Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Acid catalysis through N-protonation in undistorted carboxamides: improvement of amide proton sponge acylating ability

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Table S1. Geometric and electronic parameters of **10**(E), cation **10**H⁺(E) and cation **10**H⁺(E)' with frozen distance r_3.

Compd	E_{HB}, kcal·mol^{-1}	r_1, Å	r_2, Å	r_3, Å	α, deg	ω, deg	χ_N, deg	τ, deg	ϑ, deg	q_{NPA}, *e*	q_{MK}, *e*	q_H, *e*	δ, ppm
10(E)	-	2.789	1.372	-	-	14.81	10.60	4.32	14.92	0.6994	0.6232	0.1658	170.43
10H⁺(E)	9.15	2.697	1.423	1.708	154.66	0.55	35.65	2.09	37.74	0.7122	0.4885	0.1836	176.31
10H⁺(E)'	10.70	2.664	1.427	1.658	156.25	0.68	36.98	2.46	39.43	0.7146	0.4830	0.1855	176.74
10H⁺(E)'	12.49	2.632	1.430	1.608	157.72	0.83	38.25	2.80	41.05	0.7170	0.4833	0.1875	177.16
10H⁺(E)'	14.58	2.601	1.434	1.558	159.09	0.94	39.51	3.15	42.66	0.7196	0.4892	0.1897	177.53
10H⁺(E)'	17.03	2.572	1.439	1.508	160.31	1.14	40.69	3.54	44.23	0.7224	0.4876	0.1922	177.90
10H⁺(E)'	19.94	2.547	1.444	1.458	161.36	1.41	41.84	3.94	45.78	0.7253	0.4799	0.1950	178.22
10H⁺(E)'	23.46	2.525	1.450	1.408	162.19	1.63	42.98	4.46	47.44	0.7286	0.4784	0.1981	178.47
10H⁺(E)'	27.78	2.510	1.458	1.358	162.77	1.88	44.05	5.17	49.22	0.7321	0.4880	0.2017	178.62
10H⁺(E)'	33.17	2.502	1.466	1.308	162.99	2.19	45.05	6.12	51.17	0.7361	0.4931	0.2059	178.65

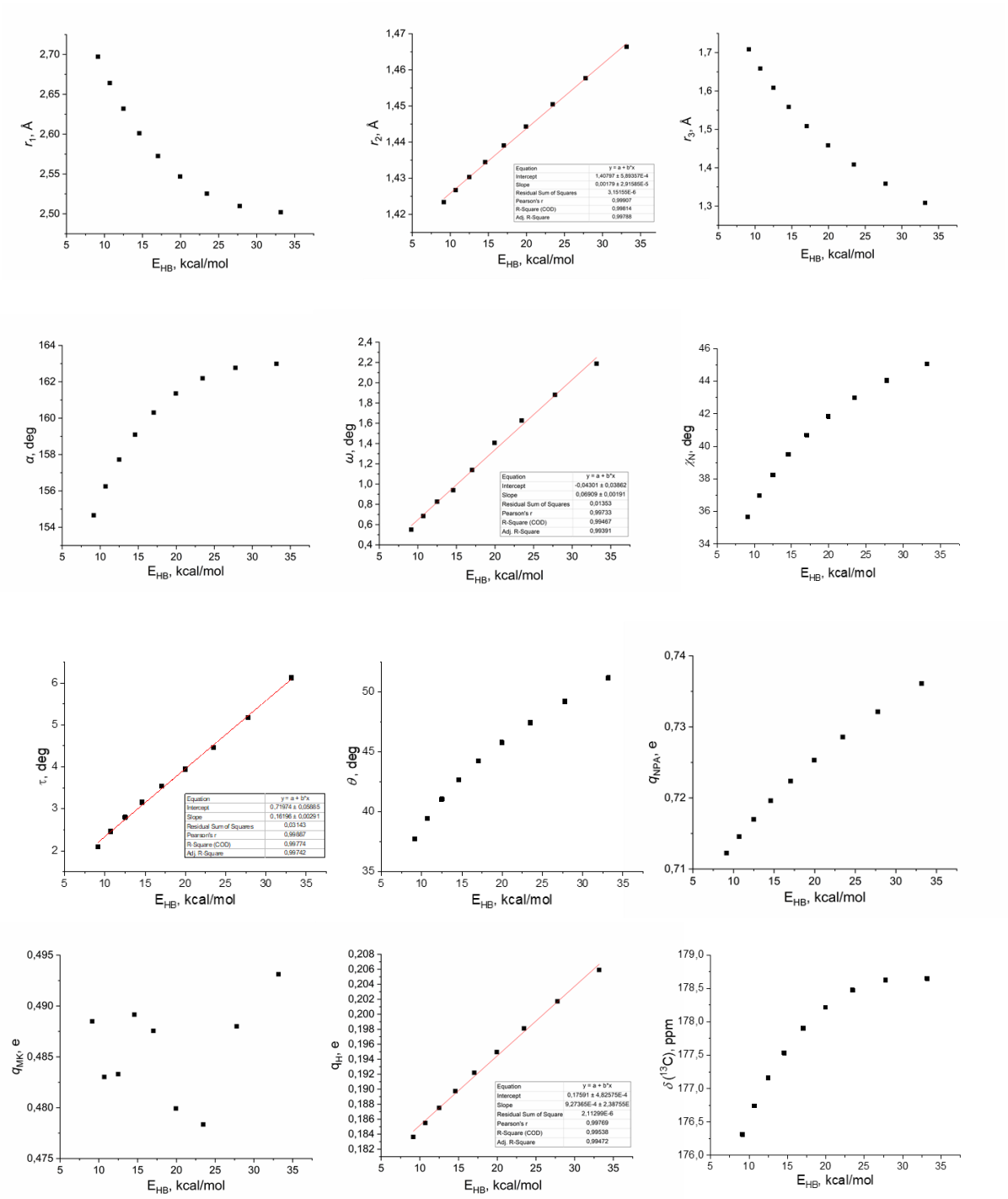

Figure S1. Correlations between parameters of activation and hydrogen bond energy for **10**H⁺(E)' with frozen distance r_3.

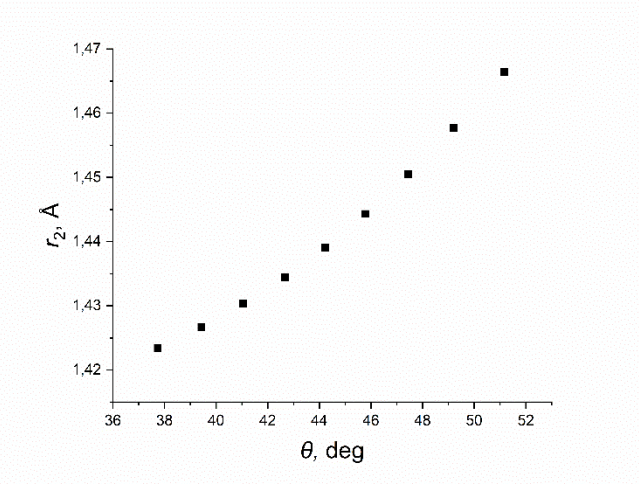

Figure S2. Correlations between ϑ and r_2 for **10**H$^+$(E)′ with frozen distance r_3.

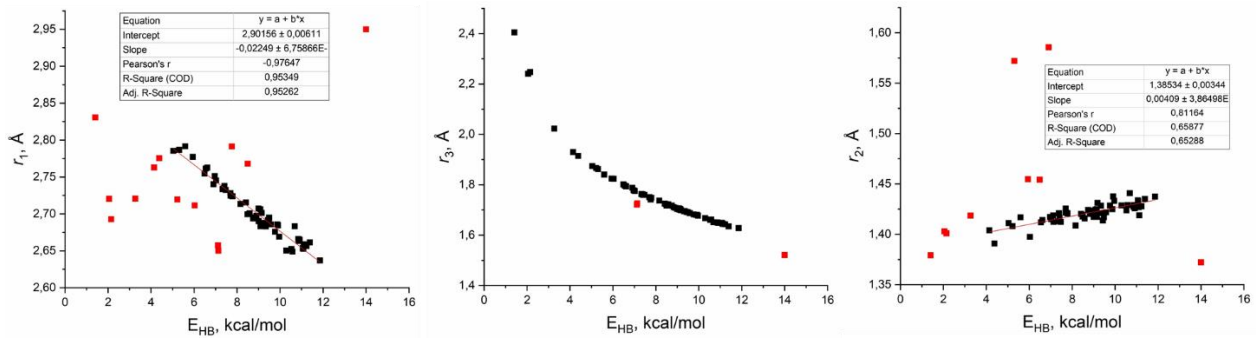

Figure S3. Correlations between parameters of activation and hydrogen bond energy for cations **9**H$^+$-**44**H$^+$

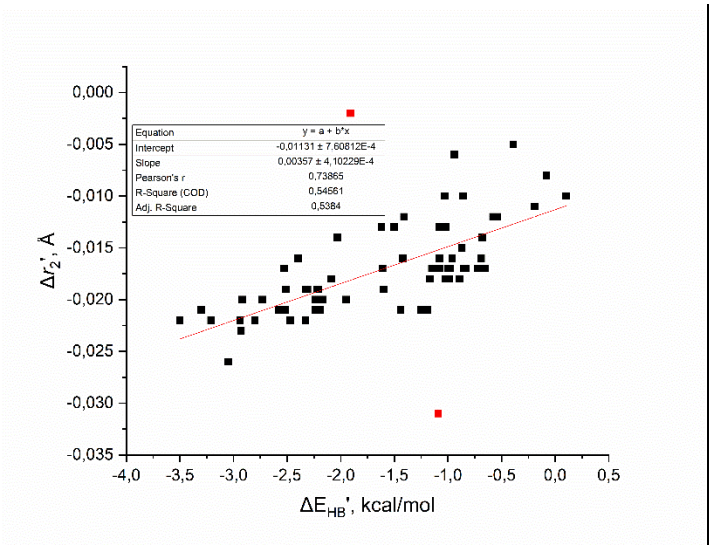

Figure S4. Correlations between parameters $\Delta r_2'$ and $\Delta E_{HB}'$.

Table S2. Geometric and electronic parameters of amide cations **9**H$^+$-**44**H$^+$ in vacuum.

Compd	E_{HB}, kcal·mol^{-1}	r_1, Å	r_2, Å	r_3, Å	α, deg	ω, deg	χ_N, deg	τ, deg	ϑ, deg	q_{NPA}	q_{MK}	q_H	δ, ppm
9H$^+$(E)	9.39*	2.687	1.431	1.698	153.88	5.32	42.29	12.8	55.09	0.6931	0.3794	0.1776	178.91
9H$^+$(Z)	7.01	2.763	1.414	1.794	153.42	5.92	25.54	19.09	44.63	0.6981	0.6123	0.1773	185.38
10H$^+$(E)	9.15	2.697	1.423	1.708	156.67	0.55	35.66	2.08	37.74	0.7123	0.4885	0.1836	180.79
10H$^+$(Z)	7.33	2.751	1.417	1.777	153.81	4.46	35.13	9.6	44.73	0.7175	0.6508	0.1862	187.24
11H$^+$(E)	11.06	2.665	1.426	1.649	159.52	5.04	36.24	2.17	38.41	0.715	0.5039	0.1854	181.44
11H$^+$(Z)	9.26	2.707	1.42	1.704	158.84	8.99	36.21	8.53	44.74	0.7196	0.6432	0.1874	187.28
12H$^+$(E)	11	2.666	1.427	1.65	159.45	0.95	36.64	2.55	39.19	0.715	0.485	0.186	180.91
12H$^+$(Z)	9.35	2.706	1.422	1.702	159.17	2.86	35.82	8.56	44.38	0.7198	0.6431	0.1881	187
13H$^+$(E)	11.02	2.663	1.429	1.65	158.89	8.95	37.15	2.93	40.07	0.7151	0.5278	0.1868	180.28
13H$^+$(Z)	9.39	2.701	1.425	1.7	157.86	12.91	37.47	5.56	43.03	0.7204	0.6565	0.1889	187
14H$^+$(E)	9.95	2.676	1.429	1.682	154.89	0.2	36.81	2.28	39.09	0.7135	0.5011	0.1855	180.63
14H$^+$(Z)	8.01	2.728	1.422	1.75	154.03	4.75	36.01	10.21	46.22	0.7197	0.6817	0.1882	187.91
15H$^+$(E)	9.06	2.695	1.42	1.711	154.12	1.57	35.68	3.41	39.09	0.7116	0.5263	0.1826	180.94
15H$^+$(Z)	7.37	2.745	1.415	1.775	153.21	10.2	35.37	9.33	44.7	0.7159	0.6596	0.185	186.97
16H$^+$(E)	9.55	2.683	1.428	1.695	154.38	0.08	36.75	2.63	39.38	0.7129	0.5125	0.1856	179.96
16H$^+$(Z)	7.72	2.735	1.421	1.762	153.54	5.51	36.06	9.18	45.24	0.7186	0.6304	0.1881	187.33
17H$^+$(E)	9.54	2.687	1.421	1.695	155.12	2.23	35.42	2.67	38.09	0.7125	0.497	0.1826	181.65
17H$^+$(Z)	7.76	2.738	1.416	1.76	154.29	7.48	34.6	9.96	44.56	0.7173	0.6326	0.185	187.25
18H$^+$(E)	9.24	2.69	1.417	1.706	154.25	0.96	31.13	1.87	32.99	0.7091	0.4786	0.1807	181.09
18H$^+$(Z)	7.81	2.732	1.412	1.76	153.55	10.69	31.31	8.55	39.86	0.7118	0.5834	0.1824	185.62
19H$^+$(E)	9.37	2.688	1.424	1.703	154.23	1.72	30.33	0.71	31.04	0.7179	0.4568	0.1776	179.47
19H$^+$(Z)	8.1	2.724	1.421	1.748	153.6	12.34	32.55	11.35	43.9	0.726	0.6704	0.1796	186.4
20H$^+$(E)	9.32	2.683	1.424	1.706	153.19	9.66	27.32	2.13	29.45	0.7161	0.4992	0.1804	177.42
20H$^+$(Z)	9	2.694	1.424	1.717	152.93	18.11	33.68	7.09	40.77	0.7328	0.6636	0.1828	186.75
21H$^+$(E)	10.67	2.652	1.424	1.66	154.79	3.36	36.32	2.35	38.67	0.7139	0.486	0.1844	181.34
21H$^+$(Z)	8.75	2.7	1.418	1.723	153.81	12.5	36.15	9.88	46.04	0.7177	0.6512	0.1862	187.12
22H$^+$(E)	10.13	2.669	1.433	1.677	154.64	3.28	37	1.45	38.45	0.714	0.5156	0.1873	179.9
22H$^+$(Z)	8.02	2.725	1.426	1.75	153.51	2.17	36.03	10.06	46.08	0.7214	0.6261	0.1904	187.68
23H$^+$(E)	9.38	2.686	1.417	1.7	154.32	7.32	35.25	4.58	39.84	0.7113	0.5302	0.1809	181.8
23H$^+$(Z)	7.66	2.734	1.413	1.763	153.17	16.69	34.32	9.9	44.22	0.7149	0.6685	0.1832	186.79
24H$^+$(E)	11.25	2.658	1.419	1.644	159.55	4.35	31.08	1.93	33.01	0.7111	0.4968	0.1821	181.86
24H$^+$(Z)	9.66	2.692	1.414	1.692	158.18	17.34	31.43	9.45	40.88	0.7207	0.6198	0.1859	184.73
25H$^+$(E)	11.34	2.656	1.428	1.643	159.34	1.37	31.15	1.19	32.34	0.7211	0.4518	0.1797	179.69
25H$^+$(Z)	10.08	2.686	1.425	1.68	158.98	10.16	32.62	10.83	43.45	0.7279	0.7009	0.1811	186.16
26H$^+$(E)	11.22	2.653	1.433	1.648	157.49	14.92	28.96	2.22	31.18	0.7208	0.501	0.1838	177.01
26H$^+$(Z)	10.11	2.685	1.437	1.681	157.79	9.25	35.11	8.3	43.41	0.7536	0.6939	0.1883	187.7
27H$^+$(E)	11.23	2.659	1.427	1.645	159.46	2.74	31.37	1.29	32.65	0.7096	0.464	0.183	180.56
27H$^+$(Z)	9.72	2.695	1.421	1.691	159	9.46	32.1	7.69	39.79	0.7135	0.633	0.1844	186.41
28H$^+$(E)	8.47	2.713	1.409	1.737	155.12	8.3	18.9	0.92	19.82	0.711	0.4688	0.1783	180.43
28H$^+$(Z)	9.7	2.691	1.417	1.691	157.52	10.25	39.26	12.21	51.47	0.7428	0.5242	0.1896	188.47
29H$^+$(E)	9.8	2.686	1.422	1.687	156.4	1.42	35.72	1.31	37.03	0.7245	0.4799	0.1833	181.69
29H$^+$(Z)	8.7	2.716	1.42	1.724	156.32	7.53	36.74	10.83	47.57	0.731	0.5974	0.1856	187.78
30H$^+$(E)	11.94	2.637	1.437	1.628	157.59	16.34	29.73	1.86	31.59	0.7212	0.5344	0.1851	176.79
30H$^+$(Z)	11.19	2.654	1.434	1.649	157.19	21.67	35.03	5.89	40.91	0.7361	0.6756	0.1864	186.71
31H$^+$(E)	8.8	2.701	1.416	1.722	153.89	0.48	30.4	2.27	32.67	0.7103	0.4934	0.1829	181.06
31H$^+$(Z)	6.91	2.761	1.412	1.796	153.09	8.67	33.64	9.9	43.55	0.7152	0.676	0.1848	186.85
32H$^+$(E)	5.51	2.787	1.572	1.862	146.87	0.24	53.28	44.02	97.29	0.775	0.4957	0.2414	175.43
32H$^+$(Z)	7.12	2.74	1.586	1.788	150.75	1	49.85	40.19	90.03	0.7721	0.6708	0.2379	174.26
33H$^+$(E)	6.24	2.711	1.397	1.823	143.35	5.81	24.18	1.05	25.23	0.7144	0.5456	0.1791	181.11
33H$^+$(Z)	4.6	2.775	1.391	1.914	140.47	6.14	27.72	6.37	34.09	None	0.6927	0.1784	184.78
34H$^+$(E)	-	2.786	1.374	2.632	87.97	5.54	10.52	13.08	23.6	0.696	0.6122	0.1706	181.45
34H$^+$(Z)	-	2.831	1.379	2.405	104.49	11.96	22.7	5.8	28.5	0.7102	0.6566	0.1697	181.7
35H$^+$(E)	5.45	2.72	1.408	1.867	138.71	1.4	28.03	0.37	28.4	0.7111	0.4963	0.1824	180.71
35H$^+$(Z)	4.39	2.763	1.404	1.93	136.83	11	29.9	6.68	36.58	0.7051	0.554	0.1779	183.94
36H$^+$(E)	5.56	2.71	1.41	1.863	138.15	1.88	24.37	0.02	24.4	0.72	0.4614	0.1787	180.09
36H$^+$(Z)	4.77	2.738	1.407	1.908	136.29	13.88	27.56	9.18	36.75	0.715	0.6827	0.1725	184.01
37H$^+$(E)	-	2.693	1.401	2.247	105.03	56.29	5.49	18.03	23.51	0.7115	0.7315	0.1749	178.2

37H⁺(Z)	-	2.72	1.403	2.24	107.45	57.78	19.16	0.25	19.4	0.708	0.4688	0.1751	174.27
38H⁺(E)	11.54	2.661	1.435	1.635	163.63	53.28	28.33	21.63	49.95	0.7347	0.587	0.1961	186.46
38H⁺(Z)	10.87	2.683	1.441	1.651	165.1	55.6	36.22	4.8	41.02	0.7209	0.5297	0.1896	177.84
39H⁺(E)	8.84	2.768	1.419	1.717	176.45	1.07	34.81	3.21	38.01	0.7164	0.4696	0.1859	184.61
39H⁺(Z)	8.15	2.791	1.421	1.741	176.68	17.66	39.22	9.41	48.63	0.7143	0.6892	0.185	186.89
40H⁺(E)	5.45	2.785	1.411	1.874	146.21	4.4	0.34	18.67	19.01	0.7106	0.7117	0.1857	181.47
40H⁺(Z)	5.98	2.791	1.417	1.84	150.85	4.15	30.24	4.79	35.03	0.7144	0.5619	0.1826	184.04
41H⁺(E)	6.78	2.755	1.454	1.801	151.25	3.25	33.17	5.1	38.28	0.7197	0.5279	0.1916	176.5
41H⁺(Z)	6.25	2.777	1.455	1.824	151.95	3.34	30.19	20.68	50.87	0.7366	0.721	0.2015	184.37
42H⁺(E)	7.61	2.65	1.412	1.726	146.56	7.47	-	-	-	0.8345	0.7352	0.2397	177.94
42H⁺(Z)	7.59	2.657	1.419	1.721	148.52	1.66	-	-	-	0.8182	0.7119	0.2313	173.3
43H⁺(E)	10.41	2.65	1.429	1.667	153.02	18.5	37.64	11.07	48.71	0.7246	0.5938	0.1881	182.49
43H⁺(Z)	10.7	2.649	1.429	1.663	154.42	17.87	29.57	21.74	51.31	0.7232	0.6157	0.1892	185.82
44H⁺(E)	3.46	2.721	1.419	2.023	122.19	0.96	32.02	2.7	34.72	0.7089	0.592	0.1814	177.07
44H⁺(Z)	-	2.95	1.372	2.544	101.5	3.35	12.79	10.42	23.2	0.7354	0.61	0.1983	187.41

* colour chart should be considered within each column

Table S3. Geometric and electronic parameters of amides **9**-**44** in vacuum.

Compd	r_1, Å	r_2, Å	ω, deg	χ_N, deg	τ, deg	ϑ, deg	q_{NPA}	q_{MK}	q_H	δ, ppm
9(E)	2.793*	1.374	4.57	17.71	6.22	23.93	0.6737	0.3285	0.1639	174.7
9(Z)	2.813	1.371	18.07	5.84	7.88	13.72	0.6805	0.5216	0.1656	178.03
10(E)	2.789	1.372	14.81	10.6	4.32	14.92	0.6994	0.6232	0.1658	174.9
10(Z)	2.792	1.374	19.41	8.56	2.02	10.58	0.7027	0.7095	0.1698	175.97
11(E)	2.766	1.369	2.43	12.33	4.14	16.46	0.6996	0.5665	0.1649	174.94
11(Z)	2.763	1.371	10.39	11.05	2.76	13.81	0.7004	0.7082	0.1677	175.59
12(E)	2.764	1.37	0.58	12.46	3.94	16.4	0.7004	0.5863	0.1659	174.56
12(Z)	2.762	1.373	10.82	12.18	2.38	14.57	0.7013	0.6724	0.1688	175.58
13(E)	2.787	1.375	9.26	14.05	5.81	19.86	0.7008	0.5761	0.1675	175.37
13(Z)	2.782	1.376	14.54	12.29	2.81	15.1	0.7032	0.6557	0.1706	176.2
14(E)	2.789	1.376	23.14	11.23	4.08	15.3	0.6998	0.6133	0.1675	175.39
14(Z)	2.789	1.377	26.26	10.05	2.35	12.39	0.7039	0.6904	0.1715	176.23
15(E)	2.777	1.372	15.76	9.72	4.39	14.11	0.6993	0.6101	0.1658	174.83
15(Z)	2.783	1.374	20.48	7.28	1.87	9.15	0.703	0.6956	0.17	175.87
16(E)	2.768	1.377	18.89	10.69	4.7	15.39	0.7006	0.5987	0.1689	174.74
16(Z)	2.77	1.378	22.78	8.56	2.12	10.67	0.7049	0.6921	0.1731	176.14
17(E)	2.78	1.371	17.02	10.05	3.8	13.86	0.6988	0.5579	0.1647	175.12
17(Z)	2.786	1.373	21.05	8.31	1.91	10.23	0.7022	0.6569	0.1687	175.7
18(E)	2.761	1.37	12.03	8.33	3.78	12.11	0.7038	0.5608	0.1664	175.73
18(Z)	2.774	1.37	18.88	4.82	2.67	7.48	0.7105	0.586	0.1723	174.73
19(E)	2.764	1.375	9.81	8.06	2.23	10.29	0.7129	0.5787	0.1634	175.22
19(Z)	2.774	1.375	13.02	9.67	4.82	14.49	0.7169	0.7832	0.1654	176.16
20(E)	2.775	1.379	14.57	9.21	0.8	10.01	0.7087	0.6059	0.1668	174.48
20(Z)	2.767	1.378	17.32	15.12	2.23	17.35	0.7186	0.7222	0.1698	178.22
21(E)	2.741	1.372	21.71	9.18	3.94	13.12	0.6986	0.6348	0.1655	174.77
21(Z)	2.749	1.374	25.31	6.92	1.61	8.53	0.7032	0.6983	0.1701	175.63
22(E)	2.802	1.382	24.13	10.32	4.85	15.17	0.7016	0.6267	0.171	175.44
22(Z)	2.799	1.383	26.79	8.47	2.62	11.09	0.7067	0.6927	0.1751	176.67
23(E)	2.759	1.37	20.89	8.34	3.69	12.02	0.6984	0.6383	0.1644	175.06
23(Z)	2.767	1.373	24.66	6.14	1.55	7.69	0.7026	0.6974	0.169	175.73
24(E)	2.746	1.368	2.21	10.96	4.12	15.08	0.7036	0.5657	0.166	175.69
24(Z)	2.747	1.367	9.4	8.83	2.98	11.81	0.7078	0.6294	0.1704	174.47
25(E)	2.748	1.373	10.2	8.58	1.63	10.21	0.7108	0.5527	0.1646	174.31
25(Z)	2.749	1.373	3.26	11.04	4.92	15.96	0.7133	0.7302	0.1651	176.55
26(E)	2.779	1.382	8.56	11.65	2.58	14.24	0.7085	0.5758	0.1677	174.72
26(Z)	2.758	1.381	13.07	17.35	2.67	20.02	0.7186	0.7469	0.17	178.58
27(E)	2.785	1.377	3.56	12.27	4.1	16.37	0.7032	0.5552	0.1678	176.7
27(Z)	2.775	1.376	10.46	11.25	2.69	13.94	0.7046	0.7329	0.1698	177.95
28(E)	2.822	1.377	1.14	1.63	9.7	11.33	0.7387	0.5277	0.1731	176.66

28(Z)	2.801	1.364	1.29	8.49	4.36	12.85	0.7297	0.5742	0.1719	178.8
29(E)	2.754	1.367	5.81	11	1.8	12.8	0.7091	0.5776	0.1657	175.03
29(Z)	2.753	1.369	0.36	12.75	2.92	15.67	0.7122	0.7631	0.167	176.05
30(E)	2.763	1.385	19.18	13.14	1.72	14.86	0.7095	0.5776	0.1686	175.15
30(Z)	2.748	1.384	21.7	19.57	2.45	22.01	0.7205	0.7171	0.1711	179.06
31(E)	2.788	1.371	16.25	10.75	3.63	14.38	0.699	0.6029	0.1678	175.12
31(Z)	2.812	1.383	18.99	13.01	5.97	18.98	0.7228	0.6168	0.17	174.44
32(E)	2.823	1.381	8.54	21.84	5.96	27.8	0.7035	0.5569	0.1633	176.59
32(Z)	2.836	1.38	1.46	18.4	2.37	20.77	0.7104	0.6047	0.1629	178.19
33(E)	2.73	1.365	12.38	10.73	0.07	10.8	0.7314	0.676	0.1705	178.37
33(Z)	2.742	1.366	21.8	0.8	4.3	5.11	0.7123	0.715	0.1676	177.01
34(E)	2.749	1.373	1.11	10.73	1.33	12.06	0.7349	0.5331	0.1715	178.73
34(Z)	2.773	1.367	5.39	13.97	1.29	15.26	0.7174	0.6641	0.1662	176.31
35(E)	2.779	1.371	3.67	6.02	3.54	9.56	0.7207	0.546	0.1735	176.65
35(Z)	2.777	1.375	20.53	11.14	3.95	15.09	0.7167	0.7142	0.1686	177.77
36(E)	2.748	1.373	2.91	5.23	0.69	5.92	0.7283	0.54	0.1725	175.9
36(Z)	2.755	1.374	18.61	9.79	5.06	14.86	0.7297	0.886	0.1667	177.77
37(E)	2.679	1.379	60.77	4.69	5.3	9.99	0.7059	0.6814	0.1673	173.52
37(Z)	2.671	1.378	61.06	5.96	3.14	9.1	0.705	0.6487	0.1663	172.01
38(E)	2.769	1.38	63.09	1.81	9.07	10.88	0.7129	0.68	0.1714	175.38
38(Z)	2.79	1.381	65.21	9.45	3.81	13.26	0.705	0.6553	0.1687	171.77
39(E)	2.927	1.384	21.08	10.9	6.53	17.43	0.7306	0.5794	0.1742	178.11
39(Z)	2.922	1.388	28.97	13.61	4.71	18.32	0.7242	0.5965	0.1709	171.58
40(E)	2.798	1.392	11.56	8.95	8.47	17.42	0.714	0.73	0.1773	175.23
40(Z)	2.825	1.389	22.93	10.02	10.99	21.02	0.7132	0.7346	0.1778	177.18
41(E)	2.801	1.414	11.48	13.48	5.03	18.5	0.738	0.5798	0.1851	176.56
41(Z)	2.776	1.417	12.95	10.41	6.11	16.52	0.7425	0.6845	0.1878	174.69
42(E)	2.737	1.38	5.19	-	-	-	0.8475	0.6931	0.2177	173.58
42(Z)	2.736	1.373	10.64	-	-	-	0.8402	0.7628	0.2164	174.57
43(E)	2.782	1.379	31.49	18.64	4.7	23.34	0.715	0.6641	0.172	177.8
43(Z)	2.785	1.381	32.72	12.15	7.12	19.27	0.7085	0.6622	0.1686	174.17
44(E)	2.899	1.382	1.37	8.83	2.15	10.98	0.711	0.5638	0.1723	175.96
44(Z)	2.832	1.375	4.72	7.8	3.86	11.66	0.6971	0.6724	0.168	176.19

* colour chart should be considered within each column

Table S4. Change of geometric and electronic parameters during transition from **9**-**44** to **9**H^+-**44**H^+ in vacuum.

Compd	Δr_1, Å	Δr_2, Å	$\Delta\omega$, deg	$\Delta\chi_N$, deg	$\Delta\tau$, deg	$\Delta\vartheta$, deg	Δq_{NPA}	Δq_{MK}	Δq_H	$\Delta\delta$, ppm
9H^+(E)	-0.106*	0.057	0.75	24.58	6.59	31.17	0.0194	0.0509	0.0137	4.21
9H^+(Z)	-0.051	0.043	-12.15	19.7	11.21	30.91	0.0176	0.0907	0.0117	7.34
10H^+(E)	-0.092	0.052	-14.25	25.06	-2.24	22.82	0.0129	-0.1347	0.0178	5.89
10H^+(Z)	-0.041	0.044	-14.95	26.57	7.58	34.15	0.0148	-0.0586	0.0164	11.27
11H^+(E)	-0.101	0.057	2.61	23.91	-1.97	21.94	0.0153	-0.0626	0.0205	6.5
11H^+(Z)	-0.055	0.049	-1.4	25.16	5.77	30.93	0.0193	-0.065	0.0197	11.68
12H^+(E)	-0.098	0.057	0.37	24.18	-1.39	22.8	0.0146	-0.1014	0.0201	6.35
12H^+(Z)	-0.056	0.049	-7.97	23.64	6.18	29.81	0.0186	-0.0293	0.0193	11.43
13H^+(E)	-0.124	0.054	-0.32	23.1	-2.89	20.22	0.0142	-0.0483	0.0193	4.91
13H^+(Z)	-0.081	0.048	-1.63	25.18	2.75	27.93	0.0173	0.0009	0.0183	10.79
14H^+(E)	-0.113	0.053	-22.94	25.59	-1.8	23.79	0.0137	-0.1122	0.018	5.23
14H^+(Z)	-0.061	0.044	-21.5	25.96	7.87	33.83	0.0157	-0.0087	0.0166	11.69
15H^+(E)	-0.081	0.049	-14.19	25.96	-0.98	24.98	0.0123	-0.0838	0.0168	6.11
15H^+(Z)	-0.038	0.041	-10.29	28.09	7.47	35.55	0.0129	-0.036	0.015	11.09
16H^+(E)	-0.085	0.051	-18.81	26.05	-2.06	23.99	0.0123	-0.0862	0.0167	5.22
16H^+(Z)	-0.035	0.043	-17.27	27.5	7.06	34.57	0.0137	-0.0617	0.015	11.19
17H^+(E)	-0.093	0.05	-14.79	25.37	-1.13	24.24	0.0137	-0.0609	0.0178	6.54
17H^+(Z)	-0.048	0.043	-13.56	26.28	8.05	34.33	0.0152	-0.0243	0.0163	11.55
18H^+(E)	-0.071	0.047	-11.07	22.79	-1.91	20.88	0.0053	-0.0822	0.0143	5.37
18H^+(Z)	-0.042	0.043	-8.2	26.49	5.88	32.38	0.0013	-0.0026	0.0101	10.9
19H^+(E)	-0.076	0.049	-8.08	22.27	-1.52	20.75	0.0051	-0.1218	0.0142	4.25
19H^+(Z)	-0.05	0.046	-0.68	22.88	6.53	29.4	0.0091	-0.1128	0.0142	10.24

20H⁺(E)	-0.091	0.046	-4.91	18.11	1.33	19.45	0.0074	-0.1068	0.0136	2.94
20H⁺(Z)	-0.073	0.047	0.79	18.56	4.86	23.42	0.0142	-0.0586	0.0131	8.53
21H⁺(E)	-0.089	0.052	-18.35	27.15	-1.59	25.56	0.0152	-0.1489	0.0189	6.57
21H⁺(Z)	-0.049	0.044	-12.81	29.23	8.27	37.51	0.0145	-0.0471	0.0162	11.49
22H⁺(E)	-0.133	0.052	-20.84	26.68	-3.41	23.28	0.0124	-0.1111	0.0163	4.46
22H⁺(Z)	-0.074	0.043	-24.62	27.56	7.44	35	0.0146	-0.0667	0.0154	11
23H⁺(E)	-0.073	0.047	-13.56	26.92	0.9	27.82	0.0129	-0.1081	0.0165	6.73
23H⁺(Z)	-0.033	0.04	-7.96	28.18	8.35	36.53	0.0123	-0.0289	0.0142	11.07
24H⁺(E)	-0.088	0.051	2.14	20.12	-2.19	17.93	0.0075	-0.0689	0.0161	6.17
24H⁺(Z)	-0.055	0.046	7.94	22.6	6.47	29.07	0.013	-0.0096	0.0155	10.26
25H⁺(E)	-0.091	0.055	-8.83	22.57	-0.44	22.13	0.0103	-0.1009	0.0151	5.38
25H⁺(Z)	-0.063	0.051	6.9	21.58	5.91	27.49	0.0146	-0.0293	0.016	9.61
26H⁺(E)	-0.127	0.051	6.36	17.31	-0.37	16.94	0.0123	-0.0747	0.0161	2.3
26H⁺(Z)	-0.074	0.057	-3.82	17.77	5.63	23.39	0.035	-0.053	0.0184	9.12
27H⁺(E)	-0.126	0.05	-0.83	19.1	-2.81	16.28	0.0064	-0.0913	0.0152	3.86
27H⁺(Z)	-0.08	0.046	-1	20.85	5	25.85	0.009	-0.0998	0.0147	8.46
28H⁺(E)	-0.109	0.032	7.16	17.27	-8.78	8.48	-0.0277	-0.0589	0.0052	3.77
28H⁺(Z)	-0.11	0.053	8.96	30.77	7.85	38.63	0.0131	-0.0501	0.0177	9.66
29H⁺(E)	-0.068	0.055	-4.39	24.73	-0.49	24.24	0.0154	-0.0976	0.0176	6.65
29H⁺(Z)	-0.038	0.052	7.17	23.99	7.91	31.9	0.0188	-0.1657	0.0186	11.73
30H⁺(E)	-0.126	0.052	-2.84	16.59	0.14	16.73	0.0118	-0.0432	0.0165	1.64
30H⁺(Z)	-0.094	0.05	-0.03	15.46	3.44	18.9	0.0156	-0.0416	0.0153	7.66
31H⁺(E)	-0.087	0.045	-15.78	19.64	-1.36	18.28	0.0114	-0.1095	0.0151	5.94
31H⁺(Z)	-0.051	0.028	-10.32	20.63	3.93	24.56	-0.0076	0.0592	0.0148	12.41
32H⁺(E)	-0.036	0.191	-8.3	31.44	38.06	69.5	0.0715	-0.0612	0.0781	-1.15
32H⁺(Z)	-0.096	0.206	-0.46	31.45	37.81	69.26	0.0617	0.0661	0.0749	-3.93
33H⁺(E)	-0.019	0.032	-6.57	13.45	0.97	14.43	-0.017	-0.1304	0.0086	2.74
33H⁺(Z)	0.034	0.025	-15.67	26.91	2.07	28.98	None	-0.0223	0.0107	7.78
34H⁺(E)	0.037	0.001	4.43	-0.21	11.75	11.54	-0.0389	0.0791	-0.0009	2.72
34H⁺(Z)	0.058	0.012	6.56	8.73	4.51	13.24	-0.0072	-0.0076	0.0035	5.38
35H⁺(E)	-0.059	0.037	-2.27	22.01	-3.17	18.84	-0.0096	-0.0497	0.0089	4.06
35H⁺(Z)	-0.014	0.029	-9.53	18.76	2.73	21.48	-0.0115	-0.1602	0.0093	6.17
36H⁺(E)	-0.038	0.037	-1.04	19.14	-0.67	18.47	-0.0083	-0.0786	0.0062	4.19
36H⁺(Z)	-0.017	0.032	-4.73	17.77	4.12	21.89	-0.0147	-0.2033	0.0059	6.24
37H⁺(E)	0.013	0.022	-4.48	0.8	12.73	13.53	0.0057	0.0501	0.0076	4.67
37H⁺(Z)	0.05	0.025	-3.27	13.2	-2.89	10.31	0.003	-0.1799	0.0088	2.25
38H⁺(E)	-0.108	0.055	-9.81	26.52	12.56	39.08	0.0218	-0.0929	0.0248	11.09
38H⁺(Z)	-0.107	0.06	-9.61	26.77	0.99	27.77	0.0159	-0.1256	0.0209	6.08
39H⁺(E)	-0.159	0.035	-20.01	23.91	-3.33	20.58	-0.0142	-0.1099	0.0117	6.5
39H⁺(Z)	-0.131	0.034	-11.31	25.61	4.7	30.31	-0.0099	0.0926	0.0141	15.31
40H⁺(E)	-0.013	0.019	-7.16	-8.61	10.2	1.58	-0.0034	-0.0183	0.0085	6.24
40H⁺(Z)	-0.033	0.028	-18.78	20.22	-6.21	14.01	0.0013	-0.1727	0.0048	6.86
41H⁺(E)	-0.046	0.041	-8.23	19.7	0.08	19.77	-0.0183	-0.0519	0.0065	-0.06
41H⁺(Z)	0.001	0.038	-9.6	19.78	14.57	34.36	-0.006	0.0365	0.0138	9.68
42H⁺(E)	-0.087	0.033	2.28	-	-	-	-0.013	0.0421	0.022	4.36
42H⁺(Z)	-0.078	0.045	-8.98	-	-	-	-0.022	-0.051	0.0149	-1.27
43H⁺(E)	-0.132	0.049	-12.98	19.01	6.37	25.37	0.0097	-0.0704	0.0161	4.69
43H⁺(Z)	-0.136	0.048	-14.84	17.42	14.62	32.04	0.0147	-0.0464	0.0207	11.65
44H⁺(E)	-0.179	0.037	-0.42	23.19	0.55	23.74	-0.0021	0.0282	0.0091	1.11
44H⁺(Z)	0.118	-0.003	-1.36	4.98	6.56	11.55	0.0383	-0.0624	0.0303	11.22

* colour chart should be considered within each column

Table S5. Geometric and electronic parameters of cations **9**H⁺-**44**H⁺ in acetonitrile (PCM).

Compd	E_{HB}, kcal·mol^{-1}	r_1, Å	r_2, Å	r_3, Å	α, deg	ω, deg	χ_N, deg	τ, deg	ϑ, deg	q_{NPA}	q_{MK}	q_H	δ, ppm
9H⁺(E)	6.34*	2.758	1.405	1.815	149.37	3.4	39.08	10.18	49.27	0.7052	0.4563	0.1806	184.49
9H⁺(Z)	5.76	2.792	1.393	1.848	150.34	3.45	24.42	9.64	34.06	0.7046	0.4105	0.1783	187.1
10H⁺(E)	6.35	2.763	1.401	1.815	150.22	1.01	34.65	4.95	39.61	0.7304	0.5783	0.1866	186.8
10H⁺(Z)	6.34	2.768	1.399	1.819	150.66	0.28	31.52	2.07	33.59	0.729	0.6241	0.1872	189.88
11H⁺(E)	8.59	2.716	1.404	1.725	157.27	1.1	36.06	6.25	42.31	0.731	0.5772	0.1873	186.79

11H⁺(Z)	8.28	2.721	1.403	1.737	156.31	4.23	33.41	1.79	35.2	0.7333	0.6365	0.1896	190.5
12H⁺(E)	8.81	2.711	1.407	1.717	157.55	0.61	36.47	6.26	42.72	0.7318	0.5632	0.1885	186.69
12H⁺(Z)	8.66	2.714	1.406	1.723	157.29	2.99	33.17	1.29	34.45	0.7338	0.6447	0.1905	190.45
13H⁺(E)	9.07	2.702	1.409	1.707	157.11	8.83	36.89	5.45	42.33	0.7321	0.5862	0.1895	186.59
13H⁺(Z)	8.74	2.707	1.408	1.72	155.86	8	34.89	0.01	34.89	0.7364	0.6495	0.1927	191.13
14H⁺(E)	7.02	2.737	1.406	1.785	150.24	1.36	36.55	4.95	41.5	0.7328	0.5816	0.1898	186.77
14H⁺(Z)	7.12	2.738	1.404	1.784	150.86	2.44	33.16	2.08	35.24	0.7321	0.6105	0.1903	190.61
15H⁺(E)	6.89	2.745	1.4	1.792	150.86	3.28	34.31	7.28	41.59	0.7282	0.579	0.1851	186.36
15H⁺(Z)	6.37	2.762	1.398	1.817	149.95	3.22	32.41	2.27	34.68	0.7292	0.6358	0.1871	189.95
16H⁺(E)	6.82	2.743	1.408	1.794	150.14	2.68	36.68	5.88	42.56	0.7327	0.6053	0.1906	186.09
16H⁺(Z)	6.87	2.745	1.404	1.795	150.7	3.44	33.32	1.49	34.82	0.7316	0.6171	0.191	190.28
17H⁺(E)	6.6	2.753	1.399	1.804	150.28	3.06	34.61	5.39	40	0.7303	0.585	0.1857	187.39
17H⁺(Z)	6.74	2.757	1.398	1.8	151.67	4.48	31.35	1.63	32.98	0.7282	0.6297	0.1861	190
18H⁺(E)	6.93	2.745	1.398	1.792	151.17	0.63	30.19	4.92	35.11	0.7232	0.5216	0.1815	186.36
18H⁺(Z)	6.73	2.753	1.396	1.803	151.05	3.59	27.17	1.74	28.91	0.7238	0.5338	0.1835	188.34
19H⁺(E)	6.85	2.746	1.403	1.797	150.7	3.5	29.49	5.81	35.3	0.731	0.5018	0.1759	184.82
19H⁺(Z)	6.5	2.759	1.402	1.812	150.38	6.56	28.94	4.52	33.46	0.7344	0.6326	0.179	188.84
20H⁺(E)	6.02	2.765	1.403	1.834	148.12	8.03	27.72	5.16	32.88	0.7287	0.5442	0.1785	183.12
20H⁺(Z)	6.91	2.741	1.406	1.795	150.14	13.49	30.5	1.17	31.67	0.7385	0.6132	0.1824	187.62
21H⁺(E)	8.34	2.697	1.402	1.734	152.03	0.39	35.33	6.49	41.83	0.7297	0.5436	0.1861	186.67
21H⁺(Z)	8.03	2.706	1.401	1.748	151.83	2.73	32.62	2.18	34.8	0.7306	0.6256	0.1882	189.82
22H⁺(E)	7.62	2.719	1.414	1.762	150.94	2.6	37.12	5.69	42.81	0.733	0.5669	0.1921	185.2
22H⁺(Z)	7.19	2.731	1.409	1.781	150.22	5.8	33.7	2.8	36.5	0.7345	0.6699	0.1937	190.76
23H⁺(E)	6.8	2.745	1.396	1.796	150.21	11.67	33.34	8.36	41.7	0.7267	0.5943	0.1825	187.03
23H⁺(Z)	6.58	2.754	1.396	1.807	150.19	13.14	31.61	3.29	34.9	0.7282	0.6272	0.1852	189.68
24H⁺(E)	9.04	2.701	1.4	1.711	157.46	4.27	30.1	4.73	34.83	0.7252	0.5389	0.1831	186.72
24H⁺(Z)	8.79	2.706	1.399	1.72	156.79	10.56	28.09	3.11	31.2	0.7332	0.6314	0.1886	187.58
25H⁺(E)	9.12	2.7	1.409	1.708	157.54	0.32	30.43	4.7	35.13	0.7342	0.4696	0.1788	185.3
25H⁺(Z)	8.93	2.706	1.408	1.716	157.43	4.73	30	4.48	34.48	0.7383	0.6641	0.1815	189.21
26H⁺(E)	8.98	2.696	1.413	1.714	155.34	15	29.5	5.22	34.72	0.7324	0.5092	0.1814	182.42
26H⁺(Z)	8.67	2.707	1.416	1.726	154.91	6.21	31.34	4.03	35.37	0.7588	0.6732	0.1867	191.19
27H⁺(E)	8.7	2.71	1.41	1.722	156.94	1.71	30.99	3.98	34.97	0.7243	0.5125	0.1857	185.7
27H⁺(Z)	8.64	2.713	1.408	1.725	156.94	5.7	29.51	1.34	30.85	0.7269	0.5979	0.1878	190.14
28H⁺(E)	7.05	2.749	1.393	1.79	153.21	10.09	20.29	3.23	23.52	0.7238	0.4439	0.1779	185.3
28H⁺(Z)	8.74	2.707	1.401	1.722	156.09	4.79	35.28	5.37	40.65	0.7482	0.5233	0.1899	190.49
29H⁺(E)	7.61	2.735	1.401	1.762	153.94	1.59	34.73	5.22	39.95	0.739	0.5485	0.1819	187.85
29H⁺(Z)	7.53	2.739	1.402	1.766	154.18	3.42	33.4	3.29	36.69	0.7389	0.5627	0.1845	189.91
30H⁺(E)	9.61	2.679	1.418	1.694	155.64	17.94	30.76	6.55	37.31	0.7328	0.5148	0.1834	182.41
30H⁺(Z)	9.58	2.678	1.417	1.695	154.92	18.25	32.88	0.48	33.36	0.7447	0.6571	0.188	189.57
31H⁺(E)	6.4	2.76	1.4	1.813	150.08	1.14	34.41	4.57	38.98	0.7299	0.6036	0.1864	186.83
31H⁺(Z)	6.23	2.772	1.398	1.824	150.86	1.73	31.97	1.99	33.97	0.7289	0.63	0.187	190.06
32H⁺(E)	4.57	2.822	1.566	1.912	145.35	2.61	53.65	43.94	97.58	0.7932	0.5708	0.2518	179.03
32H⁺(Z)	5.21	2.804	1.584	1.874	148.03	1.31	50.43	22.98	73.4	0.7904	0.5981	0.2462	181.17
33H⁺(E)	5.21	2.735	1.387	1.874	140.26	3.23	27.61	6.03	33.64	0.7234	0.5768	0.1792	184.14
33H⁺(Z)	4.52	2.764	1.383	1.917	138.91	0.73	25.65	4.6	30.26	0.7286	0.6855	0.1783	188.01
34H⁺(E)	-	2.766	1.365	2.778	78.87	0.52	8.89	0.57	9.46	0.7078	0.5333	0.1668	180.79
34H⁺(Z)	-	2.773	1.366	2.562	91.2	0.74	12.09	0.82	12.91	0.721	0.6849	0.1686	182.72
35H⁺(E)	4.87	2.741	1.396	1.895	138.22	1.06	30.26	3.18	33.44	0.7256	0.533	0.1845	186.48
35H⁺(Z)	4.49	2.754	1.394	1.918	136.99	8.42	30.48	2.74	33.22	0.7208	0.6322	0.1808	188.3
36H⁺(E)	5.02	2.729	1.398	1.888	137.6	1.06	25.6	3.64	29.24	0.7292	0.4754	0.1764	185.64
36H⁺(Z)	4.58	2.74	1.396	1.915	135.85	11.9	26.38	5.88	32.26	0.7256	0.6256	0.1716	187.16
37H⁺(E)	-	2.751	1.382	2.38	100.5	61.29	15.42	4.68	20.11	0.718	0.6504	0.1731	180.66
37H⁺(Z)	-	2.746	1.386	2.367	100.97	61.47	18.61	1.62	20.24	0.7209	0.5781	0.1748	179.77
38H⁺(E)	8.33	2.736	1.413	1.732	161.48	56.65	31.81	3.79	35.6	0.7366	0.6329	0.1913	186.64
38H⁺(Z)	7.37	2.762	1.419	1.769	158.86	59.96	34.66	6.01	40.67	0.7379	0.5775	0.1908	184.82
39H⁺(E)	7.22	2.816	1.406	1.776	175.36	0.52	37.55	4.12	41.67	0.729	0.511	0.1868	188.2
39H⁺(Z)	7.13	2.822	1.408	1.78	176.16	5.31	38.32	3.99	42.31	0.7306	0.667	0.1878	190.84
40H⁺(E)	5.06	2.806	1.406	1.888	147.1	2.9	15.9	9.48	25.38	0.7237	0.6976	0.1877	183.29
40H⁺(Z)	5.12	2.811	1.407	1.884	148.01	9.44	29.75	7.1	36.85	0.7301	0.6704	0.1865	187.76
41H⁺(E)	4.75	2.822	1.44	1.902	147.41	0.35	33.61	5.12	38.73	0.7437	0.6142	0.2007	184.03
41H⁺(Z)	4.75	2.827	1.442	1.902	148.48	4.53	31.51	4.44	35.95	0.744	0.7037	0.2045	185.9

42H$^+$(E)	6.2	2.691	1.4	1.773	146.43	6.03	-	-	-	0.8405	0.76	0.2366	179.24
42H$^+$(Z)	6.4	2.688	1.398	1.765	147.43	2.55	-	-	-	0.8432	0.8083	0.2419	178.62
43H$^+$(E)	8.17	2.694	1.408	1.74	150.29	18.98	34.81	10.81	45.62	0.7394	0.6534	0.1907	187.46
43H$^+$(Z)	7.78	2.702	1.409	1.757	149.09	22.18	31.12	5.12	36.24	0.7354	0.7038	0.189	189.38
44H$^+$(E)	2.37	2.785	1.388	2.149	118.01	0.6	25.13	2.66	27.79	0.7227	0.6019	0.1807	183.11
44H$^+$(Z)	-	2.924	1.366	2.567	99.04	3.09	11	7.63	18.63	0.7369	0.6129	0.1955	186.99

* colour chart should be considered within each column

Table S6. Geometric and electronic parameters of **9**-**44** in acetonitrile (PCM).

Compd	r_1, Å	r_2, Å	ω, deg	χ_N, deg	τ, deg	ϑ, deg	q_{NPA}	q_{MK}	q_H	δ, ppm
9(E)	2.793*	1.363	2.59	16.47	4.95	21.42	0.6819	0.4253	0.1621	178.62
9(Z)	2.808	1.36	15.7	7.8	7.04	14.84	0.6923	0.4162	0.1649	182
10(E)	2.786	1.361	15.07	10.82	5	15.83	0.7103	0.6477	0.1652	179.92
10(Z)	2.79	1.363	16.43	9.23	2.09	11.32	0.7151	0.6936	0.1699	181.45
11(E)	2.758	1.358	2.45	12.38	4.95	17.33	0.7091	0.5924	0.1633	179.69
11(Z)	2.76	1.36	6.55	11.38	2.59	13.97	0.7125	0.6407	0.1671	181.17
12(E)	2.759	1.358	3.24	12.19	4.44	16.62	0.7098	0.592	0.1641	179.54
12(Z)	2.761	1.361	3.03	11.97	2.79	14.76	0.7133	0.6152	0.1678	181.44
13(E)	2.79	1.364	10.19	14.82	6.34	21.16	0.7123	0.5922	0.1675	180.64
13(Z)	2.787	1.367	14.13	14.2	3.27	17.48	0.7162	0.6578	0.1716	181.79
14(E)	2.826	1.368	27.96	12.22	5.61	17.83	0.713	0.6406	0.1694	180.82
14(Z)	2.824	1.371	28.94	11.03	2.65	13.68	0.7183	0.6987	0.1741	181.75
15(E)	2.77	1.36	15.77	9.99	4.97	14.96	0.7097	0.6166	0.1648	179.79
15(Z)	2.777	1.363	17.91	8.11	2	10.11	0.715	0.6858	0.17	181.29
16(E)	2.772	1.368	20.49	11.21	5.71	16.92	0.7135	0.6262	0.1704	179.98
16(Z)	2.773	1.37	21.9	9.57	2.67	12.24	0.7188	0.6645	0.1754	181.62
17(E)	2.777	1.36	17.66	10.43	4.54	14.97	0.7094	0.5936	0.1638	180.12
17(Z)	2.781	1.362	18.68	9.07	1.94	11	0.7142	0.6462	0.1686	181.1
18(E)	2.758	1.359	12.25	8.24	4.19	12.43	0.7143	0.5569	0.165	180.54
18(Z)	2.77	1.361	15.36	6.63	2.83	9.46	0.7213	0.5529	0.1721	179.99
19(E)	2.761	1.363	10.29	8.35	3.88	12.24	0.7213	0.572	0.1598	180.33
19(Z)	2.769	1.365	11.81	8.05	3.54	11.6	0.7271	0.6806	0.1639	181.25
20(E)	2.77	1.367	15.54	10.2	3.93	14.13	0.7179	0.6062	0.1629	179.5
20(Z)	2.768	1.368	17.94	11.66	0.31	11.97	0.7272	0.6402	0.168	182.47
21(E)	2.736	1.36	21.68	9.79	4.72	14.51	0.7091	0.6626	0.1644	179.73
21(Z)	2.741	1.364	22.89	8.03	1.61	9.64	0.7147	0.6986	0.1698	180.79
22(E)	2.848	1.377	29.72	10.99	6.53	17.52	0.7166	0.6559	0.1752	180.98
22(Z)	2.846	1.379	20.59	9.27	3.37	12.64	0.7227	0.6821	0.18	182.25
23(E)	2.756	1.358	20.59	8.77	4.4	13.17	0.7081	0.6631	0.1624	180.08
23(Z)	2.762	1.362	22.16	6.89	1.79	8.68	0.7137	0.6901	0.168	180.96
24(E)	2.741	1.357	2.57	10.62	5.04	15.66	0.713	0.5623	0.1639	180.21
24(Z)	2.746	1.358	3.78	9.44	3.3	12.74	0.7183	0.5794	0.1695	180.21
25(E)	2.744	1.362	11.51	9.14	3.18	12.32	0.718	0.5201	0.1604	179.51
25(Z)	2.746	1.362	5.85	9.77	3.64	13.41	0.7223	0.6292	0.1625	181.68
26(E)	2.777	1.371	10.05	12.94	5.16	18.1	0.7176	0.5568	0.164	180.01
26(Z)	2.765	1.371	14.89	15.41	1.26	16.66	0.7273	0.6376	0.1685	182.95
27(E)	2.794	1.369	6.91	12.3	5.38	17.68	0.7137	0.5653	0.1679	181.48
27(Z)	2.788	1.369	14.43	11.48	1.64	13.12	0.7188	0.6211	0.172	183.7
28(E)	2.82	1.364	6.99	2.85	7.43	10.28	0.7355	0.5869	0.1685	181.87
28(Z)	2.783	1.356	8.95	5.84	2.95	8.79	0.7344	0.5236	0.1695	183.07
29(E)	2.752	1.354	6.38	10.29	2.98	13.27	0.7154	0.5932	0.16	180.41
29(Z)	2.754	1.356	5.33	7.95	2.04	9.98	0.7183	0.6201	0.1628	181.08
30(E)	2.776	1.377	1.22	15.06	4.59	19.65	0.7192	0.5604	0.1659	180.36
30(Z)	2.767	1.377	25.33	17.17	0.97	18.14	0.7306	0.6435	0.1714	183.52
31(E)	2.788	1.361	16.31	12.09	5.17	17.27	0.7095	0.6192	0.1674	180.01
31(Z)	2.823	1.371	19.84	11.83	7.28	19.11	0.734	0.6667	0.1678	180.73
32(E)	2.83	1.367	8.65	19.18	4.04	23.22	0.7131	0.5764	0.1611	181.66
32(Z)	2.845	1.367	0.92	18.97	0.05	19.02	0.717	0.5986	0.1616	183.69
33(E)	2.736	1.357	11.94	8.37	1.05	9.42	0.7332	0.6163	0.1668	181.4

33(Z)	2.738	1.357	18.64	1.65	5.64	7.29	0.7221	0.7065	0.1649	181.89
34(E)	2.749	1.359	3.18	6.69	0.88	7.57	0.7334	0.6072	0.1649	182.17
34(Z)	2.76	1.36	9.37	11.52	1.84	13.36	0.7257	0.6242	0.1645	181.55
35(E)	2.774	1.361	1.1	2.88	3.55	6.43	0.7251	0.5543	0.1701	180.49
35(Z)	2.775	1.361	17.88	7.33	4.18	11.52	0.7254	0.6627	0.1654	182.75
36(E)	2.748	1.363	5.24	4.58	1.37	5.95	0.732	0.5295	0.1676	180.33
36(Z)	2.755	1.362	17.78	6.93	4.12	11.05	0.7376	0.7362	0.1626	182.94
37(E)	2.692	1.365	61.48	7.45	3.48	10.92	0.7121	0.6799	0.1637	178.22
37(Z)	2.676	1.367	61.26	7.99	4.26	12.25	0.7148	0.6897	0.1643	177.78
38(E)	2.789	1.365	64.13	6.78	4.14	10.93	0.7152	0.6516	0.1658	178.74
38(Z)	2.788	1.367	63.93	10.08	3.98	14.06	0.7158	0.6456	0.1655	178.25
39(E)	2.936	1.37	24.09	11.21	4.09	15.3	0.7339	0.5867	0.1701	182.14
39(Z)	2.93	1.375	28.66	12.6	5.42	18.02	0.7358	0.6222	0.169	177.94
40(E)	2.807	1.382	16.6	12.08	9.51	21.59	0.7246	0.7172	0.1767	180.21
40(Z)	2.834	1.379	22.65	11.36	9.2	20.57	0.7264	0.7547	0.1795	181.67
41(E)	2.808	1.404	12.26	11.94	3.05	14.99	0.7511	0.6099	0.1867	182.62
41(Z)	2.78	1.411	13.06	10.91	8.47	19.38	0.7562	0.6724	0.1897	179.96
42(E)	2.739	1.37	4.71	-	-	-	0.8613	0.7481	0.2168	179.57
42(Z)	2.729	1.367	10.45	-	-	-	0.8584	0.7776	0.2182	179.93
43(E)	2.799	1.367	32.3	17.35	5.42	22.76	0.7203	0.7357	0.1687	181.26
43(Z)	2.808	1.367	33.23	13.5	4.66	18.16	0.7179	0.7565	0.1658	180.87
44(E)	2.893	1.366	0.73	8.94	0.93	9.87	0.7171	0.5628	0.1678	181.05
44(Z)	2.849	1.365	3.52	7.68	3.72	11.4	0.7101	0.6752	0.1687	182.24

* colour chart should be considered within each column

Table S7. Change of geometric and electronic parameters during transition from **9**-**44** to cations **9**H$^+$-**44**H$^+$ in acetonitrile (PCM).

Compd	Δr_1, Å	Δr_2, Å	$\Delta\omega$, deg	$\Delta\chi_N$, deg	$\Delta\tau$, deg	$\Delta\vartheta$, deg	Δq_{NPA}	Δq_{MK}	Δq_H	$\Delta\delta$, ppm
9H$^+$(E)	-0.036*	0.042	0.81	22.61	5.23	27.85	0.0233	0.0309	0.0185	5.86
9H$^+$(Z)	-0.016	0.032	-12.26	16.62	2.6	19.22	0.0123	-0.0057	0.0134	5.11
10H$^+$(E)	-0.023	0.04	-14.07	23.83	-0.05	23.78	0.0201	-0.0694	0.0214	6.88
10H$^+$(Z)	-0.021	0.035	-16.15	22.28	-0.01	22.27	0.0139	-0.0695	0.0172	8.43
11H$^+$(E)	-0.042	0.047	-1.35	23.68	1.31	24.98	0.0219	-0.0153	0.024	7.11
11H$^+$(Z)	-0.038	0.043	-2.33	22.03	-0.8	21.23	0.0209	-0.0042	0.0225	9.34
12H$^+$(E)	-0.048	0.048	-2.64	24.28	1.82	26.1	0.022	-0.0288	0.0243	7.15
12H$^+$(Z)	-0.047	0.045	-0.04	21.2	-1.5	19.7	0.0205	0.0295	0.0226	9.01
13H$^+$(E)	-0.088	0.045	-1.37	22.07	-0.9	21.17	0.0197	-0.006	0.022	5.95
13H$^+$(Z)	-0.08	0.041	-6.13	20.68	-3.27	17.42	0.0202	-0.0083	0.021	9.34
14H$^+$(E)	-0.089	0.038	-26.6	24.33	-0.66	23.67	0.0199	-0.059	0.0204	5.95
14H$^+$(Z)	-0.086	0.033	-26.5	22.13	-0.57	21.56	0.0138	-0.0882	0.0162	8.85
15H$^+$(E)	-0.026	0.039	-12.49	24.32	2.31	26.64	0.0185	-0.0376	0.0202	6.57
15H$^+$(Z)	-0.016	0.035	-14.69	24.3	0.26	24.56	0.0142	-0.05	0.017	8.66
16H$^+$(E)	-0.029	0.04	-17.82	25.47	0.17	25.64	0.0192	-0.0209	0.0203	6.11
16H$^+$(Z)	-0.027	0.033	-18.46	23.75	-1.18	22.57	0.0128	-0.0474	0.0156	8.66
17H$^+$(E)	-0.023	0.04	-14.61	24.18	0.85	25.03	0.021	-0.0086	0.0219	7.27
17H$^+$(Z)	-0.024	0.036	-14.2	22.28	-0.31	21.97	0.014	-0.0165	0.0175	8.9
18H$^+$(E)	-0.013	0.039	-11.62	21.96	0.73	22.68	0.0089	-0.0353	0.0165	5.82
18H$^+$(Z)	-0.017	0.035	-11.77	20.54	-1.09	19.45	0.0025	-0.019	0.0114	8.35
19H$^+$(E)	-0.014	0.04	-6.79	21.14	1.92	23.07	0.0097	-0.0702	0.0161	4.49
19H$^+$(Z)	-0.01	0.037	-5.25	20.89	0.98	21.87	0.0074	-0.0481	0.0152	7.59
20H$^+$(E)	-0.005	0.036	-7.51	17.52	1.24	18.75	0.0108	-0.062	0.0156	3.62
20H$^+$(Z)	-0.027	0.038	-4.45	18.84	0.85	19.69	0.0113	-0.027	0.0144	5.15
21H$^+$(E)	-0.039	0.042	-21.29	25.54	1.77	27.32	0.0205	-0.119	0.0217	6.94
21H$^+$(Z)	-0.034	0.037	-20.16	24.59	0.57	25.16	0.0159	-0.073	0.0184	9.03
22H$^+$(E)	-0.13	0.037	-27.12	26.14	-0.84	25.3	0.0164	-0.089	0.0169	4.22
22H$^+$(Z)	-0.115	0.03	-14.8	24.43	-0.57	23.86	0.0118	-0.0122	0.0137	8.5
23H$^+$(E)	-0.011	0.038	-8.92	24.57	3.96	28.53	0.0186	-0.0689	0.0201	6.95
23H$^+$(Z)	-0.008	0.034	-9.02	24.72	1.5	26.22	0.0145	-0.0629	0.0172	8.72
24H$^+$(E)	-0.04	0.044	1.71	19.48	-0.31	19.17	0.0122	-0.0234	0.0193	6.5
24H$^+$(Z)	-0.04	0.042	6.78	18.65	-0.19	18.45	0.0149	0.052	0.0191	7.37

25H⁺(E)	-0.044	0.047	-11.19	21.3	1.52	22.82	0.0161	-0.0505	0.0183	5.79
25H⁺(Z)	-0.04	0.046	-1.12	20.23	0.84	21.07	0.0159	0.0349	0.0191	7.53
26H⁺(E)	-0.082	0.042	4.95	16.56	0.06	16.62	0.0148	-0.0477	0.0174	2.41
26H⁺(Z)	-0.058	0.044	-8.68	15.93	2.77	18.7	0.0315	0.0356	0.0182	8.24
27H⁺(E)	-0.084	0.042	-5.2	18.69	-1.4	17.29	0.0106	-0.0528	0.0178	4.22
27H⁺(Z)	-0.075	0.039	-8.73	18.03	-0.3	17.73	0.0081	-0.0231	0.0158	6.45
28H⁺(E)	-0.07	0.029	3.11	17.45	-4.2	13.24	-0.0117	-0.143	0.0094	3.43
28H⁺(Z)	-0.076	0.045	-4.17	29.44	2.42	31.86	0.0139	-0.0004	0.0203	7.41
29H⁺(E)	-0.017	0.047	-4.79	24.44	2.24	26.68	0.0236	-0.0447	0.0218	7.44
29H⁺(Z)	-0.015	0.046	-1.92	25.45	1.25	26.7	0.0206	-0.0574	0.0218	8.83
30H⁺(E)	-0.186	0.041	16.72	15.7	1.96	17.66	0.0136	-0.0456	0.0175	2.05
30H⁺(Z)	-0.089	0.04	-7.08	15.7	-0.49	15.22	0.0141	0.0136	0.0167	6.05
31H⁺(E)	-0.028	0.039	-15.18	22.32	-0.61	21.71	0.0203	-0.0156	0.019	6.81
31H⁺(Z)	-0.051	0.027	-18.11	20.14	-5.28	14.86	-0.0051	-0.0367	0.0192	9.34
32H⁺(E)	-0.009	0.199	-6.04	34.46	39.9	74.36	0.0801	-0.0056	0.0907	-2.63
32H⁺(Z)	-0.041	0.216	0.38	31.46	22.93	54.39	0.0735	-0.0005	0.0846	-2.52
33H⁺(E)	-0.001	0.03	-8.71	19.24	4.98	24.22	-0.0097	-0.0395	0.0124	2.74
33H⁺(Z)	0.026	0.027	-17.91	24	-1.04	22.96	0.0064	-0.021	0.0135	6.12
34H⁺(E)	0.017	0.006	-2.66	2.2	-0.31	1.89	-0.0256	-0.0738	0.0019	-1.39
34H⁺(Z)	0.014	0.007	-8.62	0.58	-1.02	-0.44	-0.0047	0.0607	0.0042	1.17
35H⁺(E)	-0.033	0.035	-0.04	27.38	-0.36	27.01	0.0006	-0.0213	0.0144	6
35H⁺(Z)	-0.021	0.034	-9.46	23.15	-1.44	21.7	-0.0046	-0.0305	0.0154	5.55
36H⁺(E)	-0.02	0.034	-4.18	21.03	2.27	23.3	-0.0028	-0.0541	0.0088	5.31
36H⁺(Z)	-0.015	0.034	-5.88	19.45	1.76	21.21	-0.0119	-0.1106	0.009	4.23
37H⁺(E)	0.059	0.017	-0.19	7.97	1.21	9.18	0.0059	-0.0295	0.0094	2.45
37H⁺(Z)	0.07	0.02	0.21	10.62	-2.64	7.98	0.006	-0.1116	0.0106	1.98
38H⁺(E)	-0.053	0.048	-7.48	25.03	-0.35	24.68	0.0215	-0.0187	0.0254	7.9
38H⁺(Z)	-0.026	0.051	-3.97	24.58	2.03	26.61	0.0221	-0.0681	0.0252	6.57
39H⁺(E)	-0.12	0.035	-23.57	26.34	0.04	26.37	-0.0049	-0.0756	0.0167	6.06
39H⁺(Z)	-0.108	0.033	-23.35	25.72	-1.43	24.29	-0.0052	0.0448	0.0188	12.91
40H⁺(E)	-0.002	0.024	-13.71	3.82	-0.03	3.79	-0.0009	-0.0196	0.011	3.08
40H⁺(Z)	-0.022	0.028	-13.2	18.39	-2.11	16.28	0.0037	-0.0843	0.007	6.09
41H⁺(E)	0.014	0.036	-11.91	21.68	2.07	23.74	-0.0074	0.0043	0.014	1.41
41H⁺(Z)	0.047	0.031	-8.54	20.6	-4.03	16.57	-0.0122	0.0313	0.0148	5.93
42H⁺(E)	-0.048	0.03	1.32	-	-	-	-0.0208	0.0119	0.0198	-0.33
42H⁺(Z)	-0.041	0.032	-7.9	-	-	-	-0.0153	0.0307	0.0237	-1.31
43H⁺(E)	-0.105	0.041	-13.32	17.46	5.39	22.86	0.0191	-0.0823	0.022	6.19
43H⁺(Z)	-0.106	0.042	-11.04	17.62	0.46	18.09	0.0175	-0.0527	0.0232	8.52
44H⁺(E)	-0.108	0.022	-0.13	16.19	1.73	17.92	0.0056	0.0391	0.0129	2.07
44H⁺(Z)	0.074	0.001	-0.43	3.31	3.92	7.23	0.0268	-0.0623	0.0268	4.75

* colour chart should be considered within each column

Table S8. Change of geometric and electronic parameters in cations **9**H⁺-**44**H⁺ during transition from vacuum to acetonitrile (PCM).

Compd	**Δ'E$_{HB}$,** kcal·mol^{-1}	**Δ'r_1,** Å	**Δ'r_2,** Å	**Δ'r_3,** Å	**Δ'α,** deg	**Δ'ω,** deg	**Δ'χ_N,** deg	**Δ'τ,** deg	**Δ'ϑ,** deg	**Δ'q_{NPA}**	**Δ'q_{MK}**	**Δ'q_H**	**Δ'δ,** ppm
9H⁺(E)	-3.05*	0.071	-0.026	0.117	-4.51	-1.92	-3.21	-2.62	-5.82	0.0121	0.0769	0.003	5.58
9H⁺(Z)	-1.25	0.029	-0.021	0.054	-3.08	-2.47	-1.12	-9.45	-10.57	0.0065	-0.2018	0.001	1.72
10H⁺(E)	-2.8	0.066	-0.022	0.107	-6.45	0.46	-1.01	2.87	1.87	0.0181	0.0898	0.003	6.01
10H⁺(Z)	-0.99	0.017	-0.018	0.042	-3.15	-4.18	-3.61	-7.53	-11.14	0.0115	-0.0267	0.001	2.64
11H⁺(E)	-2.47	0.051	-0.022	0.076	-2.25	-3.94	-0.18	4.08	3.9	0.016	0.0733	0.0019	5.35
11H⁺(Z)	-0.98	0.014	-0.017	0.033	-2.53	-4.76	-2.8	-6.74	-9.54	0.0137	-0.0067	0.0022	3.22
12H⁺(E)	-2.19	0.045	-0.02	0.067	-1.9	-0.34	-0.17	3.71	3.53	0.0168	0.0782	0.0025	5.78
12H⁺(Z)	-0.69	0.008	-0.016	0.021	-1.88	0.13	-2.65	-7.27	-9.93	0.014	0.0016	0.0024	3.45
13H⁺(E)	-1.95	0.039	-0.02	0.057	-1.78	-0.12	-0.26	2.52	2.26	0.017	0.0584	0.0027	6.31
13H⁺(Z)	-0.65	0.006	-0.017	0.02	-2	-4.91	-2.58	-5.55	-8.14	0.016	-0.007	0.0038	4.13
14H⁺(E)	-2.93	0.061	-0.023	-0.643	-4.65	1.16	-0.26	2.67	2.41	0.0193	0.0805	0.0043	6.14
14H⁺(Z)	-0.89	0.01	-0.018	0.034	-3.17	-2.31	-2.85	-8.13	-10.98	0.0124	-0.0712	0.0021	2.7
15H⁺(E)	-2.17	0.05	-0.02	0.081	-3.26	1.71	-1.37	3.87	2.5	0.0166	0.0527	0.0025	5.42
15H⁺(Z)	-1	0.017	-0.017	0.042	-3.26	-6.98	-2.96	-7.06	-10.02	0.0133	-0.0238	0.0021	2.98

16H⁺(E)	-2.73	0.06	-0.02	0.089	-4.24	2.6	-0.07	3.25	3.18	0.0198	0.0928	0.005	6.13
16H⁺(Z)	-0.85	0.01	-0.017	0.033	-2.84	-2.07	-2.74	-7.69	-10.42	0.013	-0.0133	0.0029	2.95
17H⁺(E)	-2.94	0.066	-0.022	0.109	-4.84	0.83	-0.81	2.72	1.91	0.0178	0.088	0.0031	5.74
17H⁺(Z)	-1.02	0.019	-0.018	0.04	-2.62	-3	-3.25	-8.33	-11.58	0.0109	-0.0029	0.0011	2.75
18H⁺(E)	-2.31	0.055	-0.019	0.086	-3.08	-0.33	-0.94	3.05	2.12	0.0141	0.043	0.0008	5.27
18H⁺(Z)	-1.08	0.021	-0.016	0.043	-2.5	-7.1	-4.14	-6.81	-10.95	0.012	-0.0496	0.0011	2.72
19H⁺(E)	-2.52	0.058	-0.021	0.094	-3.53	1.78	-0.84	5.1	4.26	0.0131	0.045	-0.0017	5.35
19H⁺(Z)	-1.6	0.035	-0.019	0.064	-3.22	-5.78	-3.61	-6.83	-10.44	0.0084	-0.0378	-0.0006	2.44
20H⁺(E)	-3.3	0.082	-0.021	0.128	-5.07	-1.63	0.4	3.03	3.43	0.0126	0.045	-0.0019	5.7
20H⁺(Z)	-2.09	0.047	-0.018	0.078	-2.79	-4.62	-3.18	-5.92	-9.1	0.0057	-0.0504	-0.0004	0.87
21H⁺(E)	-2.33	0.045	-0.022	0.074	-2.76	-2.97	-0.99	4.14	3.16	0.0158	0.0576	0.0017	5.33
21H⁺(Z)	-0.72	0.006	-0.017	0.025	-1.98	-9.77	-3.53	-7.7	-11.24	0.0129	-0.0256	0.002	2.7
22H⁺(E)	-2.51	0.05	-0.019	0.085	-3.7	-0.68	0.12	4.24	4.36	0.019	0.0513	0.0048	5.3
22H⁺(Z)	-0.83	0.006	-0.017	0.031	-3.29	3.63	-2.33	-7.26	-9.58	0.0131	0.0438	0.0033	3.08
23H⁺(E)	-2.58	0.059	-0.021	0.096	-4.11	4.35	-1.91	3.78	1.86	0.0154	0.0641	0.0016	5.23
23H⁺(Z)	-1.08	0.02	-0.017	0.044	-2.98	-3.55	-2.71	-6.61	-9.32	0.0133	-0.0413	0.002	2.89
24H⁺(E)	-2.21	0.043	-0.019	0.067	-2.09	-0.08	-0.98	2.8	1.82	0.0141	0.0421	0.001	4.86
24H⁺(Z)	-0.87	0.014	-0.015	0.028	-1.39	-6.78	-3.34	-6.34	-9.68	0.0125	0.0116	0.0027	2.85
25H⁺(E)	-2.22	0.044	-0.019	0.065	-1.8	-1.05	-0.72	3.51	2.79	0.0131	0.0178	-0.0009	5.61
25H⁺(Z)	-1.15	0.02	-0.017	0.036	-1.55	-5.43	-2.62	-6.35	-8.97	0.0104	-0.0368	0.0004	3.05
26H⁺(E)	-2.24	0.043	-0.02	0.066	-2.15	0.08	0.54	3	3.54	0.0116	0.0082	-0.0024	5.41
26H⁺(Z)	-1.44	0.022	-0.021	0.045	-2.88	-3.04	-3.77	-4.27	-8.04	0.0052	-0.0207	-0.0016	3.49
27H⁺(E)	-2.53	0.051	-0.017	0.077	-2.52	-1.03	-0.38	2.69	2.32	0.0147	0.0485	0.0027	5.14
27H⁺(Z)	-1.08	0.018	-0.013	0.034	-2.06	-3.76	-2.59	-6.35	-8.94	0.0134	-0.0351	0.0034	3.73
28H⁺(E)	-1.42	0.036	-0.016	0.053	-1.91	1.79	1.39	2.31	3.7	0.0128	-0.0249	-0.0004	4.87
28H⁺(Z)	-0.96	0.016	-0.016	0.031	-1.43	-5.46	-3.98	-6.84	-10.82	0.0054	-0.0009	0.0003	2.02
29H⁺(E)	-2.19	0.049	-0.021	0.075	-2.46	0.17	-0.99	3.91	2.92	0.0145	0.0686	-0.0014	6.16
29H⁺(Z)	-1.17	0.023	-0.018	0.042	-2.14	-4.11	-3.34	-7.54	-10.88	0.0079	-0.0347	-0.0011	2.13
30H⁺(E)	-2.33	0.042	-0.019	0.066	-1.95	1.6	1.03	4.69	5.72	0.0116	-0.0196	-0.0017	5.62
30H⁺(Z)	-1.61	0.024	-0.017	0.046	-2.27	-3.42	-2.15	-5.41	-7.55	0.0086	-0.0185	0.0016	2.86
31H⁺(E)	-2.4	0.059	-0.016	0.091	-3.81	0.66	4.01	2.3	6.31	0.0196	0.1102	0.0035	5.77
31H⁺(Z)	-0.68	0.011	-0.014	0.028	-2.23	-6.94	-1.67	-7.91	-9.58	0.0137	-0.046	0.0022	3.21
32H⁺(E)	-0.94	0.035	-0.006	0.05	-1.52	2.37	0.37	-0.08	0.29	0.0182	0.0751	0.0104	3.6
32H⁺(Z)	-1.91	0.064	-0.002	0.086	-2.72	0.31	0.58	-17.21	-16.63	0.0183	-0.0727	0.0083	6.91
33H⁺(E)	-1.03	0.024	-0.01	0.051	-3.09	-2.58	3.43	4.98	8.41	0.009	0.0312	1.00E-04	3.03
33H⁺(Z)	-0.08	-0.011	-0.008	0.003	-1.56	-5.41	-2.07	-1.77	-3.83	None	-0.0072	-0.0001	3.23
34H⁺(E)	-	-0.02	-0.009	0.146	-9.1	-5.02	-1.63	-12.51	-14.14	0.0118	-0.0789	-0.0038	-0.66
34H⁺(Z)	-	-0.058	-0.013	0.157	-13.29	-11.22	-10.61	-4.98	-15.59	0.0108	0.0283	-0.0011	1.02
35H⁺(E)	-0.58	0.021	-0.012	0.028	-0.49	-0.34	2.23	2.81	5.04	0.0145	0.0367	0.0021	5.77
35H⁺(Z)	0.1	-0.009	-0.01	-0.012	0.16	-2.58	0.58	-3.94	-3.36	0.0157	0.0782	0.0029	4.36
36H⁺(E)	-0.54	0.019	-0.012	0.025	-0.55	-0.82	1.23	3.62	4.84	0.0092	0.014	-0.0023	5.55
36H⁺(Z)	-0.19	0.002	-0.011	0.007	-0.44	-1.98	-1.18	-3.3	-4.49	0.0106	-0.0571	-0.0009	3.15
37H⁺(E)	-	0.058	-0.019	0.133	-4.53	5	9.93	-13.35	-3.4	0.0065	-0.0811	-0.0018	2.46
37H⁺(Z)	-	0.026	-0.017	0.127	-6.48	3.69	-0.55	1.37	0.84	0.0129	0.1093	-0.0003	5.5
38H⁺(E)	-3.21	0.075	-0.022	0.097	-2.15	3.37	3.48	-17.84	-14.35	0.0019	0.0459	-0.0048	0.18
38H⁺(Z)	-3.5	0.079	-0.022	0.118	-6.24	4.36	-1.56	1.21	-0.35	0.017	0.0478	0.0012	6.98
39H⁺(E)	-1.62	0.048	-0.013	0.059	-1.09	-0.55	2.74	0.91	3.66	0.0126	0.0414	0.0009	3.59
39H⁺(Z)	-1.02	0.031	-0.013	0.039	-0.52	-12.35	-0.9	-5.42	-6.32	0.0163	-0.0222	0.0028	3.95
40H⁺(E)	-0.39	0.021	-0.005	0.014	0.89	-1.5	15.56	-9.19	6.37	0.0131	-0.0141	0.002	1.82
40H⁺(Z)	-0.86	0.02	-0.01	0.044	-2.84	5.29	-0.49	2.31	1.82	0.0157	0.1085	0.0039	3.72
41H⁺(E)	-2.03	0.067	-0.014	0.101	-3.84	-2.9	0.44	0.02	0.45	0.024	0.0863	0.0091	7.53
41H⁺(Z)	-1.5	0.05	-0.013	0.078	-3.47	1.19	1.32	-16.24	-14.92	0.0074	-0.0173	0.003	1.53
42H⁺(E)	-1.41	0.041	-0.012	0.047	-0.13	-1.44	-	-	-	0.006	0.0248	-0.0031	1.3
42H⁺(Z)	-1.19	0.031	-0.021	0.044	-1.09	0.89	-	-	-	0.025	0.0964	0.0106	5.32
43H⁺(E)	-2.24	0.044	-0.021	0.073	-2.73	0.48	-2.83	-0.26	-3.09	0.0148	0.0596	0.0026	4.97
43H⁺(Z)	-2.92	0.053	-0.02	0.094	-5.33	4.31	1.55	-16.62	-15.07	0.0122	0.0881	-0.0002	3.56
44H⁺(E)	-1.09	0.064	-0.031	0.126	-4.18	-0.36	-6.89	-0.04	-6.93	0.0138	0.0099	-0.0007	6.04
44H⁺(Z)	-	-0.026	-0.006	0.023	-2.46	-0.26	-1.79	-2.79	-4.57	0.0015	0.0029	-0.0028	-0.42

* colour chart should be considered within each column

Table S9. Change of geometric and electronic parameters in **9**-**44** during transition from vacuum to acetonitrile (PCM).

Compd	r_1, Å	r_2, Å	ω, deg	χ_N, deg	τ, deg	ϑ, deg	q_{NPA}	q_{MK}	q_H	δ, ppm
9(E)	0*	-0.011	-1.98	-1.24	-1.27	-2.51	0.0082	0.0968	-0.0018	3.92
9(Z)	-0.005	-0.011	-2.37	1.96	-0.84	1.12	0.0118	-0.1054	-0.0007	3.97
10(E)	-0.003	-0.011	0.26	0.22	0.68	0.91	0.0109	0.0245	-0.0006	5.02
10(Z)	-0.002	-0.011	-2.98	0.67	0.07	0.74	0.0124	-0.0159	1.00E-04	5.48
11(E)	-0.008	-0.011	0.02	0.05	0.81	0.87	0.0095	0.0259	-0.0016	4.75
11(Z)	-0.003	-0.011	-3.84	0.33	-0.17	0.16	0.0121	-0.0675	-0.0006	5.58
12(E)	-0.005	-0.012	2.66	-0.27	0.5	0.22	0.0094	0.0057	-0.0018	4.98
12(Z)	-0.001	-0.012	-7.79	-0.21	0.41	0.19	0.012	-0.0572	-0.001	5.86
13(E)	0.003	-0.011	0.93	0.77	0.53	1.3	0.0115	0.0161	0	5.27
13(Z)	0.005	-0.009	-0.41	1.91	0.46	2.38	0.013	0.0021	0.001	5.59
14(E)	0.037	-0.008	4.82	0.99	1.53	2.53	0.0132	0.0273	0.0019	5.43
14(Z)	0.035	-0.006	2.68	0.98	0.3	1.29	0.0144	0.0083	0.0026	5.52
15(E)	-0.007	-0.012	0.01	0.27	0.58	0.85	0.0104	0.0065	-0.001	4.96
15(Z)	-0.006	-0.011	-2.57	0.83	0.13	0.96	0.012	-0.0098	0	5.42
16(E)	0.004	-0.009	1.6	0.52	1.01	1.53	0.0129	0.0275	0.0015	5.24
16(Z)	0.003	-0.008	-0.88	1.01	0.55	1.57	0.0139	-0.0276	0.0023	5.48
17(E)	-0.003	-0.011	0.64	0.38	0.74	1.11	0.0106	0.0357	-0.0009	5
17(Z)	-0.005	-0.011	-2.37	0.76	0.03	0.77	0.012	-0.0107	-1.00E-04	5.4
18(E)	-0.003	-0.011	0.22	-0.09	0.41	0.32	0.0105	-0.0039	-0.0014	4.81
18(Z)	-0.004	-0.009	-3.52	1.81	0.16	1.98	0.0108	-0.0331	-0.0002	5.26
19(E)	-0.003	-0.012	0.48	0.29	1.65	1.95	0.0084	-0.0067	-0.0036	5.11
19(Z)	-0.005	-0.01	-1.21	-1.62	-1.28	-2.89	0.0102	-0.1026	-0.0015	5.09
20(E)	-0.005	-0.012	0.97	0.99	3.13	4.12	0.0092	0.0003	-0.0039	5.02
20(Z)	0.001	-0.01	0.62	-3.46	-1.92	-5.38	0.0086	-0.082	-0.0018	4.25
21(E)	-0.005	-0.012	-0.03	0.61	0.78	1.39	0.0105	0.0278	-0.0011	4.96
21(Z)	-0.008	-0.01	-2.42	1.11	0	1.11	0.0115	0.0003	-0.0003	5.16
22(E)	0.046	-0.005	5.59	0.67	1.68	2.35	0.015	0.0292	0.0042	5.54
22(Z)	0.047	-0.004	-6.2	0.8	0.75	1.55	0.016	-0.0106	0.0049	5.58
23(E)	-0.003	-0.012	-0.3	0.43	0.71	1.15	0.0097	0.0248	-0.002	5.02
23(Z)	-0.005	-0.011	-2.5	0.75	0.24	0.99	0.0111	-0.0073	-0.001	5.23
24(E)	-0.005	-0.011	0.36	-0.34	0.92	0.58	0.0094	-0.0034	-0.0021	4.52
24(Z)	-0.001	-0.009	-5.62	0.61	0.32	0.93	0.0105	-0.05	-0.0009	5.74
25(E)	-0.004	-0.011	1.31	0.56	1.55	2.11	0.0072	-0.0326	-0.0042	5.2
25(Z)	-0.003	-0.011	2.59	-1.27	-1.28	-2.55	0.009	-0.101	-0.0026	5.13
26(E)	-0.002	-0.011	1.49	1.29	2.58	3.86	0.0091	-0.019	-0.0037	5.29
26(Z)	0.007	-0.01	1.82	-1.94	-1.41	-3.36	0.0087	-0.1093	-0.0015	4.37
27(E)	0.009	-0.008	3.35	0.03	1.28	1.31	0.0105	0.0101	1.00E-04	4.78
27(Z)	0.013	-0.007	3.97	0.23	-1.05	-0.82	0.0142	-0.1118	0.0022	5.75
28(E)	-0.002	-0.013	5.85	1.22	-2.27	-1.05	-0.0032	0.0592	-0.0046	5.21
28(Z)	-0.018	-0.008	7.66	-2.65	-1.41	-4.06	0.0047	-0.0506	-0.0024	4.27
29(E)	-0.002	-0.013	0.57	-0.71	1.18	0.47	0.0063	0.0156	-0.0057	5.38
29(Z)	0.001	-0.013	4.97	-4.8	-0.88	-5.69	0.0061	-0.143	-0.0042	5.03
30(E)	-0.013	-0.008	-17.96	1.92	2.87	4.79	0.0097	-0.0172	-0.0027	5.21
30(Z)	0.019	-0.007	3.63	-2.4	-1.48	-3.87	0.0101	-0.0736	0.0003	4.46
31(E)	0	-0.01	0.06	1.34	1.54	2.89	0.0105	0.0163	-0.0004	4.89
31(Z)	0.011	-0.012	0.85	-1.18	1.31	0.13	0.0112	0.0499	-0.0022	6.29
32(E)	0.007	-0.014	0.11	-2.66	-1.92	-4.58	0.0096	0.0195	-0.0022	5.07
32(Z)	0.009	-0.013	-0.54	0.57	-2.32	-1.75	0.0066	-0.0061	-0.0013	5.5
33(E)	0.006	-0.008	-0.44	-2.36	0.98	-1.38	0.0018	-0.0597	-0.0037	3.03
33(Z)	-0.004	-0.009	-3.16	0.85	1.34	2.18	0.0098	-0.0085	-0.0027	4.88
34(E)	0	-0.014	2.07	-4.04	-0.45	-4.49	-0.0015	0.0741	-0.0066	3.44
34(Z)	-0.013	-0.007	3.98	-2.45	0.55	-1.9	0.0083	-0.0399	-0.0017	5.24
35(E)	-0.005	-0.01	-2.57	-3.14	0.01	-3.13	0.0044	0.0083	-0.0034	3.84
35(Z)	-0.002	-0.014	-2.65	-3.81	0.23	-3.57	0.0087	-0.0515	-0.0032	4.98
36(E)	0	-0.01	2.33	-0.65	0.68	0.03	0.0037	-0.0105	-0.0049	4.43
36(Z)	0	-0.012	-0.83	-2.86	-0.94	-3.81	0.0079	-0.1498	-0.0041	5.17
37(E)	0.013	-0.014	0.71	2.76	-1.82	0.93	0.0062	-0.0015	-0.0036	4.7
37(Z)	0.005	-0.011	0.2	2.03	1.12	3.15	0.0098	0.041	-0.002	5.77

38(E)	0.02	-0.015	1.04	4.97	-4.93	0.05	0.0023	-0.0284	-0.0056	3.36
38(Z)	-0.002	-0.014	-1.28	0.63	0.17	0.8	0.0108	-0.0097	-0.0032	6.48
39(E)	0.009	-0.014	3.01	0.31	-2.44	-2.13	0.0033	0.0073	-0.0041	4.03
39(Z)	0.008	-0.013	-0.31	-1.01	0.71	-0.3	0.0116	0.0257	-0.0019	6.36
40(E)	0.009	-0.01	5.04	3.13	1.04	4.17	0.0106	-0.0128	-0.0006	4.98
40(Z)	0.009	-0.01	-0.28	1.34	-1.79	-0.45	0.0132	0.0201	0.0017	4.49
41(E)	0.007	-0.01	0.78	-1.54	-1.98	-3.51	0.0131	0.0301	0.0016	6.06
41(Z)	0.004	-0.006	0.11	0.5	2.36	2.86	0.0137	-0.0121	0.0019	5.27
42(E)	0.002	-0.01	-0.48	-	-	-	0.0138	0.055	-0.0009	5.99
42(Z)	-0.007	-0.006	-0.19	-	-	-	0.0182	0.0148	0.0018	5.36
43(E)	0.017	-0.012	0.81	-1.29	0.72	-0.58	0.0053	0.0716	-0.0033	3.46
43(Z)	0.023	-0.014	0.51	1.35	-2.46	-1.11	0.0094	0.0943	-0.0028	6.7
44(E)	-0.006	-0.016	-0.64	0.11	-1.22	-1.11	0.0061	-0.001	-0.0045	5.09
44(Z)	0.017	-0.01	-1.2	-0.12	-0.14	-0.26	0.013	0.0028	0.0007	6.05

* colour chart should be considered within each column

Table S10. Geometric and electronic parameters of perchlorates in acetonitrile (PCM).

Compd	E_{HB}, kcal·mol^{-1}	r_1, Å	r_2, Å	r_3, Å	r_4, Å	α, deg	ω, deg	χ_N, deg	τ, deg	ϑ, deg	q_{NPA}	q_{MK}	q_H	δ, ppm
10H$^+$(E)	4.65*	2.811	1.401	1.901	2.249	144.68	-7.77	40.07	16.35	56.42	0.7412	0.5995	0.1811	182.61
10H$^+$(Z)	5.03	2.804	1.398	1.884	2.423	146.25	6.67	32.8	6.77	39.56	0.7353	0.5925	0.1845	187.1
12H$^+$(E)	7.43	2.735	1.41	1.766	2.444	152.25	-9.81	42.36	19.93	62.29	0.7485	0.5822	0.1844	183.21
12H$^+$(Z)	7.3	2.745	1.405	1.774	2.689	153.61	7.74	34.79	5.88	40.67	0.7395	0.6542	0.1884	188.13
14H$^+$(E)	5.36	2.774	1.408	1.863	2.223	144.53	-9.84	41.32	19.08	60.39	0.746	0.6055	0.1837	182.75
14H$^+$(Z)	5.61	2.774	1.402	1.853	2.425	146.23	6.94	33.59	6.87	40.47	0.7379	0.6204	0.1874	187.42
16H$^+$(E)	4.81	2.788	1.407	1.894	2.2	142.39	-16.48	40.14	19.43	59.56	0.7471	0.6257	0.1827	182.52
16H$^+$(Z)	5.36	2.782	1.403	1.867	2.398	145.66	7.5	33.87	6.7	40.57	0.7377	0.6046	0.1881	187.33
18H$^+$(E)	5.41	2.785	1.398	1.862	2.414	146.56	-1.16	34.41	10.38	44.79	0.7285	0.5181	0.1784	181.6
18H$^+$(Z)	5.21	2.793	1.396	1.875	2.507	146.24	1.68	29.14	8.15	37.29	0.7304	0.4859	0.181	186.26
19H$^+$(E)	4.71	2.807	1.404	1.901	2.352	144.53	-1.15	34.22	10.59	44.82	0.7396	0.5049	0.1723	180.55
19H$^+$(Z)	4.79	2.802	1.401	1.899	2.428	144.28	-1.02	30.22	8.75	38.97	0.7411	0.7524	0.1759	186.86
24H$^+$(E)	8.33	2.715	1.4	1.735	2.949	155.46	5.81	31.89	8.32	40.21	0.7266	0.5693	0.1815	181.7
24H$^+$(Z)	8.22	2.718	1.4	1.739	3.198	155.64	-4.24	28.36	6.73	35.09	0.7381	0.5686	0.1865	185.57
25H$^+$(E)	8.05	2.721	1.411	1.744	2.649	154.28	-3.51	34.86	11.81	46.67	0.742	0.5166	0.1744	180.33
25H$^+$(Z)	8.06	2.723	1.409	1.746	2.827	154.99	2	30.7	7.74	38.44	0.7437	0.7028	0.1795	187.04
26H$^+$(E)	5.94	2.765	1.415	1.835	2.398	147.05	-20.75	34.04	17.81	51.84	0.7442	0.5393	0.173	179.9
26H$^+$(Z)	6.97	2.74	1.415	1.791	2.683	150.05	2.12	32.21	6.82	39.03	0.7617	0.6103	0.1843	188.7
29H$^+$(E)	6.23	2.769	1.403	1.819	2.472	150.13	-2.36	38.86	12.17	51.03	0.749	0.5178	0.1783	183.08
29H$^+$(Z)	6.5	2.765	1.404	1.808	2.531	151.28	-2.81	36.78	13.52	50.29	0.7544	0.6219	0.1821	189.64
31H$^+$(E)	5.77	2.779	1.399	1.843	3.086	148.97	-3.19	36.28	8.11	44.39	0.728	0.6259	0.1833	181.63
31H$^+$(Z)	4.35	2.829	1.395	1.925	2.534	144.62	-3.93	34.15	4.92	39.06	0.7335	0.6134	0.1847	187.6
32H$^+$(E)	2.81	2.865	1.568	2.047	2.075	134.62	-3.22	53.63	33.26	86.89	0.8164	0.575	0.2348	175.83
32H$^+$(Z)	5.05	2.808	1.588	1.883	3.951	147.19	2.03	50.4	20.35	70.75	0.794	0.5909	0.2446	178.74
33H$^+$(E)	2.72	2.754	1.381	2.071	2.176	122.6	4.1	26.42	6.43	32.85	0.7303	0.6283	0.1705	180.33
33H$^+$(Z)	1.43	2.809	1.367	2.365	1.986	105.21	-3.58	20.81	0.02	20.82	0.73	0.7694	0.171	180.64
35H$^+$(E)	3.83	2.765	1.391	1.966	2.616	133.42	8.92	27.29	0.73	28.02	0.7228	0.5073	0.1807	181.95
35H$^+$(Z)	4.55	2.752	1.391	1.913	3.574	137.38	-7.64	29.78	2.73	32.51	0.7204	0.6373	0.1786	183.93
36H$^+$(E)	4.98	2.726	1.393	1.891	3.396	137.17	-2.09	24.56	4.15	28.71	None	0.4874	0.1738	181.17
36H$^+$(Z)	4.31	2.748	1.292	1.933	3.007	135.1	-14.01	25.39	5.73	31.12	0.7247	0.5692	0.17	182.93
38H$^+$(E)	8.39	2.734	1.412	1.729	3.861	161.63	56.36	32.82	0.25	33.07	0.7363	0.6592	0.1904	181.49
38H$^+$(Z)	7.85	2.748	1.418	1.749	3.771	159.79	58.29	33.98	4.4	38.38	0.738	0.5315	0.189	181.15
43H$^+$(E)	3.31	2.781	1.402	2.009	2.169	129.25	24.97	35.38	9.7	45.08	0.755	0.6392	0.178	183.93
43H$^+$(Z)	3.19	2.787	1.403	2.021	2.129	128.77	29.28	32.45	4.69	37.14	0.7515	0.662	0.1764	186.01

* colour chart should be considered within each column

Table S11. Change of geometric and electronic parameters during transition from base forms to perchlorates$^-$ in acetonitrile (PCM).

Compd	Δr_1, Å	Δr_2, Å	$\Delta\omega$, deg	$\Delta\chi_N$, deg	$\Delta\tau$, deg	$\Delta\vartheta$, deg	Δq_{NPA}	Δq_{MK}	Δq_H	$\Delta\delta$, ppm
10H$^+$(E)	0.025	0.04	-7.3	29.24	11.35	40.59	0.0309	-0.0482	0.0159	7.11
10H$^+$(Z)	0.014	0.035	-9.77	23.56	4.68	28.24	0.0202	-0.1011	0.0146	10.06
12H$^+$(E)	-0.024	0.051	6.56	30.17	15.5	45.67	0.0386	-0.0097	0.0203	8.09
12H$^+$(Z)	-0.016	0.045	4.71	22.82	3.09	25.92	0.0262	0.0389	0.0206	11.11
14H$^+$(E)	-0.052	0.04	-18.12	29.1	13.46	42.56	0.033	-0.0351	0.0143	6.35
14H$^+$(Z)	-0.049	0.032	-22	22.56	4.22	26.78	0.0196	-0.0783	0.0133	10.09
16H$^+$(E)	0.016	0.039	-4.02	28.92	13.72	42.64	0.0336	-0.0006	0.0124	6.96
16H$^+$(Z)	0.01	0.032	-14.4	24.3	4.03	28.33	0.019	-0.0599	0.0128	10.13
18H$^+$(E)	0.027	0.039	-11.09	26.18	6.19	32.37	0.0143	-0.0389	0.0134	5.47
18H$^+$(Z)	0.023	0.035	-13.68	22.52	5.32	27.84	0.0092	-0.0669	0.0089	10.69
19H$^+$(E)	0.047	0.041	-9.14	25.87	6.71	32.58	0.0182	-0.067	0.0125	4.64
19H$^+$(Z)	0.033	0.036	-10.79	22.17	5.2	27.37	0.014	0.0717	0.0121	10.03
24H$^+$(E)	-0.027	0.044	3.24	21.26	3.28	24.55	0.0136	0.007	0.0177	5.9
24H$^+$(Z)	-0.028	0.042	0.45	18.92	3.43	22.35	0.0198	-0.0108	0.017	9.77
25H$^+$(E)	-0.023	0.05	-8	25.72	8.63	34.35	0.024	-0.0035	0.014	5.24
25H$^+$(Z)	-0.022	0.047	-3.85	20.93	4.1	25.03	0.0214	0.0736	0.017	9.78
26H$^+$(E)	-0.013	0.044	10.7	21.1	12.65	33.75	0.0266	-0.0175	0.0089	4.31
26H$^+$(Z)	-0.025	0.043	-12.76	16.81	5.56	22.37	0.0344	-0.0274	0.0159	10.17
29H$^+$(E)	0.017	0.048	-4.02	28.58	9.19	37.76	0.0336	-0.0753	0.0182	7.09
29H$^+$(Z)	0.011	0.049	-2.53	28.83	11.48	40.31	0.0361	0.0018	0.0193	12.98
31H$^+$(E)	-0.009	0.038	-13.13	24.19	2.94	27.12	0.0185	0.0068	0.0159	6.04
31H$^+$(Z)	0.006	0.024	-15.91	22.31	-2.36	19.95	-0.0005	-0.0533	0.0168	11.29
32H$^+$(E)	0.035	0.201	-5.43	34.44	29.23	63.67	0.1033	-0.0014	0.0737	-1.42
32H$^+$(Z)	-0.037	0.221	1.11	31.43	20.3	51.74	0.077	-0.0077	0.083	-0.53
33H$^+$(E)	0.017	0.023	-7.84	-325.21	5.38	-319.83	-0.0028	0.012	0.0037	3.34
33H$^+$(Z)	0.071	0.011	-15.06	19.15	-5.62	13.53	0.0079	0.0628	0.0061	3.17
35H$^+$(E)	-0.009	0.03	7.82	-329.83	-2.81	-332.64	-0.0022	-0.047	0.0106	5.89
35H$^+$(Z)	-0.023	0.03	-10.24	-322.88	-1.46	-324.34	-0.005	-0.0254	0.0132	5.6
36H$^+$(E)	-0.022	0.03	-3.15	24.56	4.15	28.71	None	-0.0421	0.0063	5.26
36H$^+$(Z)	-0.006	-0.071	-3.77	25.39	5.73	31.12	-0.0129	-0.167	0.0074	4.41
38H$^+$(E)	-0.055	0.047	-7.77	26.04	-3.89	22.14	0.0211	0.0076	0.0246	7.17
38H$^+$(Z)	-0.04	0.05	-5.64	23.9	0.42	24.32	0.0223	-0.1141	0.0235	7.32
43H$^+$(E)	-0.018	0.035	-7.33	18.03	4.28	22.32	0.0347	-0.0965	0.0093	7.08
43H$^+$(Z)	-0.022	0.036	-3.94	18.95	0.03	18.98	0.0336	-0.0945	0.0106	9.56

* colour chart should be considered within each column

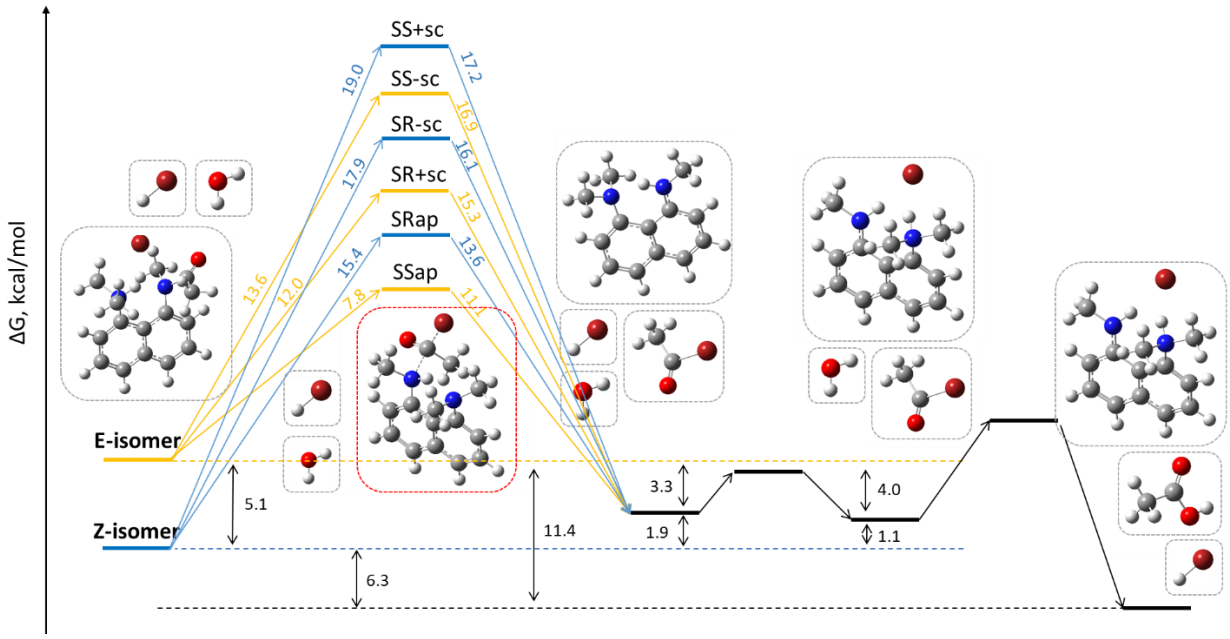

Figure 5. Energy profile for reaction of cation **10**H$^+$ with Br$^-$ anion in vacuum.

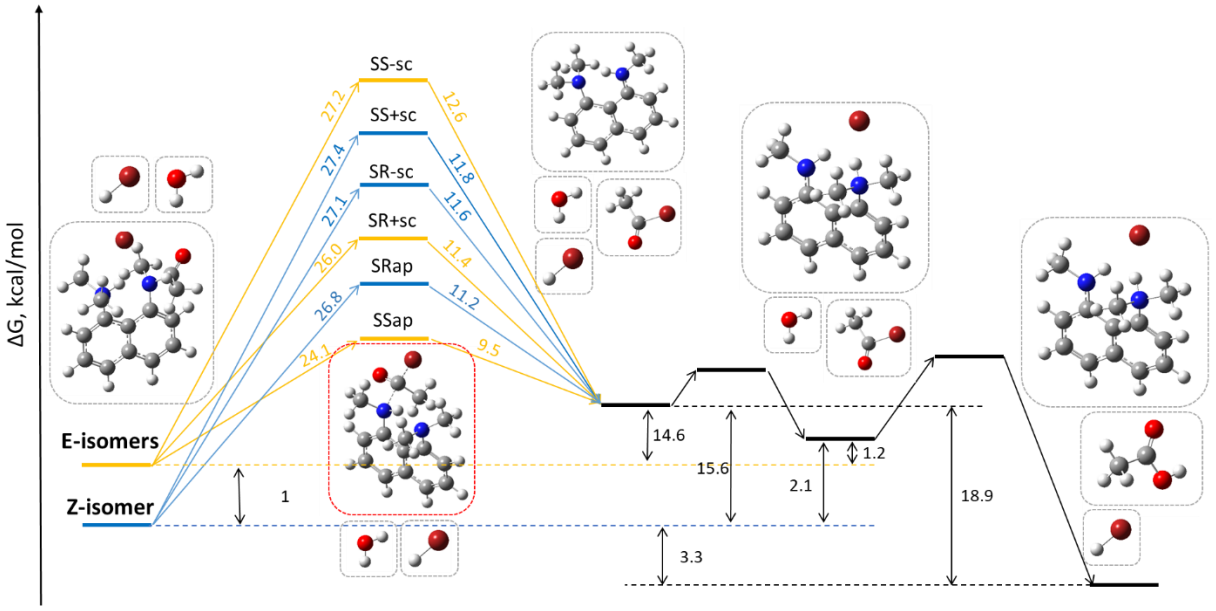

Figure 6. Energy profile for reaction of cation **10**H$^+$ with Br$^-$ anion in acetonitrile (PCM).

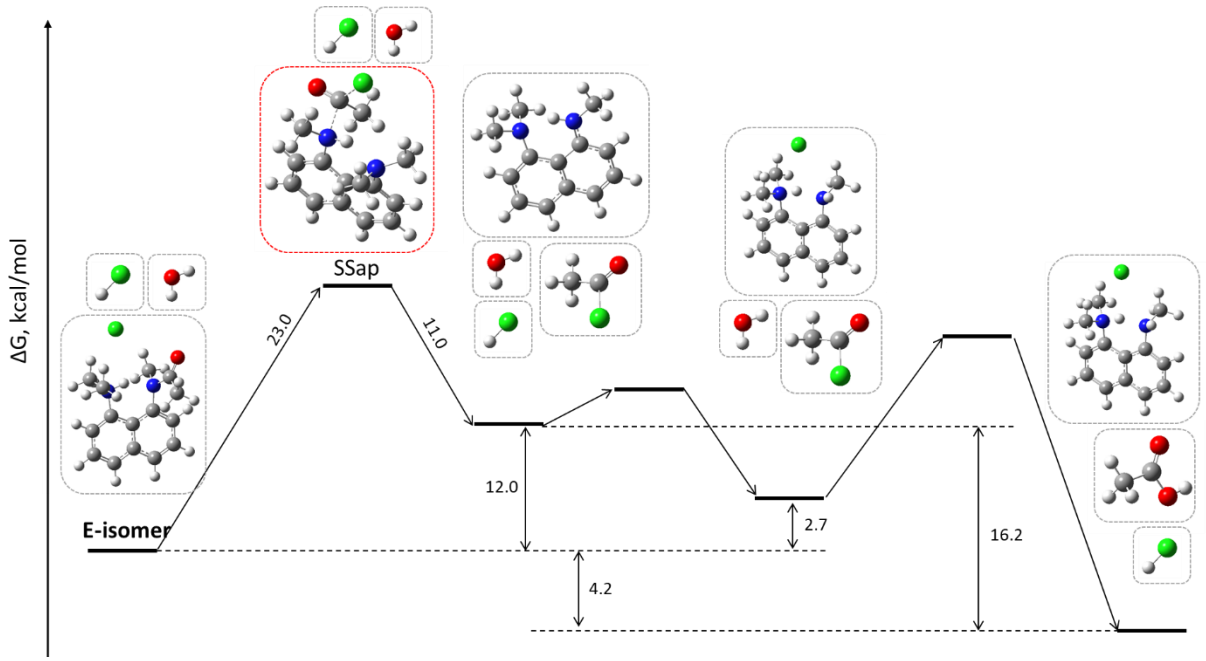

Figure 7. Energy profile for reaction of cation **10**H^+ with Cl^- anion in acetonitrile (PCM).

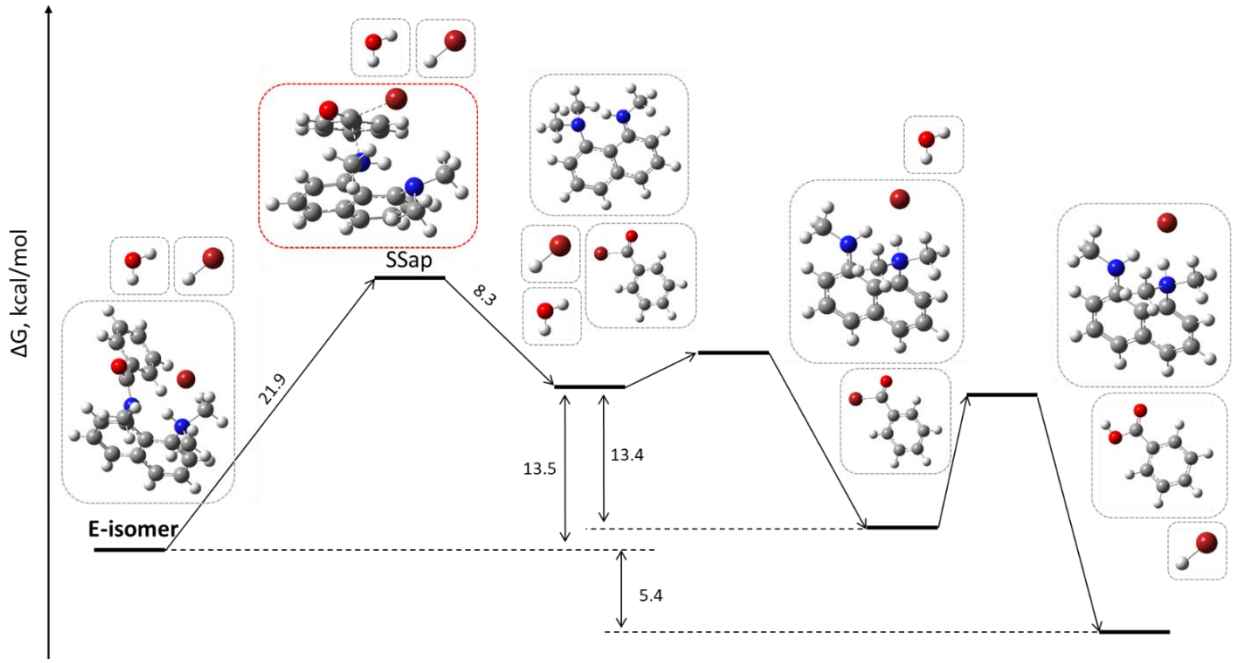

Figure 8. Energy profile for reaction of cation **9**H^+ with Br^- anion in acetonitrile (PCM).

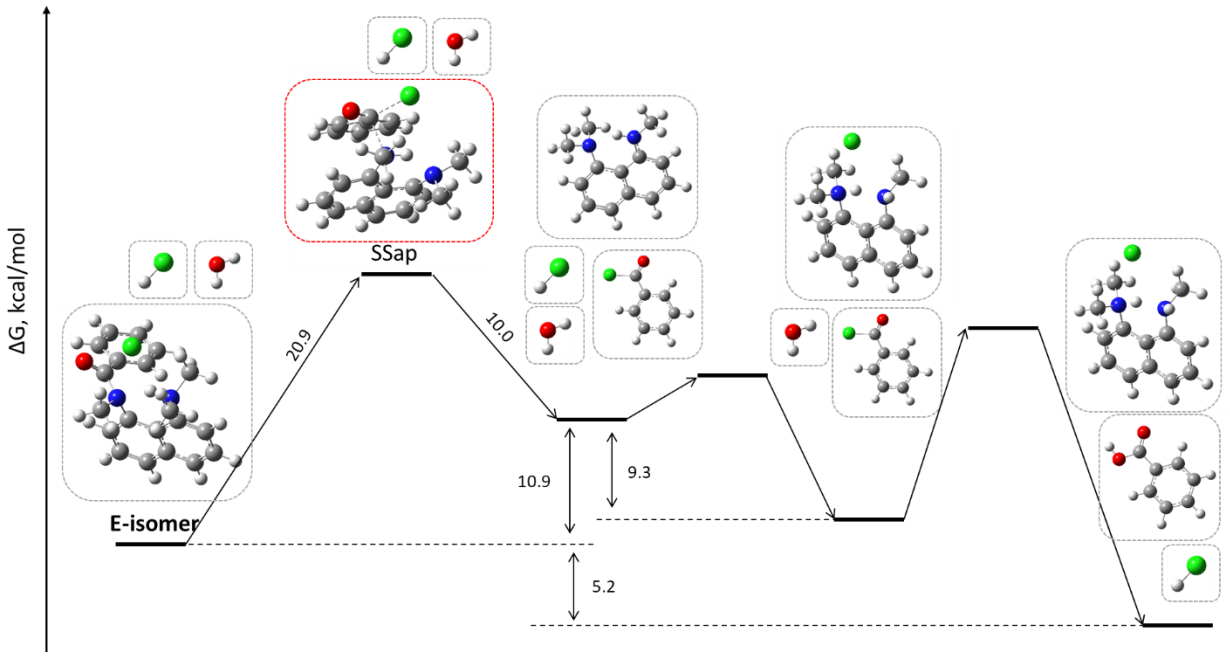

Figure 9. Energy profile for reaction of cation **9**H$^+$ with Cl$^-$ anion in acetonitrile (PCM).

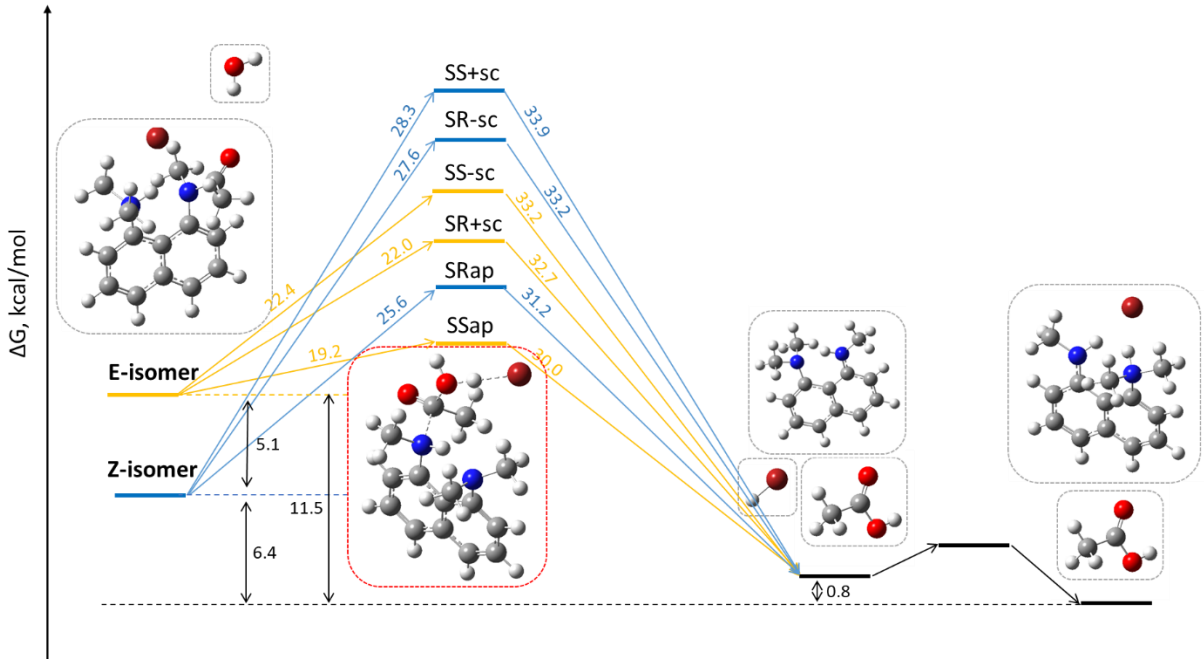

Figure 10. Energy profile for Br$^-$ assisted reaction of cation **10**H$^+$ with H_2O molecule in vacuum.

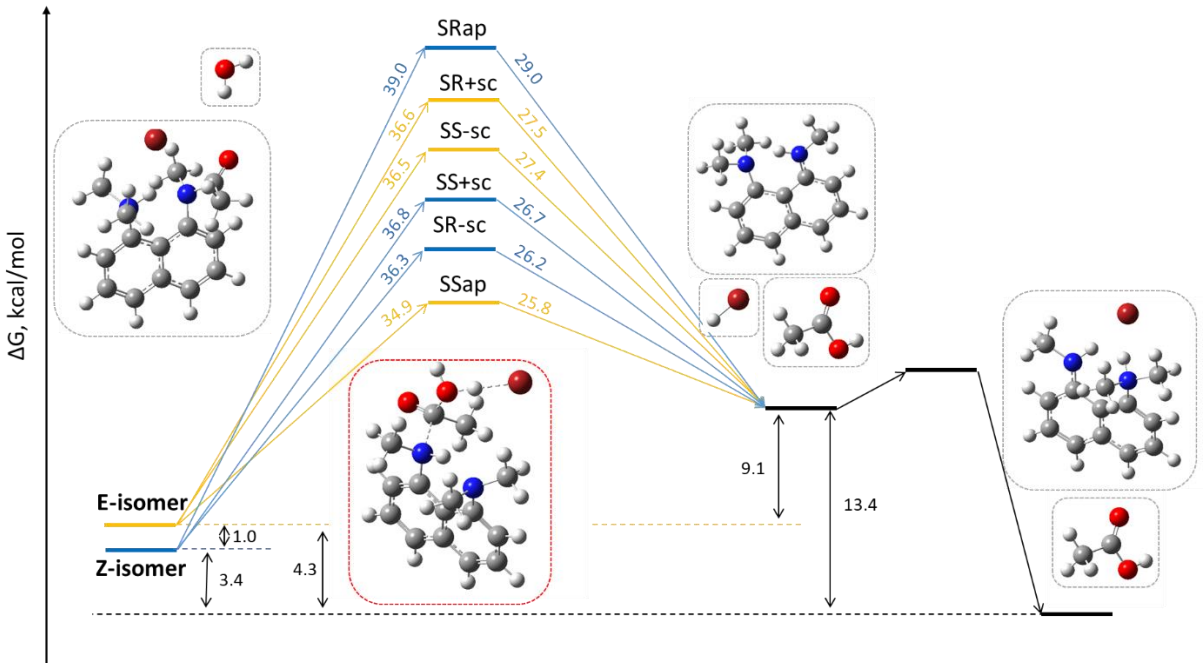

Figure 11. Energy profile for Br^- assisted reaction of cation **10**H^+ with H_2O molecule in acetonitrile (PCM).

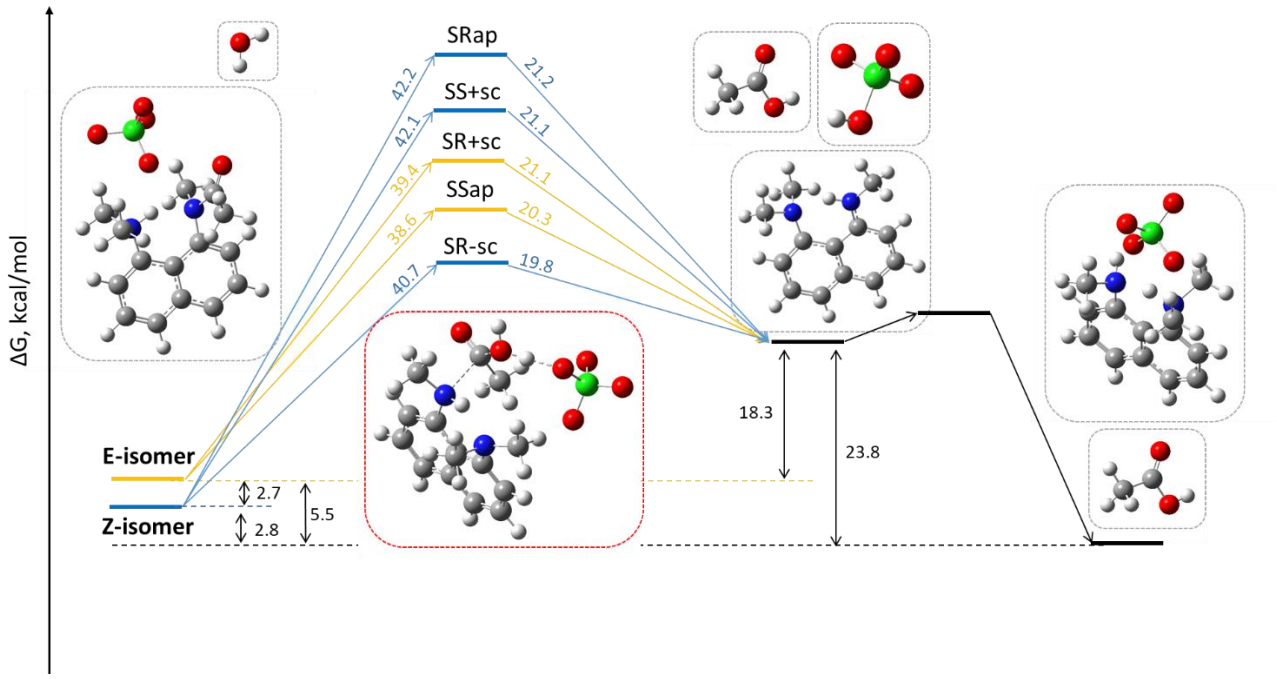

Figure 12. Energy profile for $ClO4^-$ assisted reaction of cation **10**H^+ with H_2O molecule in acetonitrile (PCM).

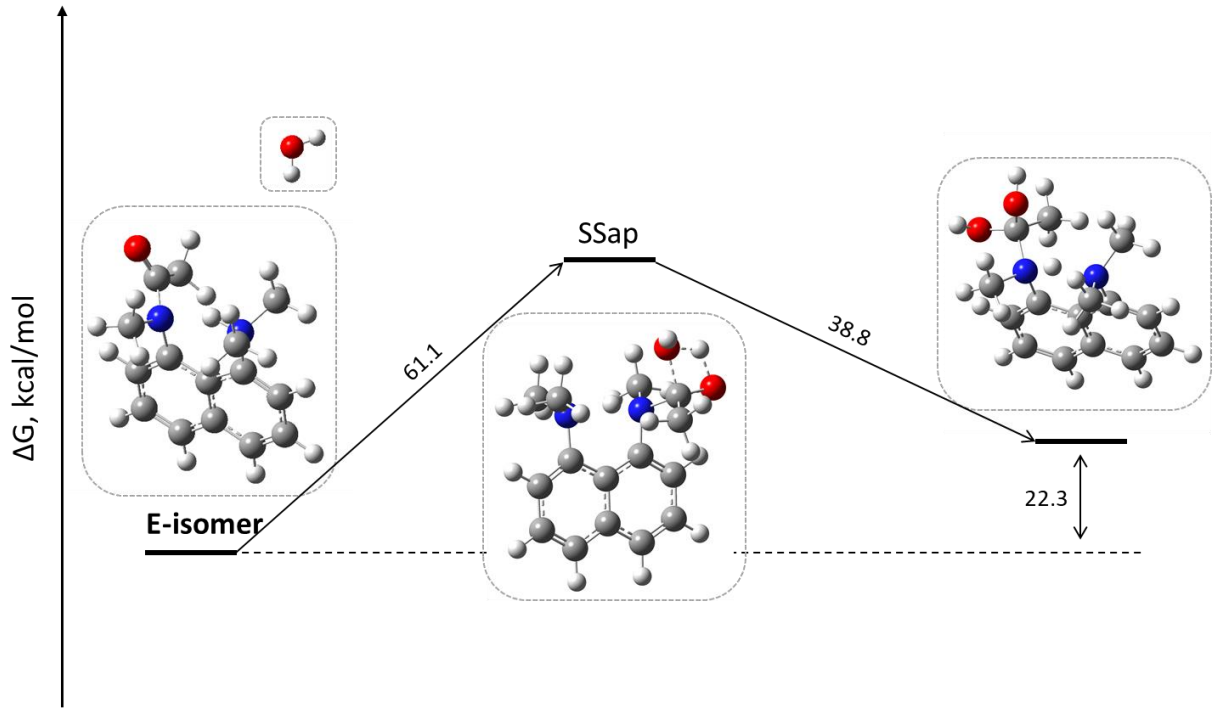

Figure 13. Energy profile for reaction of cation **10**H^+ and H_2O molecule with concerted CO group protonation in acetonitrile (PCM) without assistance of an anion.

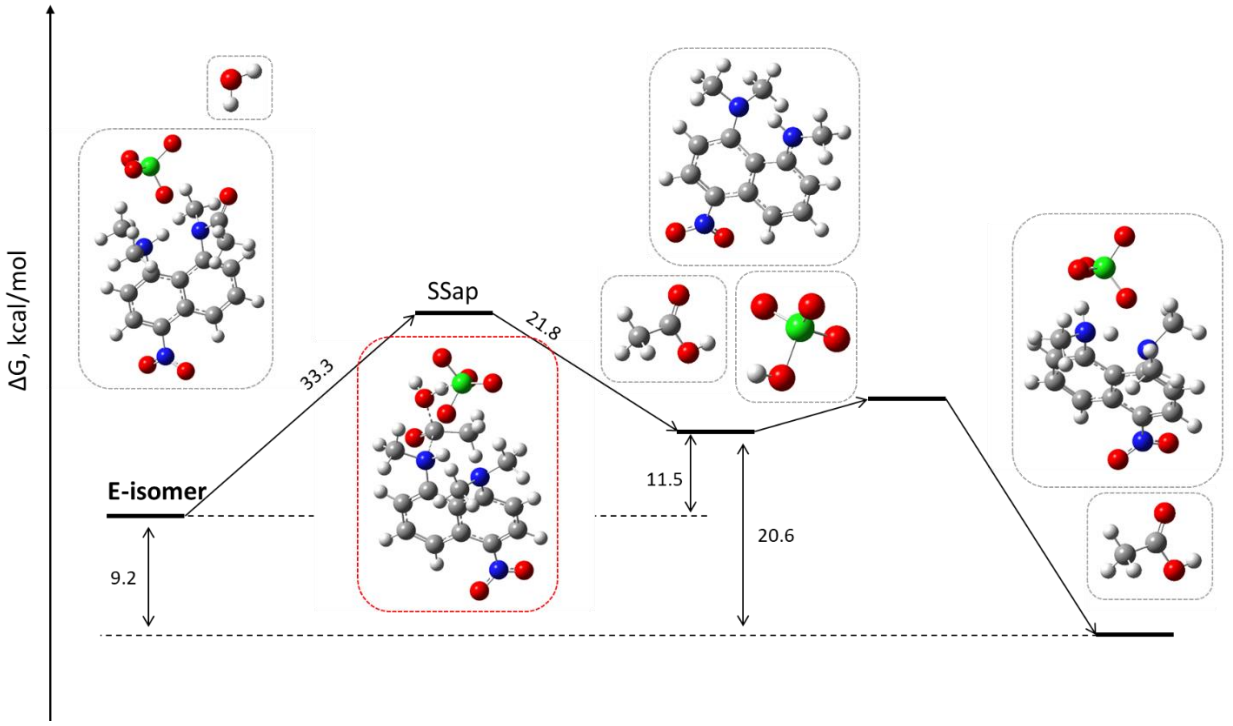

Figure 14. Energy profile for $ClO4^-$ assisted reaction of cation **14**H^+ with H_2O molecule in acetonitrile (PCM).

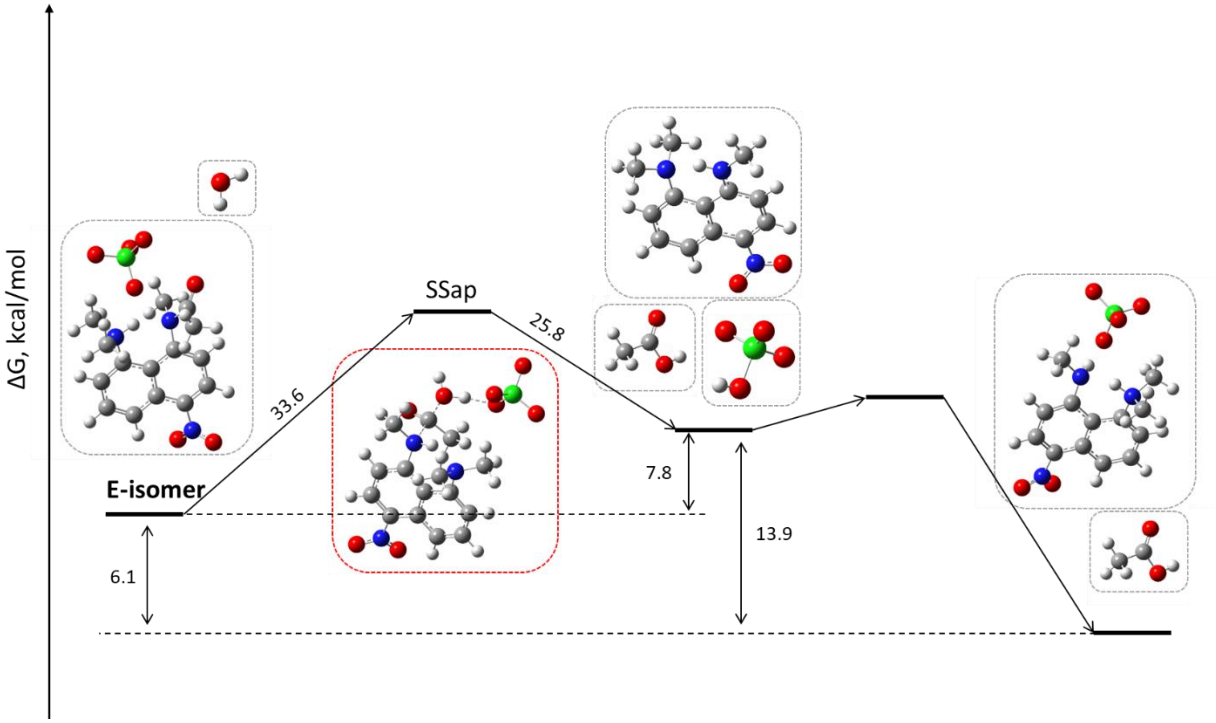

Figure 15. Energy profile for $ClO4^-$ assisted reaction of cation **16**H^+ with H_2O molecule in acetonitrile (PCM).

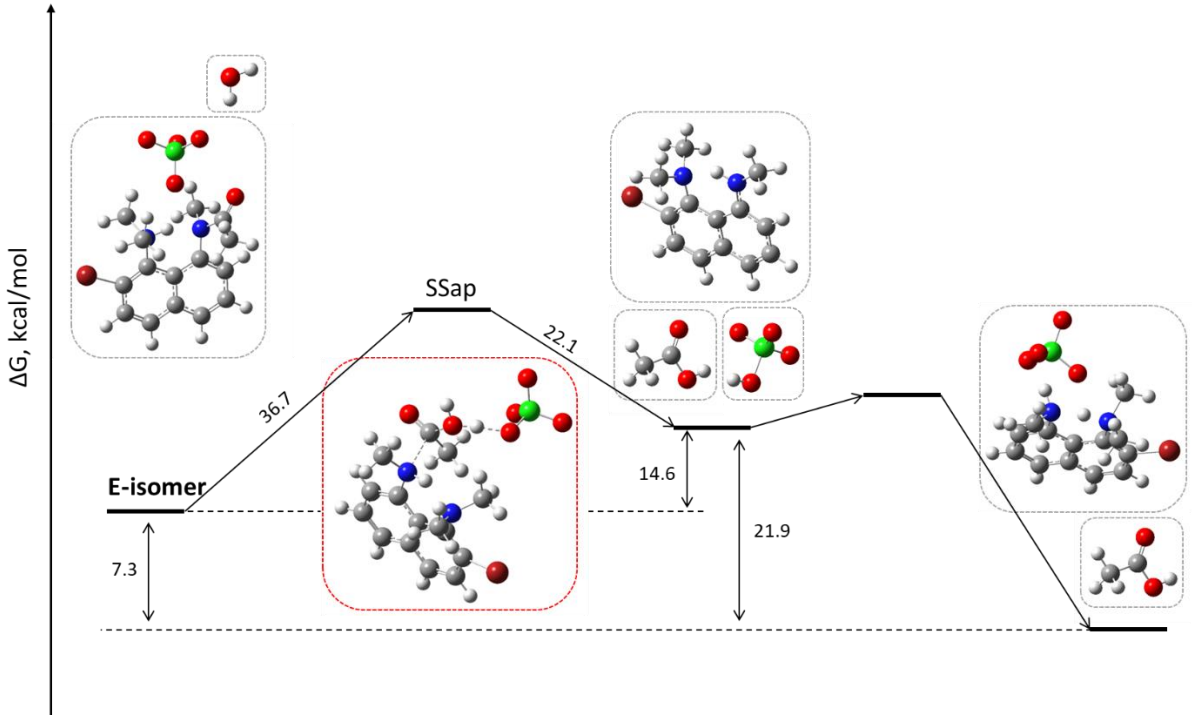

Figure 16. Energy profile for $ClO4^-$ assisted reaction of cation **12**H^+ with H_2O molecule in acetonitrile (PCM).

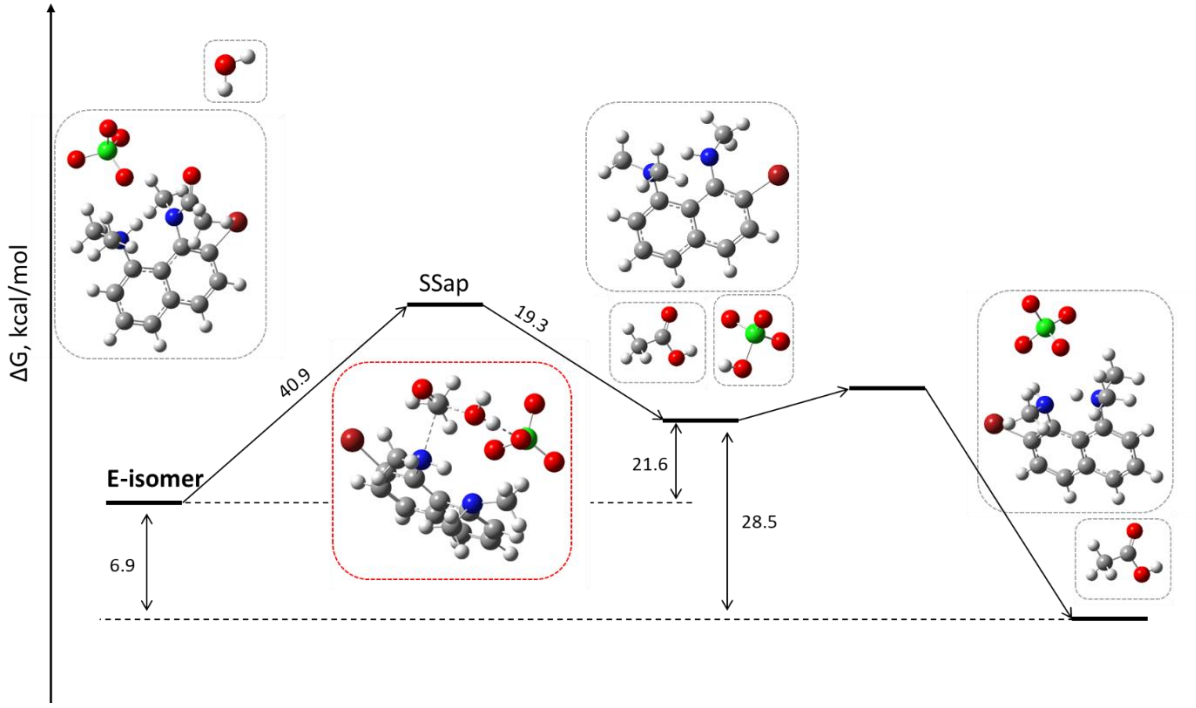

Figure 17. Energy profile for $ClO4^-$ assisted reaction of cation **19**H^+ with H_2O molecule in acetonitrile (PCM).

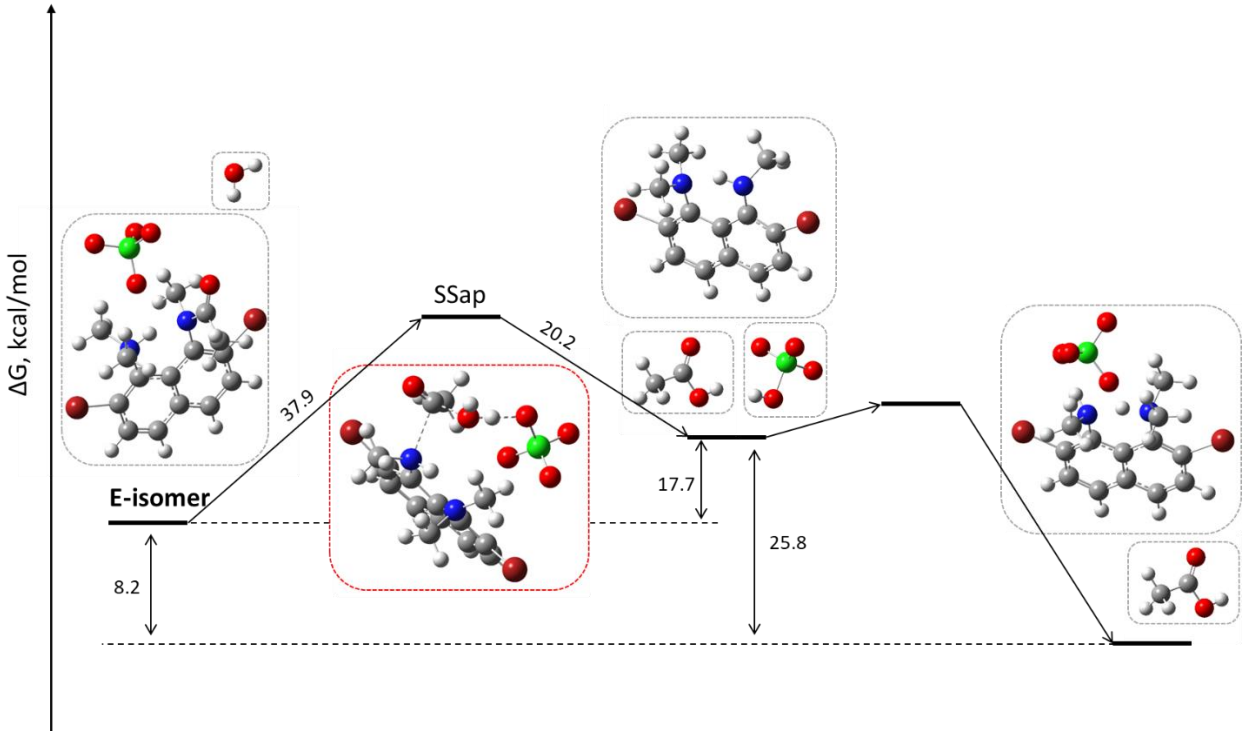

Figure 18. Energy profile for $ClO4^-$ assisted reaction of cation **25**H^+ with H_2O molecule in acetonitrile (PCM).

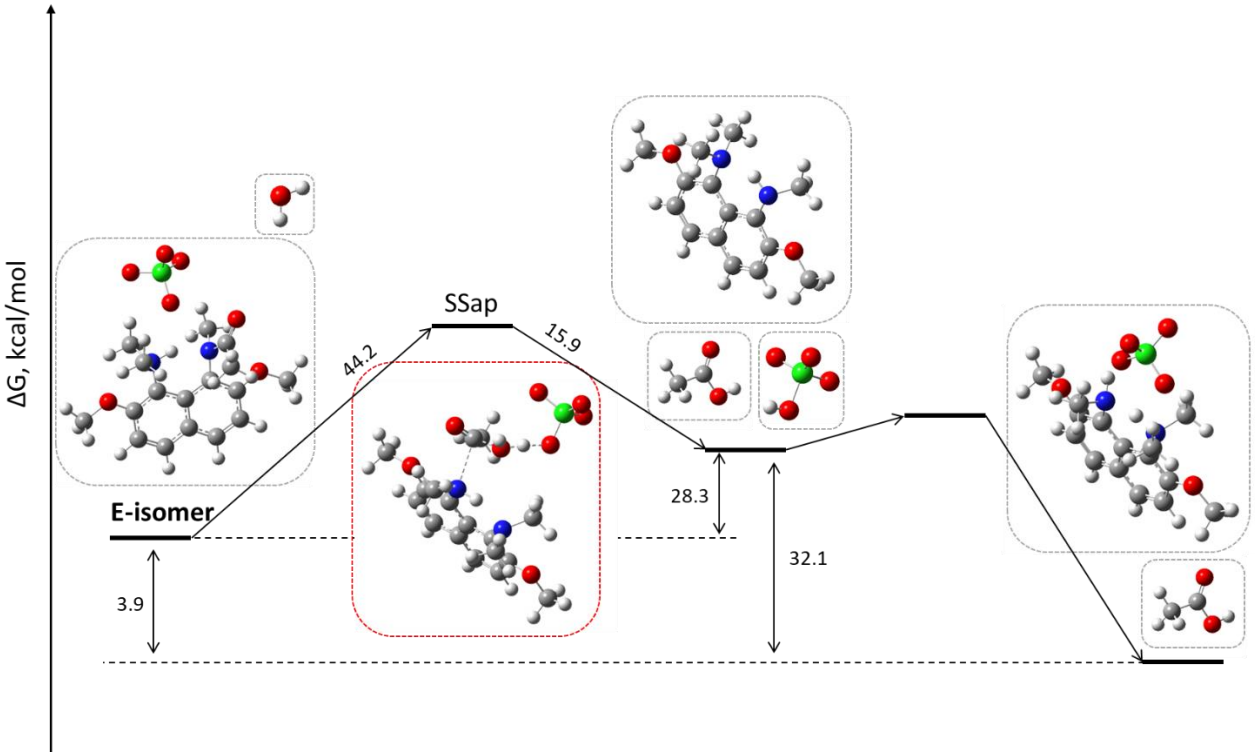

Figure 19. Energy profile for $ClO4^-$ assisted reaction of cation **29**H^+ with H_2O molecule in acetonitrile (PCM).

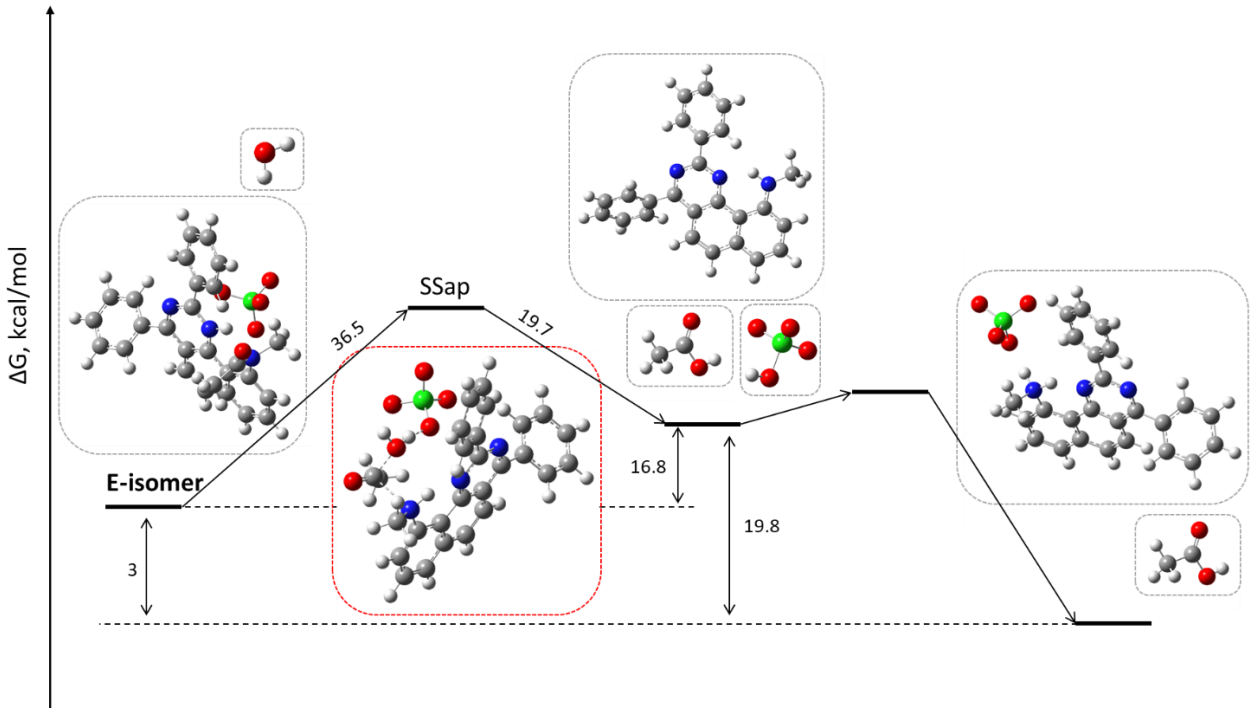

Figure 20. Energy profile for $ClO4^-$ assisted reaction of cation **35**H^+ with H_2O molecule in acetonitrile (PCM).

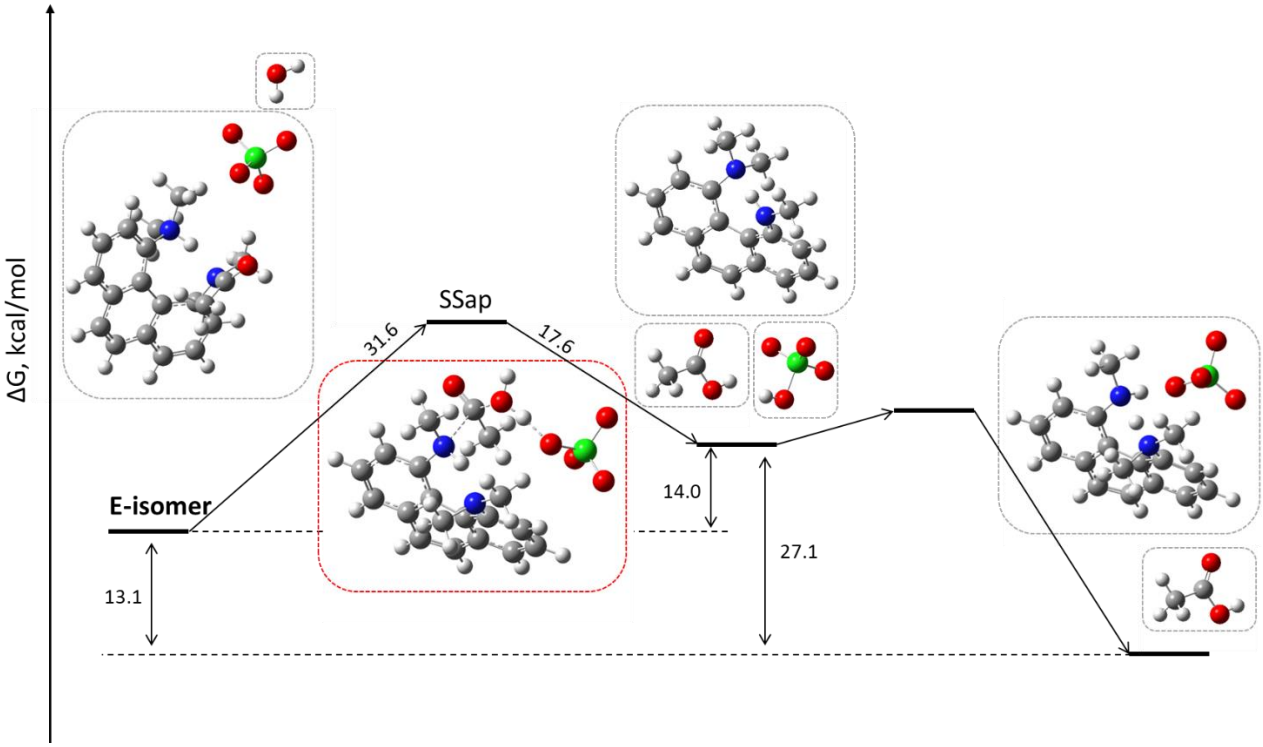

Figure 21. Energy profile for $ClO4^-$ assisted reaction of cation **38**H^+ with H_2O molecule in acetonitrile (PCM).

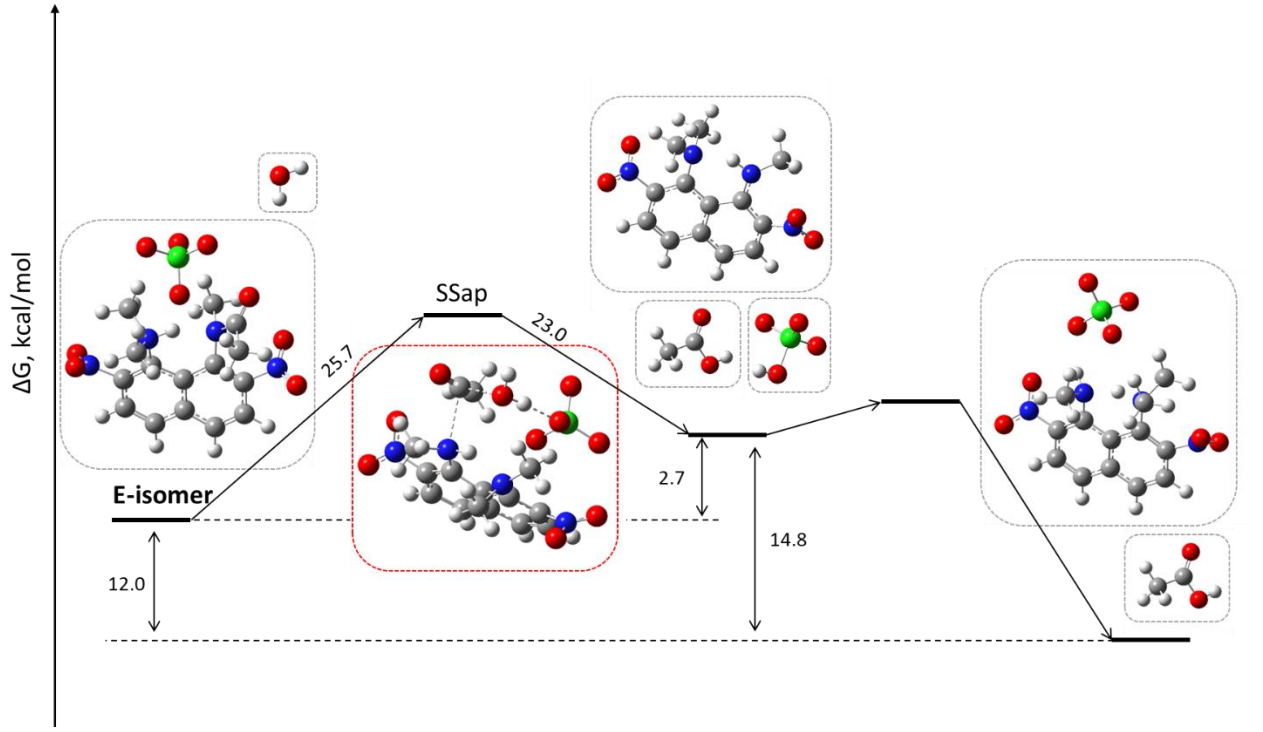

Figure 22. Energy profile for $ClO4^-$ assisted reaction of cation **26**H^+ with H_2O molecule in acetonitrile (PCM).

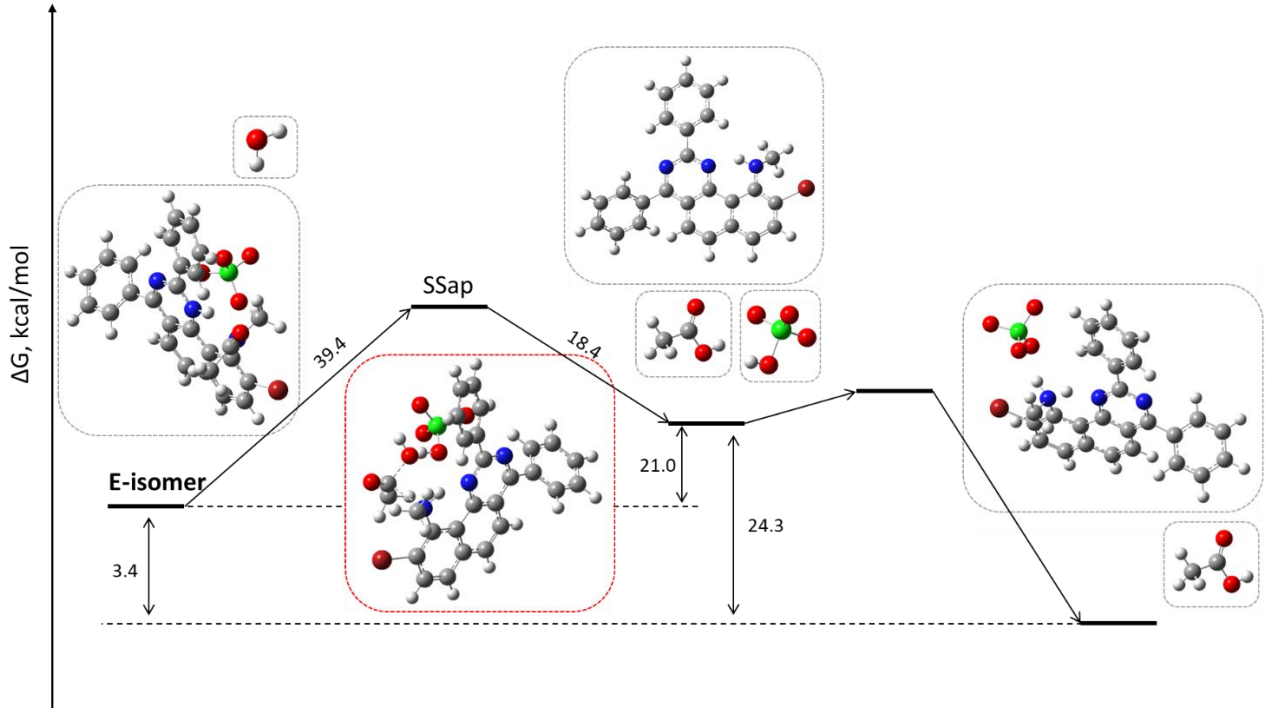

Figure 23. Energy profile for $ClO4^-$ assisted reaction of cation **36**H^+ with H_2O molecule in acetonitrile (PCM).

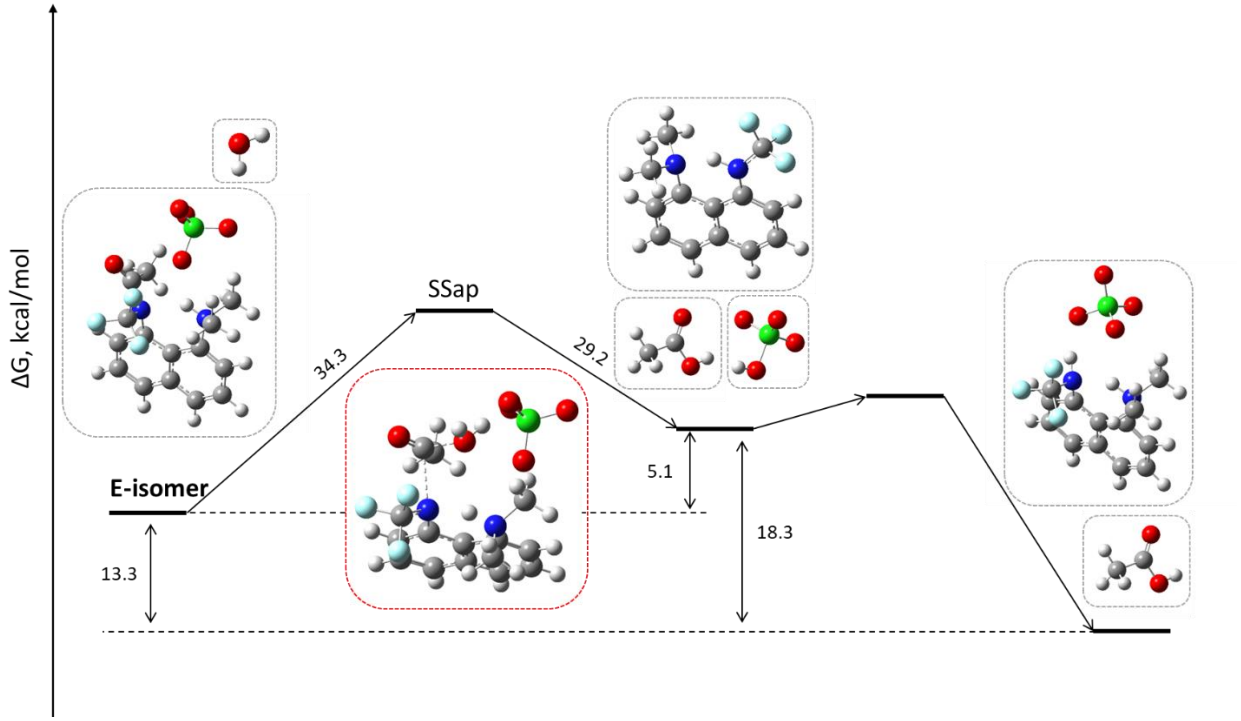

Figure 24. Energy profile for $ClO4^-$ assisted reaction of cation **41**H^+ with H_2O molecule in acetonitrile (PCM).