01	-1.26	-1.33	-1.29	-1.34	-1.01	-1.36	-1.28
N_{10}—H_b	-1.32	-1.36	-1.28	-1.02	-1.33	-1.11	-1.32	-1.34	-1.31	-1.09	-1.09	-1.30
	Electron Density at NCP of H atom											
	Group T			**Group G⁻**			**Group T´**			**Group G⁺**		
Bond	**A⁺TG⁻**	**A⁺TG⁺**	**A⁺TT**	**A⁺G⁻G⁻**	**A⁺G⁻G⁺**	**CG⁻T**	**CTG⁻**	**CTG⁺**	**CTT**	**A⁺G⁺G⁻**	**A⁺G⁺T**	**A⁺G⁺G⁺**
C_8—H_a	-0.19	0.06	-0.19	-0.15	-0.23	-0.50	-0.21	0.06	-0.18	-0.14	0.08	0.23
C_8—H_b	-0.31	-0.32	-0.05	-0.31	-0.11	-0.15	-0.19	-0.20	0.05	-0.30	-0.33	-0.61
C_9—H_a	-0.03	-0.10	-0.07	-0.03	-0.06	-0.02	-0.12	-0.18	-0.12	-0.13	-0.15	-0.25
C_9—H_b	0.03	-0.03	-0.08	-0.10	-0.15	-0.13	-0.11	-0.12	-0.17	-0.07	-0.05	0.08
N_{10}—H_a	-1.86	-1.77	-1.85	-1.93	-1.87	-1.59	-1.81	-1.86	-1.86	-1.23	-1.87	-1.77
N_{10}—H_b	-1.86	-1.93	-1.83	-1.20	-1.16	-1.77	-1.81	-1.78	-1.80	-1.99	-1.08	-1.66
	Polarization of X—H bond, % of electron density on H											
	Group T			**Group G⁻**			**Group T´**			**Group G⁺**		
Bond	**A⁺TG⁻**	**A⁺TG⁺**	**A⁺TT**	**A⁺G⁻G⁻**	**A⁺G⁻G⁺**	**CG⁻T**	**CTG⁻**	**CTG⁺**	**CTT**	**A⁺G⁺G⁻**	**A⁺G⁺T**	**A⁺G⁺G⁺**
C_8—H_a	0.35	-0.59	0.48	0.17	0.33	0.36	0.40	-0.56	0.53	0.42	-0.35	0.10
C_8—H_b	0.73	0.83	-0.54	0.72	-0.15	0.48	0.40	0.53	-0.54	0.46	0.70	0.97
C_9—H_a	-0.10	0.24	-0.03	-0.17	0.22	-0.15	0.13	0.48	0.19	0.22	0.27	0.31
C_9—H_b	-0.25	-0.13	0.95	0.22	0.29	0.51	0.12	0.19	0.48	0.07	0.31	-0.52
N_{10}—H_a	1.54	1.94	1.17	1.75	1.16	1.00	1.53	1.50	1.51	0.79	1.46	1.67
N_{10}—H_b	1.62	1.12	1.57	0.94	1.24	1.57	1.53	1.52	1.50	1.68	0.65	0.81

Table S4a. Summation of second-order stabilization energies, $E^{(2)}$, calculated at B3LYP/6-311++G** level of theory for donation and back-donation transferences in solution related to C—H and N—H bonds[a,b]

	Donation transferences											
	Group T						**Group G^-**					
Donor	**A^+TG^-**	**%Δ**	**A^+TG^+**	**%Δ**	**A^+TT**	**%Δ**	**$A^+G^-G^-$**	**%Δ**	**$A^+G^-G^+$**	**%Δ**	**CG^-T**	**%Δ**
$\sigma_{C8—Ha}$	8.50	0.35	8.70	-1.15	8.60	-0.81	10.37	1.25	9.79	2.25	10.27	5.94
$\sigma_{C8—Hb}$	7.97	1.51	8.07	1.86	8.13	0.25	8.08	2.10	8.11	1.85	8.34	9.23
$\sigma_{C9—Ha}$	6.21	-6.44	2.69	3.72	6.17	-6.16	6.16	-6.01	2.70	2.96	6.07	-4.78
$\sigma_{C9—Hb}$	6.13	-6.69	6.10	-6.56	2.64	2.65	6.62	-1.36	6.56	-0.91	3.36	4.46
$\sigma_{N10—Ha}$	2.33	5.58	2.19	5.94	2.60	6.54	2.34	4.27	2.21	0.90	2.81	7.83
$\sigma_{N10—Hb}$	2.30	5.22	2.61	6.51	2.23	5.38	2.32	0.43	2.85	6.67	2.27	6.61
	Back-Donation transferences											
	Group T						**Group G^-**					
Acceptor	**A^+TG^-**	**%Δ**	**A^+TG^+**	**%Δ**	**A^+TT**	**%Δ**	**$A^+G^-G^-$**	**%Δ**	**$A^+G^-G^+$**	**%Δ**	**CG^-T**	**%Δ**
$\sigma^*_{C8—Ha}$	5.57	-2.69	5.38	2.79	5.63	-2.31	3.63	-12.40	3.34	3.59	2.85	30.53
$\sigma^*_{C8—Hb}$	3.65	-5.48	3.71	-2.96	3.51	1.42	3.73	-5.63	3.48	2.30	6.81	-8.96
$\sigma^*_{C9—Ha}$	4.94	3.64	2.70	0.00	4.92	2.44	4.94	4.05	2.69	0.37	5.15	2.52
$\sigma^*_{C9—Hb}$	4.93	3.45	4.87	3.29	2.71	0.00	3.49	0.00	3.48	-0.86	1.06	-12.26
$\sigma^*_{N10—Ha}$	3.38	-9.76	3.29	-10.33	1.79	-11.73	3.35	-8.36	3.19	-4.70	1.82	-12.09
$\sigma^*_{N10—Hb}$	3.38	-9.76	1.79	-11.73	3.29	-10.03	3.33	-6.01	1.88	-12.77	3.18	-8.81

[a] All values are expressed in Kcal mol^{-1}

[b] %Δ represents the percentage values of summation of $E^{(2)}$ in solution with respect to vacuum

Table S4b. Summation of second-order stabilization energies, $E^{(2)}$, calculated at B3LYP/6-311++G** level of theory for donation and back-donation transferences in solution related to C—H and N—H bonds[a,b]

	Donation transferences											
	Group G^+						**Group T´**					
Donor	**$A^+G^+G^-$**	**%Δ x** [b]	**A^+G^+T**	**%Δ x**	**$A^+G^+G^+$**	**%Δ x**	**CTG^-**	**%Δ x**	**CTG^+**	**%Δ x**	**CTT**	**%Δ x**
σ_{N1-H}	3.75	10.40	3.72	9.95	3.68	10.05	3.66	10.93	3.66	10.93	3.66	10.93
σ_{C2-H}	6.82	2.20	6.65	1.50	6.55	2.29	6.50	1.85	6.50	2.00	6.50	2.00
σ_{C4-H}	10.07	1.99	10.33	-11.04	10.50	-12.57	9.00	1.89	9.02	1.66	9.02	1.66
σ_{C5-H}	8.17	1.22	8.21	6.94	8.20	6.71	8.55	1.64	8.56	1.52	8.56	1.52
σ_{C6-H}	8.13	1.48	8.11	3.08	8.04	3.73	8.23	1.82	8.22	1.95	8.22	1.95
σ_{C7-H}	9.52	2.84	9.50	3.26	9.47	3.17	9.44	3.28	9.43	3.39	9.43	3.39
σ_{C8-Ha}	8.24	0.36	8.55	-2.81	8.83	-4.53	9.38	-0.21	9.61	-1.46	9.49	-0.84
σ_{C8-Hb}	10.26	1.95	9.79	1.63	9.93	0.60	9.37	-0.11	9.48	-0.84	9.61	-1.56
σ_{C9-Ha}	6.68	-2.10	6.71	-2.09	3.45	4.93	6.21	-5.48	2.71	4.80	6.19	-5.01
σ_{C9-Hb}	6.23	-5.14	2.75	4.73	5.42	8.30	6.21	-5.15	6.19	-5.01	2.71	4.80
σ_{N10-Ha}	2.33	0.43	3.43	-9.62	2.22	8.56	2.29	4.37	2.22	3.60	2.61	6.51
σ_{N10-Hb}	2.38	2.52	2.21	1.36	3.28	-4.88	2.29	4.37	2.61	6.51	2.22	4.05
	Back-Donation transferences											
	Group G^+						**Group T´**					
Acceptor	**$A^+G^+G^-$**	**%Δ x**	**A^+G^+T**	**%Δ x**	**$A^+G^+G^+$**	**%Δ x**	**CTG^-**	**%Δ x**	**CTG^+**	**%Δ x**	**CTT**	**%Δ x**
σ^*_{N1-H}	8.66	-13.97	8.61	-14.05	8.70	-14.71	8.60	-14.07	8.61	-14.17	7.39	-14.17
σ^*_{C2-H}	8.70	-5.17	8.55	-5.85	8.62	-6.26	8.64	-4.86	8.71	-5.63	8.22	-5.63
σ^*_{C4-H}	7.35	-2.45	7.09	-3.10	7.15	-3.92	6.93	-1.59	6.90	-1.16	6.82	-1.16
σ^*_{C5-H}	5.86	-1.02	5.89	-1.02	5.93	-1.52	5.92	-1.52	5.92	-1.52	5.83	-1.52
σ^*_{C6-H}	5.89	-1.36	5.92	-1.18	6.00	-2.33	5.91	-1.35	5.92	-1.52	5.83	-1.52
σ^*_{C7-H}	6.85	-3.80	6.88	-4.07	6.94	-4.76	6.85	-3.94	6.86	-4.08	6.58	-4.08
σ^*_{C8-Ha}	4.68	-5.98	4.89	-10.22	5.50	-21.27	5.91	0.17	5.75	4.00	5.74	-1.20
σ^*_{C8-Hb}	2.34	3.42	1.82	41.76	2.16	17.59	5.91	-1.18	5.81	-0.17	6.04	5.04
σ^*_{C9-Ha}	3.50	-0.29	3.96	-12.63	1.50	-26.00	5.14	1.95	2.93	-1.71	5.17	1.57
σ^*_{C9-Hb}	4.96	2.42	2.71	-1.85	5.28	-2.46	5.14	1.95	5.09	1.38	2.88	-1.71
σ^*_{N10-Ha}	3.32	-5.72	1.85	-11.89	3.02	-0.66	3.33	-9.01	3.27	-9.17	1.58	-12.22
σ^*_{N10-Hb}	3.33	-7.21	3.23	-5.26	1.74	-5.75	3.33	-8.71	1.80	-12.22	2.97	-9.17

[a] All values are expressed in Kcal mol^{-1}

[b] %Δ x : Percentage values of summation of $E^{(2)}$ in solution with respect to vacuum