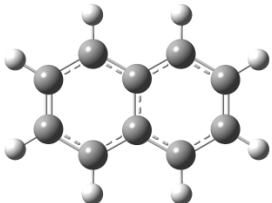


Structure, coordinates and energies of various species under investigation.

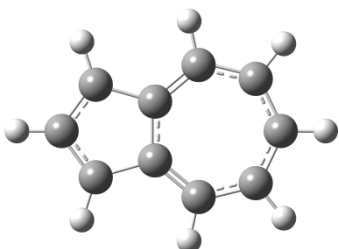
Supplementary material for "Fragmentation of multiply charged  $C_{10}H_8$  isomers produced in keV range proton collision" by Vinitha M. V. *et al.*

I.  $C_{10}H_8$  parent di and trication isomers (coordinates in a.u. and energies in hartree):

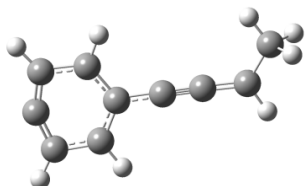
1) Naphthalene dication:

	C	-5.3974	-0.04555	0.000337	Energy: -385.132119
	C	-3.95737	-0.03335	0.000137	
	C	-3.24324	1.183423	0.000241	
	C	-3.96716	2.419757	0.000511	
	C	-5.3777	2.39242	0.000684	
	C	-6.09304	1.14251	0.000608	
	H	-1.26824	0.279451	-0.00014	
	H	-5.91913	-0.99894	0.000259	
	H	-3.42137	-0.98133	-5.9E-05	
	C	-1.83271	1.21076	0.000078	
	C	-3.25303	3.63653	0.000603	
	H	-5.94217	3.323729	0.000916	
	H	-7.17979	1.154096	0.000751	
	C	-1.81301	3.648736	0.000414	
	C	-1.11737	2.460672	0.000144	
	H	-3.78904	4.58451	0.000824	
	H	-1.29128	4.602121	0.000496	
	H	-0.03062	2.449089	-0.00001	

2) Azulene dication:

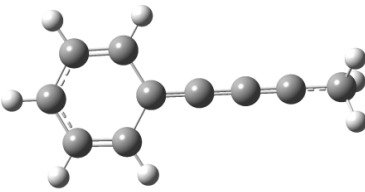
	C	3.393954	-4.66344	0.000257	Energy: -385.117838
	C	4.795856	-4.65366	-0.00034	
	C	5.690108	-3.54391	-0.00034	
	C	2.509076	-3.57634	0.001055	
	C	5.337811	-2.21045	0.000315	
	C	2.795992	-2.18006	0.001489	
	C	4.048648	-1.60286	0.001142	
	H	2.930414	-5.64776	0.000081	
	H	5.274099	-5.63194	-0.0009	
	H	6.750721	-3.78887	-0.00092	
	H	1.45006	-3.82975	0.001413	
	H	1.931799	-1.51817	0.002149	
	C	6.321845	-1.0841	0.000281	
	H	7.401765	-1.22307	-0.00025	
	C	5.65871	0.141558	0.001069	
	H	6.121125	1.122521	0.001245	
	C	4.291046	-0.1271	0.001588	
	H	3.49656	0.617441	0.002263	

3) Table S1a: Structure A dication:

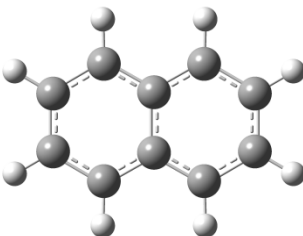
	C	1.220908	1.230404	-0.0237	Energy: -385.019151
	C	0.635173	-0.06166	-0.01466	
	C	1.444424	-1.22712	-0.01571	
	C	2.86808	-1.14444	-0.02576	
	C	3.110237	0.162534	-0.03258	
	C	2.635899	1.404569	-0.03424	
	H	0.618642	2.136964	-0.0231	
	H	1.015167	-2.22742	-0.00886	
	H	3.54311	-1.99785	-0.02707	
	H	3.147185	2.364998	-0.0416	

	C	-0.77317	-0.19343	-0.00448	
	C	-1.9987	-0.31476	0.00451	
	C	-3.3554	-0.48718	0.014591	
	H	-3.71453	-1.52115	0.021195	
	C	-4.35202	0.57805	0.017341	
	H	-5.03527	0.414469	-0.83905	
	H	-3.94891	1.589759	0.010319	
	H	-5.0227	0.421556	0.884953	

4) Table S1b: Structure B dication:

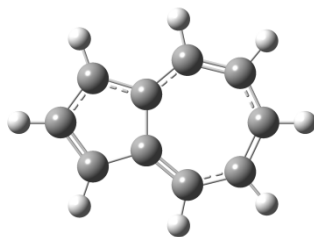
	C	1.520733	-0.46004	-0.66175	Energy: -385.060797
	C	0.51484	-1.31065	-0.02629	
	C	0.885278	-2.60247	0.551018	
	C	2.196875	-2.99431	0.482111	
	C	3.159285	-2.15764	-0.13685	
	C	2.817066	-0.90353	-0.70191	
	H	1.22708	0.494956	-1.0843	
	H	0.125025	-3.21976	1.017701	
	H	2.499969	-3.94869	0.903011	
	H	3.584558	-0.29218	-1.16791	
	C	-0.7546	-0.90294	0.028155	
	C	-1.98029	-0.5081	0.081345	
	C	-3.17458	-0.12005	0.134384	
	C	-4.51506	0.306902	0.188192	
	H	-4.70571	0.9851	1.035097	
	H	-4.79695	0.791647	-0.76781	
	H	-5.17162	-0.58508	0.277118	
	H	4.194565	-2.4888	-0.17938	

5) Naphthalene trication:

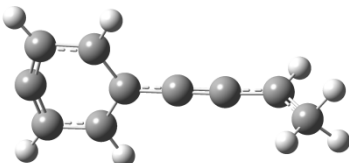
	C	-6.05914	-0.53835	0.000325	Energy: -384.441350
	C	-4.61326	-0.5364	0.000144	
	C	-3.90151	0.686997	0.00024	
	C	-4.65097	1.966927	0.000524	
	C	-6.06616	1.94488	0.000698	
	C	-6.7754	0.684886	0.000607	
	H	-1.91131	-0.2202	-0.00014	
	H	-6.59723	-1.48987	0.000234	
	H	-4.08425	-1.49256	-4.9E-05	
	C	-2.4863	0.709043	0.000066	
	C	-3.93921	3.190319	0.000621	
	H	-6.64117	2.874112	0.00093	
	H	-7.86853	0.681261	0.000744	
	C	-2.49333	3.192259	0.000413	
	C	-1.77707	1.969024	0.000134	
	H	-4.46822	4.146485	0.000842	
	H	-1.95524	4.143785	0.00048	
	H	-0.68394	1.972653	-2.4E-05	

6) Azulene trication:

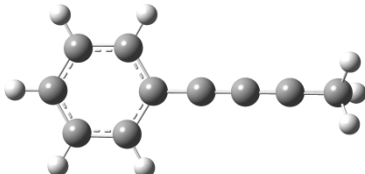
	C	3.394514	-4.66233	0.0002	
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	C	4.823014	-4.66323	-0.00031	Energy: - 384.430155
	C	5.722622	-3.55732	-0.00035	
	C	2.484547	-3.56145	0.001053	
	C	5.367459	-2.20172	0.000296	
	C	2.765021	-2.16363	0.001552	
	C	4.036611	-1.57459	0.001183	
	H	2.928734	-5.65137	-0.00007	
	H	5.289836	-5.65193	-0.00079	
	H	6.78636	-3.80505	-0.00092	
	H	1.424785	-3.83042	0.001389	
	H	1.896858	-1.50091	0.002247	
	C	6.343435	-1.11474	0.000244	
	H	7.430456	-1.23769	-0.00032	
	C	5.659752	0.144191	0.001042	
	H	6.125372	1.132141	0.001174	
	C	4.253548	-0.12996	0.001629	
	H	3.466666	0.630009	0.002333	

7) Table S1c: Structure A trication:

	C	1.36369	1.243737	0.43447	Energy: - 384.360372
	C	0.645453	0.030108	0.074214	
	C	1.355349	-1.14871	-0.4001	
	C	2.765632	-1.1377	-0.52167	
	C	3.118409	0.090797	-0.12442	
	C	2.77413	1.302038	0.32924	
	H	0.849477	2.137534	0.793573	
	H	0.834822	-2.06875	-0.67364	
	H	3.377621	-1.97904	-0.86899	
	H	3.392068	2.173041	0.5793	
	C	-0.73984	-0.00702	0.194607	
	C	-1.98512	-0.04154	0.306511	
	C	-3.36737	-0.10673	0.507374	
	H	-3.66799	-0.45573	1.511106	
	C	-4.38835	0.227734	-0.43999	
	H	-5.10603	-0.63837	-0.48037	
	H	-4.08387	0.571047	-1.42799	
	H	-5.09997	0.93585	0.06888	

8) Table S1d: Structure B trication:

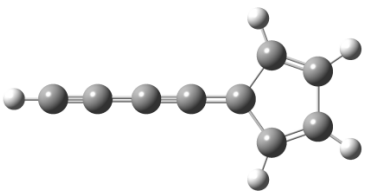
	C	1.504019	-0.48621	-0.64982
	C	0.495426	-1.30605	-0.02649
	C	0.886802	-2.57262	0.539901
	C	2.262888	-2.99177	0.474098
	C	3.239767	-2.18164	-0.13801
	C	2.869353	-0.94197	-0.69593
	H	1.249421	0.478382	-1.08896
	H	0.154625	-3.22184	1.020017
	H	2.532668	-3.95473	0.910624
	H	3.613011	-0.30281	-1.17454
	C	-0.81406	-0.88728	0.027802
	C	-2.02153	-0.49975	0.079209
	C	-3.24044	-0.10484	0.134483
	C	-4.55177	0.318039	0.192621
	H	-4.75771	0.968981	1.073226
	H	-4.83395	0.855141	-0.75274
	H	-5.23967	-0.572	0.226435

Energy: -384.399503

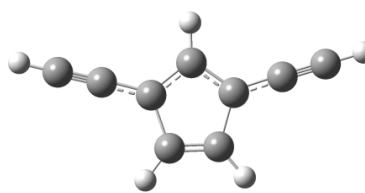
	H	4.277626	-2.51265	-0.18	
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II. C<sub>9</sub>H<sub>5</sub> mono and di-cation isomers (coordinates in a.u. and energies in hartree):

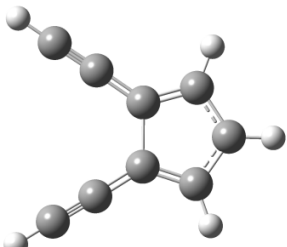
1) Table S2a: structure A monocation:

	C	1.57314	-1.20183	0.000064	Energy: -345.518991
	H	1.202599	-2.22335	0.000095	
	C	2.84981	-0.76153	0.000078	
	H	3.751998	-1.37322	0.000122	
	C	1.573056	1.201852	0.000095	
	H	1.202445	2.223345	0.000154	
	C	2.849757	0.761644	0.000097	
	H	3.751903	1.373394	0.000162	
	C	0.719268	-1.8E-05	-0.0001	
	C	-0.64502	-6.7E-05	-6.2E-05	
	C	-1.88878	-8.8E-05	-3.2E-05	
	C	-3.23233	-5.1E-05	0.000084	
	C	-4.45841	0.000005	0.000186	
	H	-5.5373	0.000087	0.000311	

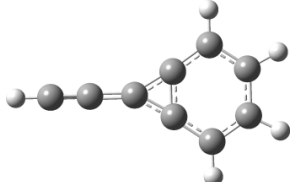
2) Table S2b: structure B monocation:

	C	0.000005	-0.84652	0.000142	Energy: -345.511259
	C	1.123878	-0.00633	0.000078	
	C	0.668826	1.441741	-0.00022	
	H	1.351532	2.288526	-0.00038	
	C	-1.12388	-0.00634	0.000068	
	C	-0.66884	1.441735	-0.0002	
	H	-1.35155	2.288513	-0.00036	
	C	-2.45617	-0.39343	0.000103	
	C	-3.64058	-0.70259	0.000129	
	H	-4.68197	-0.9839	0.000141	
	C	2.456177	-0.39341	0.000095	
	C	3.640592	-0.70255	0.000103	
	H	4.681984	-0.98384	0.000101	
	H	0.00001	-1.93267	0.000264	

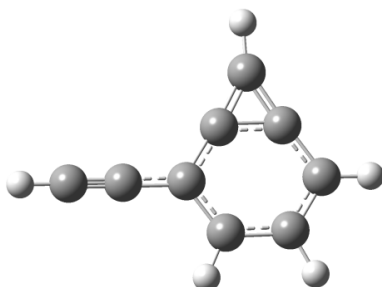
3) Table S2c: structure C monocation:

	C	2.317386	-1.7E-05	-0.0001	Energy: -345.503234
	C	1.519074	1.1849	-0.00017	
	H	1.889934	2.206634	-0.00024	
	C	1.519083	-1.18494	0.000005	
	H	1.889952	-2.20667	0.000049	
	C	0.202072	-0.79133	0.000142	
	C	0.202066	0.791278	-0.00021	
	C	-0.95699	1.550515	-0.00023	
	C	-1.99463	2.199575	-0.00022	
	H	-2.90055	2.783918	0.000013	
	C	-0.95698	-1.55057	0.000226	
	C	-1.99463	-2.19961	0.000272	
	H	-2.90072	-2.7837	0.000645	
	H	3.410351	-1.3E-05	-0.00015	

4) Table S2d: structure D monocation:

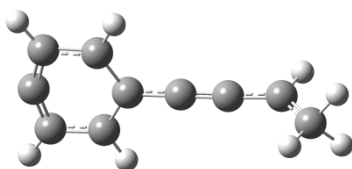
	C	2.31433	-0.72312	-2.6E-05	Energy: - 345.552081
	C	2.314333	0.7231	-4.1E-05	
	C	1.162447	1.496036	-4.2E-05	
	C	0.003625	0.700253	-4.8E-05	
	C	0.003622	-0.70026	-3.2E-05	
	C	1.162441	-1.49605	-9E-06	
	H	3.287094	-1.22113	-0.00002	
	H	3.287099	1.221106	-4.4E-05	
	H	1.171725	2.585818	-4.4E-05	
	H	1.171713	-2.58583	0.000014	
	C	-1.19753	0	-7.5E-05	
	C	-2.58312	0	0.000009	
	C	-3.80014	0.000005	0.000084	
	H	-4.87847	-1.1E-05	0.000115	

5) Table S2e: structure E monocation:

	C	1.349993	-1.51414	-0.00013
	C	-0.08478	-1.38795	-0.00011
	C	-0.76896	-0.16475	-1.8E-05
	C	1.554179	0.78385	0.000119
	C	2.235688	-0.44233	-4.3E-05
	H	1.751762	-2.53085	-0.00024
	H	-0.67147	-2.30909	-0.00021
	H	3.31922	-0.55757	-8.2E-05
	C	-2.17656	-0.02215	-2.3E-05
	H	-4.45483	0.221888	-0.0001
	C	0.149915	0.919437	0.000134
	C	0.955878	2.025092	0.000331
	C	-3.38428	0.10936	-2.9E-05
	H	1.052977	3.113982	0.00027

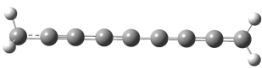
Energy: -345.542245

6) Table S2f: structure F monocation:

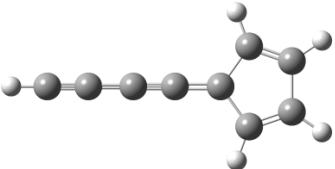
	C	-0.24381	1.285262	-6.7E-05	Energy: - 345.544013
	C	-0.84587	-0.05551	-0.00022	
	C	-0.07086	-1.22463	-0.00026	
	C	1.868341	0.340272	-3.5E-05	
	C	1.112205	1.531955	-2E-06	
	H	-0.94292	2.124659	0.000103	
	H	1.533792	2.537454	0.000086	
	C	1.299414	-0.95222	-0.00016	
	C	2.666548	-0.77118	0.000095	
	H	3.669485	-1.20516	0.000448	
	H	-0.51393	-2.21982	-0.00036	
	C	-3.476	-0.17056	0.000141	
	H	-4.55182	-0.21564	0.000265	
	C	-2.2611	-0.12639	-2.3E-05	

7) Table S2g: structure G monocation:

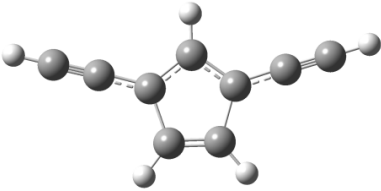
	C	-5.16535	-0.00712	-3.9E-05	Energy: - 345.495600
	H	-5.56179	-0.50477	-0.90071	
	H	-5.56192	-0.5018	0.902199	
	H	-5.52363	1.03883	-0.00186	
	C	-3.72622	-0.01187	-1.5E-05	
	C	-2.49141	-0.00833	-3.5E-05	

	C	-1.15966	-0.00615	-2.1E-05	
	C	0.093094	-0.00422	0.000068	
	C	1.404486	-0.0022	0.000132	
	C	2.670967	-0.00015	-5E-06	
	C	3.967233	0.001864	-8.6E-05	
	C	5.273575	0.003737	-0.00017	
	H	5.83706	-0.93763	-0.00017	
	H	5.834353	0.94672	-0.00017	

8) Table S2h: structure A dication:

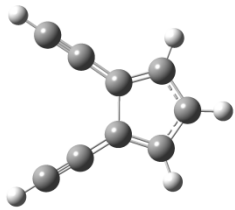
	C	1.566494	-1.18177	0.000107	Energy: - 345.045920
	H	1.232955	-2.22217	0.000136	
	C	2.893055	-0.71946	0.000025	
	H	3.785305	-1.35193	-2.9E-05	
	C	1.566164	1.181644	0.000076	
	H	1.232335	2.221957	0.000079	
	C	2.892855	0.719713	0.000007	
	H	3.784929	1.352425	-6.3E-05	
	C	0.681179	-0.00019	0.000177	
	C	-0.66726	-0.00038	0.000248	
	C	-1.92794	-0.00041	0.000309	
	C	-3.254	-6.3E-05	0.000189	
	C	-4.49303	0.000246	0.000073	
	H	-5.5809	0.000545	-8.3E-05	

9) Table S2i: structure B dication:

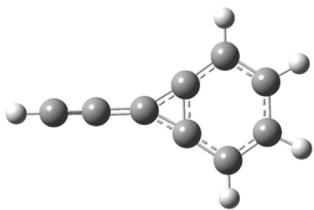
	C	-2E-06	-0.82321	0.000008	Energy: - 345.029230
	C	1.162157	0.033904	0.000002	
	C	0.690743	1.431434	0.000019	
	H	1.343629	2.307757	0.000024	
	C	-1.16216	0.033906	0.000014	
	C	-0.69074	1.431435	0.000016	
	H	-1.34363	2.30776	0.000022	
	C	-2.47292	-0.37413	0.000013	
	C	-3.65512	-0.72933	0.000011	
	H	-4.69629	-1.04412	0.000062	
	C	2.472914	-0.37414	0.000005	
	C	3.655116	-0.72933	0.000008	
	H	4.696287	-1.04411	0.000032	
	H	-3E-06	-1.91526	0.000005	

10) Table S2j: structure C dication:

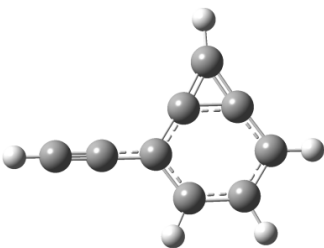
	C	-2.315491	-0.000336	0.000437	Energy: - 345.026773
	C	-1.502083	1.170233	0.000351	
	H	-1.857357	2.203059	0.00034	
	C	-1.501731	-1.170665	0.000365	
	H	-1.856699	-2.203596	0.000381	

	C	-0.13956	-0.76787	0.000177	
	C	-0.13979	0.767845	0.000378	
	C	0.968498	1.570416	0.000209	
	C	1.951272	2.32011	0.000073	
	H	2.812379	2.984894	-0.000066	
	C	0.96897	-1.570108	0.000082	
	C	1.951965	-2.319512	-0.000009	
	H	2.813263	-2.984048	-0.000064	
	H	-3.410007	-0.000501	0.000501	

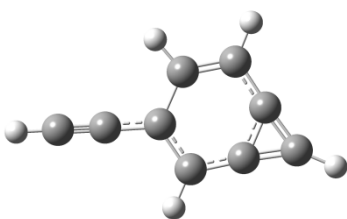
11) Table S2k: structure D dication:

	C	-2.36614	0.706635	0.000002	Energy: - 345.027791
	C	-2.36622	-0.70655	-1.4E-05	
	C	-1.17015	-1.48959	-2.9E-05	
	C	0.029237	-0.68105	-2.6E-05	
	C	0.02932	0.680839	-1.1E-05	
	C	-1.16996	1.489528	0.000004	
	H	-3.32833	1.230417	0.000013	
	H	-3.32848	-1.23022	-1.4E-05	
	H	-1.17943	-2.58522	-0.00004	
	H	-1.17911	2.58516	0.000018	
	C	1.265522	-0.00018	-3.9E-05	
	C	2.627305	-0.00027	-2.5E-05	
	C	3.853395	-0.00031	-8E-06	
	H	4.93962	0.00084	0.000261	

12) Table S2l: structure E dication:

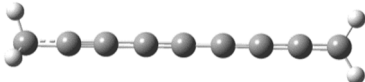
	C	-1.35914	-1.51922	0.000215	Energy: - 345.045245
	C	0.070845	-1.39685	0.000135	
	C	0.766874	-0.14664	-0.00013	
	C	-1.52242	0.822283	-0.00015	
	C	-2.22561	-0.42731	0.000041	
	H	-1.77507	-2.5318	0.000391	
	H	0.663134	-2.31813	0.000252	
	H	-3.31536	-0.52095	0.000062	
	C	2.150851	-0.0445	-0.00026	
	H	4.476134	0.121876	0.000661	
	C	-0.14447	0.968833	-0.00022	
	C	-0.95919	2.081283	0.000058	
	C	3.390203	0.045285	-0.00035	
	H	-1.06924	3.173456	-0.00034	

13) Table S2m: structure F dication:

	C	-0.2488	1.328084	0.000084	Energy: - 345.003401
	C	-0.84366	-0.01921	0.000031	
	C	-0.0679	-1.22573	-1.3E-05	
	C	1.859226	0.345635	0.000063	
	C	1.110086	1.55773	0.000094	
	H	-0.9432	2.17317	0.000116	
	H	1.549241	2.558212	0.000125	
	C	1.329037	-0.9397	0.000017	
	C	2.692627	-0.76652	0.000045	
	H	3.702953	-1.1971	0.000067	
	H	-0.51352	-2.22497	-7.2E-05	

	C	-3.47464	-0.25709	0.000027	
	H	-4.55954	-0.35584	0.000025	
	C	-2.23666	-0.14444	0.000029	

14) Table S2n: structure G dication:

	C	5.161271	0.006982	-0.00029	Energy: - 345.038617
	H	5.54622	0.527377	-0.90317	
	H	5.546375	0.526428	0.903071	
	H	5.541417	-1.03677	-0.00087	
	C	3.748328	0.006654	-0.0002	
	C	2.489683	0.005874	-0.00025	
	C	1.187592	0.004799	-0.00023	
	C	-0.09335	0.003549	-5.4E-05	
	C	-1.37752	0.00212	0.000081	
	C	-2.67041	0.000601	-0.00015	
	C	-3.94809	-0.00086	-0.00033	
	C	-5.27559	-0.00238	-0.00052	
	H	-5.84043	0.944744	-0.00174	
	H	-5.83824	-0.95081	0.000545	