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SUPPLEMENTARY MATERIAL

Conformational and stereoelectronic investigation of Tryptamine. An AIM/NBO Study

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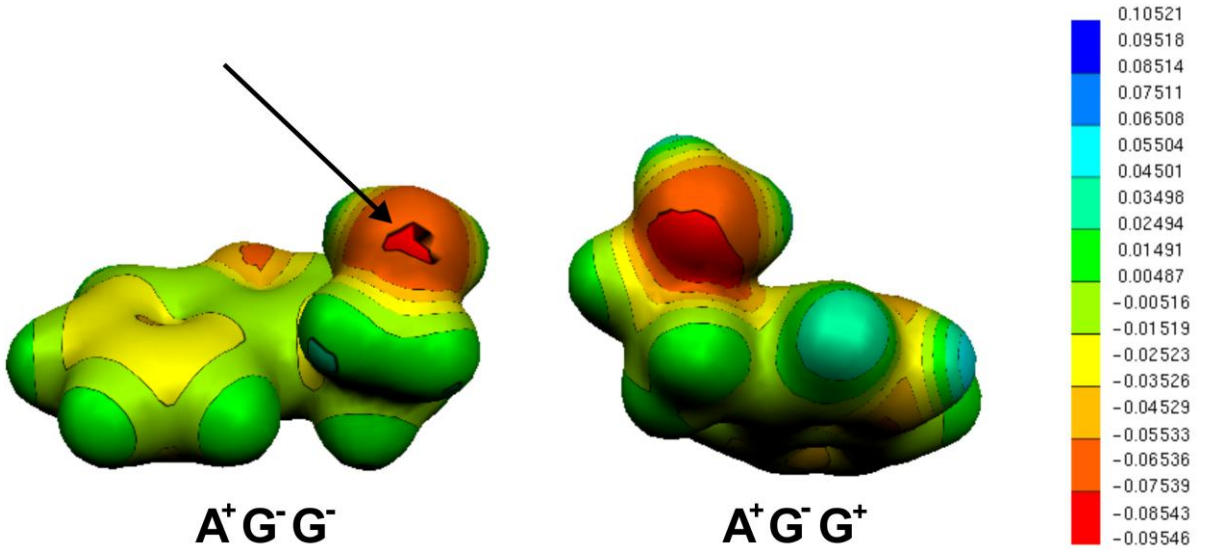

Figure S1. Molecular electrostatic potential (MEPs) for $A^+G^-G^-$, and $A^+G^-G^+$ conformers of TRA. Changes on negative $V(r)$ values on N_{10} can be observed: the negative values of $V(r)$ on N_{10} in $A^+G^-G^-$ conformer (*oblique line*) become less negative (higher) than $V(r)$ on N_{10} in the other conformer. Values in a.u.

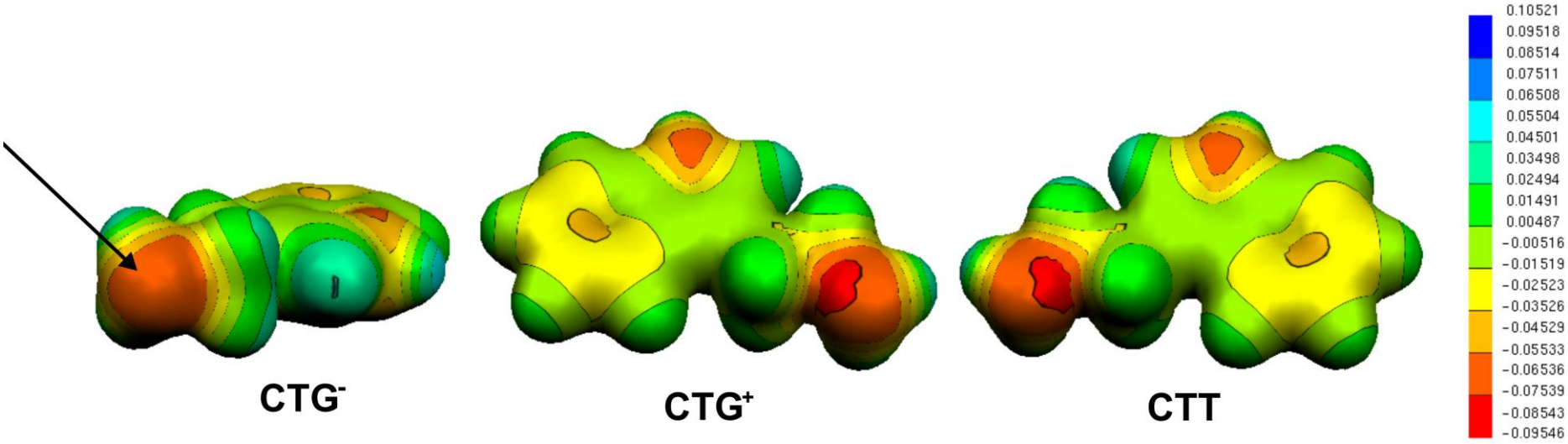

Figure S2. Molecular electrostatic potential (MEPs) for CTG^-, CTG^+ and CTT conformers of TRA. Changes on negative $V(r)$ values on N_{10} can be observed: the negative values of $V(r)$ on N_{10} in CTG^- conformer (*oblique line*) become less negative (higher) than $V(r)$ on N_{10} in the other conformers. Values in a.u.

Table S1a. Bond lengths and topological properties at bond critical points in the $A^+G^-G^+$ conformer of TRA 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	ε	$\lvert\lambda_1\rvert/\lambda_3$	G_b/ρ_b
Ring A	N_1—C_{7a}	1.381	0.299	-0.735	-0.597	-0.533	0.396	0.120	1.509	0.751
	N_1—C_2	1.386	0.295	-0.699	-0.585	-0.509	0.394	0.150	1.483	0.773
	C_2—C_3	1.386	0.319	-0.877	-0.682	-0.508	0.313	0.343	2.179	0.378
	C_3—C_{3a}	1.446	0.279	-0.691	-0.558	-0.477	0.344	0.170	1.621	0.303
	C_{3a}—C_{7a}	1.424	0.298	-0.803	-0.625	-0.521	0.343	0.200	1.822	0.310
	N_1—H	1.007	0.340	-1.657	-1.298	-1.235	0.877	0.051	1.481	0.153
	C_2—H	1.081	0.283	-0.982	-0.775	-0.743	0.537	0.043	1.444	0.127
Ring B	C_{3a}—C_4	1.408	0.299	-0.810	-0.618	-0.522	0.330	0.183	1.871	0.311
	C_4—C_5	1.391	0.309	-0.851	-0.650	-0.525	0.324	0.236	2.004	0.335
	C_5—C_6	1.412	0.298	-0.801	-0.617	-0.517	0.333	0.192	1.854	0.311
	C_6—C_7	1.392	0.308	-0.845	-0.646	-0.522	0.323	0.239	2.000	0.336
	C_7—C_{7a}	1.400	0.303	-0.831	-0.634	-0.522	0.324	0.215	1.956	0.323
	C_4—H	1.086	0.279	-0.953	-0.743	-0.727	0.517	0.021	1.437	0.138
	C_5—H	1.086	0.280	-0.952	-0.743	-0.724	0.515	0.025	1.443	0.141
	C_6—H	1.086	0.280	-0.955	-0.745	-0.728	0.517	0.023	1.441	0.139
	C_7—H	1.087	0.278	-0.942	-0.736	-0.718	0.511	0.026	1.440	0.142
Aminoethyl	C_3—C_8	1.504	0.251	-0.590	-0.479	-0.460	0.349	0.041	1.371	0.239
Moiety	C_8—C_9	1.540	0.239	-0.531	-0.452	-0.443	0.364	0.021	1.242	0.225
	C_9—N_{10}	1.467	0.262	-0.677	-0.520	-0.498	0.340	0.043	1.526	0.404
	C_8—H_a	1.098	0.272	-0.896	-0.700	-0.694	0.499	0.009	1.403	0.155
	C_8—H_b	1.096	0.275	-0.912	-0.714	-0.708	0.511	0.008	1.398	0.150
	C_9—H_a	1.103	0.273	-0.901	-0.713	-0.697	0.509	0.023	1.401	0.149
	C_9—H_b	1.096	0.278	-0.935	-0.733	-0.716	0.514	0.024	1.427	0.143
	N_{10}—H_a	1.017	0.335	-1.473	-1.219	-1.162	0.908	0.048	1.342	0.180
	N_{10}—H_b	1.016	0.336	-1.458	-1.214	-1.157	0.913	0.049	1.330	0.183

[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 S1b Bond lengths and topological properties at bond critical points (BCPs) in the $A^{+}G^{-}G^{-}$ conformer of TRA 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	ε	$\lvert\lambda_1\rvert/\lambda_3$	G_b/ρ_b
Ring A	N_1—C_{7a}	1.381	0.299	-0.733	-0.597	-0.533	0.397	0.119	1.505	0.753
	N_1—C_2	1.386	0.295	-0.702	-0.586	-0.508	0.392	0.154	1.497	0.768
	C_2—C_3	1.375	0.319	-0.876	-0.681	-0.507	0.313	0.342	2.176	0.378
	C_3—C_{3a}	1.446	0.279	-0.691	-0.558	-0.477	0.344	0.169	1.621	0.302
	C_{3a}—C_{7a}	1.423	0.299	-0.804	-0.626	-0.521	0.343	0.201	1.825	0.310
	N_1—H	1.007	0.340	-1.657	-1.298	-1.235	0.876	0.051	1.481	0.153
	C_2—H	1.082	0.283	-0.977	-0.771	-0.738	0.533	0.045	1.448	0.129
Ring B	C_{3a}—C_4	1.408	0.299	-0.810	-0.618	-0.522	0.330	0.183	1.872	0.311
	C_4—C_5	1.391	0.309	-0.852	-0.650	-0.526	0.324	0.236	2.006	0.335
	C_5—C_6	1.412	0.298	-0.802	-0.617	-0.518	0.333	0.192	1.854	0.311
	C_6—C_7	1.392	0.308	-0.845	-0.646	-0.522	0.323	0.239	2.001	0.336
	C_7—C_{7a}	1.400	0.303	-0.831	-0.634	-0.522	0.324	0.215	1.956	0.323
	C_4—H	1.086	0.279	-0.953	-0.743	-0.727	0.517	0.021	1.437	0.138
	C_5—H	1.086	0.280	-0.953	-0.744	-0.725	0.516	0.025	1.442	0.140
	C_6—H	1.086	0.280	-0.956	-0.745	-0.728	0.517	0.023	1.440	0.139
	C_7—H	1.087	0.278	-0.943	-0.736	-0.718	0.512	0.026	1.440	0.142
Aminoethyl moiety	C_3—C_8	1.502	0.252	-0.594	-0.482	-0.462	0.349	0.043	1.379	0.239
	C_8—C_9	1.551	0.234	-0.502	-0.440	-0.430	0.368	0.025	1.198	0.228
	C_9—N_{10}	1.462	0.264	-0.688	-0.520	-0.506	0.338	0.027	1.538	0.412
	C_8—H_a	1.100	0.271	-0.888	-0.696	-0.690	0.499	0.008	1.396	0.156
	C_8—H_b	1.098	0.272	-0.893	-0.697	-0.691	0.495	0.008	1.407	0.158
	C_9—H_a	1.096	0.278	-0.938	-0.738	-0.720	0.520	0.025	1.419	0.141
	C_9—H_b	1.097	0.277	-0.932	-0.733	-0.714	0.515	0.026	1.423	0.143
	N_{10}—H_a	1.017	0.335	-1.441	-1.207	-1.147	0.913	0.052	1.321	0.185
	N_{10}—H_b	1.017	0.335	-1.471	-1.219	-1.161	0.908	0.050	1.342	0.180

[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 S1c Bond lengths and topological properties at bond critical points (BCPs) in the $A^{+}TG^{-}$ conformer of TRA 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	ε	$\lvert\lambda_1\rvert/\lambda_3$	G_b/ρ_b
Ring A	N_1—C_{7a}	1.380	0.299	-0.733	-0.597	-0.533	0.397	0.120	1.503	0.754
	N_1—C_2	1.386	0.295	-0.701	-0.586	-0.508	0.393	0.155	1.492	0.771
	C_2—C_3	1.375	0.319	-0.876	-0.682	-0.507	0.313	0.344	2.180	0.378
	C_3—C_{3a}	1.446	0.279	-0.694	-0.559	-0.478	0.344	0.170	1.625	0.303
	C_{3a}—C_{7a}	1.423	0.299	-0.804	-0.626	-0.521	0.343	0.201	1.825	0.310
	N_1—H	1.007	0.340	-1.657	-1.299	-1.235	0.877	0.051	1.481	0.153
	C_2—H	1.085	0.283	-0.977	-0.771	-0.738	0.532	0.044	1.448	0.129
Ring B	C_{3a}—C_4	1.408	0.299	-0.811	-0.618	-0.522	0.330	0.183	1.873	0.311
	C_4—C_5	1.391	0.309	-0.852	-0.650	-0.526	0.324	0.237	2.007	0.335
	C_5—C_6	1.412	0.298	-0.801	-0.617	-0.517	0.333	0.192	1.853	0.311
	C_6—C_7	1.392	0.308	-0.845	-0.646	-0.522	0.323	0.239	2.001	0.336
	C_7—C_{7a}	1.400	0.303	-0.831	-0.634	-0.522	0.324	0.215	1.956	0.323
	C_4—H	1.087	0.279	-0.951	-0.741	-0.726	0.516	0.021	1.438	0.139
	C_5—H	1.086	0.280	-0.953	-0.743	-0.725	0.515	0.025	1.443	0.140
	C_6—H	1.086	0.280	-0.956	-0.745	-0.728	0.517	0.023	1.441	0.139
	C_7—H	1.087	0.278	-0.943	-0.736	-0.718	0.511	0.026	1.440	0.142
Aminoethyl Moiety	C_3—C_8	1.502	0.251	-0.592	-0.480	-0.461	0.349	0.042	1.376	0.239
	C_8—C_9	1.549	0.235	-0.509	-0.448	-0.429	0.367	0.046	1.220	0.228
	C_9—N_{10}	1.464	0.262	-0.682	-0.514	-0.502	0.334	0.024	1.539	0.415
	C_8—H_a	1.100	0.271	-0.889	-0.696	-0.690	0.497	0.008	1.399	0.157
	C_8—H_b	1.098	0.272	-0.895	-0.698	-0.692	0.495	0.007	1.408	0.158
	C_9—H_a	1.096	0.278	-0.937	-0.738	-0.718	0.520	0.028	1.420	0.141
	C_9—H_b	1.096	0.278	-0.940	-0.740	-0.720	0.521	0.027	1.421	0.141
	N_{10}—H_a	1.017	0.335	-1.451	-1.211	-1.151	0.912	0.052	1.328	0.183
	N_{10}—H_b	1.017	0.335	-1.449	-1.211	-1.151	0.913	0.052	1.327	0.184

[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 S1d Bond lengths and topological properties at bond critical points (BCPs) in the $A^{+}G^{+}T$ conformer of TRA 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	ε	$\lvert\lambda_1\rvert/\lambda_3$	G_b/ρ_b
Ring A	N_1—C_{7a}	1.380	0.299	-0.730	-0.597	-0.533	0.399	0.120	1.494	0.757
	N_1—C_2	1.385	0.295	-0.698	-0.586	-0.507	0.395	0.155	1.483	0.775
	C_2—C_3	1.375	0.318	-0.874	-0.680	-0.507	0.313	0.342	2.174	0.378
	C_3—C_{3a}	1.447	0.278	-0.688	-0.557	-0.476	0.345	0.171	1.616	0.302
	C_{3a}—C_{7a}	1.424	0.298	-0.802	-0.625	-0.520	0.343	0.201	1.822	0.310
	N_1—H	1.007	0.340	-1.656	-1.298	-1.235	0.877	0.051	1.480	0.153
	C_2—H	1.082	0.282	-0.976	-0.770	-0.737	0.532	0.045	1.448	0.130
Ring B	C_{3a}—C_4	1.409	0.298	-0.807	-0.616	-0.522	0.330	0.180	1.863	0.311
	C_4—C_5	1.391	0.309	-0.852	-0.650	-0.526	0.324	0.234	2.005	0.335
	C_5—C_6	1.412	0.298	-0.801	-0.616	-0.517	0.333	0.191	1.851	0.311
	C_6—C_7	1.392	0.308	-0.845	-0.647	-0.522	0.323	0.239	2.002	0.336
	C_7—C_{7a}	1.400	0.303	-0.830	-0.633	-0.521	0.324	0.215	1.955	0.323
	C_4—H	1.086	0.281	-0.966	-0.756	-0.741	0.530	0.020	1.424	0.132
	C_5—H	1.086	0.280	-0.953	-0.743	-0.725	0.515	0.025	1.442	0.140
	C_6—H	1.086	0.280	-0.955	-0.744	-0.727	0.516	0.023	1.441	0.139
	C_7—H	1.087	0.278	-0.941	-0.735	-0.717	0.510	0.026	1.440	0.142
Aminoethyl moiety	C_3—C_8	1.506	0.250	-0.585	-0.476	-0.459	0.349	0.037	1.362	0.238
	C_8—C_9	1.540	0.239	-0.532	-0.453	-0.444	0.364	0.019	1.243	0.225
	C_9—N_{10}	1.467	0.262	-0.677	-0.520	-0.499	0.341	0.043	1.525	0.403
	C_8—H_a	1.097	0.274	-0.907	-0.712	-0.706	0.511	0.008	1.393	0.150
	C_8—H_b	1.097	0.273	-0.899	-0.702	-0.695	0.497	0.009	1.410	0.156
	C_9—H_a	1.097	0.277	-0.934	-0.732	-0.716	0.513	0.023	1.426	0.143
	C_9—H_b	1.104	0.273	-0.897	-0.710	-0.695	0.508	0.022	1.398	0.149
	N_{10}—H_a	1.016	0.336	-1.458	-1.215	-1.157	0.914	0.050	1.329	0.183
	N_{10}—H_b	1.017	0.336	-1.479	-1.221	-1.165	0.907	0.048	1.346	0.179

[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 S1e Bond lengths and topological properties at bond critical points (BCPs) in the A^+TG^+ conformer of TRA 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	ε	$\lvert\lambda_1\rvert/\lambda_3$	G_b/ρ_b
Ring A	N_1—C_{7a}	1.380	0.299	-0.733	-0.597	-0.533	0.397	0.120	1.504	0.753
	N_1—C_2	1.386	0.295	-0.701	-0.586	-0.507	0.392	0.154	1.494	0.770
	C_2—C_3	1.374	0.319	-0.878	-0.683	-0.508	0.312	0.345	2.185	0.379
	C_3—C_{3a}	1.445	0.279	-0.694	-0.560	-0.479	0.344	0.170	1.626	0.302
	C_{3a}—C_{7a}	1.423	0.299	-0.805	-0.626	-0.521	0.343	0.200	1.826	0.310
	N_1—H	1.007	0.340	-1.656	-1.298	-1.235	0.877	0.051	1.480	0.153
	C_2—H	1.082	0.282	-0.976	-0.770	-0.738	0.532	0.045	1.449	0.130
Ring B	C_{3a}—C_4	1.408	0.299	-0.811	-0.618	-0.523	0.330	0.183	1.873	0.311
	C_4—C_5	1.391	0.309	-0.852	-0.650	-0.526	0.324	0.236	2.006	0.335
	C_5—C_6	1.412	0.298	-0.801	-0.617	-0.517	0.333	0.192	1.853	0.311
	C_6—C_7	1.392	0.308	-0.845	-0.646	-0.522	0.323	0.239	2.000	0.336
	C_7—C_{7a}	1.400	0.303	-0.831	-0.634	-0.521	0.324	0.215	1.956	0.323
	C_4—H	1.087	0.280	-0.954	-0.744	-0.728	0.518	0.021	1.435	0.138
	C_5—H	1.086	0.280	-0.953	-0.743	-0.725	0.515	0.025	1.443	0.140
	C_6—H	1.086	0.280	-0.955	-0.744	-0.727	0.517	0.023	1.441	0.139
	C_7—H	1.087	0.278	-0.942	-0.736	-0.717	0.511	0.026	1.440	0.142
Aminoethyl moiety	C_3—C_8	1.503	0.251	-0.594	-0.480	-0.463	0.349	0.038	1.377	0.237
	C_8—C_9	1.539	0.239	-0.535	-0.460	-0.439	0.364	0.047	1.262	0.226
	C_9—N_{10}	1.468	0.260	-0.672	-0.514	-0.494	0.336	0.041	1.531	0.408
	C_8—H_a	1.097	0.274	-0.907	-0.713	-0.707	0.514	0.009	1.388	0.150
	C_8—H_b	1.099	0.272	-0.893	-0.696	-0.691	0.494	0.007	1.410	0.159
	C_9—H_a	1.103	0.274	-0.902	-0.715	-0.697	0.510	0.026	1.403	0.148
	C_9—H_b	1.096	0.279	-0.942	-0.739	-0.722	0.519	0.024	1.425	0.141
	N_{10}—H_a	1.017	0.335	-1.447	-1.210	-1.151	0.914	0.051	1.324	0.183
	N_{10}—H_b	1.016	0.336	-1.463	-1.217	-1.158	0.912	0.051	1.334	0.182

[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 S1f Bond lengths and topological properties at bond critical points (BCPs) in the $A^{+}TT$ conformer of TRA 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	ε	$\lvert\lambda_1\rvert/\lambda_3$	G_b/ρ_b
Ring A	N_1—C_{7a}	1.380	0.299	-0.734	-0.597	-0.533	0.397	0.120	1.505	0.753
	N_1—C_2	1.386	0.295	-0.700	-0.586	-0.508	0.394	0.153	1.487	0.772
	C_2—C_3	1.374	0.319	-0.878	-0.683	-0.508	0.313	0.345	2.185	0.378
	C_3—C_{3a}	1.445	0.279	-0.694	-0.560	-0.478	0.344	0.170	1.626	0.303
	C_{3a}—C_{7a}	1.424	0.298	-0.804	-0.625	-0.521	0.343	0.200	1.824	0.310
	N_1—H	1.007	0.340	-1.657	-1.298	-1.235	0.877	0.051	1.481	0.153
	C_2—H	1.082	0.283	-0.978	-0.772	-0.739	0.533	0.044	1.447	0.129
Ring B	C_{3a}—C_4	1.408	0.299	-0.811	-0.618	-0.523	0.330	0.183	1.873	0.311
	C_4—C_5	1.391	0.309	-0.851	-0.650	-0.525	0.324	0.237	2.006	0.335
	C_5—C_6	1.412	0.298	-0.801	-0.617	-0.517	0.333	0.192	1.853	0.311
	C_6—C_7	1.392	0.308	-0.845	-0.646	-0.522	0.323	0.239	2.000	0.336
	C_7—C_{7a}	1.400	0.303	-0.831	-0.634	-0.522	0.324	0.215	1.956	0.323
	C_4—H	1.087	0.279	-0.951	-0.741	-0.726	0.515	0.021	1.438	0.139
	C_5—H	1.086	0.280	-0.952	-0.743	-0.724	0.515	0.026	1.443	0.141
	C_6—H	1.086	0.280	-0.955	-0.744	-0.727	0.517	0.023	1.441	0.139
	C_7—H	1.087	0.278	-0.942	-0.736	-0.718	0.511	0.026	1.440	0.142
Aminoethyl moiety	C_3—C_8	1.503	0.251	-0.594	-0.480	-0.463	0.349	0.038	1.377	0.237
	C_8—C_9	1.539	0.240	-0.536	-0.460	-0.440	0.364	0.047	1.264	0.225
	C_9—N_{10}	1.469	0.260	-0.671	-0.514	-0.493	0.336	0.044	1.529	0.407
	C_8—H_a	1.100	0.271	-0.886	-0.693	-0.688	0.495	0.008	1.400	0.158
	C_8—H_b	1.096	0.275	-0.913	-0.716	-0.709	0.512	0.009	1.398	0.150
	C_9—H_a	1.096	0.278	-0.940	-0.738	-0.720	0.518	0.024	1.424	0.141
	C_9—H_b	1.102	0.274	-0.906	-0.717	-0.699	0.510	0.025	1.405	0.148
	N_{10}—H_a	1.016	0.336	-1.462	-1.216	-1.158	0.912	0.051	1.333	0.182
	N_{10}—H_b	1.017	0.335	-1.447	-1.209	-1.151	0.914	0.050	1.323	0.183

[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 S1g Bond lengths and topological properties at bond critical points (BCPs) in the $A^+G^+G^-$ conformer of TRA 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	ε	$\lvert\lambda_1\rvert/\lambda_3$	G_b/ρ_b
Ring A	N_1—C_{7a}	1.380	0.301	-0.732	-0.600	-0.536	0.404	0.120	1.485	0.762
	N_1—C_2	1.385	0.296	-0.697	-0.589	-0.510	0.402	0.154	1.465	0.783
	C_2—C_3	1.376	0.320	-0.881	-0.683	-0.509	0.312	0.341	2.192	0.379
	C_3—C_{3a}	1.446	0.279	-0.691	-0.558	-0.477	0.344	0.171	1.622	0.303
	C_{3a}—C_{7a}	1.424	0.298	-0.804	-0.626	-0.521	0.343	0.200	1.823	0.310
	N_1—H	1.007	0.341	-1.666	-1.303	-1.240	0.877	0.051	1.486	0.152
	C_2—H	1.082	0.283	-0.978	-0.772	-0.739	0.533	0.044	1.448	0.129
Ring B	C_{3a}—C_4	1.409	0.299	-0.812	-0.619	-0.523	0.330	0.183	1.876	0.312
	C_4—C_5	1.391	0.310	-0.858	-0.653	-0.528	0.323	0.237	2.024	0.337
	C_5—C_6	1.412	0.299	-0.809	-0.620	-0.520	0.332	0.191	1.868	0.312
	C_6—C_7	1.391	0.309	-0.853	-0.650	-0.525	0.322	0.239	2.019	0.337
	C_7—C_{7a}	1.400	0.304	-0.836	-0.636	-0.524	0.323	0.214	1.966	0.324
	C_4—H	1.086	0.279	-0.952	-0.742	-0.726	0.516	0.022	1.437	0.140
	C_5—H	1.086	0.280	-0.953	-0.744	-0.725	0.515	0.025	1.443	0.140
	C_6—H	1.086	0.280	-0.957	-0.745	-0.728	0.517	0.023	1.441	0.139
	C_7—H	1.087	0.278	-0.944	-0.737	-0.719	0.512	0.025	1.440	0.142
Aminoethyl moiety	C_3—C_8	1.505	0.251	-0.590	-0.479	-0.460	0.349	0.040	1.372	0.239
	C_8—C_9	1.550	0.235	-0.506	-0.442	-0.431	0.367	0.024	1.202	0.228
	C_9—N_{10}	1.462	0.265	-0.691	-0.523	-0.511	0.343	0.024	1.526	0.407
	C_8—H_a	1.098	0.272	-0.891	-0.697	-0.691	0.497	0.009	1.403	0.158
	C_8—H_b	1.099	0.272	-0.893	-0.699	-0.692	0.498	0.009	1.404	0.157
	C_9—H_a	1.097	0.277	-0.930	-0.731	-0.713	0.514	0.025	1.421	0.143
	C_9—H_b	1.097	0.278	-0.933	-0.735	-0.717	0.518	0.024	1.417	0.142
	N_{10}—H_a	1.017	0.336	-1.472	-1.218	-1.163	0.908	0.047	1.341	0.180
	N_{10}—H_b	1.017	0.335	-1.433	-1.202	-1.146	0.915	0.049	1.314	0.186

[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 S1h Bond lengths and topological properties at bond critical points (BCPs) in the CTG^- conformer of TRA 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	ε	$\lvert\lambda_1\rvert/\lambda_3$	G_b/ρ_b
Ring A	N_1—C_{7a}	1.380	0.300	-0.736	-0.599	-0.535	0.398	0.119	1.506	0.753
	N_1—C_2	1.387	0.294	-0.703	-0.584	-0.506	0.387	0.154	1.508	0.764
	C_2—C_3	1.375	0.318	-0.867	-0.677	-0.503	0.313	0.347	2.164	0.380
	C_3—C_{3a}	1.445	0.280	-0.696	-0.561	-0.480	0.345	0.169	1.629	0.302
	C_{3a}—C_{7a}	1.423	0.299	-0.806	-0.627	-0.522	0.343	0.201	1.830	0.311
	N_1—H	1.007	0.340	-1.657	-1.299	-1.235	0.877	0.052	1.481	0.153
	C_2—H	1.081	0.284	-0.983	-0.775	-0.743	0.535	0.044	1.450	0.129
Ring B	C_{3a}—C_4	1.407	0.299	-0.812	-0.619	-0.523	0.330	0.184	1.878	0.312
	C_4—C_5	1.391	0.309	-0.850	-0.649	-0.525	0.324	0.236	2.002	0.335
	C_5—C_6	1.412	0.298	-0.801	-0.617	-0.517	0.333	0.193	1.854	0.312
	C_6—C_7	1.382	0.308	-0.844	-0.646	-0.521	0.323	0.239	1.998	0.335
	C_7—C_{7a}	1.400	0.303	-0.831	-0.634	-0.522	0.324	0.215	1.956	0.323
	C_4—H	1.087	0.279	-0.952	-0.742	-0.726	0.516	0.021	1.436	0.138
	C_5—H	1.086	0.280	-0.953	-0.743	-0.724	0.515	0.025	1.443	0.141
	C_6—H	1.086	0.280	-0.956	-0.745	-0.728	0.517	0.023	1.441	0.139
	C_7—H	1.087	0.278	-0.943	-0.736	-0.718	0.511	0.026	1.440	0.142
Aminoethyl	C_3—C_8	1.505	0.250	-0.588	-0.479	-0.457	0.349	0.048	1.375	0.237
Moiety	C_8—C_9	1.538	0.241	-0.537	-0.461	-0.443	0.367	0.042	1.258	0.227
	C_9—N_{10}	1.465	0.262	-0.677	-0.514	-0.502	0.339	0.025	1.518	0.408
	C_8—H_a	1.101	0.270	-0.883	-0.692	-0.686	0.495	0.009	1.398	0.159
	C_8—H_b	1.101	0.270	-0.883	-0.692	-0.686	0.495	0.009	1.398	0.159
	C_9—H_a	1.097	0.278	-0.934	-0.735	-0.716	0.517	0.026	1.420	0.143
	C_9—H_b	1.097	0.278	-0.934	-0.735	-0.716	0.517	0.026	1.420	0.143
	N_{10}—H_a	1.017	0.335	-1.453	-1.212	-1.152	0.912	0.052	1.329	0.183
	N_{10}—H_b	1.017	0.335	-1.453	-1.212	-1.152	0.912	0.052	1.329	0.183

[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 S1i Bond lengths and topological properties at bond critical points (BCPs) in the CG$^-$T conformer of TRA 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	ε	$\lvert\lambda_1\rvert/\lambda_3$	G_b/ρ_b
Ring A	N_1—C_{7a}	1.379	0.300	-0.740	-0.600	-0.536	0.396	0.121	1.517	0.749
	N_1—C_2	1.386	0.294	-0.687	-0.578	-0.509	0.401	0.135	1.442	0.784
	C_2—C_3	1.375	0.318	-0.873	-0.681	-0.507	0.315	0.344	2.164	0.376
	C_3—C_{3a}	1.445	0.279	-0.694	-0.561	-0.477	0.344	0.175	1.629	0.304
	C_{3a}—C_{7a}	1.424	0.298	-0.803	-0.625	-0.522	0.343	0.198	1.820	0.309
	N_1—H	1.007	0.340	-1.654	-1.298	-1.235	0.879	0.051	1.477	0.153
	C_2—H	1.080	0.286	-1.005	-0.797	-0.766	0.559	0.040	1.427	0.119
Ring B	C_{3a}—C_4	1.408	0.299	-0.811	-0.618	-0.522	0.330	0.183	1.874	0.312
	C_4—C_5	1.391	0.309	-0.849	-0.649	-0.524	0.324	0.237	2.001	0.335
	C_5—C_6	1.412	0.298	-0.801	-0.617	-0.517	0.333	0.194	1.855	0.312
	C_6—C_7	1.392	0.308	-0.843	-0.645	-0.521	0.323	0.239	1.996	0.335
	C_7—C_{7a}	1.400	0.303	-0.832	-0.634	-0.521	0.324	0.216	1.957	0.323
	C_4—H	1.087	0.279	-0.949	-0.740	-0.724	0.515	0.022	1.438	0.140
	C_5—H	1.086	0.279	-0.951	-0.741	-0.723	0.513	0.026	1.444	0.141
	C_6—H	1.086	0.280	-0.953	-0.743	-0.726	0.515	0.024	1.442	0.140
	C_7—H	1.087	0.278	-0.941	-0.735	-0.716	0.510	0.026	1.441	0.142
Aminoethyl	C_3—C_8	1.506	0.250	-0.588	-0.480	-0.458	0.350	0.046	1.370	0.234
Moiety	C_8—C_9	1.534	0.242	-0.548	-0.462	-0.449	0.363	0.027	1.271	0.223
	C_9—N_{10}	1.472	0.258	-0.660	-0.510	-0.488	0.338	0.045	1.508	0.405
	C_8—H_a	1.098	0.273	-0.901	-0.705	-0.696	0.500	0.012	1.409	0.156
	C_8—H_b	1.102	0.269	-0.872	-0.688	-0.679	0.494	0.013	1.391	0.160
	C_9—H_a	1.096	0.278	-0.939	-0.738	-0.722	0.521	0.023	1.417	0.140
	C_9—H_b	1.103	0.274	-0.902	-0.713	-0.696	0.507	0.024	1.406	0.149
	N_{10}—H_a	1.017	0.335	-1.455	-1.213	-1.156	0.913	0.050	1.328	0.182
	N_{10}—H_b	1.018	0.334	-1.445	-1.207	-1.150	0.912	0.050	1.323	0.183

[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 S1j Bond lengths and topological properties at bond critical points (BCPs) in the CTG^+ conformer of TRA 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	ε	$\lvert\lambda_1\rvert/\lambda_3$	G_b/ρ_b
Ring A	N_1—C_{7a}	1.380	0.300	-0.735	-0.598	-0.535	0.398	0.119	1.504	0.753
	N_1—C_2	1.387	0.294	-0.702	-0.583	-0.505	0.386	0.156	1.512	0.762
	C_2—C_3	1.375	0.318	-0.868	-0.678	-0.503	0.313	0.347	2.168	0.380
	C_3—C_{3a}	1.445	0.280	-0.697	-0.562	-0.480	0.345	0.169	1.630	0.302
	C_{3a}—C_{7a}	1.423	0.299	-0.806	-0.627	-0.522	0.343	0.201	1.830	0.311
	N_1—H	1.007	0.340	-1.656	-1.298	-1.235	0.877	0.052	1.480	0.153
	C_2—H	1.081	0.283	-0.981	-0.774	-0.741	0.533	0.045	1.451	0.130
Ring B	C_{3a}—C_4	1.407	0.299	-0.813	-0.619	-0.523	0.330	0.184	0.254	1.587
	C_4—C_5	1.391	0.309	-0.850	-0.649	-0.525	0.324	0.235	1.878	0.312
	C_5—C_6	1.412	0.298	-0.801	-0.617	-0.517	0.333	0.193	2.002	0.335
	C_6—C_7	1.392	0.308	-0.844	-0.646	-0.521	0.323	0.239	1.854	0.312
	C_7—C_{7a}	1.400	0.303	-0.831	-0.634	-0.522	0.324	0.215	1.998	0.335
	C_4—H	1.087	0.279	-0.953	-0.743	-0.728	0.517	0.021	1.956	0.323
	C_5—H	1.086	0.280	-0.952	-0.743	-0.724	0.515	0.026	1.435	0.138
	C_6—H	1.086	0.280	-0.955	-0.744	-0.727	0.516	0.023	1.443	0.141
	C_7—H	1.087	0.278	-0.942	-0.736	-0.717	0.511	0.026	1.441	0.139
Aminoethyl	C_3—C_8	1.504	0.251	-0.592	-0.482	-0.459	0.348	0.050	1.440	0.142
moiety	C_8—C_9	1.531	0.244	-0.558	-0.470	-0.451	0.363	0.043	0.178	1.467
	C_9—N_{10}	1.468	0.261	-0.672	-0.516	-0.495	0.339	0.042	1.384	0.236
	C_8—H_a	1.098	0.273	-0.902	-0.711	-0.703	0.512	0.010	1.294	0.224
	C_8—H_b	1.101	0.270	-0.882	-0.691	-0.684	0.493	0.009	1.522	0.404
	C_9—H_a	1.104	0.273	-0.899	-0.711	-0.695	0.507	0.024	1.387	0.151
	C_9—H_b	1.097	0.278	-0.935	-0.733	-0.717	0.515	0.023	1.400	0.160
	N_{10}—H_a	1.016	0.336	-1.464	-1.218	-1.159	0.912	0.051	1.403	0.150
	N_{10}—H_b	1.017	0.335	-1.451	-1.211	-1.153	0.913	0.051	1.424	0.143

[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 S1k Bond lengths and topological properties at bond critical points (BCPs) in the CTT conformer of TRA 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	ε	$\lvert\lambda_1\rvert/\lambda_3$	G_b/ρ_b
Ring A	N_1—C_{7a}	1.380	0.300	-0.735	-0.598	-0.535	0.398	0.119	1.504	0.753
	N_1—C_2	1.387	0.294	-0.702	-0.583	-0.505	0.386	0.156	1.512	0.762
	C_2—C_3	1.375	0.318	-0.868	-0.678	-0.503	0.313	0.347	2.168	0.380
	C_3—C_{3a}	1.445	0.280	-0.697	-0.562	-0.480	0.345	0.169	1.630	0.302
	C_{3a}—C_{7a}	1.423	0.299	-0.806	-0.627	-0.522	0.343	0.201	1.830	0.311
	N_1—H	1.007	0.340	-1.656	-1.298	-1.235	0.877	0.052	1.480	0.153
	C_2—H	1.081	0.283	-0.981	-0.774	-0.741	0.533	0.045	1.451	0.130
Ring B	C_{3a}—C_4	1.407	0.299	-0.813	-0.619	-0.523	0.330	0.184	1.878	0.312
	C_4—C_5	1.391	0.309	-0.850	-0.649	-0.525	0.324	0.235	2.002	0.335
	C_5—C_6	1.412	0.298	-0.801	-0.617	-0.517	0.333	0.193	1.854	0.312
	C_6—C_7	1.392	0.308	-0.844	-0.646	-0.521	0.323	0.239	1.998	0.335
	C_7—C_{7a}	1.400	0.303	-0.831	-0.634	-0.522	0.324	0.215	1.956	0.323
	C_4—H	1.087	0.279	-0.953	-0.743	-0.728	0.517	0.021	1.435	0.138
	C_5—H	1.086	0.280	-0.952	-0.743	-0.724	0.515	0.026	1.443	0.141
	C_6—H	1.086	0.280	-0.955	-0.744	-0.727	0.516	0.023	1.441	0.139
	C_7—H	1.087	0.278	-0.942	-0.736	-0.717	0.511	0.026	1.440	0.142
Aminoethyl moiety	C_3—C_8	1.504	0.251	-0.592	-0.482	-0.459	0.348	0.050	1.384	0.236
	C_8—C_9	1.531	0.244	-0.558	-0.470	-0.451	0.363	0.043	1.294	0.224
	C_9—N_{10}	1.468	0.261	-0.672	-0.516	-0.495	0.339	0.042	1.522	0.404
	C_8—H_a	1.101	0.270	-0.882	-0.691	-0.684	0.493	0.009	1.400	0.160
	C_8—H_b	1.098	0.273	-0.902	-0.711	-0.703	0.512	0.010	1.387	0.151
	C_9—H_a	1.097	0.278	-0.935	-0.733	-0.717	0.515	0.023	1.424	0.143
	C_9—H_b	1.104	0.273	-0.899	-0.711	-0.695	0.507	0.024	1.403	0.150
	N_{10}—H_a	1.016	0.336	-1.464	-1.218	-1.159	0.912	0.051	1.335	0.182
	N_{10}—H_b	1.017	0.335	-1.451	-1.211	-1.153	0.913	0.051	1.326	0.183

[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 S1l Bond lengths and topological properties at bond critical points (BCPs) in the $A^+G^+G^+$ conformer of TRA 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	ε	$\lvert\lambda_1\rvert/\lambda_3$	G_b/ρ_b
Ring A	N_1—C_{7a}	1.380	0.299	-0.727	-0.595	-0.532	0.400	0.118	1.488	0.759
	N_1—C_2	1.384	0.296	-0.702	-0.589	-0.509	0.396	0.156	1.486	0.774
	C_2—C_3	1.375	0.319	-0.875	-0.682	-0.506	0.313	0.348	2.180	0.378
	C_3—C_{3a}	1.448	0.277	-0.685	-0.555	-0.475	0.345	0.168	1.609	0.301
	C_{3a}—C_{7a}	1.424	0.298	-0.801	-0.624	-0.519	0.343	0.202	1.822	0.311
	N_1—H	1.007	0.340	-1.653	-1.297	-1.234	0.878	0.051	1.477	0.153
	C_2—H	1.082	0.282	-0.973	-0.768	-0.735	0.529	0.046	1.451	0.131
Ring B	C_{3a}—C_4	1.409	0.299	-0.812	-0.617	-0.525	0.330	0.177	1.870	0.311
	C_4—C_5	1.391	0.309	-0.853	-0.649	-0.527	0.324	0.231	2.004	0.335
	C_5—C_6	1.412	0.298	-0.801	-0.617	-0.517	0.333	0.192	1.853	0.311
	C_6—C_7	1.391	0.308	-0.845	-0.647	-0.522	0.323	0.240	2.003	0.336
	C_7—C_{7a}	1.401	0.303	-0.830	-0.633	-0.521	0.324	0.216	1.954	0.323
	C_4—H	1.084	0.283	-0.982	-0.770	-0.757	0.545	0.018	1.414	0.127
	C_5—H	1.086	0.279	-0.949	-0.740	-0.722	0.513	0.026	1.444	0.142
	C_6—H	1.086	0.280	-0.953	-0.742	-0.725	0.515	0.023	1.442	0.140
	C_7—H	1.087	0.277	-0.939	-0.733	-0.714	0.508	0.027	1.442	0.144
Aminoethyl moiety	C_3—C_8	1.506	0.250	-0.586	-0.477	-0.460	0.351	0.037	1.360	0.235
	C_8—C_9	1.544	0.237	-0.526	-0.451	-0.440	0.364	0.025	1.237	0.222
	C_9—N_{10}	1.470	0.259	-0.665	-0.512	-0.491	0.338	0.043	1.515	0.406
	C_8—H_a	1.100	0.271	-0.886	-0.695	-0.690	0.499	0.008	1.393	0.157
	C_8—H_b	1.097	0.273	-0.901	-0.704	-0.696	0.498	0.012	1.413	0.157
	C_9—H_a	1.103	0.273	-0.899	-0.711	-0.694	0.507	0.024	1.404	0.150
	C_9—H_b	1.095	0.279	-0.943	-0.740	-0.725	0.523	0.020	1.416	0.140
	N_{10}—H_a	1.017	0.335	-1.446	-1.209	-1.151	0.914	0.050	1.323	0.184
	N_{10}—H_b	1.016	0.336	-1.462	-1.217	-1.158	0.912	0.051	1.334	0.182

[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 B3LYP/6-311++G** level of theory for donation transferences related to the group T [a]

Donor	Acceptor	$E^{(2)}$		
		A^+TG^-	A^+TG^+	A^+TT
LP_{N10}	$\sigma^*_{C3—C8}$	0.78	-	-
	$\sigma^*_{C8—C9}$	8.51	1.15	1.13
	$\sigma^*_{C9—Ha}$	1.54	7.67	1.09
	$\sigma^*_{C9—Hb}$	1.42	1.07	7.59
$\sigma_{C3—C3a}$	$\sigma^*_{C3—C8}$	1.38	1.36	1.32
	$\sigma^*_{C8—Hb}$	0.9	0.9	0.87
$\sigma_{C2—C3}$	$\sigma^*_{C3—C8}$	1.85	1.84	1.85
	$\sigma^*_{C8—Ha}$	0.58	0.53	0.57
$\pi_{C2—C3}$	$\sigma^*_{C8—C9}$	3.73	3.63	3.64
$\sigma_{N1—C2}$	$\sigma^*_{C3—C8}$	4.11	4.1	3.96
$\sigma_{C3a—C7a}$	$\sigma^*_{C3—C8}$	5.01	4.97	5.51
$\sigma_{C3—C8}$	$\sigma^*_{C3a—C7a}$	1.56	1.57	1.15
	$\sigma^*_{C9—N10}$	2.29	1.94	1.91
$\sigma_{C8—C9}$	$\pi^*_{C2—C3}$	2.69	2.64	2.54
	$\sigma^*_{C3—C8}$	0.90	0.79	0.78
$\sigma_{C8—Ha}$	$\sigma^*_{C2—C3}$	3.56	3.53	3.45
	$\pi^*_{C2—C3}$	2.33	2.47	2.46
$\sigma_{C8—Hb}$	$\sigma^*_{C3a—C3}$	5.34	5.39	5.42
$\sigma_{C9—Ha}$	$\sigma^*_{C8—Ha}$	2.83	2.69	2.88
	$\sigma^*_{N10—Ha}$	3.38	-	-
	$\sigma^*_{N10—Hb}$	-	-	3.29
$\sigma_{C9—Hb}$	$\sigma^*_{C8—Hb}$	2.75	2.81	2.64
	$\sigma^*_{N10—Ha}$	-	3.29	-
	$\sigma^*_{N10—Hb}$	3.38	-	-
$\sigma_{N10—Ha}$	$\sigma^*_{C8—C9}$	-	-	2.6
	$\sigma^*_{C9—Ha}$	2.33	2.19	-
$\sigma_{N10—Hb}$	$\sigma^*_{C8—C9}$	-	2.61	-
	$\sigma^*_{C9—Ha}$	-	-	2.23
	$\sigma^*_{C9—Hb}$	2.3	-	-
	Σ	**65.45**	**59.14**	**58.88**

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

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

Donor	Acceptor	$E^{(2)}$		
		A^+G^+T	$A^+G^+G^-$	$A^+G^+G^+$
LP_{N10}	$\sigma^*_{C4—H}$	-	-	1.22
	$\sigma^*_{C8—C9}$	1.03	9.07	1.58
	$\sigma^*_{C8—Hb}$	-	0.65	-
	$\sigma^*_{C9—Ha}$	1.18	1.30	6.76
	$\sigma^*_{C9—Hb}$	7.95	1.72	-
$\sigma_{C3—C3a}$	$\sigma^*_{C3a—C7a}$	1.41	1.39	1.35
	$\sigma^*_{C3—C8}$	1.68	1.36	1.74
	$\sigma^*_{C8—Hb}$	0.68	0.68	0.67
$\sigma_{C2—C3}$	$\sigma^*_{C3—C8}$	2.11	1.78	2.07
$\pi_{C2—C3}$	$\sigma^*_{C8—C9}$	3.68	3.58	3.58
$\sigma_{N1—C2}$	$\sigma^*_{C3—C8}$	4.02	4.05	3.95
$\sigma_{C3a—C7a}$	$\sigma^*_{C3—C8}$	5.13	5.06	5.33
$\sigma_{C3—C8}$	$\sigma^*_{C3a—C7a}$	1.62	1.59	1.47
	$\sigma^*_{N1—C2}$	1.63	1.70	1.68
	$\sigma^*_{C9—Ha}$	1.23	1.17	0.94
$\sigma_{C8—C9}$	$\pi^*_{C2—C3}$	2.56	2.82	1.88
$\sigma_{C9—N10}$	$\sigma^*_{C8—Hb}$	1.14	0.86	0.96
$\sigma_{C8—Ha}$	$\sigma^*_{C2—C3}$	4.05	4.56	2.31
	$\sigma^*_{C9—Hb}$	2.71	2.58	2.45
$\sigma_{C8—Hb}$	$\sigma^*_{C3—C3a}$	5.17	4.62	6.12
	$\pi^*_{C2—C3}$	0.74	1.19	-
$\sigma_{C9—Ha}$	$\sigma^*_{C3—C8}$	3.48	3.36	2.92
	$\sigma^*_{N10—Hb}$	3.23	-	-
$\sigma_{C9—Hb}$	$\sigma^*_{C8—Ha}$	2.75	2.90	2.4
$\sigma_{N10—Ha}$	$\sigma^*_{C8—C9}$	2.91	-	-
	$\sigma^*_{C9—Ha}$	0.52	2.33	2.22
$\sigma_{N10—Hb}$	$\sigma^*_{C9—Ha}$	2.21	-	-
	$\sigma^*_{C9—Hb}$	-	2.38	0.61
	Σ	**64.82**	**62.70**	**54.21**

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

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

Donor	Acceptor	$E^{(2)}$		
		CTG^-	**CTG^+**	**CTT**
LP_{N10}	**$\sigma^*_{C3—C8}$**	0.82	-	-
	$\sigma^*_{C8—C9}$	8.25	1.09	1.09
	$\sigma^*_{C9—Ha}$	1.47	7.63	1.12
	$\sigma^*_{C9—Hb}$	1.47	1.12	7.63
$\sigma_{C3—C3a}$	**$\sigma^*_{C2—C3}$**	2.28	2.27	2.27
	$\sigma^*_{C3—C8}$	1.74	1.73	1.73
$\pi_{C2—C3}$	**$\sigma^*_{C8—Ha}$**	3.03	3.04	2.89
	$\sigma^*_{C8—Hb}$	3.03	2.89	3.04
$\sigma_{C3a—C7a}$	**$\sigma^*_{C3—C8}$**	4.97	4.91	4.91
$\sigma_{C3—C8}$	**$\sigma^*_{C3—C3a}$**	2.16	2.15	2.15
	$\sigma^*_{C9—N10}$	2.12	1.74	1.74
$\sigma_{C8—C9}$	**$\sigma^*_{C3—C8}$**	0.95	0.84	0.84
$\sigma_{C8—Ha}$	**$\sigma^*_{C9—Ha}$**	2.85	2.93	2.87
$\sigma_{C8—Hb}$	**$\sigma^*_{C9—Hb}$**	2.85	2.87	2.93
$\sigma_{C9—Ha}$	**$\sigma^*_{C8—Ha}$**	2.88	2.71	2.92
	$\sigma^*_{N10—Ha}$	3.33	-	-
	$\sigma^*_{N10—Hb}$	-	-	3.27
$\sigma_{C9—Hb}$	**$\sigma^*_{C8—Hb}$**	2.88	2.92	2.71
	$\sigma^*_{N10—Hb}$	3.33	3.27	-
$\sigma_{N10—Ha}$	**$\sigma^*_{C8—C9}$**	-	2.61	2.61
	$\sigma^*_{C9—Ha}$	2.29	-	-
$\sigma_{N10—Hb}$	**$\sigma^*_{C9—Ha}$**	-	-	2.22
	$\sigma^*_{C9—Hb}$	2.29	2.22	-
	Σ	**54.99**	**48.94**	**48.94**

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