Topology of Electrostatic Potential and Electron Density Reveals Covalent to Non-Covalent Carbon-Carbon Bond Continuum

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Supporting Information

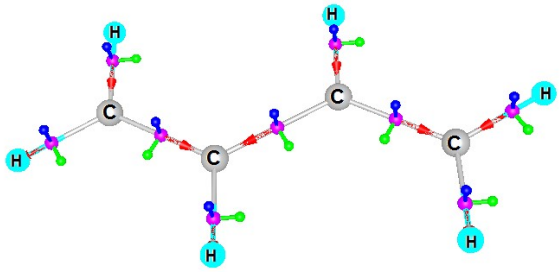

Figure S1. Distribution of (3, -1) BCPs with the directions of corresponding eigenvectors for the 1, 3-butadiene molecule. The red, blue and green arrows represent eigenvector corresponding to λ_{v1}, λ_{v2} and λ_{v3} respectively.

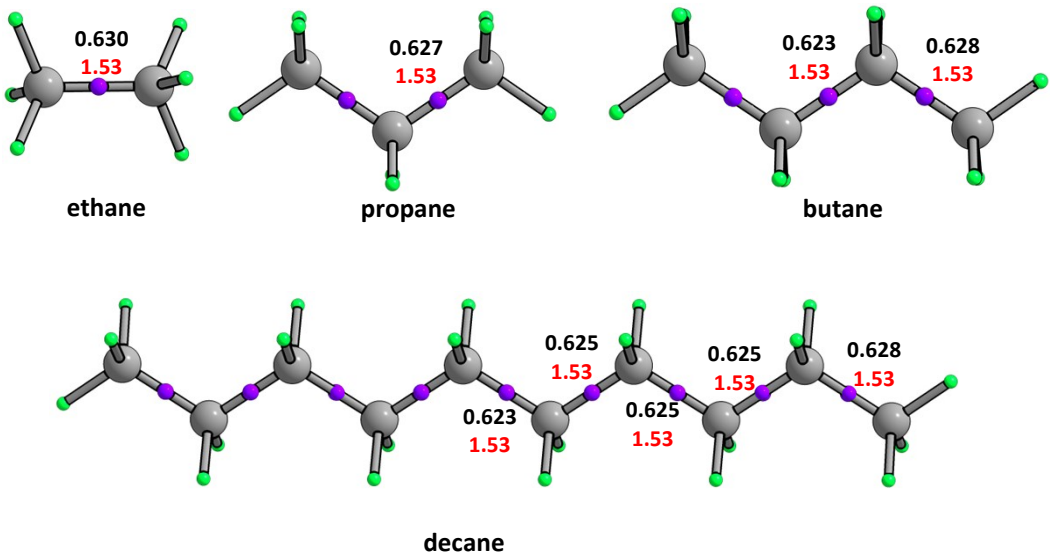

Figure S2. The MESP (3, -1) CP distribution of CC bonds in alkanes. The MESP value at the CP (in au) and bond length (in Å) are represented in black and red fonts, respectively.

Table S1. The CC bond distance (Å) and the MESP data V_{bnp}, V_ρ, $V(r)$ and eigenvalues (in au) of alkanes.

system	d_{CC}	V_{bnp}	V_ρ	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}	λ'_{v1}
ethane	1.53	10.376	-9.746	0.630	5.174	-1.094	-1.094	-12.100
propane	1.53	12.302	-11.675	0.627	5.177	-1.089	-1.077	-12.096
	1.53	12.302	-11.675	0.627	5.177	-1.089	-1.077	-12.096
butane	1.53	13.538	-12.910	0.628	5.183	-1.091	-1.080	-12.111
	1.53	13.538	-12.910	0.628	5.183	-1.091	-1.080	-12.111
	1.53	14.216	-13.594	0.623	5.175	-1.081	-1.058	-12.082
decane	1.53	17.061	-16.434	0.628	5.180	-1.091	-1.080	-12.105
	1.53	17.061	-16.434	0.628	5.180	-1.091	-1.080	-12.105

	1.53	19.389	-18.764	0.625	5.184	-1.086	-1.065	-12.105
	1.53	19.389	-18.764	0.625	5.184	-1.086	-1.065	-12.105
	1.53	19.793	-19.168	0.625	5.182	-1.085	-1.065	-12.100
	1.53	19.793	-19.168	0.625	5.181	-1.085	-1.065	-12.100
	1.53	19.918	-19.293	0.625	5.181	-1.085	-1.065	-12.100
	1.53	18.588	-17.965	0.623	5.178	-1.083	-1.062	-12.091
	1.53	18.588	-17.965	0.623	5.178	-1.083	-1.062	-12.091

Cycloalkanes

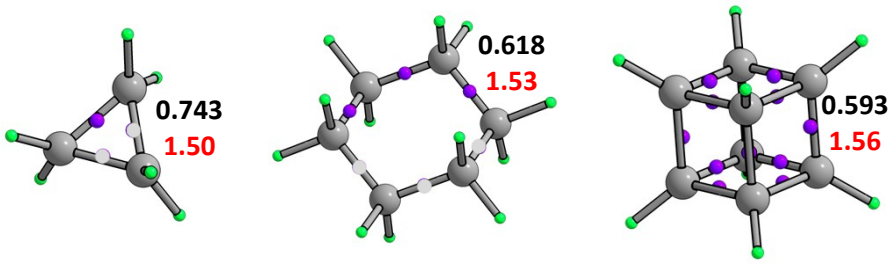

Figure S3. The MESP (3, -1) CP distribution of CC bonds in cycloalkanes. The MESP value at the CP (in au) and bond length (in Å) are represented in black and red fonts, respectively.

Table S2. The CC bond distance (Å) and the MESP data V_{bnp}, V_{ρ}, $V(r)$ and eigenvalues (in au) of cycloalkanes.

system	d_{CC}	V_{bnp}	V_{ρ}	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}	λ'_{v1}
cyclopropane	1.50	12.837	-12.093	0.743	5.311	-1.221	-1.172	-12.820
cyclobutane	1.55	14.205	-13.596	0.609	4.878	-1.013	-0.986	-11.567
cyclohexane	1.53	16.826	-16.208	0.618	5.130	-1.066	-1.052	-11.989
adamentane	1.54	22.306	-21.698	0.608	5.058	-1.034	-1.029	-11.828
cubane	1.56	20.022	-19.429	0.593	4.643	-0.949	-0.902	-11.153

Sterically crowded C-C bonds

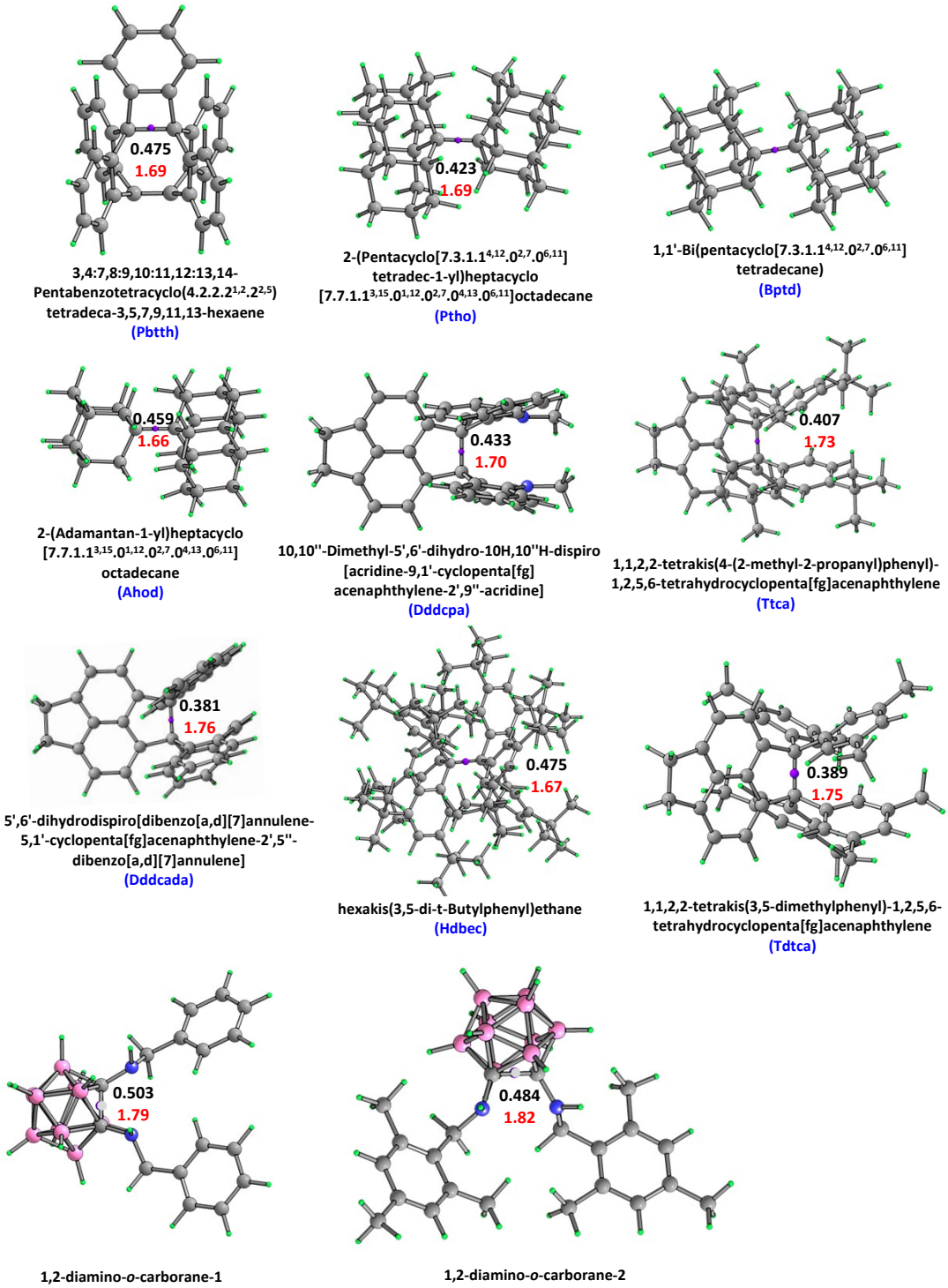

Figure S4. The MESP (3, -1) CP distribution of C-C bonds in sterically crowded systems. The MESP value at the CP (in au) and bond length (in Å) are represented in black and red fonts, respectively.

Table S3. The CC bond distance (Å) and the MESP data V_{bnp}, V_p, $V(r)$ and eigenvalues (in au) of sterically crowded systems.

system	d_{CC}	V_{bnp}	V_p	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}	λ'_{v1}
Pbtth	1.69	43.655	-43.180	0.475	3.428	-0.664	-0.613	-8.351
Ptho	1.69	43.655	-43.180	0.475	3.428	-0.664	-0.613	-8.351
Bptd	1.65	41.323	-40.857	0.467	3.889	-0.740	-0.736	-9.172
Ahod	1.66	41.302	-40.843	0.459	3.836	-0.726	-0.721	-9.042
Dddcpa	1.70	50.370	-49.937	0.433	3.407	-0.628	-0.605	-8.112
Ttca	1.73	55.861	-55.454	0.407	3.194	-0.573	-0.559	-7.588
Dddcada	1.76	49.381	-49.000	0.381	2.980	-0.517	-0.511	-7.081
Hdbec	1.67	80.666	-80.191	0.475	3.709	-0.700	-0.700	-8.735
Tdtca	1.75	52.219	-51.831	0.389	3.061	-0.543	-0.529	-7.275
1,2-diamino-o-carborane-1	1.79	35.917	-35.415	0.503	2.693	-0.501	-0.455	-6.626
1,2-diamino-o-carborane-2	1.82	40.123	-39.649	0.474	2.536	-0.464	-0.405	-6.265

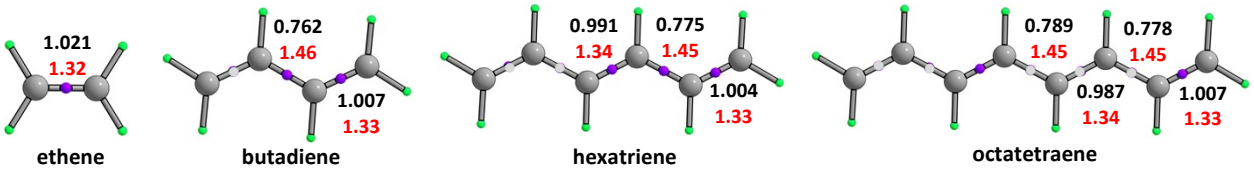

Figure S5. The MESP (3, -1) CP distribution of alkenes. The MESP value at the CP (in au) and bond length (in Å) are represented in black and red fonts, respectively.

Table S4. The CC bond distance (Å) and the MESP data V_{bnp}, V_p, $V(r)$ and eigenvalues (in au) of alkenes.

system	d_{CC}	V_{bnp}	V_p	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}	λ'_{v1}
ethene	1.32	10.966	-9.946	1.021	8.637	-2.256	-2.060	-19.170
butadiene	1.33	13.780	-12.773	1.007	8.470	-2.194	-1.996	-18.842
	1.33	13.780	-12.773	1.007	8.470	-2.194	-1.996	-18.842
	1.46	13.664	-12.902	0.762	6.098	-1.356	-1.320	-14.066
hexatriene	1.33	15.230	-14.227	1.004	8.431	-2.181	-1.985	-18.768
	1.33	15.230	-14.227	1.004	8.431	-2.181	-1.985	-18.768
	1.34	16.586	-15.595	0.991	8.275	-2.121	-1.926	-18.461
	1.45	15.629	-14.855	0.775	6.190	-1.390	-1.345	-14.261
	1.45	15.629	-14.855	0.775	6.190	-1.390	-1.345	-14.261
octatetraene	1.33	16.209	-15.207	1.003	8.418	-2.176	-1.982	-18.742
	1.33	16.209	-15.207	1.003	8.418	-2.176	-1.982	-18.742
	1.34	18.035	-17.048	0.987	8.225	-2.104	-1.912	-18.363
	1.34	18.035	-17.048	0.987	8.225	-2.104	-1.912	-18.363
	1.45	17.604	-16.815	0.789	6.301	-1.431	-1.376	-14.495
	1.45	16.813	-16.035	0.778	6.214	-1.399	-1.352	-14.312
	1.45	16.813	-16.035	0.778	6.214	-1.399	-1.352	-14.312
decapentaene	1.33	16.948	-15.946	1.002	8.412	-2.174	-1.980	-18.732

	1.33	16.948	-15.946	1.002	8.412	-2.174	-1.980	-18.732
	1.34	19.013	-18.028	0.985	8.206	-2.097	-1.907	-18.327
	1.34	19.013	-18.028	0.985	8.206	-2.097	-1.907	-18.327
	1.35	19.484	-18.501	0.982	8.169	-2.084	-1.896	-18.254
	1.45	18.791	-17.998	0.793	6.333	-1.442	-1.385	-14.563
	1.45	18.791	-17.998	0.793	6.333	-1.442	-1.385	-14.563
	1.45	17.661	-16.882	0.779	6.223	-1.402	-1.354	-14.330
	1.45	17.661	-16.882	0.779	6.223	-1.402	-1.354	-14.330

Polycyclic benzenoid hydrocarbons

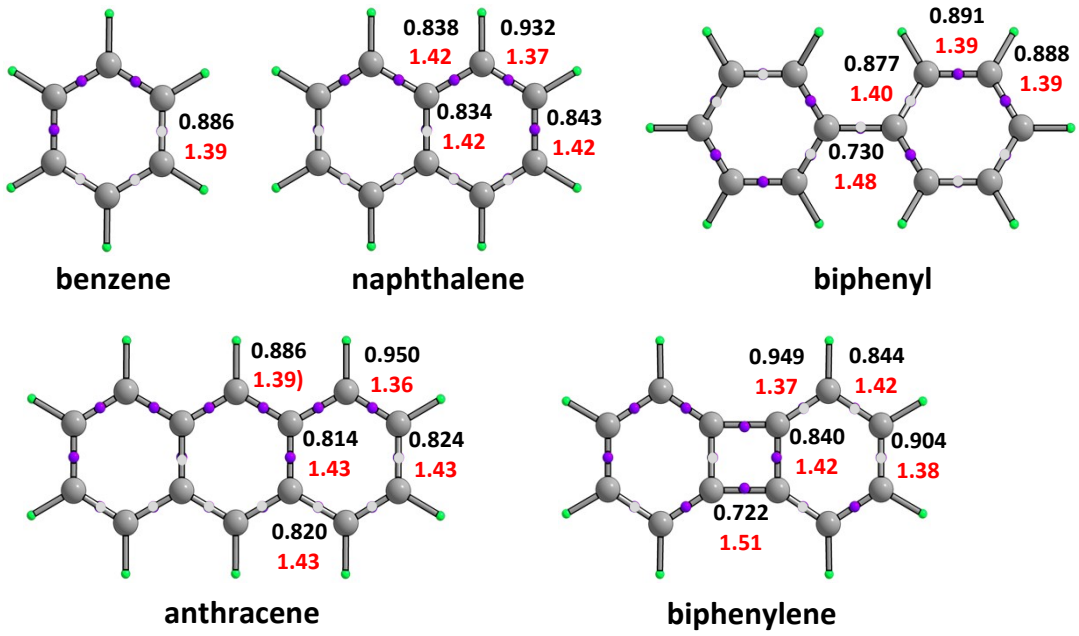

Figure S6. The MESP (3, -1) CP distribution of polycyclic benzenoid hydrocarbons. The MESP value at the CP (in au) and bond length (in Å) are represented in black and red fonts, respectively.

Table S5. The CC bond distance (Å) and the MESP data V_{bnp}, V_ρ, $V(r)$ and eigenvalues (in au) of polycyclic benzenoid hydrocarbons.

system	d_{CC}	V_{bnp}	V_ρ	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}	λ'_{v1}
benzene	1.39	15.598	-14.713	0.886	7.272	-1.764	-1.638	-16.489
naphthalene	1.37	19.961	-19.029	0.932	7.697	-1.914	-1.757	-17.335
	1.37	19.961	-19.029	0.932	7.697	-1.914	-1.757	-17.335
	1.37	19.961	-19.029	0.932	7.697	-1.914	-1.757	-17.335
	1.37	19.961	-19.029	0.932	7.697	-1.914	-1.757	-17.335
	1.42	19.361	-18.517	0.843	6.833	-1.616	-1.517	-15.601
	1.42	19.361	-18.517	0.843	6.833	-1.616	-1.517	-15.601
	1.42	20.978	-20.140	0.839	6.772	-1.591	-1.490	-15.472

	1.42	20.978	-20.140	0.839	6.772	-1.591	-1.490	-15.472
	1.42	20.978	-20.144	0.839	6.772	-1.591	-1.490	-15.472
	1.42	20.978	-20.140	0.839	6.772	-1.591	-1.490	-15.472
	1.42	22.113	-21.279	0.834	6.725	-1.575	-1.463	-15.373
biphenyl	1.39	21.193	-20.302	0.891	7.300	-1.775	-1.646	-16.547
	1.39	21.193	-20.302	0.891	7.300	-1.775	-1.646	-16.547
	1.39	21.193	-20.302	0.891	7.300	-1.775	-1.646	-16.547
	1.39	21.193	-20.302	0.891	7.300	-1.775	-1.646	-16.547
	1.39	20.385	-19.497	0.888	7.272	-1.763	-1.638	-16.489
	1.39	20.385	-19.497	0.888	7.272	-1.763	-1.638	-16.489
	1.39	20.385	-19.497	0.888	7.272	-1.763	-1.638	-16.489
	1.39	20.385	-19.497	0.888	7.272	-1.763	-1.638	-16.489
	1.40	22.803	-21.926	0.877	7.142	-1.725	-1.596	-16.224
	1.40	22.803	-21.926	0.877	7.142	-1.725	-1.596	-16.224
	1.40	22.803	-21.926	0.877	7.142	-1.725	-1.596	-16.224
	1.40	22.803	-21.926	0.877	7.142	-1.725	-1.596	-16.224
	1.48	22.857	-22.128	0.730	5.762	-1.253	-1.213	-13.351
anthracene	1.36	22.131	-21.169	0.950	7.860	-1.972	-1.803	-17.656
	1.36	22.131	-21.169	0.950	7.860	-1.972	-1.803	-17.656
	1.36	22.131	-21.169	0.950	7.860	-1.972	-1.803	-17.656
	1.36	22.131	-21.169	0.950	7.860	-1.972	-1.803	-17.656
	1.39	24.480	-23.601	0.886	7.199	-1.738	-1.609	-16.338
	1.39	24.480	-23.601	0.886	7.199	-1.738	-1.609	-16.338
	1.39	24.480	-23.601	0.886	7.199	-1.738	-1.609	-16.338
	1.39	24.480	-23.601	0.886	7.199	-1.738	-1.609	-16.338
	1.43	21.276	-20.449	0.821	6.584	-1.527	-1.439	-15.086
	1.43	21.276	-20.449	0.821	6.584	-1.527	-1.439	-15.086
	1.43	23.518	-22.705	0.821	6.584	-1.527	-1.439	-15.086
	1.43	23.518	-22.705	0.821	6.584	-1.527	-1.439	-15.086
	1.43	23.518	-22.705	0.821	6.584	-1.527	-1.439	-15.086
	1.43	23.518	-22.705	0.821	6.584	-1.527	-1.439	-15.086
	1.43	25.040	-24.197	0.814	6.509	-1.503	-1.405	-14.928
	1.43	25.040	-24.197	0.814	6.509	-1.503	-1.405	-14.928
biphenylene	1.37	22.290	-21.341	0.949	7.710	-1.933	-1.789	-17.387
	1.37	22.290	-21.341	0.949	7.710	-1.933	-1.789	-17.387
	1.37	22.290	-21.341	0.949	7.710	-1.933	-1.789	-17.387
	1.37	22.290	-21.341	0.949	7.710	-1.933	-1.789	-17.387
	1.38	20.393	-19.489	0.904	7.419	-1.827	-1.680	-16.775
	1.38	20.393	-19.489	0.904	7.419	-1.827	-1.680	-16.775
	1.42	20.603	-19.759	0.844	6.819	-1.625	-1.512	-15.567
	1.42	20.603	-19.759	0.844	6.819	-1.625	-1.512	-15.567

	1.42	20.603	-19.758	0.844	6.819	-1.625	-1.512	-15.567
	1.42	20.602	-19.758	0.844	6.819	-1.625	-1.512	-15.567
	1.42	23.714	-22.873	0.840	6.772	-1.577	-1.405	-15.535
	1.42	23.714	-22.873	0.840	6.772	-1.577	-1.405	-15.535
	1.51	22.862	-22.140	0.722	5.301	-1.194	-1.147	-12.624
	1.51	22.861	-22.139	0.722	5.301	-1.194	-1.147	-12.624

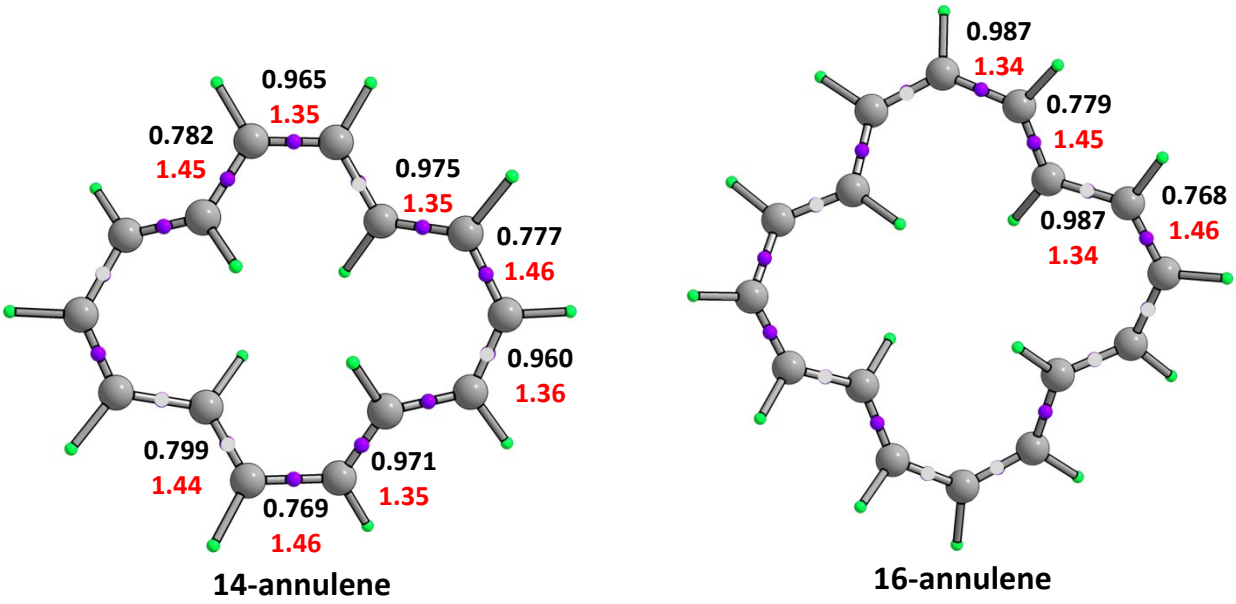

Figure S7. The MESP (3, -1) CP distribution of annulenes. The MESP value at the CP (in au) and bond length (in Å) are represented in black and red fonts, respectively.

Table S6. The CC bond distance (Å) and the MESP data V_{bnp}, V_{ρ}, $V(r)$ and eigenvalues (in au) of annulenes.

system	d_{CC}	V_{bnp}	V_{ρ}	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}	λ'_{v1}
14-annulene	1.35	23.116	-22.141	0.975	8.081	-2.056	-1.883	-18.086
	1.35	23.116	-22.141	0.975	8.081	-2.056	-1.883	-18.086
	1.35	23.159	-22.188	0.971	8.054	-2.053	-1.875	-18.036
	1.35	23.159	-22.188	0.971	8.054	-2.053	-1.875	-18.036
	1.35	22.424	-21.460	0.965	8.012	-2.038	-1.849	-17.943
	1.36	22.056	-21.095	0.960	7.933	-2.017	-1.840	-17.796
	1.36	22.056	-21.095	0.960	7.933	-2.017	-1.840	-17.796
	1.44	22.508	-21.709	0.799	6.384	-1.459	-1.406	-14.673
	1.44	22.508	-21.762	0.799	6.384	-1.459	-1.406	-14.673
	1.45	22.561	-21.779	0.782	6.232	-1.416	-1.361	-14.355
	1.45	22.561	-20.799	0.782	6.232	-1.416	-1.361	-14.355
	1.46	21.582	-20.804	0.777	6.177	-1.404	-1.347	-14.236
	1.46	21.582	-21.177	0.777	6.177	-1.404	-1.347	-14.236

	1.46	21.955	-21.739	0.769	6.140	-1.388	-1.329	-14.151
16-anuulene	1.34	24.266	-23.279	0.987	8.216	-2.107	-1.919	-18.350
	1.34	24.266	-23.279	0.987	8.216	-2.107	-1.919	-18.350
	1.34	24.266	-23.279	0.987	8.216	-2.107	-1.919	-18.350
	1.34	24.266	-23.279	0.987	8.216	-2.107	-1.919	-18.350
	1.34	23.259	-22.272	0.987	8.198	-2.111	-1.920	-18.321
	1.34	23.259	-22.272	0.987	8.198	-2.111	-1.920	-18.321
	1.34	23.259	-22.272	0.987	8.198	-2.111	-1.920	-18.321
	1.34	23.259	-22.272	0.987	8.198	-2.111	-1.920	-18.321
	1.45	23.607	-22.828	0.779	6.210	-1.404	-1.356	-14.308
	1.45	23.607	-22.828	0.779	6.210	-1.404	-1.356	-14.308
	1.45	23.607	-22.828	0.779	6.210	-1.404	-1.356	-14.308
	1.45	23.607	-22.828	0.779	6.210	-1.404	-1.356	-14.308
	1.46	22.676	-21.908	0.768	6.097	-1.369	-1.326	-14.072
	1.46	22.676	-21.908	0.768	6.097	-1.369	-1.326	-14.072
	1.46	22.676	-21.908	0.768	6.097	-1.369	-1.326	-14.072
	1.46	22.676	-21.908	0.768	6.097	-1.369	-1.326	-14.072

Table S7. The CC bond distance (Å) and the MESP data V_{bnp}, V_{ρ}, $V(r)$ and eigenvalues (in au) of fullerene, graphene, cyclophane and carbon nanotube systems.

system	d_{CC}	V_{bnp}	V_{ρ}	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}	λ'_{v1}
fullerene	1.39	53.132	-52.178	0.954	7.370	-1.819	-1.670	-16.687
	1.39	53.132	-52.178	0.954	7.370	-1.819	-1.670	-16.687
	1.45	52.960	-52.128	0.832	6.241	-1.450	-1.335	-14.399
	1.45	52.960	-52.128	0.832	6.241	-1.450	-1.335	-14.399
ovalene	1.36	31.916	-30.950	0.966	7.965	-2.012	-1.833	-17.863
	1.36	31.916	-30.950	0.966	7.965	-2.012	-1.833	-17.863
	1.36	31.916	-30.950	0.966	7.965	-2.012	-1.833	-17.863
	1.36	31.916	-30.950	0.966	7.965	-2.012	-1.833	-17.863
	1.37	31.371	-30.445	0.927	7.579	-1.875	-1.724	-17.103
	1.37	31.371	-30.445	0.927	7.579	-1.875	-1.724	-17.103
	1.40	34.551	-33.662	0.889	7.183	-1.735	-1.604	-16.305
	1.40	34.551	-33.662	0.889	7.183	-1.735	-1.604	-16.305
	1.40	34.551	-33.662	0.889	7.183	-1.735	-1.604	-16.305
	1.40	34.551	-33.662	0.889	7.183	-1.735	-1.604	-16.305
	1.41	38.875	-38.009	0.866	6.917	-1.641	-1.518	-15.771
	1.41	38.875	-38.009	0.866	6.917	-1.641	-1.518	-15.771
	1.41	38.875	-38.009	0.866	6.917	-1.641	-1.518	-15.771
	1.41	38.875	-38.009	0.866	6.917	-1.641	-1.518	-15.771
	1.41	36.042	-35.181	0.861	6.901	-1.634	-1.512	-15.735

	1.41	36.042	-35.181	0.861	6.901	-1.634	-1.512	-15.735
	1.41	36.042	-35.181	0.861	6.901	-1.634	-1.512	-15.735
	1.41	36.042	-35.181	0.861	6.901	-1.634	-1.512	-15.735
	1.41	32.735	-31.876	0.859	6.913	-1.640	-1.530	-15.760
	1.41	32.735	-31.876	0.859	6.913	-1.640	-1.530	-15.760
	1.41	32.735	-31.876	0.859	6.913	-1.640	-1.530	-15.760
	1.41	32.735	-31.876	0.859	6.913	-1.640	-1.530	-15.760
	1.42	37.592	-36.748	0.845	6.726	-1.578	-1.466	-15.382
	1.42	37.592	-36.748	0.845	6.726	-1.578	-1.466	-15.382
	1.42	36.937	-36.097	0.840	6.696	-1.566	-1.456	-15.316
	1.42	36.937	-36.097	0.840	6.696	-1.566	-1.456	-15.316
	1.42	36.937	-36.097	0.840	6.696	-1.566	-1.456	-15.316
	1.42	36.937	-36.097	0.840	6.696	-1.566	-1.456	-15.316
	1.43	37.883	-37.047	0.835	6.634	-1.546	-1.441	-15.193
	1.43	37.883	-37.047	0.835	6.634	-1.546	-1.441	-15.193
	1.43	37.883	-37.047	0.835	6.634	-1.546	-1.441	-15.193
	1.43	37.883	-37.047	0.835	6.634	-1.546	-1.441	-15.193
	1.44	39.329	-38.507	0.822	6.494	-1.499	-1.403	-14.904
	1.44	32.748	-31.931	0.816	6.498	-1.500	-1.416	-14.908
	1.44	32.748	-31.931	0.816	6.498	-1.500	-1.416	-14.908
	1.44	32.748	-31.931	0.816	6.498	-1.500	-1.416	-14.908
	1.44	32.748	-31.931	0.816	6.498	-1.500	-1.416	-14.908
	1.44	33.446	-32.632	0.814	6.476	-1.492	-1.409	-14.862
	1.44	33.446	-32.632	0.814	6.476	-1.492	-1.409	-14.862
	1.44	33.446	-32.632	0.814	6.476	-1.492	-1.409	-14.862
	1.44	33.446	-32.632	0.814	6.476	-1.492	-1.409	-14.862
cyclophane_$C_{13}H_{18}$	1.39	24.795	-23.901	0.895	7.340	-1.804	-1.670	-16.646
	1.39	24.454	-23.570	0.884	7.249	-1.781	-1.645	-16.458
	1.39	25.302	-24.428	0.875	7.221	-1.742	-1.615	-16.380
	1.39	25.302	-24.428	0.875	7.221	-1.742	-1.615	-16.380
	1.40	25.092	-24.224	0.868	7.145	-1.723	-1.599	-16.228
	1.40	25.092	-24.224	0.868	7.145	-1.723	-1.599	-16.228
	1.50	23.764	-23.083	0.682	5.474	-1.176	-1.156	-12.752
	1.50	23.764	-23.083	0.682	5.474	-1.176	-1.156	-12.752
	1.55	23.456	-22.863	0.593	4.948	-1.032	-1.009	-11.588
	1.55	23.456	-22.863	0.593	4.948	-1.032	-1.009	-11.588
	1.55	22.661	-22.069	0.591	4.886	-1.002	-0.999	-11.442
	1.55	22.661	-22.069	0.591	4.886	-1.002	-0.999	-11.442
	1.56	22.335	-21.749	0.586	4.759	-0.983	-0.966	-11.172
	1.56	22.335	-21.749	0.586	4.759	-0.983	-0.966	-11.172
cyclophane_$C_{16}H_{16}$	1.39	26.835	-25.952	0.883	7.284	-1.789	-1.651	-16.527

	1.39	26.835	-25.952	0.883	7.284	-1.789	-1.651	-16.526
	1.39	26.835	-25.952	0.883	7.283	-1.789	-1.651	-16.525
	1.39	26.835	-25.951	0.883	7.283	-1.789	-1.651	-16.525
	1.39	27.427	-26.557	0.870	7.196	-1.740	-1.609	-16.331
	1.39	27.427	-26.557	0.870	7.196	-1.739	-1.609	-16.331
	1.39	27.427	-26.557	0.870	7.196	-1.739	-1.609	-16.330
	1.39	27.427	-26.557	0.870	7.196	-1.739	-1.609	-16.329
	1.40	27.393	-26.527	0.866	7.173	-1.733	-1.601	-16.281
	1.40	27.393	-26.527	0.866	7.172	-1.733	-1.601	-16.281
	1.40	27.393	-26.527	0.866	7.172	-1.733	-1.601	-16.280
	1.40	27.393	-26.527	0.866	7.172	-1.733	-1.601	-16.280
	1.51	25.820	-25.150	0.670	5.377	-1.143	-1.131	-12.528
	1.51	25.820	-25.150	0.670	5.377	-1.143	-1.131	-12.527
	1.51	25.820	-25.150	0.670	5.377	-1.143	-1.131	-12.527
	1.51	25.820	-25.150	0.670	5.376	-1.143	-1.131	-12.525
	1.59	24.258	-23.701	0.557	4.427	-0.906	-0.884	-10.439
	1.59	24.258	-23.701	0.557	4.427	-0.906	-0.884	-10.438
CNT_C24H12	1.41	32.013	-31.135	0.878	6.898	-1.684	-1.547	-15.744
	1.41	32.013	-31.135	0.878	6.898	-1.684	-1.546	-15.744
	1.41	32.013	-31.135	0.878	6.898	-1.684	-1.546	-15.744
	1.41	32.013	-31.135	0.878	6.898	-1.684	-1.546	-15.744
	1.41	32.013	-31.135	0.878	6.897	-1.684	-1.546	-15.744
	1.41	32.013	-31.135	0.878	6.897	-1.684	-1.546	-15.744
	1.41	32.013	-31.135	0.878	6.897	-1.684	-1.546	-15.744
	1.41	32.013	-31.135	0.878	6.897	-1.684	-1.546	-15.744
	1.41	32.012	-31.135	0.878	6.896	-1.684	-1.546	-15.744
	1.41	32.012	-31.135	0.878	6.896	-1.684	-1.546	-15.744
	1.41	37.377	-31.135	0.878	6.895	-1.684	-1.546	-15.744
	1.41	32.011	-31.134	0.878	6.895	-1.684	-1.546	-15.744
	1.41	32.012	-31.134	0.877	6.895	-1.684	-1.546	-15.744
	1.41	32.012	-36.500	0.877	6.895	-1.684	-1.546	-15.744
	1.41	32.012	-31.134	0.877	6.895	-1.684	-1.546	-15.744
	1.41	32.012	-31.135	0.877	6.895	-1.684	-1.546	-15.744
	1.41	32.011	-31.135	0.877	6.895	-1.683	-1.546	-15.744
	1.41	32.011	-31.135	0.877	6.895	-1.683	-1.546	-15.744
	1.41	32.011	-31.135	0.877	6.895	-1.683	-1.546	-15.744
	1.41	32.011	-31.134	0.877	6.895	-1.683	-1.546	-15.744
	1.41	32.012	-31.134	0.877	6.894	-1.683	-1.545	-15.744
	1.41	32.012	-31.134	0.877	6.894	-1.683	-1.545	-15.744
	1.41	32.012	-31.134	0.877	6.893	-1.683	-1.545	-15.744
	1.41	32.012	-31.134	0.877	6.893	-1.683	-1.545	-15.744

	1.45	32.755	-31.134	0.805	6.298	-1.425	-1.347	-14.475
	1.45	32.755	-31.134	0.805	6.298	-1.425	-1.347	-14.475
	1.45	32.754	-31.134	0.805	6.296	-1.424	-1.347	-14.475
	1.45	32.754	-31.950	0.805	6.296	-1.424	-1.347	-14.475
	1.45	32.755	-31.950	0.805	6.295	-1.424	-1.347	-14.475
	1.45	32.755	-31.949	0.805	6.295	-1.424	-1.347	-14.475

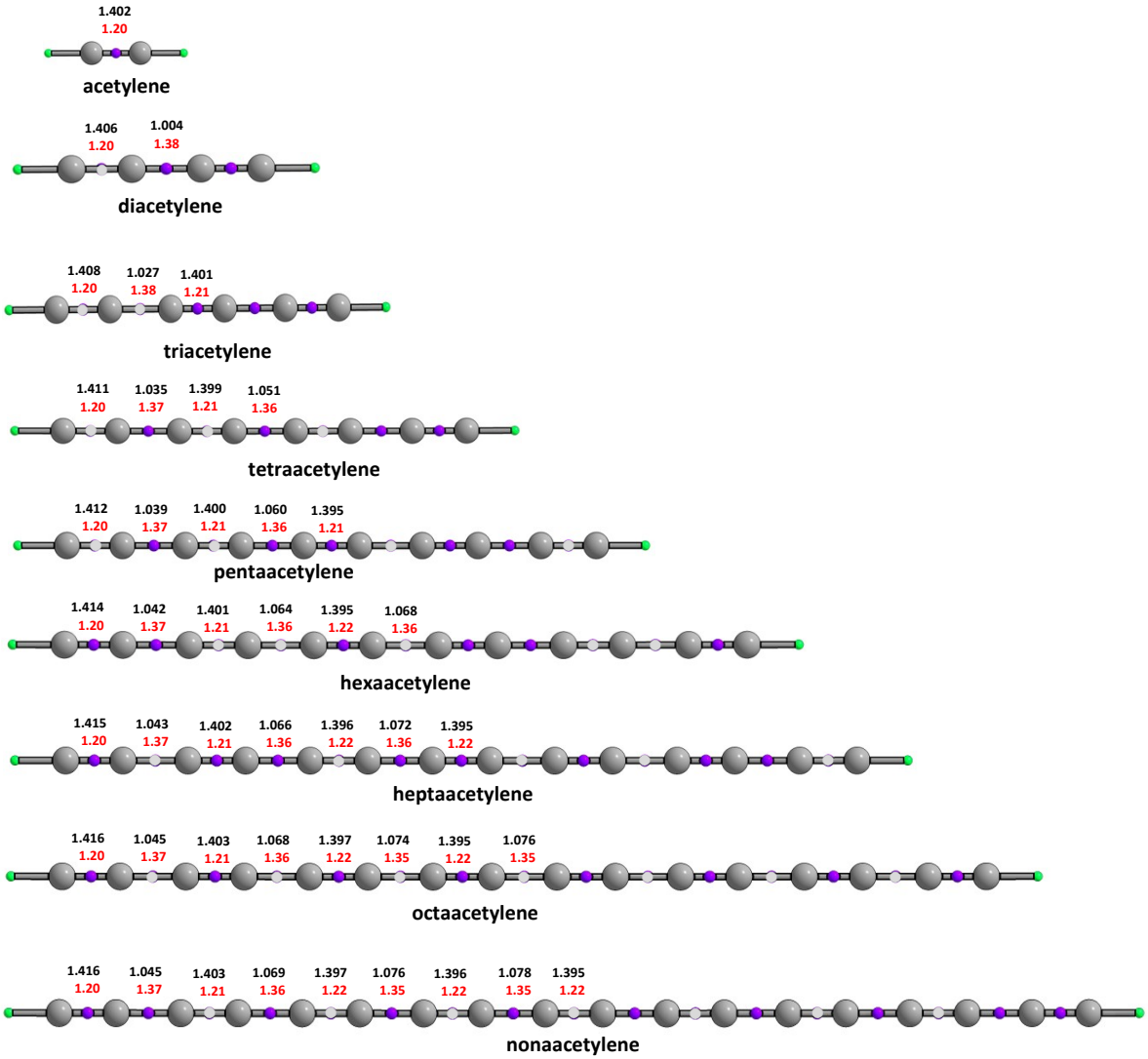

Figure S8. The MESP (3, -1) CP distribution of alkynes. The MESP value at the CP (in au) and bond length (in Å) are represented in black and red fonts, respectively.

Table S8. The CC bond distance (Å) and the MESP data V_{bnp}, V_p, $V(r)$ and eigenvalues (in au) of alkynes.

system	d_{CC}	V_{bnp}	V_p	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}	λ'_{v1}
acetylene	1.20	11.255	-9.853	1.402	12.151	-3.500	-3.500	-25.649
diacetylene	1.20	13.612	-12.206	1.406	11.951	-3.435	-3.435	-25.310
	1.20	13.612	-12.206	1.406	11.951	-3.435	-3.435	-25.310

	1.38	12.938	-11.934	1.004	7.447	-1.844	-1.844	-16.996
triacetylene	1.20	14.806	-13.398	1.408	11.898	-3.414	-3.414	-25.218
	1.20	14.806	-13.398	1.408	11.898	-3.414	-3.414	-25.218
	1.21	15.963	-14.562	1.401	11.697	-3.348	-3.348	-24.872
	1.37	14.588	-13.560	1.027	7.597	-1.894	-1.894	-17.290
	1.37	14.588	-13.560	1.027	7.597	-1.894	-1.894	-17.290
tetraacetylene	1.20	15.610	-14.200	1.411	11.883	-3.408	-3.408	-25.191
	1.20	15.610	-14.200	1.411	11.883	-3.408	-3.408	-25.191
	1.21	17.152	-15.753	1.399	11.620	-3.319	-3.319	-24.738
	1.21	17.152	-15.753	1.399	11.620	-3.319	-3.319	-24.738
	1.36	16.250	-15.198	1.051	7.775	-1.954	-1.954	-17.642
	1.37	15.567	-14.532	1.035	7.637	-1.907	-1.907	-17.370
	1.37	15.567	-14.532	1.035	7.637	-1.907	-1.907	-17.370
pentaacetylene	1.20	16.217	-14.805	1.412	11.878	-3.405	-3.405	-25.183
	1.20	16.217	-14.805	1.412	11.878	-3.405	-3.405	-25.183
	1.21	17.955	-16.556	1.400	11.595	-3.309	-3.309	-24.695
	1.21	17.955	-16.556	1.400	11.595	-3.309	-3.309	-24.695
	1.21	18.341	-16.946	1.395	11.535	-3.286	-3.286	-24.590
	1.36	17.234	-16.175	1.060	7.827	-1.971	-1.971	-17.744
	1.36	17.234	-16.175	1.060	7.827	-1.971	-1.971	-17.744
	1.37	16.266	-15.227	1.039	7.653	-1.912	-1.912	-17.400
	1.37	16.266	-15.227	1.039	7.653	-1.912	-1.912	-17.400
hexaacetylene	1.20	16.704	-15.291	1.414	11.876	-3.404	-3.404	-25.193
	1.20	16.704	-15.291	1.414	11.876	-3.404	-3.404	-25.193
	1.21	18.562	-17.161	1.401	11.585	-3.305	-3.305	-24.683
	1.21	18.562	-17.161	1.401	11.585	-3.305	-3.305	-24.683
	1.22	19.143	-17.748	1.395	11.505	-3.275	-3.275	-24.515
	1.22	19.143	-17.748	1.395	11.505	-3.275	-3.275	-24.515
	1.36	18.221	-17.153	1.068	7.884	-1.990	-1.990	-17.838
	1.36	17.935	-16.872	1.064	7.848	-1.978	-1.978	-17.798
	1.36	17.935	-16.872	1.064	7.848	-1.978	-1.978	-17.798
	1.37	16.809	-15.768	1.042	7.659	-1.914	-1.914	-17.398
	1.37	16.809	-15.768	1.042	7.659	-1.914	-1.914	-17.398
heptaacetylene	1.20	17.111	-15.697	1.415	11.876	-3.404	-3.404	-25.193
	1.20	17.111	-15.696	1.415	11.876	-3.404	-3.404	-25.193
	1.21	19.049	-17.647	1.402	11.582	-3.304	-3.304	-24.683
	1.21	19.049	-17.647	1.402	11.582	-3.304	-3.304	-24.683
	1.22	19.750	-18.354	1.396	11.494	-3.271	-3.271	-24.515
	1.22	19.750	-18.354	1.396	11.494	-3.271	-3.271	-24.515
	1.22	19.946	-18.551	1.395	11.474	-3.263	-3.263	-24.460
	1.36	18.923	-17.851	1.072	7.906	-1.997	-1.997	-17.879

	1.36	18.923	-17.851	1.072	7.906	-1.997	-1.997	-17.879
	1.36	18.480	-17.413	1.066	7.856	-1.981	-1.981	-17.798
	1.36	18.480	-17.413	1.066	7.856	-1.981	-1.981	-17.798
	1.37	17.254	-16.211	1.043	7.662	-1.915	-1.915	-17.438
	1.37	17.254	-16.211	1.043	7.662	-1.915	-1.915	-17.438
octaacetylene	1.20	17.461	-16.045	1.416	11.876	-3.404	-3.404	-25.193
	1.20	17.461	-16.045	1.416	11.876	-3.404	-3.404	-25.193
	1.21	19.456	-18.054	1.403	11.580	-3.303	-3.303	-24.683
	1.21	19.456	-18.054	1.403	11.580	-3.303	-3.303	-24.683
	1.22	20.237	-18.840	1.397	11.489	-3.269	-3.269	-24.515
	1.22	20.237	-18.840	1.397	11.489	-3.269	-3.269	-24.515
	1.22	20.552	-19.156	1.395	11.462	-3.258	-3.258	-24.460
	1.22	20.552	-19.156	1.395	11.462	-3.258	-3.258	-24.460
	1.35	19.625	-18.549	1.076	7.929	-2.005	-2.005	-17.960
	1.35	19.468	-18.393	1.074	7.916	-2.000	-2.000	-17.920
	1.35	19.468	-18.393	1.074	7.916	-2.000	-2.000	-17.920
	1.36	18.925	-17.857	1.068	7.860	-1.982	-1.982	-17.798
	1.36	18.925	-17.857	1.068	7.860	-1.982	-1.982	-17.798
	1.37	17.631	-16.586	1.045	7.664	-1.915	-1.915	-17.438
	1.37	17.631	-16.586	1.045	7.664	-1.915	-1.915	-17.438
nonaacetylene	1.20	17.767	-16.351	1.416	11.876	-3.404	-3.404	-25.193
	1.20	17.767	-16.351	1.416	11.876	-3.404	-3.404	-25.193
	1.21	19.806	-18.402	1.403	11.580	-3.303	-3.303	-24.683
	1.21	19.806	-18.402	1.403	11.580	-3.303	-3.303	-24.683
	1.22	20.644	-19.246	1.398	11.487	-3.268	-3.268	-24.515
	1.22	20.644	-19.246	1.398	11.487	-3.268	-3.268	-24.515
	1.22	21.039	-19.643	1.396	11.457	-3.256	-3.256	-24.460
	1.22	21.039	-19.643	1.396	11.457	-3.256	-3.256	-24.460
	1.22	21.158	-19.762	1.395	11.449	-3.253	-3.253	-24.460
	1.35	20.170	-19.092	1.078	7.939	-2.008	-2.008	-17.960
	1.35	20.170	-19.092	1.078	7.939	-2.008	-2.008	-17.960
	1.35	19.913	-18.838	1.076	7.920	-2.002	-2.002	-17.920
	1.35	19.913	-18.838	1.076	7.920	-2.002	-2.002	-17.920
	1.36	19.302	-18.233	1.069	7.862	-1.983	-1.983	-17.798
	1.36	19.302	-18.233	1.069	7.862	-1.983	-1.983	-17.798
	1.37	17.958	-16.912	1.045	7.665	-1.916	-1.916	-17.438
	1.37	17.958	-16.912	1.045	7.665	-1.916	-1.916	-17.438

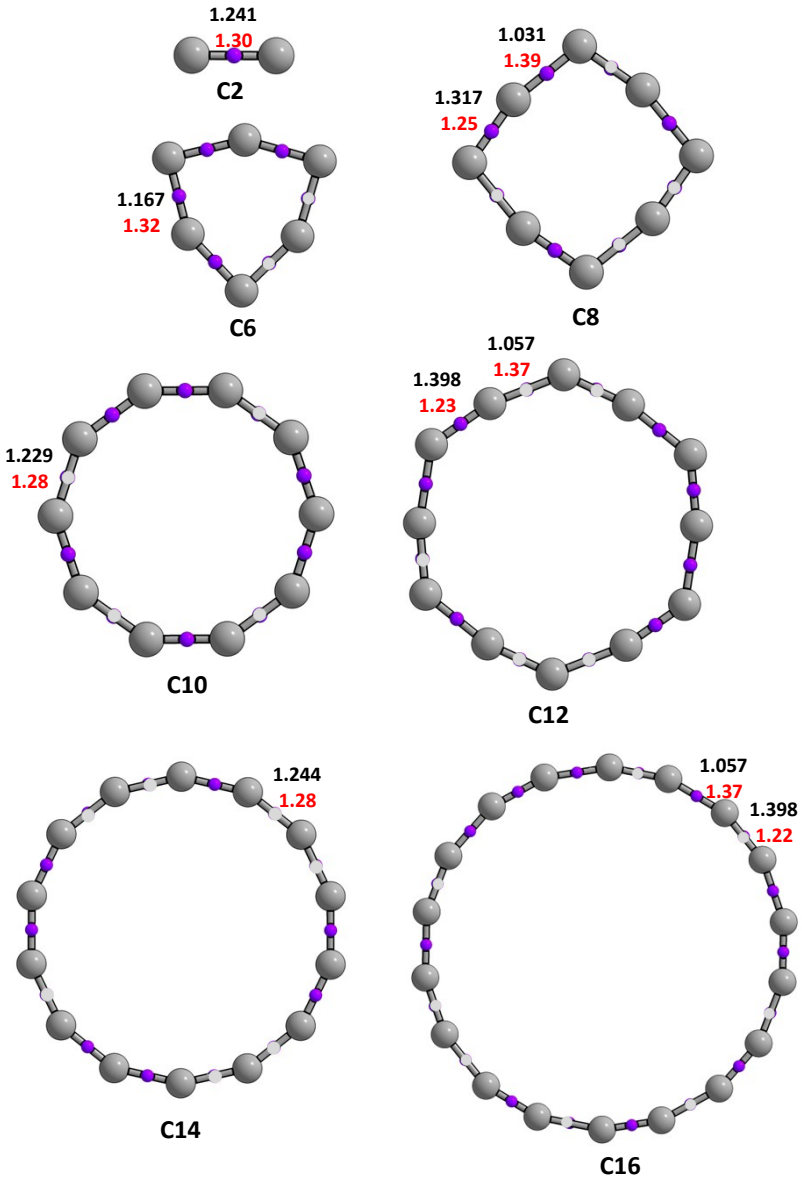

Figure S9. The MESP (3, -1) CP distribution of C2 and carbon rings. The MESP value at the CP (in au) and bond length (in Å) are represented in black and red fonts, respectively.

Table S9. The CC bond distance (Å) and the MESP data V_{bnp}, V_{ρ}, $V(r)$ and eigenvalues (in au) of C2 and carbon rings.

system	d_{CC}	V_{bnp}	V_{ρ}	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}	λ'_{v1}
C2	1.30	9.745	-8.504	1.241	9.118	-2.691	-2.337	-20.108
C6	1.32	16.221	-15.054	1.167	8.651	-2.322	-2.215	-19.276
	1.32	16.222	-15.055	1.167	8.651	-2.322	-2.215	-19.276
	1.32	16.221	-15.054	1.167	8.651	-2.322	-2.215	-19.276
	1.32	16.221	-15.054	1.167	8.651	-2.322	-2.215	-19.276
	1.32	16.221	-15.054	1.167	8.651	-2.322	-2.215	-19.276

	1.32	16.221	-15.054	1.167	8.651	-2.322	-2.215	-19.276
C8	1.39	18.043	-17.012	1.031	7.320	-1.863	-1.831	-16.678
	1.39	18.043	-17.012	1.031	7.320	-1.863	-1.831	-16.678
	1.39	18.043	-17.012	1.031	7.320	-1.863	-1.831	-16.678
	1.39	18.043	-17.012	1.031	7.320	-1.863	-1.831	-16.678
	1.25	17.242	-15.924	1.317	10.483	-2.944	-2.777	-22.642
	1.25	17.242	-15.924	1.317	10.483	-2.944	-2.777	-22.642
	1.25	17.242	-15.924	1.317	10.483	-2.944	-2.777	-22.642
	1.25	17.242	-15.924	1.317	10.483	-2.944	-2.777	-22.642
C10	1.28	18.905	-17.675	1.229	9.572	-2.593	-2.583	-21.055
C12	1.23	20.161	-18.794	1.366	11.121	-3.141	-3.075	-23.823
	1.37	19.258	-18.200	1.058	7.656	-1.958	-1.931	-17.383
C14	1.28	20.629	-19.385	1.244	9.668	-2.620	-2.612	-21.247
C16	1.22	21.622	-20.224	1.398	11.480	-3.262	-3.254	-24.486
	1.37	20.611	-19.555	1.057	7.656	-1.950	-1.934	-17.409

Table S10. The CC bond distance (Å) and the MESP data V_{bnp}, V_p, $V(r)$ and eigenvalues (in au) of heterocyclic systems.

system	d_{CC}	V_{bnp}	V_p	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}	λ'_{v1}
pyrazine	1.39	16.922	-16.005	0.917	7.268	-1.734	-1.598	-16.445
	1.39	16.922	-16.005	0.917	7.268	-1.734	-1.598	-16.445
pyrrole	1.37	15.970	-15.060	0.910	7.611	-1.941	-1.692	-17.189
	1.37	15.970	-15.060	0.910	7.611	-1.941	-1.692	-17.189
	1.42	15.626	-14.820	0.806	6.683	-1.633	-1.463	-15.347
furan	1.35	16.240	-15.267	0.973	7.998	-2.063	-1.787	-17.933
	1.35	16.240	-15.267	0.973	7.998	-2.063	-1.787	-17.933
	1.43	15.683	-14.871	0.812	6.469	-1.562	-1.413	-14.921
thiophene	1.36	17.600	-16.640	0.960	7.849	-2.016	-1.798	-17.647
	1.36	17.600	-16.640	0.960	7.849	-2.016	-1.798	-17.647
	1.43	17.021	-16.198	0.823	6.621	-1.578	-1.447	-15.188
tetrahydropyran	1.53	17.246	-16.608	0.638	5.218	-1.075	-1.031	-12.146
	1.53	17.246	-16.608	0.638	5.218	-1.075	-1.031	-12.146
	1.53	17.023	-16.395	0.629	5.126	-1.067	-1.051	-11.988
	1.53	17.023	-16.395	0.629	5.126	-1.067	-1.051	-11.988
THF	1.53	16.005	-15.363	0.643	5.173	-1.072	-1.017	-12.078
	1.53	16.004	-15.362	0.642	5.172	-1.071	-1.017	-12.078
	1.53	15.882	-15.241	0.641	5.120	-1.075	-1.054	-12.011
thiozolidine	1.52	17.584	-16.919	0.665	5.235	-1.097	-1.053	-12.200
thioxanthene	1.39	25.760	-24.858	0.902	7.244	-1.776	-1.627	-16.428
	1.39	25.760	-24.858	0.902	7.244	-1.776	-1.627	-16.428

	1.39	23.450	-22.554	0.896	7.295	-1.781	-1.646	-16.539
	1.39	23.450	-22.554	0.896	7.295	-1.781	-1.646	-16.539
	1.39	25.359	-24.463	0.895	7.251	-1.770	-1.630	-16.447
	1.39	25.359	-24.463	0.895	7.251	-1.770	-1.630	-16.447
	1.40	27.272	-26.379	0.893	7.155	-1.740	-1.590	-16.240
	1.40	27.272	-26.379	0.893	7.155	-1.740	-1.590	-16.240
	1.39	23.312	-22.419	0.893	7.280	-1.771	-1.639	-16.507
	1.39	23.312	-22.419	0.893	7.280	-1.771	-1.639	-16.507
	1.39	22.726	-21.836	0.891	7.273	-1.767	-1.638	-16.492
	1.39	22.726	-21.836	0.891	7.273	-1.767	-1.638	-16.492
	1.51	25.658	-24.964	0.694	5.421	-1.164	-1.126	-12.633
	1.51	25.658	-24.964	0.694	5.421	-1.164	-1.126	-12.633
piperazine	1.52	17.325	-16.688	0.638	5.252	-1.078	-1.038	-12.217
	1.52	17.325	-16.688	0.638	5.252	-1.078	-1.038	-12.217
pyrrolidine	1.54	15.774	-15.157	0.616	5.052	-1.042	-1.002	-11.819
	1.54	15.774	-15.157	0.616	5.052	-1.042	-1.002	-11.819
	1.55	15.598	-15.002	0.596	4.876	-1.007	-0.981	-11.452
dioxolane	1.54	16.358	-15.708	0.650	5.075	-1.035	-0.944	-11.846
DBN	1.52	20.956	-20.287	0.669	5.339	-1.111	-1.060	-12.432
	1.53	19.861	-19.215	0.646	5.182	-1.082	-1.043	-12.098
	1.53	19.596	-18.955	0.641	5.081	-1.054	-1.008	-11.961
	1.54	19.461	-18.828	0.633	5.067	-1.058	-1.027	-11.880
	1.54	19.469	-18.844	0.625	5.128	-1.063	-1.030	-11.880
benzonitrile	1.39	18.225	-17.303	0.923	7.329	-1.781	-1.654	-16.588
	1.39	18.225	-17.302	0.923	7.329	-1.781	-1.654	-16.588
	1.39	19.021	-18.104	0.917	7.163	-1.742	-1.596	-16.475
	1.39	19.021	-18.104	0.917	7.163	-1.742	-1.596	-16.475
	1.40	17.875	-16.962	0.913	7.259	-1.754	-1.635	-16.252
	1.40	17.875	-16.962	0.913	7.259	-1.754	-1.635	-16.252
	1.44	18.060	-17.173	0.887	6.421	-1.507	-1.461	-14.841
porphyrin	1.36	27.976	-27.003	0.972	8.086	-2.071	-1.868	-17.879
	1.36	27.976	-27.003	0.972	8.086	-2.071	-1.868	-17.879
	1.37	27.941	-26.987	0.954	7.760	-1.965	-1.766	-17.478
	1.37	27.941	-26.987	0.954	7.760	-1.964	-1.766	-17.478
	1.39	29.973	-29.051	0.922	7.326	-1.795	-1.654	-16.588
	1.39	29.973	-29.051	0.922	7.326	-1.795	-1.654	-16.588
	1.39	29.973	-29.052	0.922	7.326	-1.795	-1.654	-16.588
	1.39	29.973	-29.051	0.922	7.326	-1.795	-1.653	-16.588
	1.39	29.980	-29.084	0.896	7.215	-1.746	-1.615	-16.364
	1.39	29.980	-29.084	0.896	7.215	-1.746	-1.615	-16.364
	1.39	29.980	-29.084	0.896	7.215	-1.746	-1.615	-16.364

	1.39	29.980	-29.084	0.896	7.214	-1.746	-1.615	-16.364
	1.43	29.154	-28.323	0.830	6.530	-1.526	-1.381	-14.977
	1.43	29.154	-28.323	0.830	6.530	-1.526	-1.381	-14.977
	1.43	29.154	-28.324	0.830	6.530	-1.526	-1.381	-14.977
	1.43	29.154	-28.324	0.830	6.530	-1.526	-1.381	-14.977
	1.46	29.030	-28.265	0.765	6.115	-1.385	-1.277	-14.118
	1.46	29.030	-28.265	0.765	6.115	-1.385	-1.276	-14.118
	1.46	29.030	-28.265	0.765	6.115	-1.385	-1.276	-14.118
	1.46	29.030	-28.265	0.765	6.115	-1.385	-1.276	-14.118
aziridine	1.48	13.253	-12.447	0.806	5.558	-1.326	-1.247	-13.411
cyanogen	1.39	13.183	-12.097	1.086	7.258	-1.783	-1.783	-16.648
pyramidopyramidine	1.40	22.956	-22.029	0.927	7.113	-1.675	-1.535	-16.142
	1.42	21.593	-20.709	0.885	6.744	-1.537	-1.446	-15.390
	1.42	21.593	-20.708	0.885	6.743	-1.537	-1.446	-15.390
oxirane	1.47	13.663	-12.802	0.861	5.712	-1.414	-1.274	-13.837
ethylene carbonate	1.53	17.322	-16.621	0.702	5.180	-1.067	-0.964	-12.070
furfural	1.36	18.033	-17.052	0.981	7.850	-2.001	-1.742	-17.637
	1.36	19.243	-18.266	0.977	7.816	-1.984	-1.734	-17.557
	1.42	17.852	-16.999	0.854	6.653	-1.608	-1.464	-15.286
	1.46	18.148	-17.342	0.805	6.107	-1.342	-1.255	-14.022
ethylene glycol	1.51	14.946	-14.283	0.664	5.405	-1.122	-1.023	-12.505
tetrathiafulvalene	1.33	24.712	-23.650	1.062	8.534	-2.285	-2.017	-18.966
	1.33	24.712	-23.650	1.062	8.534	-2.285	-2.017	-18.966
	1.34	29.224	-28.172	1.053	8.313	-2.265	-1.934	-18.541
dithianodithiine	1.52	30.311	-29.605	0.706	5.324	-1.133	-1.111	-12.404
	1.52	30.311	-29.605	0.706	5.324	-1.133	-1.111	-12.404
	1.53	39.159	-38.475	0.684	5.113	-1.056	-1.017	-11.891
thiirane	1.48	15.175	-14.384	0.791	5.710	-1.289	-1.245	-13.465
thietane	1.54	16.072	-15.429	0.643	5.026	-1.045	-0.995	-11.803
	1.54	16.072	-15.429	0.643	5.026	-1.045	-0.995	-11.803
thiane	1.53	18.478	-17.831	0.647	5.198	-1.086	-1.070	-12.126
	1.53	18.478	-17.831	0.647	5.198	-1.086	-1.070	-12.126
	1.53	18.145	-17.513	0.632	5.132	-1.067	-1.053	-11.993
	1.53	18.145	-17.513	0.632	5.132	-1.067	-1.053	-11.993
thiaindans	1.39	22.292	-21.384	0.908	7.314	-1.801	-1.657	-16.626
	1.39	21.852	-20.948	0.904	7.343	-1.804	-1.662	-16.588
	1.39	20.065	-19.178	0.887	7.269	-1.769	-1.636	-16.475
	1.39	23.459	-22.572	0.887	7.147	-1.733	-1.576	-16.401
	1.39	20.566	-19.680	0.887	7.234	-1.765	-1.629	-16.364
	1.40	20.389	-19.506	0.882	7.211	-1.753	-1.621	-16.216

	1.51	21.450	-20.761	0.689	5.401	-1.157	-1.113	-12.602
	1.53	20.384	-19.727	0.657	5.134	-1.078	-1.043	-11.988
SeC3Se	1.27	24.341	-23.080	1.261	9.808	-2.649	-2.649	-21.481
SC3S	1.27	17.942	-16.680	1.262	9.803	-2.654	-2.654	-21.491
C5S	1.26	16.805	-15.497	1.308	10.094	-2.742	-2.742	-22.027
	1.28	17.152	-15.880	1.272	9.587	-2.571	-2.571	-21.087
	1.29	15.909	-14.691	1.219	9.279	-2.446	-2.446	-20.534
	1.28	14.708	-13.506	1.202	9.803	-2.537	-2.537	-21.352
NCCP	1.38	14.783	-13.741	1.043	7.422	-1.828	-1.828	-16.916

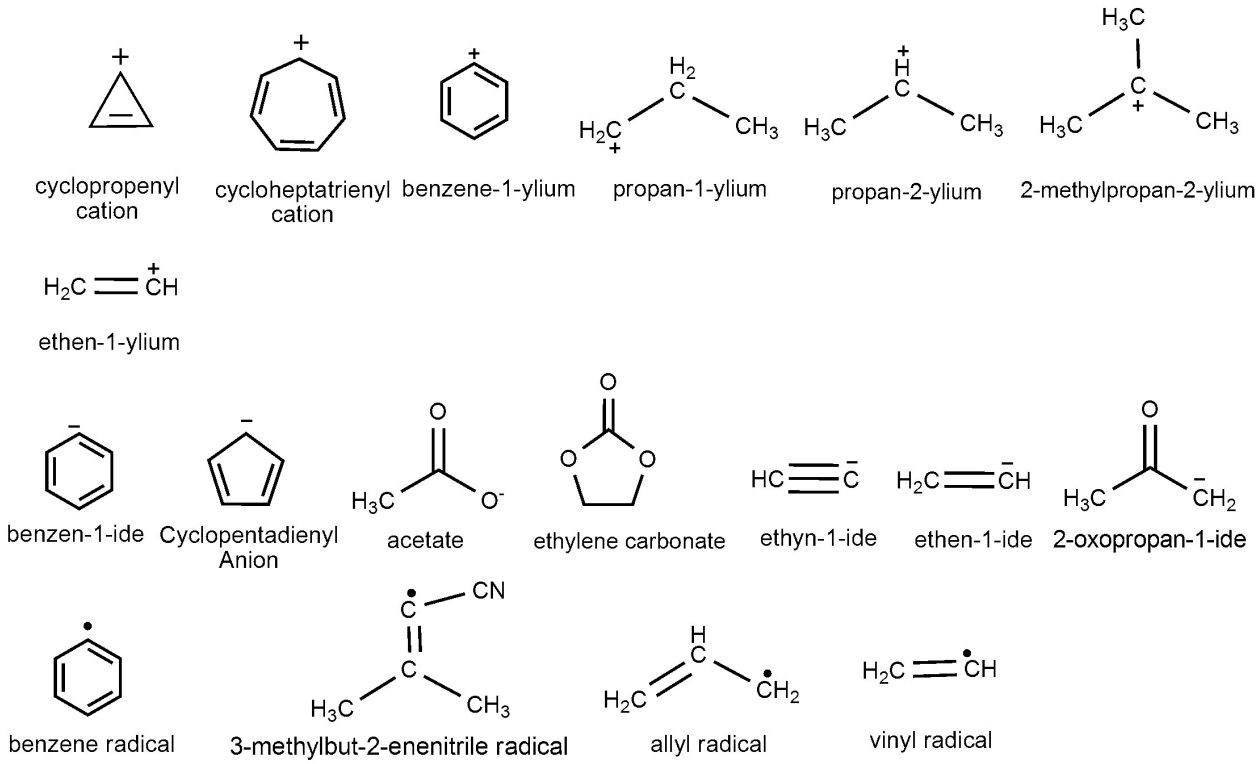

Figure S10. Selected set of cationic, anionic and radical systems.

Table S11. The CC bond distance (Å) and the MESP data V_{bnp}, V_p, $V(r)$ and eigenvalues (in au) of anions, cations and radical systems.

system	d_{CC}	V_{bnp}	V_p	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}	λ'_{v1}
acetylene cation	1.19209	10.97	-9.053	**1.914**	12.212	-3.951	-3.951	-25.883
Cyclopropenyl cation	1.36	12.989	-11.640	1.349	7.554	-2.000	-1.726	-17.665
	1.36	12.989	-11.640	1.349	7.554	-2.000	-1.726	-17.665
	1.36	12.989	-11.640	1.349	7.554	-2.000	-1.726	-17.665
cycloheptatrienyl cation	1.39	17.274	-16.163	1.110	7.237	-1.703	-1.654	-16.403
	1.39	17.274	-16.163	1.110	7.236	-1.703	-1.653	-16.402

	1.39	17.274	-16.163	1.110	7.236	-1.703	-1.653	-16.402
	1.39	17.274	-16.163	1.110	7.236	-1.703	-1.653	-16.401
	1.39	17.273	-16.163	1.110	7.236	-1.703	-1.653	-16.400
	1.39	17.273	-16.163	1.110	7.235	-1.703	-1.653	-16.400
	1.39	17.273	-16.163	1.110	7.235	-1.703	-1.653	-16.399
benzene-1-ylium	1.32	16.839	-15.477	1.362	8.708	-2.343	-2.097	-19.377
	1.32	16.839	-15.477	1.362	8.708	-2.343	-2.097	-19.377
	1.39	16.411	-15.292	1.119	7.311	-1.776	-1.638	-16.549
	1.39	16.411	-15.292	1.119	7.311	-1.776	-1.638	-16.549
	1.43	16.151	-15.052	1.100	6.567	-1.645	-1.517	-15.120
	1.43	16.151	-15.052	1.100	6.567	-1.645	-1.517	-15.120
propan-1-ylium	1.39	13.237	-12.049	1.188	7.179	-1.710	-1.704	-16.404
	1.69	12.075	-11.270	0.805	3.406	-0.780	-0.667	-8.295
	1.78	11.915	-11.161	0.754	2.753	-0.624	-0.465	-6.814
propan-2-ylium	1.44	12.486	-11.412	1.074	6.497	-1.451	-1.391	-14.850
2-methylpropan-2-ylium	1.46	14.341	-13.324	1.017	6.170	-1.348	-1.297	-14.170
	1.46	14.323	-13.308	1.015	6.156	-1.346	-1.292	-14.140
	1.46	14.317	-13.305	1.012	6.130	-1.338	-1.284	-14.085
ethen-1-ylium	1.25	11.139	-9.569	1.570	10.449	-2.933	-2.571	-22.521
Cyclopentadienyl Anion	1.41	15.315	-14.712	0.603	6.912	-1.734	-1.530	-15.802
	1.41	15.315	-14.712	0.603	6.912	-1.734	-1.530	-15.802
	1.41	15.313	-14.711	0.602	6.902	-1.731	-1.527	-15.783
	1.41	15.311	-14.709	0.602	6.898	-1.730	-1.526	-15.774
	1.41	15.311	-14.709	0.602	6.898	-1.730	-1.526	-15.774
acetate	1.57	14.006	-13.630	0.376	4.715	-0.928	-0.924	-11.014
benzen-1-ide	1.39	16.265	-15.577	0.688	7.207	-1.766	-1.620	-16.365
	1.39	16.265	-15.577	0.688	7.207	-1.766	-1.620	-16.365
	1.40	16.208	-15.547	0.661	7.120	-1.726	-1.598	-16.174
	1.40	16.208	-15.547	0.661	7.120	-1.726	-1.598	-16.174
	1.42	15.870	-15.284	0.585	6.759	-1.564	-1.563	-15.417
	1.42	15.870	-15.284	0.585	6.759	-1.564	-1.563	-15.417
ethyn-1-ide	1.24	10.567	-9.607	0.960	10.842	-2.979	-2.979	-23.281
ethen-1-ide	1.35	10.413	-9.741	0.671	8.027	-2.043	-1.934	-17.951
2-oxopropan-1-ide	1.38	14.515	-13.853	0.663	7.498	-1.912	-1.679	-16.898
	1.55	13.799	-13.398	0.401	4.942	-1.003	-0.992	-11.543
ethan-1-ide	1.54	9.947	-9.605	0.342	5.031	-1.146	-1.055	-11.767
Benzene radical	1.37	16.293	-15.353	0.940	7.600	-1.883	-1.761	-17.148
	1.37	16.293	-15.353	0.940	7.600	-1.883	-1.761	-17.148
	1.39	16.331	-15.441	0.889	7.247	-1.760	-1.629	-16.434
	1.39	16.331	-15.441	0.889	7.247	-1.760	-1.629	-16.434
	1.40	16.255	-15.369	0.886	7.140	-1.742	-1.616	-16.235

	1.40	16.255	-15.369	0.886	7.140	-1.742	-1.616	-16.235
3-methylbut-2-enenitrile radical	1.31	17.036	-15.925	1.111	8.884	-2.380	-2.172	-19.654
	1.37	15.995	-14.963	1.032	7.614	-1.906	-1.894	-17.302
	1.51	15.317	-14.598	0.719	5.460	-1.173	-1.156	-12.711
	1.51	15.494	-14.781	0.714	5.392	-1.160	-1.147	-12.573
allyl_radical	1.38	12.348	-11.443	0.905	7.469	-1.836	-1.710	-16.876
vinyl_radical	1.30	10.749	-9.662	1.087	9.087	-2.429	-2.229	-20.033

Table S12. The CC bond distance (Å) and the MESP data V_{bnp}, V_p, $V(r)$ and eigenvalues (in au) of systems containing multiple types of bonds.

system	d_{CC}	V_{bnp}	V_p	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}	λ'_{v1}
cyclobutadiene	1.33	14.365	-13.342	1.023	8.514	-2.252	-1.978	-19.006
	1.33	14.365	-13.342	1.023	8.514	-2.252	-1.978	-19.006
	1.57	13.322	-12.708	0.614	4.546	-0.996	-0.911	-10.956
	1.57	13.322	-12.708	0.614	4.546	-0.996	-0.911	-10.956
hexa_1,5_dien_3_yne	1.21	16.771	-15.401	1.370	11.776	-3.394	-3.359	-25.012
	1.33	14.865	-13.847	1.019	8.434	-2.191	-1.989	-18.774
	1.33	14.865	-13.847	1.019	8.434	-2.191	-1.989	-18.774
	1.43	15.119	-14.256	0.864	6.616	-1.563	-1.528	-15.216
	1.43	15.119	-14.256	0.864	6.616	-1.563	-1.528	-15.216
hexpta_1_en_3,6_diyne	1.20	16.081	-16.203	1.397	12.099	-3.499	-3.496	-25.567
	1.20	17.600	-13.995	1.385	11.930	-3.450	-3.435	-25.279
	1.33	15.380	-14.707	1.022	8.466	-2.203	-1.999	-18.837
	1.43	15.728	-15.069	0.857	6.557	-1.544	-1.511	-15.097
	1.47	15.926	-14.701	0.805	5.993	-1.373	-1.350	-13.909
	1.47	15.506	-14.200	0.803	5.972	-1.363	-1.339	-13.862
2-pentene	1.33	15.003	-14.002	1.001	8.549	-2.236	-2.013	-18.990
	1.50	13.648	-12.965	0.682	5.534	-1.196	-1.179	-12.875
	1.50	15.117	-14.441	0.675	5.517	-1.178	-1.163	-12.829
	1.53	14.169	-13.543	0.626	5.110	-1.078	-1.064	-11.956
isoprene	1.33	15.250	-14.245	1.005	8.464	-2.195	-1.997	-18.833
	1.34	15.694	-14.699	0.995	8.400	-2.171	-1.964	-18.697
	1.47	15.526	-14.781	0.744	5.958	-1.313	-1.274	-13.765
	1.50	14.997	-14.313	0.684	5.476	-1.172	-1.155	-12.745
indene	1.34	19.317	-18.330	0.988	8.295	-2.141	-1.920	-18.511
	1.38	20.332	-19.432	0.900	7.383	-1.812	-1.678	-16.721
	1.39	20.264	-19.377	0.888	7.270	-1.769	-1.643	-16.495
	1.39	19.170	-18.291	0.879	7.242	-1.764	-1.629	-16.428
	1.39	18.887	-18.012	0.875	7.215	-1.752	-1.622	-16.372
	1.39	19.175	-18.300	0.874	7.192	-1.747	-1.616	-16.328

	1.40	21.365	-20.512	0.854	7.029	-1.669	-1.524	-15.997
	1.47	19.801	-19.052	0.749	5.966	-1.342	-1.271	-13.830
	1.51	19.610	-18.927	0.683	5.420	-1.160	-1.121	-12.655
	1.51	18.481	-17.801	0.680	5.412	-1.164	-1.116	-12.625
dihydroindene	1.39	20.604	-19.715	0.889	7.319	-1.786	-1.658	-16.591
	1.39	20.604	-19.715	0.889	7.319	-1.786	-1.658	-16.591
	1.39	19.110	-18.234	0.876	7.240	-1.759	-1.629	-16.423
	1.39	19.414	-18.539	0.875	7.219	-1.755	-1.624	-16.383
	1.39	19.414	-18.539	0.875	7.219	-1.755	-1.624	-16.383
	1.40	21.724	-20.859	0.865	7.177	-1.720	-1.574	-16.292
	1.51	19.908	-19.240	0.668	5.363	-1.142	-1.109	-12.526
	1.51	19.908	-19.240	0.668	5.363	-1.142	-1.109	-12.526
	1.54	18.657	-18.044	0.613	4.974	-1.030	-1.001	-11.664
	1.54	18.657	-18.044	0.613	4.974	-1.030	-1.001	-11.664
cyclopentadiene	1.34	15.835	-14.859	0.975	8.249	-2.127	-1.909	-18.428
	1.34	15.835	-14.859	0.975	8.249	-2.127	-1.909	-18.428
	1.47	15.180	-14.444	0.736	5.945	-1.346	-1.264	-13.778
	1.50	15.058	-14.375	0.683	5.501	-1.192	-1.142	-12.824
	1.50	15.058	-14.375	0.683	5.501	-1.192	-1.142	-12.824

Table S13. The CC bond distance (Å) and the MESP data V_{bnp}, V_p, $V(r)$ and eigenvalues (in au) of organometallic and hypervalent carbon compexes.

system	d_{CC}	V_{bnp}	V_p	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}	λ'_{v1}
ferrocene	1.42	26.987	-26.147	0.840	6.744	-1.643	-1.481	-15.477
Bis(benzene)chromium(0)	1.41	28.355	-27.503	0.852	6.851	-1.663	-1.522	-15.643
η3-CrCl3	1.40	27.583	-26.511	1.073	6.765	-1.762	-1.525	-16.089
metallacyclobutane	1.42	27.389	-26.389	1.001	6.789	-1.651	-1.505	-15.572
C3H4Li2	1.50	13.348	-12.690	0.658	5.379	-1.232	-1.215	-12.825
	1.53	13.290	-12.677	0.613	4.976	-1.227	-1.084	-12.042
C6H6_CrCO3	1.41	28.150	-27.253	0.897	6.929	-1.670	-1.546	-15.809
Si2C5H2	1.38	19.190	-18.274	0.916	7.520	-1.874	-1.689	-16.981
	1.42	19.612	-18.764	0.848	6.733	-1.613	-1.516	-15.417
	1.42	19.612	-18.764	0.848	6.732	-1.613	-1.516	-15.415
	1.46	21.248	-20.440	0.808	5.973	-1.446	-1.315	-13.948
	1.46	21.246	-20.439	0.807	5.964	-1.444	-1.313	-13.930
Ge2C5H2	1.38	24.399	-23.502	0.896	7.441	-1.855	-1.668	-16.826
	1.42	25.794	-24.956	0.837	6.731	-1.624	-1.523	-15.417
	1.42	25.794	-24.956	0.837	6.731	-1.624	-1.523	-15.417
	1.46	29.716	-28.913	0.803	6.103	-1.475	-1.342	-14.185
	1.46	29.716	-28.913	0.802	6.102	-1.474	-1.341	-14.185

C6Li6	1.42	18.138	-17.402	0.736	6.764	-1.600	-1.584	-15.451
C2B8	1.50	18.849	-18.020	0.829	5.426	-1.248	-1.233	-12.719

Table S14. The CC bond distance (Å) and the MESP data V_{bnp}, V_{ρ}, $V(r)$ and eigenvalues (in au) of transition states.

system	d_{CC}	V_{bnp}	V_{ρ}	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}	λ'_{v1}
TS1	2.16	20.036	-19.869	0.166	1.186	-0.222	-0.204	-2.882
	2.41	20.848	-20.764	0.084	0.641	-0.102	-0.064	-1.633
TS2	2.19	18.789	-18.657	0.133	1.096	-0.184	-0.173	-2.673
	2.30	20.191	-20.099	0.092	0.807	-0.130	-0.087	-2.085
TS3	2.18	20.237	-20.091	0.146	1.141	-0.207	-0.191	-2.773
	2.38	21.077	-21.009	0.068	0.707	-0.108	-0.085	-1.741
TS4	2.08	19.788	-19.588	0.200	1.408	-0.262	-0.244	-3.422
	2.33	19.330	-19.227	0.103	0.788	-0.122	-0.099	-1.934
TS5	2.14	18.414	-18.246	0.168	1.244	-0.231	-0.215	-3.020
	2.40	19.529	-19.451	0.078	0.657	-0.103	-0.071	-1.654
TS6	1.92	20.566	-20.420	0.145	2.021	-0.395	-0.384	-4.910
TS7	1.98	36.002	-35.573	0.428	1.782	-0.353	-0.307	-4.298
TS8	2.00	36.648	-36.239	0.408	1.678	-0.324	-0.269	-4.127
TS9	2.04	22.873	-22.627	0.246	1.534	-0.312	-0.310	-3.738
TS10	2.13	17.407	-17.299	0.108	1.312	-0.202	-0.180	-3.111
TS11	2.21	23.836	-23.701	0.135	1.051	-0.184	-0.158	-2.547
TS12	2.15	30.785	-30.632	0.153	1.214	-0.216	-0.185	-2.945
TS13	2.01	27.393	-27.149	0.244	1.662	-0.337	-0.314	-4.065
TS14	1.95	22.124	-21.888	0.236	1.928	-0.315	-0.292	-4.640
TS15	2.41	27.666	-27.566	0.101	0.683	-0.117	-0.101	-1.638
TS16	2.06	29.557	-29.380	0.177	1.496	-0.237	-0.209	-3.583
TS17	2.02	30.036	-29.772	0.264	1.647	-0.331	-0.304	-3.975
TS18	1.97	37.351	-37.238	0.113	1.831	-0.333	-0.314	-4.467
TS19	1.92	37.721	-37.564	0.157	1.998	-0.376	-0.334	-4.967
TS20	2.45	20.002	-20.101	-0.099	0.637	-0.080	-0.073	-1.504
TS21	2.21	20.840	-20.775	0.065	1.096	-0.144	-0.121	-2.554

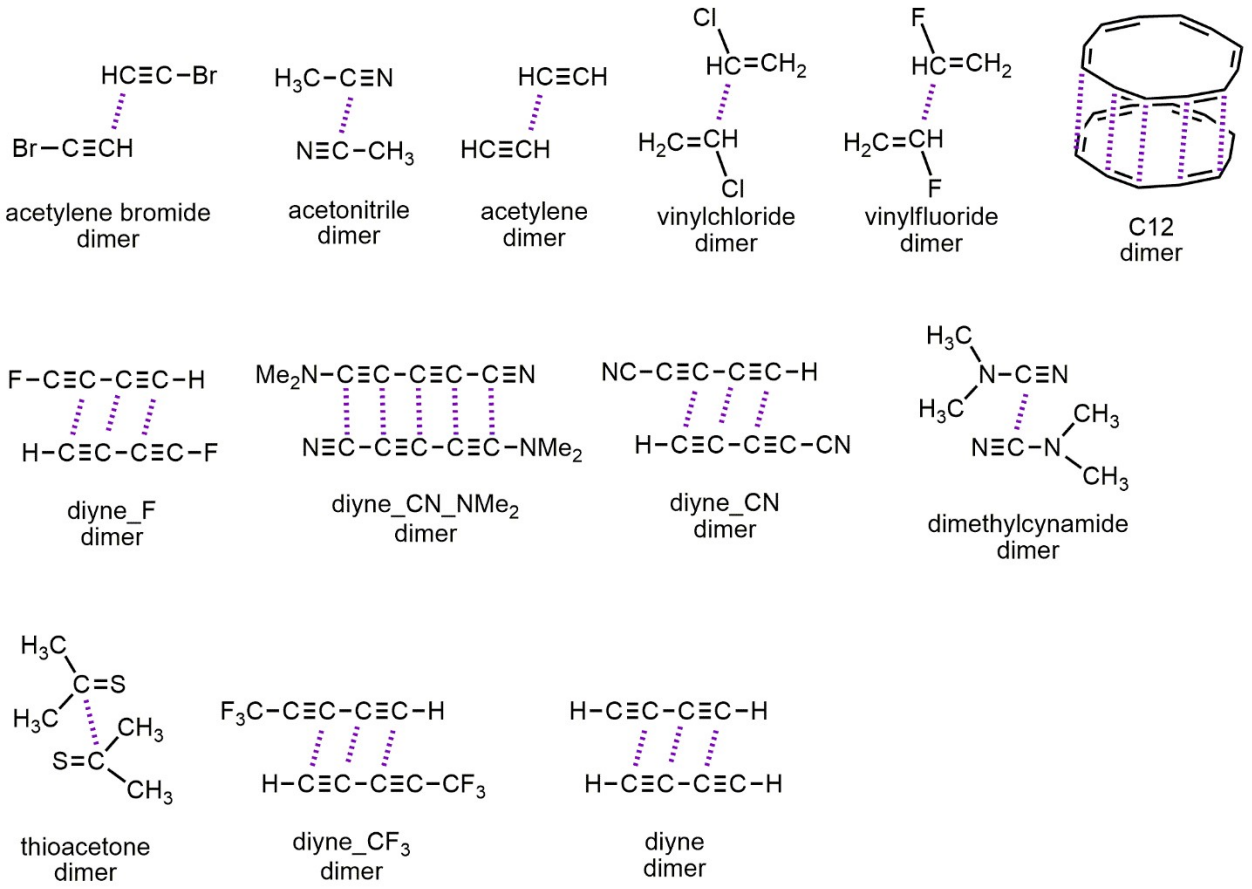

Figure S11. Selected set of π-conjugated dimers.

Table S15. The CC bond distance (Å) and the MESP data V_{bnp}, V_{ρ}, $V(r)$ and eigenvalues (in au) of π-conjugated dimers.

system	d_{CC}	V_{bnp}	V_{ρ}	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}	λ'_{v1}
Acetylenebromide dimer	1.20	23.498	-22.072	1.426	12.060	-3.520	-3.517	-25.492
	1.20	23.498	-22.072	1.426	12.060	-3.520	-3.517	-25.492
	3.31	16.206	-16.177	0.029	0.102	-0.023	-0.004	-0.212
Acetonitrile dimer	1.46	14.949	-14.106	0.843	6.096	-1.404	-1.398	-14.157
	1.46	14.949	-14.106	0.842	6.096	-1.404	-1.398	-14.157
	3.25	11.858	-11.854	0.004	0.120	-0.015	-0.015	-0.244
Acetylene dimer	3.30	7.449	-7.425	0.024	0.104	-0.024	-0.005	-0.213
Vinylchloride dimer	3.15	15.711	-15.682	0.029	0.140	-0.030	-0.009	-0.306
Diyne dimer	3.42	11.457	-11.466	-0.009	0.009	-0.004	-0.003	-0.165
	3.42	11.451	-11.459	-0.009	0.084	-0.013	-0.012	-0.164
	3.41	12.322	-12.350	-0.028	0.083	-0.008	-0.001	-0.169
Diyneflouride dimer	3.23	15.217	-15.210	0.007	0.135	-0.024	-0.020	-0.254
	3.23	15.217	-15.210	0.007	0.135	-0.024	-0.020	-0.254
	3.27	15.625	-15.627	-0.002	0.109	-0.016	-0.009	-0.232

Diynecyanide dimer	3.25	14.505	-14.474	0.031	0.122	-0.021	-0.020	-0.243
	3.25	14.505	-14.474	0.031	0.122	-0.021	-0.020	-0.243
	3.39	16.031	-16.003	0.028	0.094	-0.015	-0.013	-0.177
	3.36	15.720	-15.693	0.027	0.098	-0.015	-0.011	-0.190
	3.36	15.720	-15.693	0.027	0.098	-0.015	-0.011	-0.190
C12 dimer	3.18	24.677	-24.642	0.034	0.133	-0.018	-0.014	-0.283
	3.18	24.677	-24.643	0.034	0.133	-0.018	-0.014	-0.283
	3.18	24.678	-24.644	0.034	0.133	-0.018	-0.014	-0.283
	3.18	24.678	-24.644	0.034	0.133	-0.018	-0.014	-0.283
	3.18	24.677	-24.643	0.034	0.133	-0.018	-0.014	-0.283
	3.18	24.676	-24.643	0.034	0.132	-0.018	-0.014	-0.282
	3.19	24.508	-24.476	0.032	0.124	-0.017	-0.014	-0.275
	3.19	24.509	-24.477	0.032	0.124	-0.017	-0.014	-0.274
	3.19	24.509	-24.477	0.032	0.124	-0.017	-0.014	-0.274
	3.19	24.509	-24.477	0.032	0.125	-0.017	-0.014	-0.275
	3.19	24.509	-24.477	0.032	0.124	-0.017	-0.014	-0.274
	3.19	24.511	-24.479	0.032	0.124	-0.017	-0.014	-0.274
diyne_CN_NMe_2_dimer	3.23	21.075	-21.073	0.002	0.126	-0.022	-0.015	-0.252
	3.40	21.243	-21.260	-0.017	0.087	-0.009	-0.008	-0.171
Dimethylcynamide dimer	3.08	18.108	-18.108	0.000	0.169	-0.036	-0.017	-0.353
Thioacetone dimer	3.51	18.449	-18.407	0.042	0.080	-0.015	-0.010	-0.134
Vinylfluoride dimer	3.06	13.235	-13.195	0.040	0.180	-0.051	-0.030	-0.371
diyneCF_3 dimer	3.40	20.805	-20.767	0.039	0.131	-0.037	-0.021	-0.173
	3.40	20.802	-20.763	0.038	0.131	-0.037	-0.021	-0.173
	3.39	21.577	-21.560	0.017	0.094	-0.016	-0.015	-0.175
	3.37	21.558	-21.542	0.015	0.101	-0.016	-0.007	-0.182
	3.37	21.557	-21.541	0.015	0.101	-0.016	-0.007	-0.182
C2@C60	2.95	57.258	-57.186	0.072	0.168	-0.009	-0.003	-0.481
	2.95	57.258	-57.186	0.071	0.167	-0.009	-0.003	-0.479
	3.10	57.127	-57.061	0.067	0.120	-0.012	-0.006	-0.338
	3.11	57.126	-57.059	0.066	0.119	-0.011	-0.006	-0.336
	3.10	57.122	-57.056	0.066	0.119	-0.010	-0.005	-0.342
	3.10	57.122	-57.056	0.066	0.119	-0.010	-0.005	-0.342

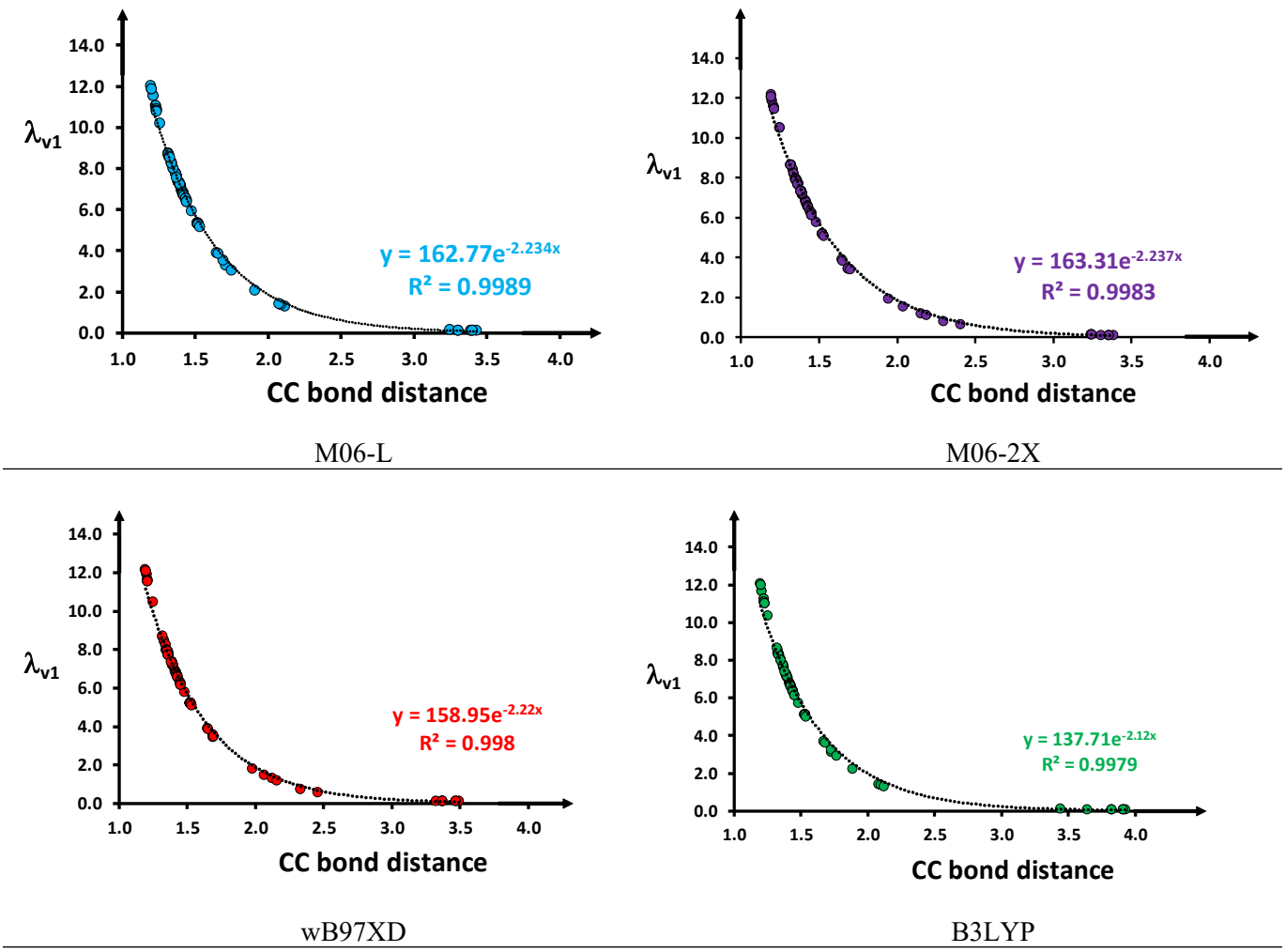

Figure S12. The exponential variation of λ_{v1} (in au) with CC bond distances (Å) using different levels of theory.

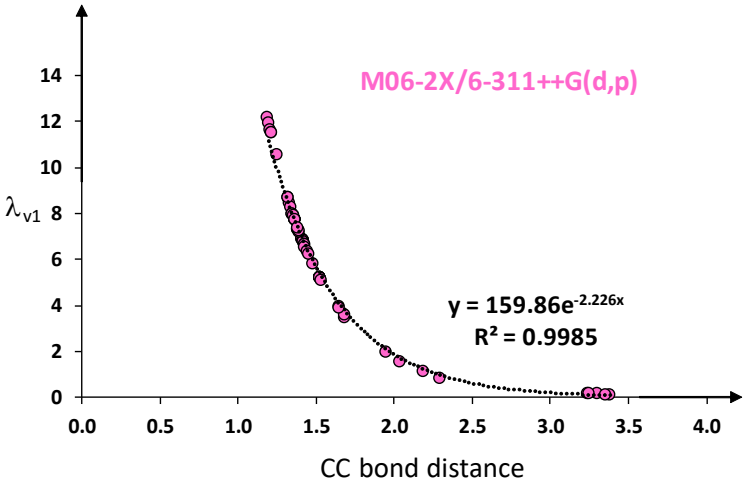

Figure S13. The exponential variation of λ_{v1} (in au) with CC bond distances (Å) using M06-2X/6-311++G(d,p) level of theory.

Table S16. The CC bond distance (Å) and the AIM data ρ(r) and eigenvalues (in au) of alkanes.

system	d_{cc}	ρ(r)	$\lambda_{\rho 1}$	$\lambda_{\rho 2}$	$\lambda_{\rho 3}$	$\nabla^2\rho$
ethane	1.53	0.238	-0.433	-0.433	0.336	-0.530
propane	1.53	0.240	-0.441	-0.437	0.340	-0.537
	1.53	0.240	-0.441	-0.437	0.340	-0.537
butane	1.53	0.242	-0.447	-0.440	0.344	-0.543
	1.53	0.240	-0.440	-0.437	0.339	-0.538
	1.53	0.240	-0.440	-0.437	0.339	-0.537
decane	1.53	0.241	-0.445	-0.440	0.343	-0.542
	1.53	0.241	-0.446	-0.440	0.343	-0.542
	1.53	0.241	-0.446	-0.440	0.344	-0.542
	1.53	0.241	-0.445	-0.440	0.343	-0.542
	1.53	0.241	-0.445	-0.440	0.343	-0.542
	1.53	0.241	-0.446	-0.440	0.343	-0.542
	1.53	0.241	-0.446	-0.440	0.344	-0.542
	1.53	0.240	-0.439	-0.437	0.339	-0.537
	1.53	0.240	-0.439	-0.437	0.339	-0.537

Table S17. The CC bond distance (Å) and the AIM data ρ(r) and eigenvalues (in au) of cycloalkanes.

system	d_{cc}	ρ(r)	$\lambda_{\rho 1}$	$\lambda_{\rho 2}$	$\lambda_{\rho 3}$	$\nabla^2\rho$
cyclopropane	1.50	0.236	-0.440	-0.288	0.314	-0.413
cyclobutane	1.55	0.233	-0.420	-0.417	0.344	-0.493
cyclohexane	1.53	0.240	-0.439	-0.437	0.343	-0.533
adamentane	1.54	0.238	-0.433	-0.433	0.344	-0.523
cubane	1.56	0.229	-0.410	-0.409	0.349	-0.470

Table S18. The CC bond distance (Å) and the AIM data ρ(r) and eigenvalues (in au) of sterically crowded systems.

system	d_{cc}	ρ(r)	$\lambda_{\rho 1}$	$\lambda_{\rho 2}$	$\lambda_{\rho 3}$	$\nabla^2\rho$
Pbtth	1.69	0.176	-0.288	-0.280	0.324	-0.244
Ptho	1.69	0.179	-0.294	-0.292	0.316	-0.270
Bptd	1.65	0.191	-0.320	-0.318	0.327	-0.312
Ahod	1.66	0.191	-0.320	-0.318	0.327	-0.312
Dddcpa	1.70	0.173	-0.280	-0.280	0.322	-0.238
Ttca	1.73	0.164	-0.261	-0.259	0.306	-0.214
Dddcada	1.76	0.156	-0.243	-0.240	0.297	-0.186

Hdbec	1.67	0.184	-0.305	-0.305	0.323	-0.287
Tdtca	1.75	0.159	-0.248	-0.247	0.299	-0.196
1,2-diamino-o-carborane-1	1.79	0.138	-0.215	-0.067	0.273	-0.009
1,2-diamino-o-carborane-2	1.82	0.133	-0.204	-0.056	0.267	-0.007

Table S19. The CC bond distance (Å) and the AIM data ρ(r) and eigenvalues (in au) of alkenes.

system	d_{cc}	ρ(r)	$\lambda_{\rho 1}$	$\lambda_{\rho 2}$	$\lambda_{\rho 3}$	$\nabla^2\rho$
ethene	1.32	0.344	-0.734	-0.550	0.256	-1.028
Butadiene	1.33	0.341	-0.727	-0.549	0.264	-1.011
	1.46	0.272	-0.541	-0.501	0.335	-0.707
hexatriene	1.33	0.339	-0.723	-0.548	0.266	-1.005
	1.34	0.336	-0.716	-0.548	0.274	-0.990
	1.45	0.275	-0.547	-0.503	0.333	-0.717
octatetraene	1.33	0.339	-0.722	-0.547	0.266	-1.003
	1.34	0.335	-0.712	-0.547	0.276	-0.984
	1.45	0.278	-0.555	-0.505	0.331	-0.730
	1.45	0.276	-0.549	-0.504	0.333	-0.720
decapentaene	1.33	0.339	-0.722	-0.547	0.266	-1.003
	1.34	0.335	-0.711	-0.547	0.276	-0.981
	1.35	0.333	-0.708	-0.546	0.278	-0.976
	1.45	0.279	-0.558	-0.506	0.330	-0.734
	1.45	0.276	-0.550	-0.504	0.333	-0.721

Table S20. The CC bond distance (Å) and the AIM data ρ(r) and eigenvalues (in au) of polycyclic benzenoid hydrocarbons.

system	d_{cc}	ρ(r)	$\lambda_{\rho 1}$	$\lambda_{\rho 2}$	$\lambda_{\rho 3}$	$\nabla^2\rho$
benzene	1.39	0.308	-0.635	-0.531	0.308	-0.858
naphthalene	1.37	0.320	-0.669	-0.540	0.295	-0.915
	1.37	0.320	-0.669	-0.540	0.295	-0.915
	1.37	0.320	-0.669	-0.540	0.295	-0.915
	1.37	0.320	-0.669	-0.540	0.295	-0.915
	1.42	0.295	-0.598	-0.518	0.320	-0.796
	1.42	0.295	-0.598	-0.518	0.320	-0.796
	1.42	0.294	-0.596	-0.519	0.324	-0.792
	1.42	0.294	-0.596	-0.519	0.324	-0.792
	1.42	0.294	-0.595	-0.516	0.328	-0.783
	1.42	0.294	-0.596	-0.519	0.324	-0.792

	1.42	0.294	-0.596	-0.519	0.324	-0.792
Anthracene	1.36	0.325	-0.682	-0.543	0.289	-0.936
	1.39	0.307	-0.631	-0.530	0.312	-0.849
	1.43	0.288	-0.581	-0.511	0.324	-0.768
	1.43	0.288	-0.581	-0.513	0.328	-0.766
	1.43	0.287	-0.576	-0.508	0.332	-0.752
biphenyl	1.39	0.309	-0.636	-0.531	0.307	-0.860
	1.39	0.308	-0.635	-0.532	0.308	-0.858
	1.40	0.304	-0.624	-0.522	0.314	-0.832
	1.48	0.262	-0.513	-0.482	0.343	-0.653
biphenylene	1.37	0.318	-0.659	-0.538	0.292	-0.904
	1.38	0.311	-0.643	-0.524	0.303	-0.864
	1.42	0.293	-0.593	-0.507	0.320	-0.780
	1.42	0.304	-0.633	-0.538	0.336	-0.835
	1.51	0.243	-0.447	-0.433	0.349	-0.530

Table S21. The CC bond distance (Å) and the AIM data ρ(r) and eigenvalues (in au) of annulenes.

system	d_{cc}	ρ(r)	$\lambda_{\rho 1}$	$\lambda_{\rho 2}$	$\lambda_{\rho 3}$	$\nabla^2\rho$
14 annulene	1.35	0.306	-0.627	-0.527	0.308	-0.846
	1.35	0.304	-0.619	-0.525	0.309	-0.835
	1.35	0.293	-0.594	-0.499	0.321	-0.772
	1.36	0.293	-0.594	-0.498	0.318	-0.774
	1.44	0.306	-0.627	-0.527	0.308	-0.846
	1.45	0.304	-0.619	-0.525	0.309	-0.835
	1.46	0.293	-0.594	-0.498	0.318	-0.774
	1.46	0.293	-0.594	-0.499	0.321	-0.772
16 annulene	1.34	0.333	-0.706	-0.540	0.276	-0.971
	1.34	0.332	-0.703	-0.535	0.277	-0.961
	1.45	0.275	-0.545	-0.499	0.332	-0.712
	1.46	0.271	-0.534	-0.494	0.334	-0.695

Table S22. The CC bond distance (Å) and the AIM data ρ(r) and eigenvalues (in au) of carbon clusters

system	d_{cc}	ρ(r)	$\lambda_{\rho 1}$	$\lambda_{\rho 2}$	$\lambda_{\rho 3}$	$\nabla^2\rho$
ovalene	1.40	0.306	-0.630	-0.529	0.312	-0.846
	1.43	0.290	-0.586	-0.514	0.328	-0.772
	1.44	0.285	-0.573	-0.510	0.329	-0.754
	1.41	0.299	-0.610	-0.524	0.321	-0.812

	1.42	0.292	-0.592	-0.516	0.327	-0.781
	1.44	0.285	-0.572	-0.509	0.329	-0.752
	1.42	0.293	-0.593	-0.517	0.326	-0.784
	1.44	0.286	-0.574	-0.510	0.331	-0.753
	1.41	0.299	-0.609	-0.523	0.322	-0.811
	1.41	0.298	-0.608	-0.522	0.320	-0.810
	1.37	0.317	-0.659	-0.537	0.298	-0.897
	1.36	0.328	-0.691	-0.543	0.285	-0.949
C60	1.45	0.276	-0.543	-0.478	0.336	-0.686
	1.39	0.309	-0.631	-0.518	0.305	-0.844

Table S23. The CC bond distance (Å) and the AIM data ρ(r) and eigenvalues (in au) of alkynes.

system	d_{cc}	ρ(r)	$\lambda_{\rho 1}$	$\lambda_{\rho 2}$	$\lambda_{\rho 3}$	$\nabla^2\rho$
acetylene	1.20	0.410	-0.657	-0.657	0.085	-1.228
diacetylene	1.20	0.404	-0.646	-0.646	0.099	-1.193
	1.38	0.299	-0.570	-0.570	0.293	-0.848
triacetylene	1.20	0.403	-0.647	-0.647	0.102	-1.193
	1.21	0.398	-0.636	-0.636	0.108	-1.163
	1.37	0.303	-0.575	-0.575	0.288	-0.863
tetracetylene	1.20	0.403	-0.648	-0.648	0.103	-1.193
	1.21	0.396	-0.637	-0.637	0.113	-1.161
	1.36	0.308	-0.581	-0.581	0.284	-0.877
	1.37	0.304	-0.577	-0.577	0.287	-0.867
penta acetylene	1.36	0.309	-0.583	-0.583	0.282	-0.883
	1.21	0.396	-0.637	-0.637	0.114	-1.161
	1.20	0.403	-0.649	-0.649	0.103	-1.194
	1.37	0.305	-0.578	-0.578	0.287	-0.869
	1.21	0.395	-0.638	-0.638	0.117	-1.159
	1.36	0.309	-0.583	-0.583	0.282	-0.883
	1.21	0.396	-0.637	-0.637	0.114	-1.161
	1.37	0.305	-0.578	-0.578	0.287	-0.869
	1.20	0.403	-0.649	-0.649	0.103	-1.194
hexa acetylene	1.22	0.394	-0.638	-0.638	0.119	-1.158
	1.36	0.310	-0.583	-0.583	0.282	-0.885
	1.21	0.396	-0.638	-0.638	0.115	-1.161
	1.36	0.311	-0.585	-0.585	0.281	-0.889
	1.37	0.305	-0.578	-0.578	0.287	-0.870
	1.20	0.403	-0.649	-0.649	0.103	-1.194
	1.22	0.394	-0.638	-0.638	0.119	-1.158

	1.36	0.310	-0.583	-0.583	0.282	-0.885
	1.21	0.396	-0.638	-0.638	0.115	-1.161
	1.37	0.305	-0.578	-0.578	0.287	-0.870
	1.20	0.403	-0.649	-0.649	0.103	-1.194
hepta acetylene	1.22	0.394	-0.639	-0.639	0.121	-1.157
	1.35	0.311	-0.586	-0.586	0.280	-0.891
	1.22	0.394	-0.639	-0.639	0.120	-1.157
	1.36	0.310	-0.584	-0.584	0.282	-0.886
	1.35	0.311	-0.586	-0.586	0.280	-0.891
	1.22	0.394	-0.639	-0.639	0.120	-1.157
	1.36	0.310	-0.584	-0.584	0.282	-0.886
	1.21	0.396	-0.638	-0.638	0.115	-1.161
	1.37	0.305	-0.578	-0.578	0.287	-0.870
	1.20	0.403	-0.649	-0.649	0.103	-1.195
	1.21	0.396	-0.638	-0.638	0.115	-1.161
	1.37	0.305	-0.578	-0.578	0.287	-0.870
	1.20	0.403	-0.649	-0.649	0.103	-1.195
octa acetylene	1.22	0.394	-0.639	-0.639	0.122	-1.157
	1.35	0.312	-0.586	-0.586	0.280	-0.892
	1.22	0.394	-0.639	-0.639	0.120	-1.158
	1.35	0.312	-0.587	-0.587	0.279	-0.894
	1.36	0.310	-0.584	-0.584	0.281	-0.887
	1.22	0.396	-0.638	-0.638	0.115	-1.161
	1.22	0.394	-0.639	-0.639	0.122	-1.157
	1.35	0.312	-0.586	-0.586	0.280	-0.892
	1.22	0.394	-0.639	-0.639	0.120	-1.158
	1.36	0.310	-0.584	-0.584	0.281	-0.887
	1.22	0.396	-0.638	-0.638	0.115	-1.161
	1.37	0.305	-0.579	-0.579	0.287	-0.871
	1.20	0.403	-0.649	-0.649	0.103	-1.195
	1.37	0.305	-0.579	-0.579	0.287	-0.871
	1.20	0.403	-0.649	-0.649	0.103	-1.195
nona acetylene	1.22	0.393	-0.639	-0.639	0.122	-1.156
	1.35	0.312	-0.587	-0.587	0.279	-0.895
	1.22	0.393	-0.639	-0.639	0.122	-1.157
	1.35	0.312	-0.586	-0.586	0.280	-0.893
	1.35	0.312	-0.587	-0.587	0.279	-0.895
	1.22	0.393	-0.639	-0.639	0.122	-1.157
	1.35	0.312	-0.586	-0.586	0.280	-0.893
	1.22	0.394	-0.639	-0.639	0.120	-1.158
	1.36	0.310	-0.584	-0.584	0.281	-0.887

1.21	0.396	-0.638	-0.638	0.115	-1.161
1.37	0.305	-0.579	-0.579	0.287	-0.871
1.20	0.403	-0.649	-0.649	0.103	-1.195
1.22	0.394	-0.639	-0.639	0.120	-1.158
1.36	0.310	-0.584	-0.584	0.281	-0.887
1.21	0.396	-0.638	-0.638	0.115	-1.161
1.37	0.305	-0.579	-0.579	0.287	-0.871
1.20	0.403	-0.649	-0.649	0.103	-1.195

Table S24. The CC bond distance (Å) and the AIM data ρ(r) and eigenvalues (in au) of carbon rings.

system	d_{cc}	ρ(r)	$\lambda_{\rho 1}$	$\lambda_{\rho 2}$	$\lambda_{\rho 3}$	$\nabla^2\rho$
C2	1.30	0.325	-0.629	-0.415	0.198	-0.846
C6	1.32	0.325	-0.531	-0.483	0.213	-0.801
C8	1.25	0.375	-0.640	-0.582	0.221	-1.001
	1.39	0.287	-0.521	-0.443	0.251	-0.713
C10	1.28	0.350	-0.605	-0.601	0.211	-0.995
C12	1.23	0.389	-0.651	-0.627	0.149	-1.129
	1.37	0.300	-0.556	-0.530	0.272	-0.814
C14	1.28	0.353	-0.618	-0.614	0.212	-1.020
C16	1.37	0.301	-0.558	-0.554	0.285	-0.827
	1.22	0.396	-0.651	-0.641	0.126	-1.166
C20	1.36	0.306	-0.570	-0.567	0.283	-0.855
	1.22	0.394	-0.645	-0.640	0.127	-1.158

Table S25. The CC bond distance (Å) and the AIM data ρ(r) and eigenvalues (in au) of heterocyclic systems

system	d_{cc}	ρ(r)	$\lambda_{\rho 1}$	$\lambda_{\rho 2}$	$\lambda_{\rho 3}$	$\nabla^2\rho$
DBN	1.53	0.243	-0.454	-0.445	0.345	-0.554
	1.53	0.242	-0.448	-0.442	0.349	-0.541
	1.53	0.240	-0.447	-0.439	0.347	-0.539
	1.53	0.237	-0.432	-0.429	0.341	-0.520
	1.52	0.252	-0.489	-0.465	0.353	-0.601
porphyrin	1.43	0.289	-0.586	-0.505	0.331	-0.760
	1.39	0.307	-0.642	-0.535	0.314	-0.863
	1.39	0.309	-0.642	-0.532	0.305	-0.870
	1.46	0.276	-0.550	-0.488	0.346	-0.693
	1.39	0.307	-0.642	-0.535	0.314	-0.863
	1.46	0.276	-0.550	-0.488	0.346	-0.693
	1.39	0.309	-0.642	-0.532	0.305	-0.870

	1.35	0.331	-0.690	-0.538	0.281	-0.948
	1.36	0.321	-0.664	-0.525	0.292	-0.898
	1.39	0.309	-0.642	-0.532	0.305	-0.870
aziridine	1.48	0.245	-0.463	-0.331	0.318	-0.476
cynogen	1.39	0.294	-0.575	-0.575	0.298	-0.851
pyramidopyramidine	1.40	0.311	-0.649	-0.550	0.327	-0.873
	1.42	0.299	-0.627	-0.545	0.338	-0.834
benzonitrile	1.44	0.273	-0.528	-0.499	0.293	-0.734
	1.40	0.304	-0.628	-0.521	0.312	-0.837
	1.39	0.310	-0.640	-0.535	0.306	-0.868
	1.39	0.308	-0.634	-0.534	0.309	-0.860
furfural	1.42	0.286	-0.562	-0.483	0.321	-0.725
	1.36	0.326	-0.688	-0.532	0.290	-0.930
	1.36	0.327	-0.690	-0.524	0.285	-0.930
	1.46	0.279	-0.587	-0.516	0.354	-0.748
ethylene glycol	1.51	0.259	-0.527	-0.488	0.360	-0.655
tetrathiafulavalene	1.33	0.337	-0.705	-0.512	0.264	-0.953
	1.34	0.327	-0.679	-0.475	0.272	-0.883
thiaindans	1.39	0.308	-0.633	-0.527	0.308	-0.852
	1.39	0.306	-0.627	-0.522	0.308	-0.840
	1.40	0.305	-0.622	-0.521	0.317	-0.826
	1.39	0.307	-0.628	-0.522	0.306	-0.844
	1.39	0.305	-0.627	-0.524	0.309	-0.842
	1.39	0.309	-0.634	-0.524	0.306	-0.852
	1.53	0.240	-0.439	-0.436	0.343	-0.532
	1.51	0.249	-0.471	-0.455	0.343	-0.582
dithianodithiine	1.52	0.245	-0.453	-0.451	0.346	-0.558
	1.34	0.329	-0.677	-0.489	0.277	-0.890
	1.53	0.242	-0.451	-0.443	0.366	-0.528
thiatane	1.54	0.239	-0.438	-0.436	0.342	-0.532
thiane	1.53	0.242	-0.445	-0.443	0.344	-0.544
	1.53	0.240	-0.440	-0.437	0.343	-0.534
SeC_3Se	1.27	0.358	-0.628	-0.628	0.199	-1.057
SC_3S	1.27	0.357	-0.617	-0.617	0.195	-1.040
NCCP	1.38	0.299	-0.577	-0.577	0.289	-0.866
C_5S	1.29	0.346	-0.623	-0.623	0.213	-1.034
	1.26	0.366	-0.635	-0.635	0.185	-1.084
	1.28	0.353	-0.620	-0.620	0.205	-1.036

Table S26. The CC bond distance (Å) and the AIM data ρ(r) and eigenvalues (in au) of cation, anion and radical systems

system	d_{cc}	$\rho(r)$	$\lambda_{\rho 1}$	$\lambda_{\rho 2}$	$\lambda_{\rho 3}$	$\nabla^2\rho$
cyclopropenyl cation	1.36	0.314	-0.540	-0.456	0.294	-0.703
tropellium cation	1.39	0.309	-0.638	-0.559	0.312	-0.884
benzene-1-ylium	1.32	0.337	-0.643	-0.548	0.217	-0.974
	1.43	0.270	-0.506	-0.431	0.296	-0.642
	1.39	0.310	-0.637	-0.533	0.304	-0.866
propan-1-ylium	1.39	0.305	-0.616	-0.535	0.298	-0.852
	1.69	0.158	-0.251	-0.107	0.263	-0.095
propan-2-ylium	1.44	0.288	-0.562	-0.528	0.292	-0.799
2-methylpropan-2-ylium	1.46	0.278	-0.541	-0.513	0.309	-0.745
	1.46	0.278	-0.539	-0.512	0.309	-0.742
	1.46	0.277	-0.536	-0.511	0.309	-0.738
acetylene cation	1.19	0.342	-0.340	-0.340	0.144	-0.536
ethen-1-ylium	1.25	0.385	-0.775	-0.623	0.340	-1.058
cyclopentadienyl anion	1.41	0.291	-0.584	-0.467	0.315	-0.736
	1.41	0.291	-0.585	-0.468	0.315	-0.738
benzen-1-ide	1.42	0.287	-0.528	-0.518	0.298	-0.747
	1.40	0.302	-0.614	-0.512	0.309	-0.817
	1.39	0.304	-0.626	-0.517	0.310	-0.833
acetate	1.57	0.227	-0.434	-0.410	0.363	-0.481
ethylene carbonate	1.53	0.251	-0.490	-0.470	0.363	-0.596
ethyn-1-ide	1.24	0.385	-0.712	-0.712	0.212	-1.212
ethan-1-ide	1.54	0.222	-0.392	-0.346	0.302	-0.436
2-oxopropan-1-ide	1.38	0.311	-0.658	-0.481	0.299	-0.840
	1.55	0.234	-0.445	-0.425	0.354	-0.516
benzene_radical	1.37	0.315	-0.637	-0.542	0.291	-0.889
	1.40	0.301	-0.612	-0.511	0.310	-0.812
	1.39	0.307	-0.632	-0.527	0.309	-0.851
3-methylbut-2-enenitrile radical	1.31	0.344	-0.705	-0.535	0.236	-1.005
	1.37	0.303	-0.570	-0.554	0.276	-0.847
	1.51	0.249	-0.471	-0.453	0.338	-0.586
	1.51	0.245	-0.459	-0.444	0.338	-0.565
allyl_radical	1.38	0.312	-0.647	-0.531	0.299	-0.879
vinyl_radical	1.30	0.352	-0.732	-0.555	0.228	-1.059

Table S27. The CC bond distance (Å) and the AIM data $\rho(r)$ and eigenvalues (in au) of systems with multiple types of CC bonds.

system	d_{cc}	$\rho(r)$	$\lambda_{\rho 1}$	$\lambda_{\rho 2}$	$\lambda_{\rho 3}$	$\nabla^2\rho$
dihydroindene	1.39	0.309	-0.634	-0.530	0.307	-0.856
	1.39	0.306	-0.628	-0.524	0.309	-0.842

	1.40	0.309	-0.637	-0.532	0.318	-0.851
	1.39	0.307	-0.630	-0.526	0.309	-0.848
	1.39	0.306	-0.628	-0.524	0.309	-0.842
	1.39	0.309	-0.634	-0.530	0.307	-0.856
	1.51	0.248	-0.465	-0.452	0.344	-0.572
	1.51	0.248	-0.465	-0.452	0.344	-0.572
	1.54	0.234	-0.425	-0.424	0.343	-0.505
	1.54	0.234	-0.425	-0.424	0.343	-0.505
isoprene	1.34	0.339	-0.724	-0.543	0.268	-0.999
	1.47	0.268	-0.531	-0.492	0.340	-0.683
	1.33	0.340	-0.723	-0.547	0.264	-1.006
	1.50	0.251	-0.474	-0.460	0.339	-0.595
2-pentene	1.50	0.251	-0.476	-0.460	0.336	-0.600
	1.33	0.342	-0.732	-0.537	0.262	-1.006
	1.50	0.253	-0.479	-0.465	0.340	-0.604
	1.53	0.236	-0.431	-0.427	0.339	-0.520
hex_1_ene_3_yne	1.43	0.278	-0.539	-0.511	0.306	-0.745
	1.33	0.339	-0.725	-0.541	0.264	-1.002
	1.20	0.401	-0.640	-0.625	0.097	-1.167
	1.46	0.261	-0.484	-0.480	0.308	-0.656
	1.53	0.235	-0.432	-0.424	0.339	-0.518
hexa_1,5_dien_3_yne	1.43	0.280	-0.543	-0.513	0.303	-0.753
	1.33	0.339	-0.723	-0.542	0.265	-1.000
	1.21	0.400	-0.654	-0.621	0.104	-1.171
	1.43	0.280	-0.543	-0.513	0.303	-0.753
	1.33	0.339	-0.723	-0.542	0.265	-1.000

Table S28. The CC bond distance (Å) and the AIM data ρ(r) and eigenvalues (in au) of organometallic and hypervalent carbon compounds.

system	d_{cc}	ρ(r)	$\lambda_{\rho 1}$	$\lambda_{\rho 2}$	$\lambda_{\rho 3}$	$\nabla^2\rho$
η3-CrCl3	1.40	0.285	-0.456	-0.384	0.298	-0.542
metallacyclobutane	1.42	0.289	-0.510	-0.480	0.310	-0.680
ferrocene	1.42	0.289	-0.574	-0.456	0.314	-0.717
Bis(benzene)chromium(0)	1.41	0.292	-0.585	-0.474	0.311	-0.747
C3H4Li2	1.50	0.236	-0.441	-0.299	0.317	-0.423
	1.53	0.214	-0.334	-0.232	0.293	-0.273
C6H6_CrCO3	1.41	0.296	-0.595	-0.491	0.311	-0.775
Si2C5H2	1.38	0.315	-0.657	-0.518	0.302	-0.873
	1.42	0.287	-0.565	-0.498	0.320	-0.744
	1.42	0.287	-0.565	-0.498	0.320	-0.744
	1.46	0.254	-0.408	-0.389	0.309	-0.487

	1.46	0.254	-0.408	-0.389	0.309	-0.487
Ge2C5H2	1.38	0.312	-0.648	-0.511	0.305	-0.854
	1.42	0.286	-0.559	-0.489	0.319	-0.729
	1.42	0.286	-0.559	-0.489	0.319	-0.729
	1.46	0.261	-0.427	-0.423	0.314	-0.537
	1.46	0.261	-0.427	-0.423	0.314	-0.537
C6Li6	1.42	0.285	-0.512	-0.498	0.319	-0.691
C2B8	1.50	0.234	-0.421	-0.388	0.337	-0.472

Table S29. The CC bond distance (Å) and the AIM data ρ(r) and eigenvalues (in au) of transition states

system	d_{cc}	ρ(r)	$\lambda_{\rho 1}$	$\lambda_{\rho 2}$	$\lambda_{\rho 3}$	$\nabla^2\rho$
TS1	2.16	0.061	-0.064	-0.061	0.164	0.039
	2.41	0.040	-0.038	-0.024	0.116	0.054
TS2	2.30	0.048	-0.045	-0.040	0.135	0.050
	2.19	0.059	-0.060	-0.058	0.161	0.043
TS3	2.18	0.059	-0.062	-0.058	0.163	0.043
	2.38	0.041	-0.038	-0.033	0.119	0.049
TS4	2.33	0.046	-0.045	-0.038	0.130	0.047
	2.08	0.072	-0.082	-0.076	0.186	0.029
TS5	2.14	0.064	-0.068	-0.065	0.170	0.037
	2.40	0.041	-0.039	-0.025	0.117	0.053
TS6	1.92	0.099	-0.127	-0.121	0.235	-0.013
	2.63	0.027	-0.022	-0.013	0.084	0.049
TS7	1.98	0.089	-0.117	-0.096	0.217	0.004
TS8	2.00	0.087	-0.110	-0.099	0.214	0.005
TS9	2.04	0.073	-0.080	-0.078	0.190	0.032
TS10	2.13	0.068	-0.076	-0.071	0.188	0.041
TS11	2.21	0.057	-0.061	-0.053	0.152	0.038
TS12	2.15	0.065	-0.074	-0.065	0.169	0.030
TS13	2.01	0.080	-0.095	-0.090	0.209	0.024
TS14	1.95	0.102	-0.140	-0.128	0.244	-0.025
TS15	2.41	0.038	-0.033	-0.031	0.114	0.051
TS16	2.06	0.077	-0.096	-0.091	0.225	0.038
TS17	2.02	0.080	-0.095	-0.085	0.196	0.016
TS19	1.97	0.093	-0.118	-0.111	0.234	0.005
TS20	1.92	0.102	-0.135	-0.128	0.255	-0.008
TS21	2.45	0.036	-0.031	-0.028	0.114	0.054
TS22	2.21	0.060	-0.063	-0.060	0.166	0.043

Table S30. The CC bond distance (Å) and the AIM data ρ(r) and eigenvalues (in au) of π-conjugate dimers

system	d_{cc}	ρ(r)	$\lambda_{\rho 1}$	$\lambda_{\rho 2}$	$\lambda_{\rho 3}$	$\nabla^2\rho$
acetyleneBr_dimer	3.31	0.006	-0.004	-0.001	0.026	0.021
acetonitrile_dimer	3.25	0.007	-0.005	-0.002	0.029	0.023
diyneCN_dimer	3.39	0.005	-0.003	-0.001	0.020	0.016
	3.36	0.006	-0.003	-0.001	0.021	0.017
	3.36	0.006	-0.003	-0.001	0.021	0.017
	3.25	0.006	-0.004	-0.002	0.026	0.020
	3.25	0.006	-0.004	-0.002	0.026	0.020
acetylene_ dimer	3.30	0.006	-0.004	-0.001	0.027	0.022
vinylCl_ dimer	3.15	0.008	-0.005	-0.002	0.034	0.027
diyne_F_dimer	3.23	0.007	-0.004	-0.002	0.028	0.021
	3.27	0.007	-0.004	-0.001	0.026	0.021
C12 dimer	3.18	0.008	-0.005	-0.002	0.031	0.024
	3.19	0.008	-0.004	-0.001	0.029	0.024
diyne_CN_NMe_2_dimer	3.40	0.006	-0.003	0.000	0.021	0.018
vinylF_dimer	3.06	0.008	-0.004	-0.003	0.035	0.028
dimethyl cynamide_dimer	3.08	0.009	-0.006	-0.001	0.040	0.033
thiacetone_dimer	3.51	0.004	0.000	0.000	0.014	0.013
diyne_CF_3_dimer	3.39	0.005	-0.003	0.000	0.019	0.016
	3.37	0.006	-0.003	-0.002	0.021	0.016
diyne_dimer	3.41	0.006	-0.003	-0.001	0.022	0.017
C60_C2	2.95	0.013	-0.005	-0.003	0.057	0.048
	2.95	0.013	-0.005	-0.003	0.056	0.048
	2.95	0.013	-0.005	-0.003	0.055	0.047
	2.95	0.013	-0.005	-0.003	0.057	0.048
	2.96	0.013	-0.005	-0.003	0.055	0.047
	2.96	0.013	-0.005	-0.003	0.055	0.047
	2.96	0.013	-0.005	-0.003	0.055	0.047
	2.95	0.013	-0.005	-0.003	0.056	0.047
	2.95	0.013	-0.005	-0.003	0.057	0.048
	2.95	0.013	-0.005	-0.003	0.056	0.048

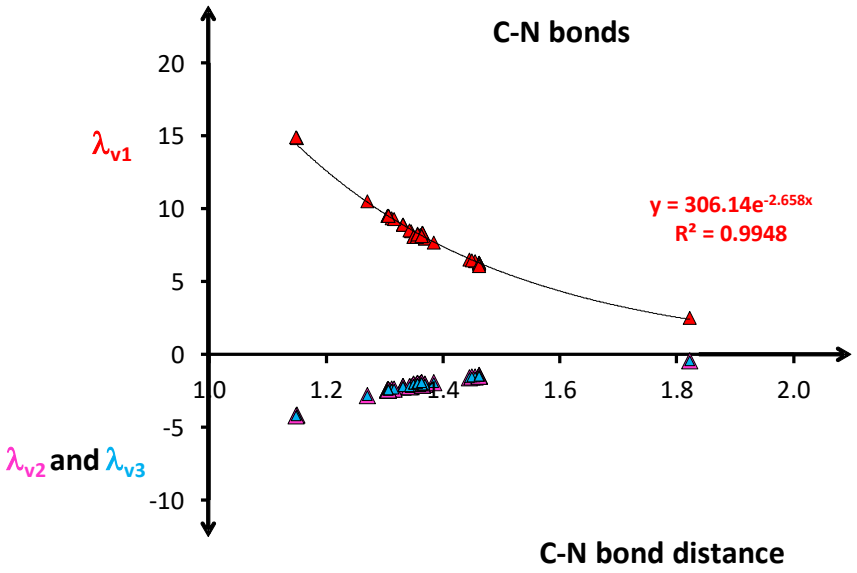

Figure S14. The exponential variation of $\lambda_{v1,}$ λ_{v2} and λ_{v3} (in au) with C-N bond distances (Å) from selected set of systems.

Table S31. MESP topology of selected set of systems containing C-N bonds. The C-N bond distance is given in Å and the MESP data V_{bnp}, V_p, $V(r)$ and eigenvalues are given in au.

system	d_{CN}	V_{bnp}	V_p	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}
Pyrrole	1.37	16.521	-15.565	0.955	7.995	-2.039	-1.786
	1.37	16.521	-15.565	0.955	7.995	-2.039	-1.786
Pyrazine	1.33	17.584	-16.534	1.050	8.911	-2.168	-2.145
	1.33	17.584	-16.534	1.050	8.911	-2.168	-2.145
	1.33	17.584	-16.534	1.050	8.911	-2.168	-2.145
	1.33	17.584	-16.534	1.050	8.911	-2.168	-2.145
Quinazoline	1.31	21.216	-20.110	1.107	9.532	-2.374	-2.323
	1.31	21.315	-20.210	1.105	9.570	-2.393	-2.321
	1.36	20.580	-19.602	0.977	8.216	-1.941	-1.937
	1.36	24.817	-23.839	0.977	8.200	-1.947	-1.938
Piperazine	1.46	17.945	-17.211	0.735	6.305	-1.464	-1.323
	1.46	17.945	-17.211	0.735	6.305	-1.464	-1.323
	1.46	17.944	-17.210	0.734	6.303	-1.464	-1.323
	1.46	17.944	-17.210	0.734	6.303	-1.464	-1.323
Pyrrolidine	1.46	16.584	-15.852	0.732	6.288	-1.458	-1.312
	1.46	16.584	-15.852	0.732	6.288	-1.458	-1.312
Thiozolidine	1.46	18.314	-17.541	0.772	6.409	-1.503	-1.347
Triazole	1.31	17.118	-16.032	1.086	9.378	-2.364	-2.207
	1.32	17.168	-16.096	1.072	9.302	-2.350	-2.103
	1.35	17.135	-16.084	1.051	8.516	-2.187	-1.900
	1.36	16.833	-15.866	0.967	8.233	-1.995	-1.881

Tetrazole	1.31	17.330	-16.206	1.124	9.540	-2.407	-2.204
	1.34	17.278	-16.191	1.087	8.571	-2.204	-1.933
DBN	1.27	22.891	-21.731	1.160	10.564	-2.791	-2.617
	1.38	23.424	-22.511	0.913	7.703	-1.917	-1.676
	1.45	21.871	-21.078	0.793	6.557	-1.557	-1.406
	1.45	21.736	-20.953	0.783	6.465	-1.534	-1.366
	1.46	20.429	-19.703	0.726	6.290	-1.408	-1.399
Benzonitrile	1.15	18.485	-16.913	1.572	14.886	-4.143	-4.142
Porphyrin	1.35	32.253	-31.269	0.984	8.100	-2.035	-1.810
	1.35	32.253	-31.269	0.984	8.100	-2.035	-1.810
	1.36	32.253	-31.269	0.984	8.100	-2.035	-1.810
	1.36	32.253	-31.269	0.983	8.100	-2.035	-1.809
	1.37	32.300	-31.341	0.960	8.365	-2.050	-1.925
	1.37	32.300	-31.340	0.960	8.364	-2.050	-1.925
	1.37	32.300	-31.340	0.960	8.364	-2.050	-1.925
	1.37	32.300	-31.340	0.960	8.363	-2.050	-1.924
Aziridine	1.46	13.557	-12.744	0.813	6.086	-1.469	-1.305
	1.46	13.557	-12.744	0.813	6.086	-1.469	-1.305
Cyanogen	1.15	14.790	-13.142	1.647	14.956	-4.172	-4.172
Pyramidopyramidine	1.31	21.251	-20.119	1.131	9.572	-2.383	-2.340
	1.31	21.250	-20.119	1.131	9.571	-2.383	-2.339
	1.31	21.400	-20.274	1.126	9.552	-2.386	-2.313
	1.31	21.400	-20.274	1.126	9.550	-2.385	-2.313
	1.36	22.289	-21.275	1.013	8.299	-1.980	-1.969
	1.36	22.288	-21.275	1.013	8.298	-1.980	-1.969
	1.36	20.653	-19.660	0.993	8.152	-1.923	-1.916
	1.36	20.652	-19.660	0.993	8.150	-1.923	-1.915
TS_{C-N}	1.82	23.157	-1.450	0.372	2.531	-0.421	-0.390

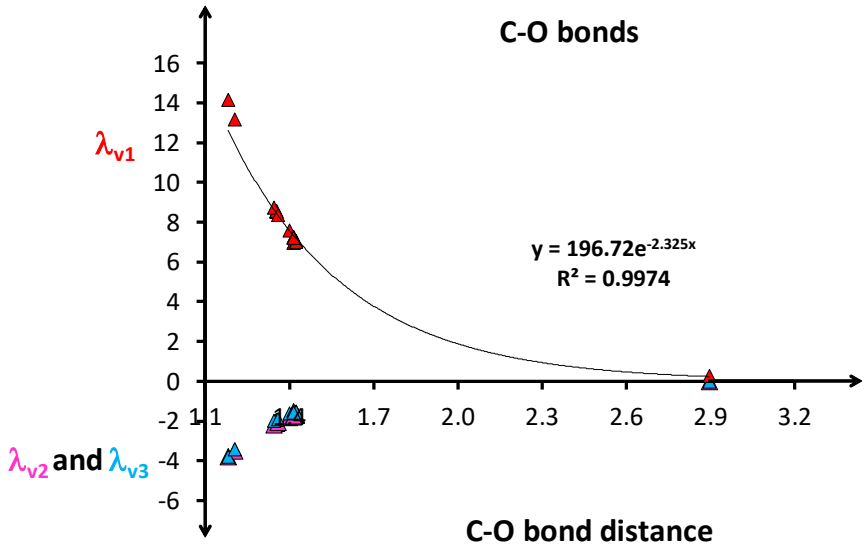

Figure S15. The exponential variation of $\lambda_{v1,}$ λ_{v2} and λ_{v3} (in au) with C-O bond distances (Å) from selected set of systems.

Table S32. MESP topology of selected set of systems containing C-O bonds. The C-O bond distance is given in Å and the MESP data V_{bnp}, V_{ρ}, $V(r)$ and eigenvalues are given in au.

system	d_{CO}	V_{bnp}	V_{ρ}	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}
Furan	1.35	17.148	-16.152	0.996	8.513	-2.127	-1.948
	1.35	17.148	-16.152	0.996	8.513	-2.127	-1.948
Tetrahydropyran	1.41	18.643	-17.824	0.820	7.221	-1.743	-1.607
	1.41	18.643	-17.824	0.820	7.221	-1.743	-1.607
THF	1.42	17.243	-16.445	0.798	7.028	-1.700	-1.542
	1.42	17.243	-16.445	0.798	7.027	-1.700	-1.541
Dioxolone	1.40	17.883	-17.006	0.877	7.556	-1.828	-1.643
	1.42	17.497	-16.677	0.820	7.036	-1.711	-1.547
Oxirane	1.41	14.329	-13.432	0.898	6.974	-1.804	-1.486
	1.41	14.329	-13.431	0.898	6.971	-1.803	-1.485
Ethylene carbonate	1.18	20.205	-18.726	1.480	14.132	-3.802	-3.787
	1.35	20.041	-19.010	1.032	8.575	-2.123	-1.939
	1.35	20.040	-19.009	1.031	8.573	-2.122	-1.938
	1.42	18.672	-17.803	0.868	7.012	-1.672	-1.540
	1.42	18.671	-17.803	0.868	7.009	-1.672	-1.539
Furfural	1.20	18.935	-17.549	1.385	13.155	-3.511	-3.431
	1.34	19.311	-18.268	1.043	8.738	-2.193	-2.015
	1.36	20.107	-19.101	1.006	8.354	-2.078	-1.897
Ethylene glycol	1.42	15.347	-14.523	0.825	7.198	-1.753	-1.605
	1.42	15.347	-14.522	0.825	7.198	-1.753	-1.605
NNDMAacetylCl	2.90	16.630	-16.680	-0.050	0.243	-0.025	-0.010

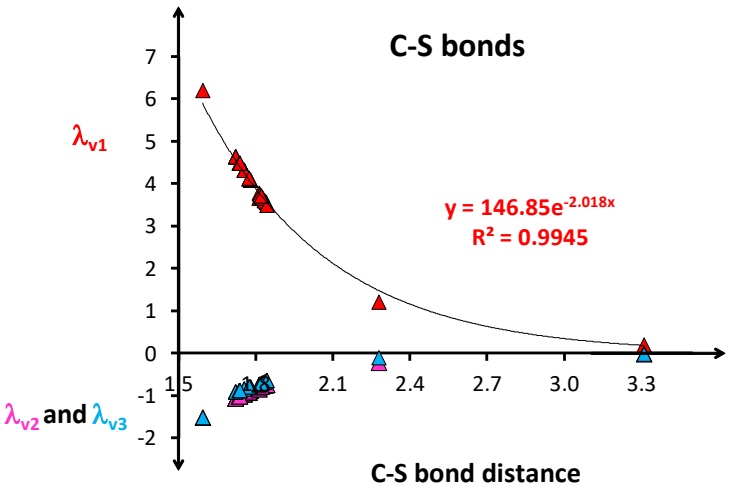

Figure S16. The exponential variation of $\lambda_{v1,}$ λ_{v2} and λ_{v3} (in au) with C-S bond distances (Å) from selected set of systems.

Table S33. MESP topology of selected set of systems containing C-S bonds. The C-S bond distance is given in Å and the MESP data V_{bnp}, V_{ρ}, $V(r)$ and eigenvalues are given in au.

system	d_{CS}	V_{bnp}	V_{ρ}	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}
thiophene	1.72	18.667	-17.945	0.723	4.641	-1.056	-0.917
	1.72	18.667	-17.945	0.723	4.641	-1.056	-0.917
thioxathene	1.78	27.181	-26.539	0.642	4.073	-0.882	-0.785
	1.78	27.181	-26.539	0.642	4.073	-0.882	-0.785
	1.83	17.804	-17.246	0.559	3.609	-0.764	-0.674
thiozolidine	1.84	17.804	-17.253	0.552	3.558	-0.744	-0.639
tetrathiafulvalene	1.75	25.759	-25.064	0.694	4.312	-0.963	-0.835
	1.75	25.759	-25.064	0.694	4.312	-0.963	-0.835
	1.75	25.759	-25.064	0.694	4.312	-0.963	-0.835
	1.75	25.759	-25.064	0.694	4.312	-0.963	-0.835
	1.77	28.322	-27.649	0.674	4.122	-0.929	-0.787
	1.77	28.322	-27.649	0.674	4.122	-0.929	-0.787
	1.77	28.322	-27.649	0.674	4.122	-0.929	-0.787
	1.77	28.322	-27.649	0.674	4.122	-0.929	-0.787
benzoyl isothiocyanate	1.59	21.146	-20.188	0.958	6.201	-1.508	-1.507
thiaindans	1.77	23.101	-22.459	0.642	4.123	-0.900	-0.789
	1.84	21.553	-20.988	0.566	3.591	-0.752	-0.669
thiirane	1.81	15.950	-15.297	0.652	3.655	-0.840	-0.747
	1.81	15.950	-15.297	0.652	3.655	-0.840	-0.747
lenthionine	1.81	26.066	-25.444	0.621	3.784	-0.792	-0.724
	1.82	25.982	-25.361	0.621	3.743	-0.797	-0.722
	1.83	25.949	-25.339	0.610	3.670	-0.779	-0.703
	1.83	26.170	-25.564	0.606	3.663	-0.764	-0.696
thietane	1.84	17.219	-16.667	0.552	3.489	-0.736	-0.649
	1.84	17.219	-16.667	0.552	3.489	-0.736	-0.649
thiane	1.82	19.781	-19.215	0.566	3.709	-0.776	-0.706
	1.82	19.781	-19.215	0.566	3.709	-0.776	-0.706
terthienyl	1.72	26.013	-25.284	0.729	4.634	-1.056	-0.915
	1.72	26.013	-25.284	0.729	4.634	-1.056	-0.915
	1.74	30.044	-29.331	0.713	4.477	-1.014	-0.868
	1.74	30.044	-29.331	0.713	4.477	-1.014	-0.868
	1.74	28.371	-27.659	0.713	4.490	-1.016	-0.872
	1.74	28.371	-27.658	0.713	4.490	-1.016	-0.872
CO_2….H_2S complex	3.31	11.710	-11.693	0.018	0.201	-0.017	-0.014
TS_{C-S}	2.28	15.521	-15.218	0.304	1.208	-0.225	-0.110

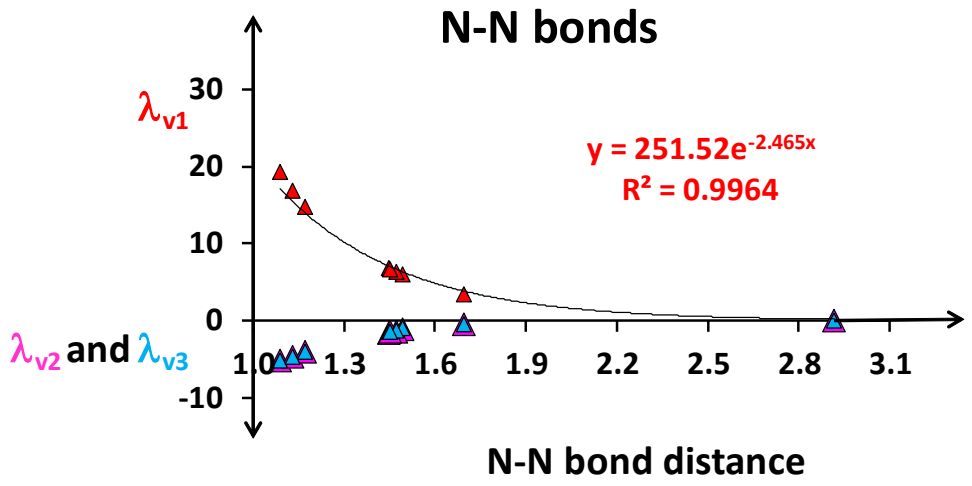

Figure S17. The exponential variation of $\lambda_{v1,}$ λ_{v2} and λ_{v3} (in au) with N-N bond distances (Å) from selected set of systems.

Table S34. MESP topology of selected set of systems containing N-N bonds. The N-N bond distance is given in Å and the MESP data V_{bnp}, V_{ρ}, $V(r)$ and eigenvalues are given in au.

system	d_{NN}	V_{bnp}	V_{ρ}	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}
N_2	1.09	13.593	-11.683	1.910	19.221	-5.267	-5.267
N_2F_4	1.50	21.362	-20.526	0.836	5.982	-1.249	-1.038
N_2O_4	1.70	18.722	-18.165	0.556	3.426	-0.599	-0.547
N_3CH_3_dimer	2.92	16.322	-16.250	0.072	0.206	-0.054	-0.048
N_3H	1.13	15.433	0.072	1.776	16.844	-4.811	-4.811
	1.17	0.000	0.072	1.637	14.681	-4.177	-4.177
hydrazine	1.47	11.590	15.433	0.722	6.334	-1.500	-1.329
Aminimide_1	1.45	39.776	-38.956	0.820	6.721	-1.596	-1.495
Aminimide_2	1.45	34.614	-33.806	0.808	6.618	-1.565	-1.460

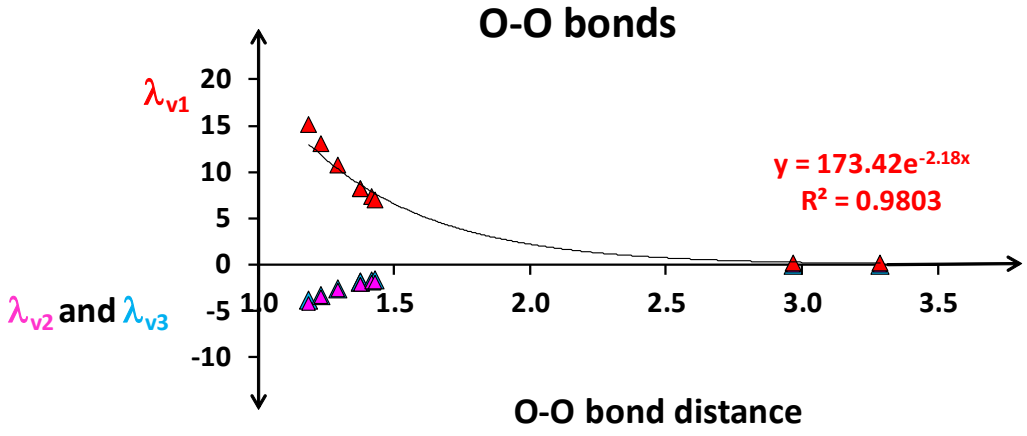

Figure S18. The exponential variation of $\lambda_{v1,}$ λ_{v2} and λ_{v3} (in au) with O-O bond distances (Å) from selected set of systems.

Table S35. MESP topology of selected set of systems containing O-O bonds. The O-O bond distance is given in Å and the MESP data V_{bnp}, V_ρ, $V(r)$ and eigenvalues are given in au.

system	d_{OO}	V_{bnp}	V_ρ	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}
CH_3COO_dimer	2.97	20.343	-20.341	0.002	0.163	-0.016	-0.012
CrO_5	1.38	24.809	-23.803	1.006	8.247	-2.165	-1.838
	1.38	24.806	-23.800	1.006	8.242	-2.164	-1.836
$H_2S_2O_8$	1.42	30.159	-29.230	0.929	7.384	-1.840	-1.739
O_2	1.19	14.253	-12.709	1.544	15.084	-4.178	-3.776
O_2F_2	1.30	18.614	-17.361	1.252	10.756	-2.687	-2.644
O_2H_2	1.43	12.639	-11.847	0.793	7.055	-1.828	-1.573
O_3	1.23	16.356	-14.928	1.428	13.062	-3.395	-3.327
cyclopentanone_dimer	3.29	21.649	-21.607	0.042	0.208	-0.045	-0.035

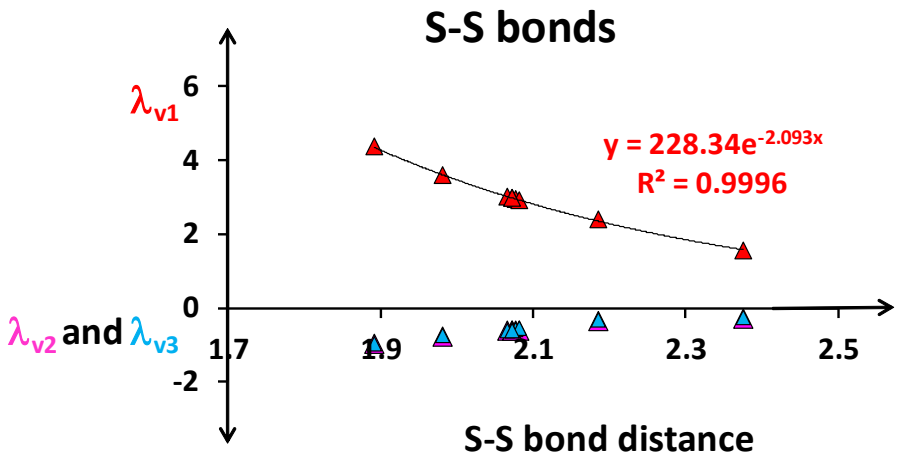

Figure S19. The exponential variation of $\lambda_{v1,}$ λ_{v2} and λ_{v3} (in au) with SS bond distances (Å) from selected set of systems.

Table S36. MESP topology of selected set of systems containing S-S bonds. The S-S bond distance is given in Å and the MESP data V_{bnp}, V_ρ, $V(r)$ and eigenvalues are given in au.

system	d_{SS}	V_{bnp}	V_ρ	$V(r)$	λ_{v1}	λ_{v2}	λ_{v3}
lenthionine	2.08	27.490	-26.889	0.601	2.938	-0.610	-0.586
S_2Cl_2	1.98	24.137	-23.380	0.757	3.596	-0.766	-0.754
$[(CH_3)_3P^+$-SCH_3...CH_3S^-...H_2O	2.07	26.309	-25.731	0.578	2.970	-0.614	-0.597
$H_2S_2O_3$	1.89	24.283	-23.422	0.861	4.373	-0.957	-0.954
$H_2S_2O_6$	2.19	28.356	-27.791	0.565	2.387	-0.342	-0.329
DHS_{red}	2.08	24.730	-24.152	0.579	2.918	-0.624	-0.560

$C_4H_{10}S_2O_2$	2.07	24.410	-23.814	0.596	3.009	-0.626	-0.614
$H_2O...(CH_3)_3P...CH_3SSCH_3...H2O$	2.07	27.050	-26.473	0.577	2.972	-0.614	-0.597
$TS_{S\text{-}S}$	2.38	29.428	-29.152	0.276	1.576	-0.297	-0.267

Table S37. SCF energy of all the geometries (in au).

system	Energy	system	Energy
ethane	-79.796880	thiane	-594.696274
propane	-119.100287	thiaindans	-707.794037
butane	-158.403661	SeC3Se	-4917.315372
decane	-394.223470	SC3S	-910.593339
cyclopropane	-117.864742	C5S	-588.447084
cyclobutane	-157.167375	NCCP	-472.214255
cyclohexane	-235.816094	Cyclopropenyl cation	-115.707274
adamentane	-390.644698	cycloheptatrienyl cation	-270.598388
cubane	-309.405831	benzene-1-ylium	-231.203103
Pbtth	-1307.380881	propan-1-ylium	-118.154223
Ptho	-1244.529849	propan-2-ylium	-118.162832
Bptd	-1089.727235	2-methylpropan-2-ylium	-157.494892
Ahod	-1089.718480	ethen-1-ylium	-77.559631
Dddcpa	-1651.585796	Cyclopentadienyl Anion	-193.477164
ttca	-2093.521684	acetate	-228.479200
Dddcada	-1617.025988	benzen-1-ide	-231.535724
Hdbec	-3352.472291	ethyn-1-ide	-76.691680
Tdtca	-1779.098667	ethen-1-ide	-77.885353
1,2-diamino-o-carborane-1	-983.377431	2-oxopropan-1-ide	-192.504273
1,2-diamino-o-carborane-2	-1219.218626	ethan-1-ide	-79.096596
ethene	-78.562427	Benzene radical	-231.510277
butadiene	-155.949214	3-methylbut-2-enenitrile radical	-248.743037
hexatriene	-233.337187	allyl_radical	-117.221332
octatetraene	-310.725613	vinyl_radical	-77.878778
decapentaene	-388.114211	cyclobutadiene	-154.643416
benzene	-232.196125	azulene	-385.750817
naphthalene	-385.811917	hexa_1,5_dien_3_yne	-232.089425
biphenyl	-463.211454	hexpta_1_en_3,6_diyne	-270.140411
anthracene	-539.420789	2-pentene	-196.480776
biphenylene	-461.938574	isoprene	-195.257750
14-annulene	-541.683061	indene	-348.910882
16-annulene	-619.076853	dihydroindene	-347.690079
fullerene	-2285.889164	cyclopentadiene	-194.057020
ovalene	-1227.792084	ferrocene	-1650.612427
cyclophane_C13H18	-506.097776	Bis(benzene)chromium(0)	-1508.784842
cyclophane_C16H16	-619.187087	η3-CrCl3	-2541.046458

CNT_C48H12	-1835.592869
acetylene	-77.314808
diacetylene	-153.457103
triacetylene	-229.601559
tetraacetylene	-305.746577
pentaacetylene	-381.891814
hexaacetylene	-458.037073
heptaacetylene	-534.182346
octaacetylene	-610.327650
nonaacetylene	-686.472917
C2	-75.900852
C6	-228.220524
C8	-304.350733
C10	-380.581430
C12	-456.702759
C14	-532.898138
C16	-609.036980
pyrazine	-264.268487
pyrrole	-210.131414
furan	-229.985749
thiophene	-552.965240
tetrahydropyran	-271.714542
THF	-232.402356
thiozolidine	-571.415322
thioxanthene	-899.507122
piperazine	-267.877714
pyrrolidine	-212.533171
dioxolane	-268.306121
DBN	-383.394409
benzonitrile	-324.433800
porphyrin	-989.379569
aziridine	-133.894596
cyanogen	-185.633370
pyramidopyramidine	-449.969604
oxirane	-153.761556
ethylene carbonate	-342.362420
furfural	-343.300442
ethylene glycol	-230.216362
tetrathiafulvalene	-1823.675339
dithianodithiine	-3572.456593
thiirane	-476.757900
thietane	-516.056385
quinazoline	-417.894235
tetrazole	-258.217682
metallacyclobutane	-2540.952757
C3H4Li2	-131.618634
η6_CrCO3	-1616.569634
Si2C5H2	-770.528246
Ge2C5H2	-4345.532159
C6Li6	-273.652599
C2B8	-274.634501
TS1	-451.882389
TS2	-432.034026
TS3	-451.886271
TS4	-489.982813
TS5	-432.012138
TS6	-564.687454
TS7	-1149.604188
TS8	-1149.611277
TS9	-655.039149
TS10	-614.794405
TS11	-983.146676
TS12	-1216.575656
TS13	-1079.948739
TS14	-550.711864
TS15	-1393.255580
TS16	-932.463615
TS17	-1393.249700
TS18	-1206.588776
TS19	-1300.025636
TS20	-555.054457
TS21	-693.407093
Acetylenebromide dimer	-5301.757651
Acetonitrile dimer	-265.472718
Acetylene dimer	-154.632348
Vinylchloride dimer	-1076.332023
Diyne dimer	-306.917012
Diyneflouride dimer	-505.346006
Diynecyanide dimer	-491.392912
C12 dimer	-913.425242
diyne_CN_NMe_2_dimer	-759.309069
Dimethylcynamide dimer	-454.736015
Thioacetone dimer	-1032.143336
Vinylfluoride dimer	-355.604764
diyneCF_3 dimer	-980.987917
C2@C60	-2361.829470
trizole	-242.217644
TS_{C-N}	-1082.891522

NNDMAacetylCl	-901.199429	benzoyl isothiocyanate	-761.921318
lenthionine	-2069.519122	terthienyl	-1656.535040
TS_{C-S}	-587.869357	CO_2….H_2S complex	-587.948893
N_2	-109.519139	CH_3COO_dimer	-536.706231
N_2F_4	-508.529589	CrO_5	-1420.201994
N_2O_4	-410.116383	$H_2S_2O_8$	-1399.050636
N_3CH_3_dimer	-408.115404	O_2	-150.243937
N_3H	-164.720542	O_2F_2	-349.767497
hydrazine	-111.839454	O_2H_2	-151.526454
Aminimide_1	-1509.604188	O_3	-225.367003
Aminimide_2	-1203.345841	cyclopentanone_dimer	-541.056785
S_2Cl_2	-1716.730468	DHS_{red}	-1104.014914
$[(CH_3)_3P^+$-SCH_3...CH_3S^-...H_2O	-1413.640953	$C_4H_{10}S_2O_2$	-1105.190601
$H_2S_2O_3$	-1023.132733	H_2O...$(CH_3)_3P$...CH_3SSCH_3...H2O	-1490.061484
$H_2S_2O_6$	-1248.711141	TS_{S-S}	-1642.920688
quinazoline	-417.894235	trizole	-242.217644

Table S38. Cartesian coordinates of all the geometries (in Å).

Coordinates of the molecules (Given in the order Atomic number (At. No.), X coordinate, Y coordinate, Z coordinate

ethane

6	0.000000	0.000000	0.758269
1	0.000000	1.015716	1.161933
1	-0.879636	-0.507857	1.161933
1	0.879635	-0.507858	1.161933
6	0.000000	0.000000	-0.758269
1	0.879636	0.507857	-1.161933
1	0.000000	-1.015716	-1.161933
1	-0.879635	0.507858	-1.161933

propane

6	0.000000	0.587344	-0.000006
1	0.000004	1.244700	0.876120
1	-0.000002	1.244677	-0.876149
6	1.270136	-0.259789	-0.000001
1	2.168661	0.362647	-0.000017
1	1.309744	-0.905302	0.883036
1	1.309733	-0.905330	-0.883019
6	-1.270135	-0.259789	0.000007
1	-1.309735	-0.905308	0.883040
1	-2.168662	0.362645	0.000005

1	-1.309743	-0.905324	-0.883014

butane

6	-0.564316	-0.514884	-0.000061
1	-0.456952	-1.164855	0.876638
1	-0.456946	-1.164666	-0.876899
6	-1.951891	0.120277	0.000002
1	-2.739789	-0.637189	-0.000108
1	-2.094247	0.750748	0.883186
1	-2.094222	0.750978	-0.883023
6	0.564316	0.514885	0.000052
1	0.456940	1.164676	0.876883
1	0.456961	1.164848	-0.876654
6	1.951890	-0.120278	0.000007
1	2.094223	-0.750949	0.883053
1	2.094241	-0.750780	-0.883157
1	2.739791	0.637185	0.000087

decane

6	-1.898734	-0.462940	-0.000009
1	-1.882260	-1.129302	0.874011
1	-1.882267	-1.129289	-0.874040
6	-3.191957	0.337026	0.000000
1	-3.209431	1.003571	0.873979
1	-3.209418	1.003615	-0.873945
6	-0.646590	0.400132	-0.000007
1	-0.663074	1.066479	0.874002
1	-0.663066	1.066471	-0.874021
6	0.646591	-0.400130	0.000002
1	0.663063	-1.066477	0.874010
1	0.663081	-1.066467	-0.874013
6	1.898734	0.462942	0.000019
1	1.882265	1.129276	0.874060
1	1.882260	1.129318	-0.873991
6	3.191957	-0.337027	-0.000004
1	3.209426	-1.003618	0.873940
1	3.209425	-1.003570	-0.873984
6	4.444858	0.526389	0.000020
1	4.425029	1.191047	0.873530
1	4.425026	1.191099	-0.873450
6	5.728723	-0.284581	-0.000006
1	5.789536	-0.931817	-0.880354
1	6.616568	0.352172	0.000029
1	5.789522	-0.931896	0.880285

6	-4.444858	-0.526390	-0.000032
1	-4.425021	-1.191114	0.873427
1	-4.425033	-1.191035	-0.873551
6	-5.728724	0.284579	0.000016
1	-5.789541	0.931789	0.880383
1	-5.789520	0.931920	-0.880256
1	-6.616569	-0.352174	-0.000043

cyclopropane

6	0.000000	0.866873	0.000000
6	0.750734	-0.433436	0.000000
6	-0.750734	-0.433436	0.000000
1	0.000000	1.451308	0.910254
1	0.000000	1.451308	-0.910254
1	1.256870	-0.725654	0.910254
1	1.256870	-0.725654	-0.910254
1	-1.256870	-0.725654	-0.910254
1	-1.256870	-0.725654	0.910254

cyclobutane

6	0.000000	1.075067	0.142191
6	-1.075067	0.000000	-0.142191
6	0.000000	-1.075067	0.142191
6	1.075067	0.000000	-0.142191
1	0.000000	1.357062	1.196934
1	0.000000	1.978209	-0.468075
1	-1.357062	0.000000	-1.196934
1	-1.978209	0.000000	0.468075
1	0.000000	-1.357062	1.196934
1	0.000000	-1.978209	-0.468075
1	1.357062	0.000000	-1.196934
1	1.978209	0.000000	0.468075

cyclohexane

6	-0.005862	-0.000586	-1.476525
6	0.229884	1.288091	-0.684293
6	-0.453888	1.227384	0.684241
6	0.005862	0.000586	1.476525
6	-0.229884	-1.288091	0.684293
6	0.453888	-1.227384	-0.684241
1	0.510016	0.045620	-2.439293
1	-1.076657	-0.095889	-1.693713
1	-0.127614	2.152757	-1.249738
1	1.308188	1.426579	-0.539378

1	-0.254844	2.141554	1.249790
1	-1.539670	1.173023	0.539300
1	-0.510016	-0.045620	2.439293
1	1.076657	0.095889	1.693713
1	0.127614	-2.152757	1.249738
1	-1.308188	-1.426579	0.539378
1	0.254844	-2.141554	-1.249790
1	1.539670	-1.173023	-0.539300

adamentane

6	0.000000	1.773706	0.000000
6	0.888832	0.888832	0.888832
6	0.000000	0.000000	1.773706
6	-0.888832	-0.888832	0.888832
6	0.000000	-1.773706	0.000000
6	0.888832	-0.888832	-0.888832
6	0.000000	0.000000	-1.773706
6	-0.888832	0.888832	-0.888832
6	-1.773706	0.000000	0.000000
6	1.773706	0.000000	0.000000
1	-0.624201	2.422322	0.624201
1	0.624201	2.422322	-0.624201
1	1.520580	1.520580	1.520580
1	0.624201	-0.624201	2.422322
1	-0.624201	0.624201	2.422322
1	-1.520580	-1.520580	1.520580
1	0.624201	-2.422322	0.624201
1	-0.624201	-2.422322	-0.624201
1	1.520580	-1.520580	-1.520580
1	0.624201	0.624201	-2.422322
1	-0.624201	-0.624201	-2.422322
1	-1.520580	1.520580	-1.520580
1	-2.422322	-0.624201	-0.624201
1	-2.422322	0.624201	0.624201
1	2.422322	0.624201	-0.624201
1	2.422322	-0.624201	0.624201

cubane

6	0.781406	0.781406	0.781406
6	0.781406	-0.78141	0.781406
6	0.781406	-0.78141	-0.78141
6	0.781406	0.781406	-0.78141
6	-0.78141	0.781406	0.781406
6	-0.78141	-0.78141	0.781406

6	-0.78141	-0.78141	-0.78141
6	-0.78141	0.781406	-0.78141
1	1.409147	-1.40915	-1.40915
1	1.409147	1.409147	-1.40915
1	1.409147	1.409147	1.409147
1	1.409147	-1.40915	1.409147
1	-1.40915	-1.40915	1.409147
1	-1.40915	1.409147	1.409147
1	-1.40915	1.409147	-1.40915
1	-1.40915	-1.40915	-1.40915

Pbtth

6	-0.000005	0.642775	0.845173
6	-0.000129	0.642558	-0.845035
6	0.000393	-1.911650	0.672976
6	0.000266	-1.911912	-0.672872
6	-1.228079	-0.024842	1.436955
6	-2.315964	0.637703	1.980806
1	-2.330199	1.721627	2.011078
6	-3.395783	-0.097594	2.473747
1	-4.245815	0.420025	2.901806
6	-3.389408	-1.483755	2.412583
1	-4.233700	-2.045855	2.793267
6	-2.302597	-2.159506	1.854289
1	-2.298091	-3.240931	1.785581
6	-1.230220	-1.432558	1.372199
6	1.228382	-0.024463	1.436737
6	2.316040	0.638439	1.980592
1	2.329919	1.722373	2.010845
6	3.396112	-0.096502	2.473516
1	4.245954	0.421394	2.901614
6	3.390205	-1.482663	2.412320
1	4.234686	-2.044484	2.792996
6	2.303621	-2.158771	1.854012
1	2.299493	-3.240196	1.785251
6	1.230991	-1.432181	1.371956
6	-1.228328	-0.025080	-1.436548
6	-2.316281	0.637515	-1.980239
1	-2.330545	1.721441	-2.010375
6	-3.396103	-0.097730	-2.473226
1	-4.246210	0.419924	-2.901095
6	-3.389671	-1.483909	-2.412328
1	-4.233910	-2.045966	-2.793191
6	-2.302830	-2.159712	-1.854168

1	-2.298306	-3.241146	-1.785584
6	-1.230509	-1.432807	-1.371911
6	1.228167	-0.024730	-1.436729
6	2.315861	0.638215	-1.980515
1	2.329739	1.722147	-2.010691
6	3.395911	-0.096676	-2.473525
1	4.245819	0.421243	-2.901461
6	3.389949	-1.482856	-2.412564
1	4.234379	-2.044648	-2.793402
6	2.303371	-2.159004	-1.854320
1	2.299205	-3.240441	-1.785763
6	1.230810	-1.432460	-1.372044
6	-0.000226	2.146667	0.692445
6	-0.000501	3.317812	1.432502
1	-0.000424	3.326709	2.516572
6	-0.000917	4.507070	0.698270
1	-0.001140	5.456230	1.221267
6	-0.001070	4.506871	-0.699209
1	-0.001405	5.455881	-1.222476
6	-0.000828	3.317378	-1.433073
1	-0.000970	3.325868	-2.517142
6	-0.000378	2.146491	-0.692622

Ptho

6	-0.617512	-0.029686	-0.125956
6	-0.960542	-1.538112	-0.419790
6	1.028997	0.189754	0.174704
6	-2.391421	-1.730789	-0.970261
6	1.198174	1.327913	1.216881
6	-1.688677	0.379239	1.001261
6	1.823036	0.588035	-1.127319
6	-1.736798	1.883876	1.357504
6	-2.445209	0.586207	-1.863457
6	2.739017	-1.736171	-1.541262
6	-1.016399	0.870502	-1.353752
6	-3.148909	0.125854	0.447744
6	-1.550956	-0.513934	2.247317
6	3.266940	1.051959	-0.793316
6	3.344936	-0.569683	1.070502
6	-0.949961	2.377840	-1.028744
6	-3.403583	-1.341563	0.115476
6	1.888447	-1.024064	0.731736
6	-3.454145	0.988461	-0.780725
6	4.067791	-0.121664	-0.212287

6	2.637667	1.750454	1.504636
6	1.931568	-0.573045	-2.134985
6	4.157767	-1.258060	-1.228307
6	2.084461	-2.213779	-0.237712
6	-1.833272	-1.989295	1.913097
6	3.387505	0.561030	2.091883
6	-1.939885	2.741781	0.091653
6	3.278338	2.215411	0.196599
6	-2.608268	-0.887282	-2.222702
6	-3.349783	2.474469	-0.443019
6	-0.866692	-2.453967	0.822463
6	-3.256225	-2.173168	1.386707
1	-0.356721	0.658026	-2.195216
1	2.773080	-2.562770	-2.257335
1	2.616592	2.575850	2.223449
1	2.913522	0.248260	3.029047
1	-1.881180	-1.168164	-2.993883
1	0.130184	-2.521007	1.236566
1	-4.469473	0.757521	-1.126164
1	-2.605363	1.202903	-2.756407
1	0.946569	-0.920225	-2.452263
1	-1.235915	2.930417	-1.931866
1	4.656581	-0.907951	-2.138965
1	4.752662	-2.083726	-0.822916
1	-3.826750	0.415980	1.262278
1	-2.609616	2.029513	2.006154
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1	-3.607440	-1.068373	-2.634475
1	-0.293539	-1.902286	-1.199367
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1	3.857802	-1.447509	1.481062
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6	-1.477244	0.632726	1.011061
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6	3.162640	0.665095	-1.001907
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6	1.693736	2.188392	0.315740
6	-2.333721	-1.674067	1.614849
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1	-1.329515	-1.484289	-1.696024

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6	-2.975781	-0.667474	-2.398194
6	-1.988253	-1.628868	-1.921888
6	-2.343773	-2.971632	-2.166099
6	-1.551151	-4.036683	-1.793752
6	-0.334163	-3.769409	-1.178866
6	0.037106	-2.457438	-0.948594
6	-0.771759	-1.352586	-1.268656
1	1.948471	-0.000145	3.212369
1	4.385385	-0.000356	2.952279
1	3.675388	0.000518	-3.663534
1	1.219732	0.000234	-3.391704
1	6.322339	-0.880027	0.581626
1	6.324549	0.876385	0.583542
1	6.067718	0.880250	-1.763535
1	6.069254	-0.876365	-1.765817
1	1.215046	2.043579	2.341012
1	0.314037	4.121898	3.187215
1	-2.095261	4.676238	2.846996
1	-3.554378	3.019943	1.732318
1	-3.860390	1.165133	0.411282
1	-3.860390	-1.165173	0.411196
1	-3.554289	-3.020171	1.731915
1	-2.095121	-4.676574	2.846350

1	0.314149	-4.122164	3.186728
1	1.215082	-2.043703	2.340828
1	0.990248	2.286715	-0.466757
1	0.324356	4.573412	-0.874119
1	-1.870434	5.053730	-1.986208
1	-3.286934	3.160936	-2.666932
1	-3.850548	1.133414	-2.842394
1	-3.850441	-1.133667	-2.842420
1	-3.286575	-3.161141	-2.667086
1	-1.869907	-5.053798	-1.986351
1	0.324790	-4.573281	-0.874149
1	0.990449	-2.286533	-0.466750

Hdbec

6	1.380722	0.052499	1.415177
6	2.482619	-0.744849	1.727573
6	3.210476	-0.597401	2.912980
6	2.800769	0.363563	3.832871
6	4.451532	-1.472334	3.119990
6	5.491555	-1.110357	2.045163
1	2.828443	-1.483140	1.020381
1	3.345934	0.486654	4.757730
1	6.380681	-1.739063	2.150787
1	5.088755	-1.253033	1.039186
1	5.796303	-0.065062	2.143040
6	-0.931760	-0.012171	0.016253
6	0.738254	0.006110	-0.013946
6	-1.489000	-1.264467	0.757122
6	-1.520036	1.236150	0.740182
6	1.329893	1.240435	-0.778382
6	1.357148	-1.254072	-0.711162
6	-1.543842	-0.028362	-1.416632
6	-2.516899	1.115203	1.705526
6	-3.089789	2.227923	2.334483
6	-2.621875	3.494446	1.997734
6	-1.656421	3.664132	0.997600
6	-1.153776	2.533674	0.362579
1	-0.457190	2.670645	-0.446210
6	-1.185555	5.051134	0.544595
6	0.317618	5.032238	0.217736
6	-1.965210	5.436405	-0.723273
6	-1.426981	6.113293	1.624761
1	-1.006177	7.067291	1.298285
1	-0.947928	5.834064	2.567585

1	-2.490938	6.274682	1.811234
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1	-1.799437	4.699331	-1.513277
1	-3.039148	5.482583	-0.521990
1	0.661823	6.048436	0.003559
1	0.547504	4.419131	-0.657064
1	0.896246	4.641271	1.058933
1	-3.023085	4.362717	2.500832
6	-4.250534	2.007957	3.311433
6	-3.893825	0.942983	4.361115
6	-5.465393	1.521404	2.500240
6	-4.636659	3.293784	4.049255
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1	-5.000868	4.061739	3.362589
1	-6.323781	1.364618	3.160074
1	-5.246631	0.578420	1.992820
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1	-4.745409	0.783254	5.028619
1	-3.647281	-0.017393	3.904082
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1	-2.883354	0.135895	1.974673
6	-1.166092	-0.993771	-2.357206
6	-1.688280	-1.021691	-3.646312
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6	-3.162769	0.814435	-3.047446
6	-2.570992	0.840752	-1.778709
1	-2.946158	1.552704	-1.059032
6	-4.357904	1.733633	-3.325339
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1	-5.586358	2.425169	-4.959111
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6	-1.200705	-2.095271	-4.626313
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1	-2.603895	-1.707412	-6.263907
1	-1.107949	-0.756990	-6.347263
1	0.670822	-2.974590	-5.278311
1	0.619608	-2.688691	-3.539884
1	0.842292	-1.327443	-4.641671
1	-1.544491	-4.221427	-4.935993
1	-1.668978	-3.708405	-3.242056
1	-2.976990	-3.336117	-4.374803
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6	2.743998	-3.500137	-1.705912
6	3.137613	-2.222141	-2.092027
6	2.426362	-1.123537	-1.598508
1	2.759269	-0.141209	-1.896787
6	4.343272	-1.960985	-3.001211
6	3.917586	-1.106800	-4.207091
6	5.411315	-1.201453	-2.194835
6	4.963478	-3.258106	-3.529042
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1	5.342201	-3.883948	-2.717098
1	6.275454	-0.977224	-2.827264
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1	5.752339	-1.802749	-1.347948
1	4.784050	-0.900599	-4.842010
1	3.493307	-0.149241	-3.895371
1	3.169685	-1.632063	-4.806177
1	3.276911	-4.361260	-2.082990
6	1.168463	-5.068880	-0.410489
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6	1.099496	-5.171639	1.122694
6	2.068349	-6.193945	-0.930077
1	1.676400	-7.157128	-0.594779
1	2.102267	-6.211985	-2.022234
1	3.089784	-6.096160	-0.552391
1	0.770390	-6.174031	1.412538
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1	2.079215	-4.989081	1.572666
1	-0.655782	-6.227373	-0.678429
1	-0.916534	-4.474105	-0.626529

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6	-2.526106	-3.490752	2.121846
6	-1.551559	-2.696644	2.738034
6	-1.080972	-1.577572	2.058929
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1	0.736659	-1.677097	4.093923
1	1.015339	-3.304691	3.469811
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6	-3.916108	-4.266476	-1.229541
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6	-4.555302	-5.194086	0.985129
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1	-6.311975	-3.471080	-0.157305
1	-5.254817	-2.054754	-0.291607
1	-5.676618	-2.691393	1.304815
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1	-3.702990	-3.384674	-1.836976
1	-3.060369	-4.942375	-1.300279
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6	1.558025	2.567270	-2.825786
6	2.656583	3.231957	-2.272422
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6	2.422027	1.940214	-0.263213
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1	4.174898	5.483879	-1.399672
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1	5.059620	1.674357	0.452195
1	5.717207	2.078732	-1.139815
1	3.164880	3.993095	-2.846907
6	0.994689	2.908570	-4.210177
6	0.883775	1.638842	-5.071161
6	-0.410626	3.502867	-4.018239
6	1.862957	3.925048	-4.957422
1	1.426437	4.124083	-5.939061
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1	1.922391	4.876036	-4.422284
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1	-1.060014	2.797302	-3.492687
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1	0.509398	1.897160	-6.066259
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1	1.858457	1.156622	-5.186099
1	0.118995	1.037452	-2.542236
6	1.693287	1.175930	3.570520
6	1.019865	1.020214	2.360511
1	0.201667	1.689391	2.156037
6	1.174369	2.218389	4.567779
6	1.052303	3.592970	3.888083
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1	3.348025	-3.243739	3.743246

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6	-0.034271	4.472572	1.186090
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6	0.000759	1.622529	1.189073
6	0.000032	2.351658	-0.000001
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6	-0.025737	0.126262	-0.875094
6	-1.318574	-0.543719	-1.348317
6	-1.565691	-1.886525	-1.040843
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6	-4.665551	0.410641	-2.896554
6	1.243851	-0.489427	-1.482478
6	2.466003	0.150472	-1.234915
6	3.675474	-0.406546	-1.619492
6	3.662630	-1.610242	-2.330003
6	2.465763	-2.227076	-2.667661
6	1.261666	-1.657830	-2.237221
6	4.975662	0.248378	-1.230905
6	2.446210	-3.488314	-3.494705
6	0.025734	0.126258	0.875085
6	-1.243876	-0.489387	1.482468
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6	-2.465842	-2.226991	2.667657
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1	0.925289	6.452282	-1.146637
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1,2-diamino-o-carborane-1

6	-0.219378	1.684287	0.896061
6	-0.219378	1.684287	-0.896061
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5	0.098434	4.419995	0.881416
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6	0.266815	-1.390445	2.988678
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6	0.259353	-3.042135	4.754260
6	0.483886	-1.740628	4.320049
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1	-0.374950	-5.019352	4.199752
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6	0.266815	-1.390445	-2.988678
6	0.483886	-1.740628	-4.320049
6	0.259353	-3.042135	-4.754260
6	-0.194991	-4.006163	-3.861314
6	-0.422532	-3.661297	-2.533223
6	-0.191843	-2.361297	-2.099761
1	0.829608	-0.988788	-5.021852
1	0.432133	-3.300963	-5.792018
1	-0.374950	-5.019352	-4.199752
1	-0.779285	-4.407240	-1.832704
1	-0.369355	-2.080695	-1.069358

1,2-diamino-o-carborane-2

6	0.895742	1.723912	0.212028
6	-0.920667	1.755326	0.228106
5	-0.025720	2.149756	-1.160387
5	1.437564	3.049647	-0.669998
5	1.459834	3.047720	1.094180
5	0.012871	2.149902	1.607185
5	-1.446160	3.097462	-0.642494
5	0.003070	3.925132	-1.207217
5	0.908339	4.482188	0.221879
5	0.035900	3.916076	1.668069
5	-1.424575	3.085900	1.122702
5	-0.853053	4.508695	0.241607
1	-0.041068	1.395068	-2.064890
1	2.417789	2.914289	-1.310898
1	2.460013	2.873813	1.697685
1	0.007221	1.366530	2.488282
1	-2.445933	2.979779	-1.257847
1	0.004485	4.497093	-2.239611
1	1.563809	5.464081	0.211648
1	0.053087	4.479722	2.704995

1	-2.416827	2.937207	1.746143
1	-1.478030	5.510256	0.250536
7	1.476319	0.461167	0.234520
7	-1.547313	0.517574	0.292456
1	1.930398	0.244513	1.111061
1	-2.072445	0.385409	1.146096
6	2.168769	-0.079641	-0.947662
1	2.530805	0.739614	-1.573110
1	1.459773	-0.653832	-1.547747
6	-2.182089	-0.076451	-0.892795
1	-1.439539	-0.669518	-1.433628
1	-2.526870	0.707930	-1.570647
6	3.329808	-0.946457	-0.517239
6	3.169282	-2.330532	-0.369182
6	4.251748	-3.101280	0.050965
6	5.488178	-2.531128	0.335235
6	5.623639	-1.151688	0.199712
6	4.565902	-0.349906	-0.219675
6	1.844133	-2.993900	-0.650015
1	4.121767	-4.173174	0.166328
6	6.657247	-3.381779	0.758858
1	6.577922	-0.686938	0.429245
6	4.764672	1.139565	-0.354589
6	-3.340967	-0.944724	-0.463042
6	-4.634814	-0.408052	-0.394574
6	-5.684360	-1.223228	0.023643
6	-5.480417	-2.551099	0.388355
6	-4.182657	-3.053561	0.348665
6	-3.109725	-2.268808	-0.065287
6	-4.901390	1.034780	-0.747930
1	-6.686120	-0.807200	0.073960
6	-6.635222	-3.425063	0.803545
1	-3.999145	-4.078524	0.657129
6	-1.710918	-2.832125	-0.060292
1	7.279704	-3.635619	-0.103580
1	6.322258	-4.314783	1.213885
1	7.287111	-2.855183	1.477638
1	1.840884	-4.020382	-0.282775
1	1.631285	-3.021561	-1.722888
1	1.029582	-2.454687	-0.165445
1	-1.674618	-3.779041	0.478713
1	-1.020630	-2.133511	0.417995
1	-1.348546	-3.011357	-1.077304
1	-5.930606	1.303112	-0.510672

1	-4.743117	1.223160	-1.813491
1	-4.239459	1.709251	-0.197766
1	-7.434317	-2.834926	1.254398
1	-6.318409	-4.181722	1.522874
1	-7.053808	-3.944744	-0.062757
1	5.738234	1.433737	0.036879
1	3.998044	1.701837	0.183973
1	4.716557	1.451768	-1.401837

ethene

6	0.000000	0.000000	0.662151
6	0.000000	0.000000	-0.662151
1	0.000000	0.923212	1.230466
1	0.000000	-0.923212	1.230466
1	0.000000	0.923212	-1.230466
1	0.000000	-0.923212	-1.230466

butadiene

6	-0.165653	0.545699	-1.749937
6	-0.082301	0.590747	-0.421426
1	-0.287686	1.443046	-2.343206
1	-0.113445	-0.398204	-2.282736
1	-0.136994	1.547395	0.092620
6	0.082301	-0.590747	0.421426
6	0.165653	-0.545699	1.749937
1	0.136994	-1.547395	-0.092620
1	0.113445	0.398204	2.282736
1	0.287686	-1.443046	2.343206

hexatriene

6	-3.058158	-0.170349	0.000002
6	-1.863716	0.422865	-0.000014
1	-3.976730	0.402373	0.000010
1	-3.147055	-1.251740	0.000023
1	-1.801684	1.508448	-0.000025
6	-0.600468	-0.298223	-0.000006
6	0.600468	0.298222	-0.000006
1	-0.654744	-1.385301	-0.000005
1	0.654743	1.385301	-0.000012
6	1.863716	-0.422866	-0.000005
6	3.058158	0.170350	0.000021
1	1.801685	-1.508448	-0.000016
1	3.147055	1.251740	0.000041
1	3.976730	-0.402372	0.000035

octatetraene

6	-4.286167	0.201287	0.000036
6	-3.103032	-0.415470	0.000011
1	-5.215689	-0.353410	0.000062
1	-4.353767	1.284189	0.000047
1	-3.063144	-1.502138	0.000011
6	-1.826799	0.279111	0.000001
6	-0.636769	-0.343887	-0.000004
1	-1.857872	1.367001	-0.000012
1	-0.609547	-1.431949	0.000001
6	0.636769	0.343888	-0.000030
6	1.826798	-0.279111	-0.000006
1	0.609548	1.431949	-0.000057
1	1.857872	-1.367001	0.000027
6	4.286168	-0.201286	-0.000006
6	3.103032	0.415469	-0.000006
1	4.353769	-1.284188	-0.000005
1	5.215689	0.353412	-0.000033
1	3.063143	1.502138	-0.000024

decapentaene

6	-4.286167	0.201287	0.000036
6	-3.103032	-0.415470	0.000011
1	-5.215689	-0.353410	0.000062
1	-4.353767	1.284189	0.000047
1	-3.063144	-1.502138	0.000011
6	-1.826799	0.279111	0.000001
6	-0.636769	-0.343887	-0.000004
1	-1.857872	1.367001	-0.000012
1	-0.609547	-1.431949	0.000001
6	0.636769	0.343888	-0.000030
6	1.826798	-0.279111	-0.000006
1	0.609548	1.431949	-0.000057
1	1.857872	-1.367001	0.000027
6	4.286168	-0.201286	-0.000006
6	3.103032	0.415469	-0.000006
1	4.353769	-1.284188	-0.000005
1	5.215689	0.353412	-0.000033
1	3.063143	1.502138	-0.000024

benzene

6	1.204329	0.695319	0.000000
6	0.000000	1.390637	0.000000

6	1.204327	-0.695318	0.000000
1	0.000000	2.474104	0.000000
1	2.142637	-1.237052	0.000000
6	-1.204329	0.695319	0.000000
6	0.000000	-1.390639	0.000000
1	-2.142638	1.237052	0.000000
1	0.000000	-2.474105	0.000000
6	-1.204327	-0.695318	0.000000
1	-2.142637	-1.237052	0.000000
1	2.142638	1.237052	0.000000

naphthalene

6	-0.000001	0.710760	0.000016
6	-1.241324	1.397593	0.000031
6	0.000005	-0.710753	-0.000007
1	-1.236594	2.482304	0.000044
6	-2.423198	0.707507	0.000020
6	-1.241315	-1.397593	-0.000013
1	-3.365175	1.242631	0.000024
1	-1.236574	-2.482304	-0.000026
6	-2.423193	-0.707516	0.000000
1	-3.365167	-1.242646	-0.000005
6	1.241312	1.397591	0.000020
1	1.236600	2.482303	0.000034
6	2.423195	0.707505	-0.000006
6	1.241315	-1.397589	-0.000028
1	3.365165	1.242643	-0.000007
1	1.236584	-2.482300	-0.000042
6	2.423200	-0.707506	-0.000029
1	3.365175	-1.242633	-0.000049

biphenyl

6	0.000000	0.000000	-0.741791
6	-0.417099	1.126655	-1.456213
6	0.417099	-1.126655	-1.456213
6	-0.417291	1.126892	-2.845312
1	-0.767750	1.998812	-0.915935
6	0.417291	-1.126892	-2.845312
1	0.767750	-1.998812	-0.915935
6	0.000000	0.000000	-3.545196
1	-0.752254	2.006426	-3.382231
1	0.752254	-2.006426	-3.382231
1	0.000000	0.000000	-4.628448
6	0.000000	0.000000	0.741791

6	-0.417099	-1.126655	1.456213
6	0.417099	1.126655	1.456213
1	0.767750	1.998812	0.915935
1	-0.767750	-1.998812	0.915935
6	0.417291	1.126892	2.845312
6	-0.417291	-1.126892	2.845312
1	0.752254	2.006426	3.382231
1	-0.752254	-2.006426	3.382231
6	0.000000	0.000000	3.545196
1	0.000000	0.000000	4.628448

anthracene

6	0.000000	2.471646	1.403093
6	0.000000	1.217090	0.717221
6	0.000000	0.000000	1.398285
6	0.000000	1.217090	-0.717221
6	0.000000	0.000000	-1.398285
6	0.000000	-1.217090	-0.717221
6	0.000000	-1.217090	0.717221
6	0.000000	3.644342	0.713286
6	0.000000	2.471646	-1.403093
1	0.000000	0.000000	-2.484148
6	0.000000	-2.471646	-1.403093
6	0.000000	-2.471646	1.403093
6	0.000000	-3.644342	0.713286
6	0.000000	-3.644342	-0.713286
1	0.000000	-2.467890	-2.487664
1	0.000000	-2.467890	2.487664
1	0.000000	-4.588318	1.244792
1	0.000000	-4.588318	-1.244792
6	0.000000	3.644342	-0.713286
1	0.000000	2.467890	2.487664
1	0.000000	0.000000	2.484148
1	0.000000	4.588318	1.244792
1	0.000000	2.467890	-2.487664
1	0.000000	4.588318	-1.244792

biphenylene

6	-3.110749	-0.691591	0.000021
6	-1.908934	-1.440331	0.000062
6	-3.110781	0.691472	-0.000044
1	-1.927614	-2.522906	0.000048
1	-4.058176	1.217188	-0.000088
6	-0.754096	-0.708328	0.000025

6	-1.909039	1.440353	-0.000054
1	-1.927998	2.522927	-0.000079
6	-0.754079	0.708550	0.000027
1	-4.058133	-1.217327	0.000038
6	0.754008	-0.708490	-0.000060
6	1.908960	-1.440339	-0.000075
6	0.754168	0.708393	-0.000042
1	1.927867	-2.522916	-0.000071
6	3.110733	-0.691529	-0.000007
6	1.909007	1.440345	0.000066
1	4.058097	-1.217305	-0.000008
1	1.927750	2.522918	0.000111
6	3.110801	0.691530	0.000069
1	4.058212	1.217213	0.000131

14-annulene

6	-0.014732	0.676555	2.727936
6	-0.163273	1.422872	1.491705
6	0.014732	-0.676555	2.727936
6	0.163273	-1.422872	1.491705
1	0.031989	1.224389	3.664592
6	0.198200	2.700998	1.250820
6	0.257606	1.419149	-1.533727
6	-0.257606	-1.419149	-1.533727
6	0.055626	2.821545	-1.265601
6	0.076551	3.381709	-0.029747
1	0.603212	3.289420	2.072001
6	-0.055626	0.726866	-2.650977
1	-0.115215	3.474094	-2.117777
1	0.005534	4.464259	0.022102
6	-0.198200	-2.700998	1.250820
6	-0.055626	-2.821545	-1.265601
6	-0.076551	-3.381709	-0.029747
1	-0.031989	-1.224389	3.664592
6	0.055626	-0.726866	-2.650977
1	-0.410606	1.239676	-3.541853
1	0.115215	-3.474094	-2.117777
1	-0.005534	-4.464259	0.022102
1	0.410606	-1.239676	-3.541853
1	-0.603212	-3.289420	2.072001
1	-0.663411	0.885023	0.695580
1	-0.728262	-0.855148	-0.737092
1	0.728262	0.855148	-0.737092
1	0.663411	-0.885023	0.695580

16-annulene

6	-0.375896	3.132998	-0.563579
6	-1.133662	2.033884	0.010271
6	1.956143	2.468680	0.119528
6	2.033885	1.133662	-0.010271
1	-0.970486	3.892089	-1.065713
6	-2.468680	1.956143	-0.119525
6	-2.033885	-1.133662	-0.010268
6	1.133662	-2.033884	0.010267
6	-3.132997	-0.375896	0.563583
6	-3.342072	0.949172	0.477176
1	-2.971746	2.749916	-0.669843
6	-1.956143	-2.468680	0.119529
1	-3.892088	-0.970485	1.065719
1	-4.283138	1.328186	0.867164
6	3.132998	0.375896	0.563577
6	2.468680	-1.956143	-0.119531
6	3.342073	-0.949172	0.477168
1	2.749916	2.971745	0.669847
6	0.375895	-3.132997	-0.563582
1	-2.749914	-2.971745	0.669850
1	2.971744	-2.749916	-0.669852
1	4.283140	-1.328186	0.867154
1	0.970483	-3.892088	-1.065718
1	3.892090	0.970484	1.065712
1	1.304877	0.606865	-0.619237
1	0.606865	-1.304877	0.619233
1	-1.304878	-0.606864	-0.619235
1	-0.606864	1.304876	0.619236
6	-0.949172	-3.342072	-0.477172
6	0.949171	3.342073	-0.477171
1	-1.328187	-4.283139	-0.867159
1	1.328185	4.283139	-0.867159

fullerene

6	0.725155	-0.998091	3.313751
6	1.173326	0.381237	3.313751
6	0.000000	1.233708	3.313751
6	-1.173326	0.381237	3.313751
6	-0.725155	-0.998091	3.313751
6	-1.417843	-1.951493	2.585416
6	-0.692688	-2.949584	1.822943
6	0.692688	-2.949584	1.822943

6	1.417843	-1.951493	2.585416
6	2.591169	-1.570257	1.822943
6	3.019273	-0.252686	1.822943
6	2.294118	0.745404	2.585416
6	2.294118	1.979112	1.822943
6	1.173326	2.793415	1.822943
6	0.000000	2.412178	2.585416
6	-1.173326	2.793415	1.822943
6	-2.294118	1.979112	1.822943
6	-2.294118	0.745404	2.585416
6	-3.019273	-0.252686	1.822943
6	-2.591169	-1.570257	1.822943
6	-2.591169	-2.332730	0.589235
6	-1.417843	-3.185201	0.589235
6	-0.725155	-3.410269	-0.589235
6	0.725155	-3.410269	-0.589235
6	1.417843	-3.185201	0.589235
6	2.591169	-2.332730	0.589235
6	3.019273	-1.743495	-0.589235
6	3.467444	-0.364167	-0.589235
6	3.467444	0.364167	0.589235
6	3.019273	1.743495	0.589235
6	2.591169	2.332730	-0.589235
6	1.417843	3.185201	-0.589235
6	0.725155	3.410269	0.589235
6	-0.725155	3.410269	0.589235
6	-1.417843	3.185201	-0.589235
6	-2.591169	2.332730	-0.589235
6	-3.019273	1.743495	0.589235
6	-3.467444	0.364167	0.589235
6	-3.467444	-0.364167	-0.589235
6	-3.019273	-1.743495	-0.589235
6	-2.294118	-1.979112	-1.822943
6	-1.173326	-2.793415	-1.822943
6	0.000000	-2.412178	-2.585416
6	1.173326	-2.793415	-1.822943
6	2.294118	-1.979112	-1.822943
6	2.294118	-0.745404	-2.585416
6	3.019273	0.252686	-1.822943
6	2.591169	1.570257	-1.822943
6	1.417843	1.951493	-2.585416
6	0.692688	2.949584	-1.822943
6	-0.692688	2.949584	-1.822943
6	-1.417843	1.951493	-2.585416

6	-2.591169	1.570257	-1.822943
6	-3.019273	0.252686	-1.822943
6	-2.294118	-0.745404	-2.585416
6	-1.173326	-0.381237	-3.313751
6	0.000000	-1.233708	-3.313751
6	1.173326	-0.381237	-3.313751
6	0.725155	0.998091	-3.313751
6	-0.725155	0.998091	-3.313751

ovalene

6	0.000000	3.527236	0.000000
6	1.218111	2.846186	0.000000
6	-1.218111	2.846186	0.000000
6	3.651405	-2.849749	0.000000
6	2.457112	-0.710613	0.000000
1	4.596359	-3.382055	0.000000
6	1.221066	1.423074	0.000000
6	0.000000	-0.717563	0.000000
6	4.888323	-0.687269	0.000000
6	4.888323	0.687269	0.000000
6	3.680003	-1.415024	0.000000
6	3.680003	1.415024	0.000000
6	3.651405	2.849749	0.000000
6	2.457112	0.710613	0.000000
6	2.480208	3.531962	0.000000
6	1.218111	-2.846186	0.000000
6	1.221066	-1.423074	0.000000
6	-1.218111	-2.846186	0.000000
6	-1.221066	-1.423074	0.000000
6	0.000000	0.717563	0.000000
6	-2.480208	-3.531962	0.000000
6	-3.651405	-2.849749	0.000000
6	-3.680003	-1.415024	0.000000
1	5.826003	-1.232173	0.000000
1	5.826003	1.232173	0.000000
1	4.596359	3.382056	0.000000
1	-4.596359	-3.382056	0.000000
6	-1.221066	1.423074	0.000000
6	-2.457112	0.710613	0.000000
6	-2.480208	3.531962	0.000000
6	-3.680003	1.415024	0.000000
6	-3.651405	2.849749	0.000000
6	-2.457112	-0.710613	0.000000
6	-4.888323	-0.687269	0.000000

1	-5.826003	-1.232173	0.000000
6	-4.888323	0.687269	0.000000
6	0.000000	-3.527236	0.000000
6	2.480208	-3.531962	0.000000
1	-5.826003	1.232173	0.000000
1	-4.596359	3.382055	0.000000
1	-2.475116	-4.616422	0.000000
1	0.000000	-4.612849	0.000000
1	2.475116	-4.616422	0.000000
1	-2.475116	4.616422	0.000000
1	0.000000	4.612849	0.000000
1	2.475116	4.616422	0.000000

cyclophane_C13H18

6	-2.722245	-0.470556	0.017271
1	-3.217790	-0.510387	0.991481
1	-3.393282	-0.929353	-0.713785
6	-1.395231	-1.173858	0.093622
6	1.395252	-1.173845	0.093612
6	-0.695728	-1.555802	-1.054548
6	-0.693222	-1.133605	1.296769
6	0.693252	-1.133597	1.296764
6	0.695745	-1.555794	-1.054554
1	-1.232728	-1.691795	-1.988523
1	-1.230238	-0.947983	2.221603
1	1.230273	-0.947968	2.221593
1	1.232738	-1.691782	-1.988534
6	2.722257	-0.470527	0.017252
1	3.217813	-0.510363	0.991456
1	3.393293	-0.929303	-0.713818
6	-2.495016	1.023409	-0.378244
1	-3.433348	1.554995	-0.198170
1	-2.319401	1.066526	-1.458835
6	-1.328153	1.760874	0.330134
1	-1.195356	1.361037	1.339612
1	-1.603951	2.811564	0.456385
6	-0.000013	1.665599	-0.455306
1	-0.000006	2.442947	-1.228215
1	-0.000013	0.728095	-0.999474
6	1.328116	1.760863	0.330154
1	1.195314	1.360989	1.339617
1	1.603901	2.811552	0.456443
6	2.494999	1.023440	-0.378236
1	3.433320	1.555042	-0.198146

1	2.319388	1.066575	-1.458827

cyclophane_C16H16

6	2.778304	0.775110	-0.180438
1	3.489990	1.274985	0.481166
1	3.149417	0.894825	-1.200699
6	1.402690	1.394452	-0.084419
6	-1.402427	1.394497	0.084547
6	0.618527	1.547762	-1.229438
6	0.768996	1.553418	1.148026
6	-0.618265	1.547527	1.229632
6	-0.768695	1.553665	-1.147822
1	1.091424	1.509760	-2.206002
1	1.355888	1.518853	2.061328
1	-1.091201	1.509284	2.206163
1	-1.355581	1.519429	-2.061138
6	-2.778163	0.775408	0.180396
1	-3.149378	0.895245	1.200616
1	-3.489694	1.275396	-0.481289
6	2.778189	-0.775395	0.180429
1	3.149296	-0.895166	1.200683
1	3.489755	-1.275315	-0.481259
6	-2.778324	-0.775131	-0.180418
1	-3.489852	-1.274873	0.481442
1	-3.149665	-0.894884	-1.200594
6	1.402455	-1.394604	0.084442
6	-0.618539	-1.547489	-1.229636
6	0.768729	-1.553523	-1.148007
1	-1.091490	-1.509258	-2.206165
1	1.355633	-1.519041	-2.061301
6	-1.402704	-1.394381	-0.084577
6	-0.768989	-1.553564	1.147812
1	-1.355905	-1.519268	2.061107
6	0.618253	-1.547783	1.229458
1	1.091142	-1.509791	2.206025

CNT_C48H12

6	-0.708534	2.369219	-0.429730
6	-1.419780	2.262665	0.811004
6	-1.419701	1.833644	-1.553850
6	-2.846616	1.832963	-1.553154
6	-1.419871	-0.428908	-2.364181
6	-2.846608	-0.428640	-2.362942
6	-0.708570	-1.557268	-1.837335

6	-1.419781	-2.262661	-0.811010
6	-2.846542	-2.261778	-0.810510
6	-2.846540	2.261776	0.810516
6	-1.419870	0.428907	2.364181
6	-2.846608	0.428649	2.362941
6	-0.708575	-0.812572	2.266639
6	-1.419702	-1.833639	1.553851
6	-2.846618	-1.832966	1.553147
6	-3.549935	1.514965	1.787086
6	-3.549785	-2.305611	0.418152
6	-3.549852	0.790726	-2.205176
6	-3.549902	-1.514908	-1.787020
6	-3.549820	-0.790696	2.205095
6	-3.549751	2.305526	-0.418137
6	-0.708534	-2.369238	0.429735
6	-0.708568	1.557277	1.837349
6	-0.708575	0.812575	-2.266652
1	-4.634021	2.330477	-0.422835
1	-4.634173	1.532020	1.807029
1	-4.634074	-0.799323	2.229041
1	-4.634052	-2.330601	0.422857
1	-4.634144	-1.531935	-1.806933
1	-4.634103	0.799369	-2.229158
6	0.708520	2.369181	-0.429723
6	1.419696	1.833644	-1.553867
6	1.419783	2.262654	0.811012
6	2.846566	2.261766	0.810523
6	1.419854	0.428906	2.364202
6	2.846609	0.428634	2.362994
6	0.708544	-0.812567	2.266624
6	1.419692	-1.833643	1.553864
6	2.846626	-1.832974	1.553189
6	2.846625	1.832980	-1.553181
6	1.419854	-0.428900	-2.364203
6	2.846609	-0.428644	-2.362993
6	0.708546	-1.557245	-1.837316
6	1.419780	-2.262650	-0.811011
6	2.846568	-2.261762	-0.810532
6	3.549828	0.790690	-2.205111
6	3.549789	-2.305424	0.418131
6	3.549921	1.514863	1.787010
6	3.549848	-0.790723	2.205195
6	3.549941	-1.514924	-1.787079
6	3.549809	2.305512	-0.418146

6	0.708518	-2.369168	0.429721
6	0.708548	0.812558	-2.266608
6	0.708548	1.557231	1.837306
1	4.634079	2.330595	-0.422871
1	4.634082	0.799358	-2.229157
1	4.634182	-1.532008	-1.807086
1	4.634062	-2.330477	0.422850
1	4.634098	-0.799397	2.229271
1	4.634166	1.531933	1.806993

acetylene

6	0.000000	0.000000	0.598045
6	0.000000	0.000000	-0.598045
1	0.000000	0.000000	-1.662231
1	0.000000	0.000000	1.662231

diacetylene

6	0.000000	0.000000	1.890610
6	0.000000	0.000000	0.688656
1	0.000000	0.000000	2.954475
6	0.000000	0.000000	-0.688656
6	0.000000	0.000000	-1.890610
1	0.000000	0.000000	-2.954475

triacetylene

6	0.000000	0.000000	-0.604822
6	0.000000	0.000000	0.604822
6	0.000000	0.000000	1.974564
6	0.000000	0.000000	3.178123
1	0.000000	0.000000	4.242093
6	0.000000	0.000000	-3.178122
6	0.000000	0.000000	-1.974564
1	0.000000	0.000000	-4.242094

tetraacetylene

6	0.000000	0.680449	0.000000
6	0.008534	1.892437	0.000000
6	0.019634	3.260125	0.000000
6	0.030232	4.464104	0.000000
1	0.039753	5.528204	0.000000
6	-0.014024	-1.892407	0.000000
6	-0.008401	-0.680403	0.000000
6	-0.018041	-3.260135	0.000000
6	-0.020748	-4.464157	0.000000

1	-0.022858	-5.528297	0.000000

pentaacetylene

6	-4.545404	-0.000403	-0.000082
6	-3.178464	0.000192	0.000010
6	-1.965675	0.000674	0.000121
6	-5.749578	-0.001117	-0.000065
6	-0.607333	0.001011	0.000074
6	0.607331	0.001070	0.000095
6	1.965674	0.000805	-0.000105
6	3.178463	0.000331	-0.000021
6	4.545408	-0.000462	-0.000149
1	-6.813783	-0.002672	0.000190
6	5.749579	-0.001281	-0.000059
1	6.813781	-0.002249	0.000894

hexaacetylene

6	-3.250713	-0.002567	-0.000098
6	-1.893370	-0.004663	-0.000002
6	-0.677781	-0.005651	0.000026
6	-4.463801	0.000146	-0.000054
6	0.677782	-0.005643	0.000046
6	1.893372	-0.004643	0.000020
6	3.250714	-0.002550	0.000005
6	4.463802	0.000151	0.000006
6	5.830407	0.003735	0.000005
6	7.034636	0.007267	0.000013
1	8.098887	0.010207	-0.000212
6	-5.830407	0.003732	-0.000003
6	-7.034640	0.007255	0.000075
1	-8.098893	0.010378	-0.000015

heptaacetylene

6	1.962799	-0.001723	0.000132
6	0.608281	-0.001914	-0.000086
6	-0.608278	-0.001967	-0.000159
6	3.178733	-0.001179	0.000365
6	-1.962797	-0.001755	-0.000238
6	-3.178730	-0.001216	-0.000061
6	-4.535675	-0.000392	-0.000056
6	-5.748871	0.000526	-0.000017
6	-7.115354	0.001586	0.000038
6	-8.319597	0.002600	0.000129
1	-9.383895	0.003601	0.000004

6	4.535674	-0.000456	0.000168
6	5.748872	0.000428	0.000094
6	7.115348	0.001584	-0.000118
6	8.319594	0.002664	-0.000208
1	9.383894	0.003679	0.000090

octaacetylene

6	3.247729	-0.003786	-0.000144
6	1.893660	-0.004988	-0.000118
6	0.676716	-0.005506	-0.000042
6	4.463810	-0.002194	-0.000100
6	-0.676716	-0.005530	0.000004
6	-1.893660	-0.005027	0.000093
6	-3.247729	-0.003891	0.000130
6	-4.463810	-0.002305	0.000149
6	-5.820551	-0.000083	0.000071
6	-7.033797	0.002285	0.000041
6	5.820551	-0.000058	-0.000059
6	7.033797	0.002251	0.000001
6	8.400163	0.005037	0.000073
6	9.604406	0.007649	0.000122
1	10.668713	0.010096	-0.000117
6	-8.400163	0.005089	-0.000062
6	-9.604407	0.007712	-0.000120
1	-10.668715	0.009974	-0.000123

nonaacetylene

6	1.961628	-0.010920	-0.000334
6	0.608666	-0.011969	-0.000174
6	-0.608665	-0.011943	0.000166
6	3.178720	-0.008938	-0.000435
6	-1.961629	-0.010934	0.000367
6	-3.178720	-0.008977	0.000508
6	-4.532576	-0.005981	0.000519
6	-5.748707	-0.002548	0.000443
6	-7.105340	0.001906	0.000239
6	-8.318595	0.006405	0.000053
6	4.532575	-0.005949	-0.000538
6	5.748706	-0.002478	-0.000425
6	7.105339	0.001926	-0.000267
6	8.318594	0.006389	-0.000053
6	-9.684908	0.011797	-0.000363
6	-10.889137	0.016759	-0.000604
1	-11.953462	0.020915	0.000278

6	9.684909	0.011752	0.000173
6	10.889139	0.016698	0.000434
1	11.953464	0.021121	0.001456
C2			
6	0.000000	0.000000	0.651636
6	0.000000	0.000000	-0.651636
C6			
6	0.997527	1.089106	0.000039
6	1.046922	-0.231823	-0.000041
6	0.444433	-1.408415	0.000040
6	-0.724204	-0.790692	-0.000040
6	-1.441999	0.319310	0.000039
6	-0.322679	1.022513	-0.000038
C8			
6	1.084386	-1.023906	0.000022
6	1.845729	-0.031241	-0.000051
6	1.023920	1.084371	0.000020
6	0.031242	1.845691	0.000013
6	-1.084386	1.023906	-0.000001
6	-1.845729	0.031241	-0.000037
6	-1.023920	-1.084371	0.000013
6	-0.031242	-1.845691	0.000022
C10			
6	-0.656286	-1.969387	-0.000017
6	-1.688602	-1.207561	0.000015
6	-2.075925	0.015556	-0.000071
6	-1.670350	1.232769	-0.000103
6	-0.626679	1.978925	0.000001
6	0.656292	1.969399	-0.000145
6	1.688529	1.207503	0.000192
6	2.076086	-0.015562	-0.000121
6	1.670262	-1.232683	0.000204
6	0.626675	-1.978959	0.000044
C12			
6	2.440116	-0.831542	-0.000067
6	1.623976	-1.749968	0.000067
6	0.499743	-2.528315	-0.000100
6	-1.940120	-1.697089	-0.000167
6	-2.327891	-0.531267	-0.000448

6	-2.440092	0.831567	0.000190
6	-1.624135	1.750141	0.000279
6	-0.499762	2.528303	0.000319
6	1.940186	1.697101	0.000120
6	2.328046	0.531300	0.000195
6	-0.703784	-2.281261	-0.000518
6	0.703718	2.281030	0.000130

C14

6	0.006087	2.875443	0.000275
6	1.251609	2.584940	0.000460
6	2.252362	1.788354	-0.000533
6	2.242124	-1.795574	0.000144
6	1.242257	-2.593328	-0.000563
6	-0.005997	-2.871914	0.000341
6	-1.253196	-2.588142	0.000065
6	-2.249461	-1.786097	0.000102
6	-2.799058	0.644966	0.000701
6	-2.244827	1.797769	-0.000044
6	2.801513	0.633263	0.000048
6	-2.804929	-0.633923	-0.000609
6	-1.240730	2.589995	-0.000598
6	2.802247	-0.645751	0.000211

C16

6	3.291295	0.355213	0.000030
6	-0.857683	-3.197562	-0.000093
6	2.867713	1.654674	0.000105
6	-2.076174	-2.578491	-0.000076
6	2.076137	2.578464	0.000077
6	0.857734	3.197725	0.000063
6	-0.355201	3.291144	0.000056
6	-2.867676	-1.654635	-0.000139
6	-1.654664	2.867622	-0.000020
6	-2.578553	2.076152	0.000032
6	-3.291392	-0.355222	-0.000113
6	-3.197679	0.857691	-0.000046
6	3.197710	-0.857706	0.000121
6	0.355226	-3.291301	-0.000040
6	2.578563	-2.076172	0.000030
6	1.654644	-2.867597	0.000013

pyrazine

6	0.000000	1.127905	0.695908

6	0.000000	1.127905	-0.695908
7	0.000000	0.000000	-1.402391
6	0.000000	-1.127905	-0.695908
6	0.000000	-1.127905	0.695908
7	0.000000	0.000000	1.402391
1	0.000000	2.059331	1.252145
1	0.000000	2.059331	-1.252145
1	0.000000	-2.059331	-1.252145
1	0.000000	-2.059331	1.252145

pyrrole

6	0.000000	0.711121	-0.979518
6	0.000000	1.120149	0.330423
7	0.000000	0.000000	1.117294
6	0.000000	-1.120149	0.330423
6	0.000000	-0.711121	-0.979518
1	0.000000	1.358703	-1.841243
1	0.000000	2.106328	0.764006
1	0.000000	-2.106328	0.764006
1	0.000000	-1.358703	-1.841243
1	0.000000	0.000000	2.122554

furan

6	0.000000	0.717313	-0.954632
6	0.000000	-0.717313	-0.954632
6	0.000000	-1.088208	0.347222
8	0.000000	0.000000	1.151549
6	0.000000	1.088208	0.347222
1	0.000000	1.374290	-1.808396
1	0.000000	-1.374290	-1.808396
1	0.000000	-2.041837	0.846661
1	0.000000	2.041837	0.846661

thiophene

6	0.000000	0.713421	-1.266620
6	0.000000	1.233734	-0.009280
16	0.000000	0.000000	1.191252
6	0.000000	-1.233734	-0.009280
6	0.000000	-0.713421	-1.266620
1	0.000000	1.320357	-2.161153
1	0.000000	2.270901	0.286536
1	0.000000	-2.270901	0.286536
1	0.000000	-1.320357	-2.161153

tetrahydropyran

6	-1.251587	0.693053	-0.226524
6	-1.172076	-0.768224	0.203272
8	-0.000229	-1.388840	-0.288891
6	1.171824	-0.768600	0.203266
6	1.251815	0.692651	-0.226519
6	0.000234	1.441512	0.239085
1	-2.157556	1.150660	0.179676
1	-1.318986	0.731270	-1.318334
1	-2.011371	-1.344848	-0.186450
1	-1.188622	-0.834004	1.302757
1	2.010929	-1.345489	-0.186471
1	1.188368	-0.834388	1.302750
1	2.157929	1.149961	0.179696
1	1.319240	0.730852	-1.318326
1	0.000407	2.467964	-0.133931
1	0.000240	1.496385	1.334283

THF

8	-0.000134	-1.243289	0.000549
6	1.158873	-0.426580	0.137699
6	-1.158757	-0.426446	-0.138405
6	0.726670	0.989509	-0.239180
6	-0.726713	0.989332	0.239473
1	-1.505837	-0.462068	-1.178021
1	1.945990	-0.822979	-0.506364
1	0.764786	1.123091	-1.323399
1	1.507478	-0.462675	1.176750
1	1.341863	1.758407	0.228226
1	-1.342001	1.758564	-0.227262
1	-0.764764	1.122035	1.323815
1	-1.946875	-0.822953	0.504339

thiozolidine

16	-1.297756	0.003271	0.018607
6	-0.042815	-1.321656	-0.152396
6	-0.005558	1.311155	0.093160
6	1.267507	-0.663109	0.259609
7	1.215894	0.658944	-0.354236
1	-0.003004	-1.646886	-1.190392
1	-0.308234	-2.155946	0.494297
1	2.026198	1.215998	-0.104012
1	-0.274475	2.123250	-0.580763
1	2.127724	-1.216401	-0.122050

1	0.043997	1.682549	1.123980
1	1.325839	-0.625842	1.358637

thioxanthene

6	-3.468650	1.006116	-0.569006
6	-2.310485	1.558104	-0.033713
6	-3.568172	-0.371112	-0.733405
1	-2.231357	2.631854	0.098604
1	-4.465893	-0.807051	-1.154524
6	-1.248440	0.747821	0.356781
6	-2.505213	-1.192589	-0.379222
1	-2.560518	-2.263509	-0.534267
6	-1.352523	-0.632322	0.164662
1	-4.290560	1.649518	-0.858167
6	2.310486	1.558104	-0.033712
6	1.248440	0.747821	0.356781
6	3.468650	1.006116	-0.569005
6	0.000000	1.299234	0.998010
1	4.290560	1.649517	-0.858166
6	1.352523	-0.632322	0.164662
6	3.568172	-0.371112	-0.733405
16	0.000000	-1.687154	0.638677
1	4.465893	-0.807051	-1.154524
6	2.505213	-1.192590	-0.379223
1	2.560518	-2.263509	-0.534267
1	2.231357	2.631853	0.098605
1	0.000000	0.995844	2.054094
1	0.000000	2.389390	0.962562

piperazine

6	0.733064	1.203206	-0.207040
6	-0.732262	1.203660	0.206915
7	-1.367371	0.000444	-0.325840
6	-0.733048	-1.203185	0.206915
6	0.732277	-1.203681	-0.207041
7	1.367285	-0.000445	0.326119
1	1.235840	2.081311	0.203947
1	0.779074	1.252310	-1.307093
1	-1.234445	2.082080	-0.204168
1	-0.778036	1.253006	1.306952
1	-2.354552	0.000766	-0.097884
1	-1.235802	-2.081279	-0.204167
1	-0.778852	-1.252500	1.306953
1	1.234483	-2.082112	0.203945

1	0.778256	-1.252814	-1.307094
1	2.354459	-0.000766	0.098156

pyrrolidine

6	0.775601	1.024615	-0.058709
6	-0.775556	1.024621	-0.058864
6	1.152908	-0.446702	0.178107
6	-1.152915	-0.446622	0.178237
7	-0.000054	-1.162679	-0.365031
1	1.195699	1.675958	0.707987
1	-1.154376	1.358177	-1.025135
1	-1.195826	1.676214	0.707526
1	-0.000054	-2.139379	-0.093129
1	1.154633	1.358512	-1.024777
1	-2.071728	-0.738265	-0.332723
1	1.285815	-0.624901	1.257848
1	2.071633	-0.738350	-0.333013
1	-1.285640	-0.624690	1.258003

dioxolane

6	-1.035190	-0.655125	-0.061423
8	0.288740	-1.178365	-0.056836
6	-0.832923	0.851548	0.160173
6	1.166386	-0.093121	0.147215
8	0.494981	1.054960	-0.285058
1	-1.628121	-1.117166	0.730702
1	-1.498575	1.480806	-0.426814
1	2.064187	-0.228757	-0.453731
1	1.416336	-0.011792	1.216399
1	-0.920152	1.111224	1.222630
1	-1.493082	-0.866882	-1.029817

DBN

7	-0.231053	0.648626	0.063742
6	-0.194629	-0.733145	-0.011731
7	0.826636	-1.484927	-0.078348
6	2.130293	-0.824358	-0.130287
6	2.140648	0.615277	0.392097
6	0.974612	1.397930	-0.207731
6	-1.558338	1.169948	-0.201719
6	-2.456662	0.022448	0.279379
6	-1.626654	-1.226597	-0.047892
1	2.837413	-1.429407	0.441991
1	2.480993	-0.844713	-1.169270

1	2.026823	0.609755	1.479485
1	3.088640	1.102778	0.155225
1	0.888607	2.389325	0.245534
1	1.118064	1.534961	-1.290393
1	-1.705373	1.369529	-1.274289
1	-1.724438	2.102017	0.343877
1	-2.596864	0.106763	1.358522
1	-3.435692	0.029877	-0.198188
1	-1.830604	-1.586131	-1.060378
1	-1.772272	-2.059655	0.637430

benzonitrile

7	-3.190259	-0.000221	-0.000727
6	-0.603062	0.000190	0.000180
6	0.089583	-1.212498	0.000122
6	0.089937	1.212675	0.000123
6	1.477185	-1.206681	0.000028
6	1.477537	1.206448	0.000029
6	2.170325	-0.000218	-0.000024
6	-2.040312	0.000414	0.000353
1	-0.463139	-2.143383	0.000168
1	-0.462515	2.143720	0.000171
1	2.018068	-2.144722	-0.000008
1	2.018693	2.144331	-0.000005
1	3.253542	-0.000376	-0.000102

porphyrin

7	2.098071	-0.015596	0.000386
7	0.015276	2.014614	-0.000001
7	-0.015306	-2.014634	-0.000105
7	-2.098053	0.015542	-0.000156
6	2.883332	1.100677	0.000017
6	1.098826	2.827403	0.000009
6	2.866297	-1.143663	0.000183
6	-1.056013	2.843534	0.000067
6	2.429780	2.412322	-0.000086
6	4.243599	0.650402	-0.000195
6	0.706194	4.232499	0.000015
6	4.233245	-0.714077	-0.000103
6	-0.642371	4.242607	0.000113
6	2.393002	-2.448348	0.000070
6	-2.392983	2.448360	-0.000041
6	1.056014	-2.843496	-0.000013
6	-2.866216	1.143658	-0.000141

6	-1.098888	-2.827462	-0.000061
6	-2.883388	-1.100689	-0.000117
6	-2.429817	-2.412333	-0.000006
6	0.642380	-4.242563	-0.000041
6	-4.233186	0.714150	0.000044
6	-0.706194	-4.232519	0.000096
6	-4.243614	-0.650363	0.000031
1	3.191860	3.182710	-0.000345
1	1.083955	-0.007803	0.000525
1	5.099586	1.307496	-0.000400
1	1.388370	5.070010	0.000038
1	5.079189	-1.384049	-0.000206
1	-1.311934	5.090234	0.000249
1	3.143393	-3.230130	0.000050
1	-3.143453	3.230064	-0.000102
1	-3.191893	-3.182730	0.000193
1	1.311958	-5.090183	-0.000010
1	-5.079060	1.384213	0.000266
1	-1.388310	-5.070080	0.000137
1	-5.099644	-1.307402	0.000133
1	-1.083933	0.007585	-0.000438

aziridine

7	-0.000001	0.849955	-0.172454
6	0.740813	-0.394428	0.023330
6	-0.740812	-0.394429	0.023330
1	1.244151	-0.558419	0.969598
1	1.278054	-0.745520	-0.848758
1	-1.278051	-0.745525	-0.848758
1	-1.244147	-0.558422	0.969599
1	-0.000001	1.391339	0.685541

cyanogen

7	0.000000	0.000000	1.841683
7	0.000000	0.000000	-1.841683
6	0.000000	0.000000	0.693206
6	0.000000	0.000000	-0.693206

pyramidopyramidine

6	-2.272346	-0.669640	0.000114
7	-2.361138	0.691829	-0.000167
6	-1.239221	1.358487	0.000037
6	0.020234	0.699699	0.000069
6	-0.020275	-0.699683	0.000067

7	-1.185832	-1.394652	0.000048
7	1.185869	1.394663	0.000055
6	2.272325	0.669682	0.000094
7	2.361133	-0.691882	-0.000164
6	1.239251	-1.358489	0.000042
1	-3.221097	-1.195177	-0.000445
1	-1.270387	2.445008	-0.000053
1	3.221118	1.195141	-0.000402
1	1.270332	-2.445017	-0.000052

oxirane

6	-0.733784	-0.366168	0.000007
6	0.734072	-0.365822	0.000009
8	-0.000296	0.843093	-0.000012
1	-1.265287	-0.588529	-0.919351
1	-1.265332	-0.588457	0.919354
1	1.265605	-0.587932	-0.919644
1	1.265655	-0.587883	0.919635

ethylene carbonate

6	-1.289531	-0.752885	0.128652
8	0.069615	-1.102825	-0.115150
6	0.845641	-0.000033	0.000038
8	0.069510	1.102788	0.115466
6	-1.289453	0.752917	-0.128801
1	-1.926093	-1.315069	-0.550368
8	2.026793	0.000049	-0.000134
1	-1.537243	0.995976	-1.163998
1	-1.926313	1.315153	0.549885
1	-1.537636	-0.996155	1.163695

furfural

6	-0.218555	-1.931509	0.000000
6	-0.938905	-0.703413	0.000000
6	0.000000	0.283993	0.000000
8	1.248573	-0.254405	0.000000
6	1.098908	-1.590009	0.000000
1	-0.619313	-2.931471	0.000000
1	-2.005435	-0.548176	0.000000
1	2.007944	-2.167828	0.000000
6	-0.104467	1.742327	0.000000
8	-1.157481	2.325244	0.000000
1	0.866180	2.272425	0.000000

ethylene glycol

8	1.768004	-0.259794	0.000012
6	0.570974	0.495818	0.000011
6	-0.570973	-0.495813	-0.000011
8	-1.768006	0.259791	-0.000012
1	2.509169	0.347718	-0.000084
1	0.487729	1.131183	0.889341
1	0.487742	1.131206	-0.889303
1	-0.487724	-1.131180	-0.889340
1	-0.487737	-1.131203	0.889302
1	-2.509168	-0.347723	0.000084

tetrathiafulvalene

16	-1.629795	1.491382	-0.000807
16	-1.629801	-1.491385	-0.000798
16	1.629799	-1.491384	-0.000815
16	1.629798	1.491385	-0.000806
6	-0.669571	0.000002	-0.000844
6	0.669570	-0.000006	-0.000847
6	-3.176538	0.664349	0.001999
6	-3.176540	-0.664343	0.002019
6	3.176540	-0.664346	0.001995
6	3.176537	0.664345	0.002015
1	-4.064783	1.279755	0.003382
1	-4.064789	-1.279742	0.003415
1	4.064787	-1.279749	0.003381
1	4.064788	1.279742	0.003414

dithianodithiine

6	-5.440283	0.594715	0.390086
6	-5.574565	-0.718193	-0.356396
16	-4.030352	-1.719597	-0.452560
6	-2.800593	-0.639926	0.179337
6	-2.798072	0.700394	0.178788
16	-4.161423	1.679440	-0.330789
16	-1.399742	-1.433594	0.922195
6	-0.336864	0.035041	0.689495
16	-1.402393	1.500872	0.919291
6	0.336830	0.035051	-0.689284
16	1.402342	1.500906	-0.919064
6	2.797974	0.700447	-0.178471
6	2.800520	-0.639892	-0.179077
16	1.399736	-1.433579	-0.921976
16	4.161523	1.679180	0.331110

6	5.439916	0.594819	-0.391215
6	5.574887	-0.718382	0.354618
16	4.030422	-1.719227	0.453076
1	-6.380051	1.144848	0.321885
1	-5.193159	0.440417	1.440326
1	-6.309744	-1.353176	0.141740
1	-5.894357	-0.533396	-1.380283
1	0.417143	0.033997	1.477481
1	-0.417183	0.033997	-1.477264
1	6.379734	1.144946	-0.323621
1	5.191888	0.440933	-1.441299
1	6.309148	-1.353392	-0.144838
1	5.896253	-0.534027	1.378095

thiirane

16	-0.861731	0.000001	-0.000005
6	0.792217	0.739927	0.000008
6	0.792212	-0.739930	0.000002
1	1.070277	1.249180	0.914020
1	1.070290	1.249184	-0.914000
1	1.070281	-1.249181	-0.914009
1	1.070273	-1.249187	0.914013

thietane

16	-1.091194	0.000000	-0.066390
6	1.331875	0.000001	-0.161358
6	0.343697	1.140661	0.134368
6	0.343698	-1.140661	0.134368
1	1.601231	0.000000	-1.217929
1	2.244590	0.000001	0.436761
1	0.402630	1.505086	1.159526
1	0.346205	1.977926	-0.559957
1	0.346207	-1.977925	-0.559957
1	0.402632	-1.505085	1.159527

thiane

16	-1.496465	-0.000003	-0.201454
6	1.714129	0.000001	0.166111
6	0.982946	1.275734	-0.259748
6	0.982950	-1.275731	-0.259752
6	-0.419106	1.366956	0.335659
6	-0.419099	-1.366955	0.335663
1	2.722538	0.000005	-0.254827
1	1.827771	0.000000	1.257179

1	1.558795	2.150710	0.057677
1	0.909235	1.310529	-1.351035
1	0.909233	-1.310522	-1.351039
1	1.558799	-2.150707	0.057669
1	-0.373681	1.367291	1.428803
1	-0.923257	2.281407	0.021207
1	-0.923248	-2.281409	0.021220
1	-0.373669	-1.367284	1.428808

thiaindans

6	2.547012	0.530348	0.048763
6	2.383688	-0.850825	0.059868
6	1.111457	-1.415722	0.018658
6	0.009697	-0.573039	-0.039133
6	0.160625	0.816320	-0.059242
6	1.432961	1.365736	-0.013139
16	-1.687305	-1.084196	-0.105522
6	-2.223552	0.610317	0.352245
6	-1.149507	1.552575	-0.197065
1	3.541094	0.957956	0.091327
1	3.251899	-1.496787	0.112078
1	0.983315	-2.491032	0.041903
1	1.557521	2.443152	-0.026608
1	-3.209792	0.792947	-0.069779
1	-2.273913	0.668632	1.440144
1	-1.150175	2.507606	0.331854
1	-1.337358	1.750399	-1.258295

SeC3Se

34	0.000000	0.000000	2.966929
6	0.000000	0.000000	1.274174
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	-1.274174
34	0.000000	0.000000	-2.966929

SC3S

16	0.000000	0.000000	2.826408
6	0.000000	0.000000	1.273983
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	-1.273983
16	0.000000	0.000000	-2.826408

C5S

6	0.000000	0.000000	-2.708296

6	0.000000	0.000000	-1.414257
6	0.000000	0.000000	-0.151139
6	0.000000	0.000000	1.131206
16	0.000000	0.000000	2.672855
6	0.000000	0.000000	-3.985128

NCCP

6	0.000000	0.000000	0.087820
6	0.000000	0.000000	-1.291565
7	0.000000	0.000000	-2.445745
15	0.000000	0.000000	1.622846

Cyclopropenyl cation

6	0.000000	0.785362	0.000000
6	0.680143	-0.392681	0.000000
6	-0.680143	-0.392681	0.000000
1	1.617489	-0.933858	0.000000
1	0.000000	1.867716	0.000000
1	-1.617489	-0.933858	0.000000

cycloheptatrienyl cation

6	-0.526927	1.516348	0.000025
6	0.857010	1.357362	0.000036
6	-1.514065	0.533444	-0.000031
1	1.436434	2.275062	0.000097
1	-2.537692	0.894123	-0.000279
6	1.595596	0.176261	-0.000043
6	-0.183186	-1.594732	0.000089
1	2.674364	0.295381	-0.000091
1	-0.307085	-2.672957	-0.000060
6	1.132627	-1.137523	-0.000022
1	1.898360	-1.906641	-0.000112
1	-0.883251	2.541505	0.000029
6	-1.361044	-0.851130	0.000019
1	-2.281199	-1.426656	-0.000020

benzene-1-ylium

6	0.000000	0.000000	1.177569
6	0.000000	-1.269702	0.818278
6	0.000000	1.269702	0.818278
1	0.000000	-2.182076	1.399070
1	0.000000	2.182076	1.399070
6	0.000000	-1.209035	-0.609242
6	0.000000	1.209035	-0.609242

1	0.000000	-2.166928	-1.119042
1	0.000000	2.166928	-1.119042
6	0.000000	0.000000	-1.293103
1	0.000000	0.000000	-2.375283

propan-1-ylium

6	0.000000	-0.895669	0.000000
1	0.232160	-1.411078	0.923155
1	0.232160	-1.411078	-0.923155
6	-0.924313	0.146380	0.000000
1	-1.358469	0.503956	0.927689
1	-1.358469	0.503956	-0.927689
6	0.797143	0.598109	0.000000
1	1.363866	0.570308	-0.925040
1	1.363866	0.570308	0.925040
1	0.287904	1.580709	0.000000

propan-2-ylium

6	0.005813	0.446424	0.000000
1	-0.014385	1.538354	0.000000
6	0.005813	-0.202287	1.281934
6	0.005813	-0.202287	-1.281934
1	0.798499	0.247193	-1.903786
1	0.061571	-1.286478	-1.255445
1	-0.905195	0.144560	-1.807865
1	0.061571	-1.286478	1.255445
1	-0.905195	0.144560	1.807865
1	0.798499	0.247193	1.903786

2-methylpropan-2-ylium

6	-0.003008	0.003794	-0.016003
6	-1.347330	0.569024	-0.015512
6	1.168508	0.875141	-0.013376
1	1.993987	0.436826	-0.581755
1	0.963997	1.902606	-0.303773
1	1.519486	0.865706	1.035504
1	-1.417826	1.493653	-0.590059
1	-1.505738	0.861461	1.041719
1	-2.124757	-0.149466	-0.270358
6	0.175727	-1.442192	0.017666
1	1.160241	-1.759775	0.357590
1	-0.640514	-1.959301	0.525071
1	0.087745	-1.726316	-1.050590

ethen-1-ylium

6	0.001308	0.671197	0.000000
6	0.001308	-0.582160	0.000000
1	-0.003369	1.754274	0.000000
1	-0.953532	-1.133000	0.000000
1	0.941207	-1.155491	0.000000

Cyclopentadienyl Anion

6	0.000000	0.704955	-0.969983
6	0.000000	-0.704955	-0.969983
6	0.000000	1.140621	0.370374
1	0.000000	2.173093	0.705470
6	0.000000	0.000000	1.199548
1	0.000000	0.000000	2.284796
6	0.000000	-1.140621	0.370374
1	0.000000	-2.173093	0.705470
1	0.000000	-1.341968	-1.848860
1	0.000000	1.341968	-1.848860

acetate

6	-1.347747	0.054668	-0.000012
1	-1.713462	1.083474	-0.000570
1	-1.725953	-0.476169	-0.879119
1	-1.725868	-0.475086	0.879797
6	0.219555	-0.001525	-0.000015
8	0.690738	-1.155805	0.000004
8	0.801066	1.099420	0.000003

benzen-1-ide

6	0.000000	0.000000	1.558356
6	0.000000	-1.167455	0.749596
6	0.000000	1.167455	0.749596
1	0.000000	-2.147077	1.242343
1	0.000000	2.147077	1.242343
6	0.000000	-1.194130	-0.649277
6	0.000000	1.194130	-0.649277
1	0.000000	-2.144170	-1.186096
1	0.000000	2.144170	-1.186096
6	0.000000	0.000000	-1.368439
1	0.000000	0.000000	-2.455819

ethyn-1-ide

6	0.000000	0.000000	0.749357
6	0.000000	0.000000	-0.489383

1	0.000000	0.000000	-1.559841

ethen-1-ide

6	0.067971	0.784430	0.000000
6	0.067971	-0.568803	0.000000
1	-1.014015	1.093595	0.000000
1	-0.812611	-1.246589	0.000000
1	1.010970	-1.140772	0.000000

2-oxopropan-1-ide

8	0.169161	1.379813	0.000022
6	0.140616	0.118903	0.000028
6	1.192287	-0.774381	-0.000017
1	2.212545	-0.403222	-0.000150
1	1.030060	-1.846273	0.000188
6	-1.278064	-0.499651	-0.000027
1	-1.818164	-0.132528	0.879502
1	-1.818146	-0.131776	-0.879262
1	-1.288614	-1.593931	-0.000353

ethan-1-ide

6	-0.065819	0.857400	0.000000
1	0.550914	1.174001	0.871814
1	0.550914	1.174001	-0.871814
6	-0.065819	-0.681816	0.000000
1	-0.610514	-1.078014	0.873844
1	-0.610514	-1.078014	-0.873844
1	0.909032	-1.245478	0.000000

Benzene radical

6	0.000000	0.000000	1.393837
6	0.000000	1.221306	0.767699
6	0.000000	-1.221306	0.767699
1	0.000000	2.154741	1.319346
1	0.000000	-2.154741	1.319346
6	0.000000	1.208741	-0.629346
6	0.000000	-1.208741	-0.629346
1	0.000000	2.146524	-1.174542
1	0.000000	-2.146524	-1.174542
6	0.000000	0.000000	-1.318431
1	0.000000	0.000000	-2.402291

3-methylbut-2-enenitrile radical

6	0.795367	0.047990	-0.000146

6	1.086671	-1.433675	0.000024
6	1.987060	0.967516	0.000180
1	1.688120	2.013953	0.000041
1	2.604245	0.772357	0.881566
1	2.605006	0.772209	-0.880617
1	1.679642	-1.690425	0.882133
1	1.679887	-1.690590	-0.881872
1	0.174010	-2.027197	-0.000058
6	-0.435203	0.506799	-0.000423
6	-1.769286	0.197563	-0.000273
7	-2.916938	0.018934	0.000376

allyl_radical

6	0.000004	0.447119	-0.000176
6	-1.220913	-0.197029	0.000035
1	-1.276062	-1.279188	0.000289
1	-2.151464	0.353198	0.000200
6	1.220890	-0.197070	-0.000004
1	2.151355	0.353337	0.000732
1	1.276175	-1.279202	-0.000384
1	0.000107	1.533727	0.000037

vinyl_radical

6	-0.706436	-0.147817	-0.000212
6	0.586186	0.030826	0.000171
1	1.027445	1.028363	-0.000486
1	1.279180	-0.806113	0.000056
1	-1.585130	0.479697	0.000678

cyclobutadiene

6	-0.785341	-0.664031	0.000486
6	-0.785289	0.664058	-0.000438
6	0.785312	0.664030	0.000453
6	0.785317	-0.664059	-0.000497
1	-1.547597	-1.429932	0.000893
1	-1.547512	1.429993	-0.000813
1	1.547562	1.429939	0.000836
1	1.547548	-1.429985	-0.000942

azulene

6	0.000000	0.000000	-2.491057
6	0.000000	1.262383	-1.902729
6	0.000000	1.590141	-0.549817
6	0.000000	-1.262383	-1.902729

6	0.000000	0.746474	0.551643
6	0.000000	-1.590141	-0.549817
6	0.000000	-0.746474	0.551643
1	0.000000	0.000000	-3.577161
1	0.000000	2.100865	-2.590754
1	0.000000	2.652857	-0.318545
1	0.000000	-2.100865	-2.590754
1	0.000000	-2.652857	-0.318545
6	0.000000	1.146765	1.893593
1	0.000000	2.171306	2.236676
6	0.000000	0.000000	2.696374
1	0.000000	0.000000	3.778226
6	0.000000	-1.146765	1.893593
1	0.000000	-2.171306	2.236676

hexa_1,5_dien_3_yne

6	1.049305	2.799513	0.000000
6	-0.039074	2.029044	0.000000
6	0.000000	0.603569	0.000000
6	0.000078	-0.603597	0.000000
6	0.039079	-2.029075	0.000000
6	-1.049356	-2.799465	0.000000
1	0.964713	3.878744	0.000000
1	2.042820	2.368218	0.000000
1	-1.025855	2.481888	0.000000
1	1.025825	-2.481993	0.000000
1	-0.964855	-3.878702	0.000000
1	-2.042838	-2.368092	0.000000

hexpta_1_en_3,6_diyne

6	3.466379	0.062473	-0.000425
6	2.337108	-0.643940	0.000078
6	1.032949	-0.058662	0.000473
6	-0.077197	0.403449	0.000717
6	-1.421390	0.987430	-0.000125
6	-2.484437	-0.023608	-0.000179
6	-3.360556	-0.839966	-0.000206
1	4.429544	-0.431637	-0.000638
1	3.452302	1.145523	-0.000617
1	2.372049	-1.729015	0.000306
1	-1.538396	1.630865	0.877417
1	-1.537658	1.630189	-0.878264
1	-4.134968	-1.568988	-0.000203

2-pentene

6	-1.300381	-0.571311	0.208621
6	0.063636	0.019799	0.417124
6	-2.312131	0.476727	-0.266339
6	1.158291	-0.333423	-0.247531
6	2.515736	0.272517	-0.050296
1	-1.654638	-1.010025	1.147801
1	-1.236177	-1.386041	-0.517930
1	0.134355	0.812666	1.162530
1	-3.305505	0.041257	-0.390267
1	-2.000874	0.902804	-1.222181
1	-2.390646	1.294740	0.454010
1	1.081724	-1.122973	-0.993955
1	3.243268	-0.484640	0.255155
1	2.490852	1.050939	0.714115
1	2.886732	0.715424	-0.978750

isoprene

6	-1.591178	-0.894549	-0.000044
6	-0.518530	-0.099289	-0.000012
6	0.828067	-0.689167	-0.000031
6	1.968176	-0.000216	0.000021
6	-0.637639	1.400043	0.000051
1	-2.597010	-0.491036	-0.000030
1	-1.488771	-1.974091	-0.000086
1	0.864206	-1.775610	-0.000091
1	2.926461	-0.504320	0.000006
1	1.984734	1.083812	0.000083
1	-1.682971	1.707206	0.000036
1	-0.150036	1.826511	0.880913
1	-0.149988	1.826590	-0.880746

dihydroindene

6	0.955004	-1.405218	0.000052
6	-0.227861	-0.685745	-0.000006
6	2.164004	-0.709343	0.000097
1	3.099040	-1.256792	-0.000617
6	-0.210377	0.718128	-0.000222
6	2.181903	0.684313	0.000217
1	3.131666	1.206098	-0.000056
6	0.994768	1.411710	-0.000038
1	0.947041	-2.489826	0.000079
6	-1.660198	-1.154787	-0.000131
6	-1.599980	1.191627	-0.000021

6	-2.431557	0.141253	0.000146
1	1.011573	2.495620	-0.000405
1	-1.891241	-1.764209	0.880124
1	-1.891405	-1.764484	-0.880247
1	-3.512091	0.187511	0.000438
1	-1.888818	2.234455	0.000128

indene

6	-1.045716	1.402096	0.005923
6	0.149212	0.697966	0.057327
6	-2.245814	0.696202	-0.050937
1	-3.185444	1.233605	-0.101409
6	0.149212	-0.697966	0.057327
6	-2.245814	-0.696202	-0.050938
1	-3.185444	-1.233605	-0.101410
6	-1.045716	-1.402096	0.005923
1	-1.047792	2.486829	0.002622
6	1.564859	1.221903	0.138503
6	1.564859	-1.221903	0.138504
6	2.404568	0.000000	-0.289156
1	-1.047792	-2.486829	0.002622
1	1.794853	-1.508615	1.171005
1	1.794853	1.508615	1.171004
1	1.734664	-2.097531	-0.490502
1	2.502421	0.000000	-1.377699
1	3.407131	0.000000	0.139411
1	1.734664	2.097531	-0.490502

cyclopentadiene

6	-1.175997	-0.280062	0.000124
6	-0.734720	0.986980	-0.000008
6	0.735018	0.986761	-0.000131
6	1.175912	-0.280412	-0.000018
6	-0.000183	-1.213583	0.000012
1	-2.206581	-0.605765	0.000255
1	-1.349094	1.877344	0.000011
1	1.349672	1.876932	-0.000207
1	2.206388	-0.606451	-0.000025
1	-0.000256	-1.870041	0.878395
1	-0.000309	-1.870125	-0.878306

ferrocene

26	0.000000	0.000000	0.000000
6	0.000000	1.206663	1.746317

6	0.709259	0.976211	-1.746317
6	1.147605	0.372879	1.746317
6	-1.147605	0.372879	1.746317
6	-0.709259	0.976211	-1.746317
6	1.147605	-0.372879	-1.746317
6	0.709259	-0.976211	1.746317
6	-0.709259	-0.976211	1.746317
6	-1.147605	-0.372879	-1.746317
6	0.000000	-1.206663	-1.746317
1	0.000000	2.285087	1.715576
1	1.343141	1.848674	-1.715576
1	2.173247	0.706131	1.715576
1	-2.173247	0.706131	1.715576
1	-1.343141	1.848674	-1.715576
1	2.173247	-0.706131	-1.715576
1	1.343141	-1.848674	1.715576
1	-1.343141	-1.848674	1.715576
1	-2.173247	-0.706131	-1.715576
1	0.000000	-2.285087	-1.715576

Bis(benzene)chromium(0)

24	-0.000097	0.000451	0.000517
6	1.638777	1.140413	-0.836385
6	1.639435	1.294203	0.568787
6	1.637730	-0.153724	-1.405583
1	1.601369	2.283691	1.004464
1	1.597190	-0.271308	-2.480305
6	1.640132	0.153373	1.404145
6	1.638214	-1.294259	-0.569991
1	1.603756	0.272161	2.478915
1	1.598372	-2.283714	-1.005704
6	1.640062	-1.140720	0.835350
1	1.600807	-2.012529	1.474633
1	1.598425	2.012307	-1.475579
6	-1.639683	1.123304	-0.857765
6	-1.638768	1.304542	0.544331
6	-1.639163	-0.181714	-1.401611
1	-1.599640	2.302460	0.960371
1	-1.600141	-0.320410	-2.473830
6	-1.638994	0.181413	1.402386
6	-1.639002	-1.305065	-0.543770
1	-1.599857	0.320089	2.474566
1	-1.598111	-2.302789	-0.960053
6	-1.638599	-1.123538	0.858347

1	-1.599415	-1.982546	1.514820
1	-1.601264	1.982389	-1.514163

η3-CrCl3

24	0.000000	0.000000	-0.001579
17	0.000000	2.037877	-0.774559
17	-1.764853	-1.018938	-0.774559
17	1.764853	-1.018938	-0.774559
6	-0.700731	-0.404567	1.842546
6	0.000000	0.809134	1.842546
6	0.700731	-0.404567	1.842546
1	-1.599728	-0.923604	2.124857
1	0.000000	1.847207	2.124857
1	1.599728	-0.923604	2.124857

metallacyclobutane

24	0.000000	0.000000	0.070215
17	2.318751	0.000000	-0.039620
17	-2.318751	0.000000	-0.039620
17	0.000000	0.000000	-2.070513
6	0.000000	1.199092	1.323606
6	0.000000	0.000000	2.076422
6	0.000000	-1.199092	1.323606
1	0.000000	2.219708	1.678706
1	0.000000	0.000000	3.161399
1	0.000000	-2.219708	1.678706

C3H4Li2

6	0.000000	0.000000	0.581005
6	0.000000	0.750651	-0.751073
6	0.000000	-0.750651	-0.751073
3	1.600750	0.000000	1.673261
3	-1.600750	0.000000	1.673261
1	0.899669	1.241815	-1.128180
1	-0.899669	1.241815	-1.128180
1	-0.899669	-1.241815	-1.128180
1	0.899669	-1.241815	-1.128180

C6H6_CrCO3

24	0.122780	-0.000030	-0.000031
6	1.189046	0.609567	-1.424250
6	1.188868	0.928546	1.240229
6	1.188706	-1.538505	0.184116
8	1.771173	1.516587	2.025100

8	1.771512	0.995462	-2.325756
8	1.770857	-2.512319	0.301048
6	-1.604401	-0.557555	1.300734
6	-1.589982	0.840278	1.123273
6	-1.590058	-1.392765	0.165843
1	-1.541167	1.487913	1.989202
1	-1.541386	-2.466501	0.293821
6	-1.604166	1.405523	-0.167483
6	-1.604331	-0.847584	-1.133488
1	-1.577817	2.478019	-0.295241
1	-1.578062	-1.494475	-1.998424
6	-1.589906	0.552864	-1.289306
1	-1.541069	0.978875	-2.283177
1	-1.578203	-0.983148	2.293434

Si2C5H2

6	-0.689609	-1.854540	0.000166
6	-1.157040	-0.513424	0.000152
6	0.000299	0.384605	-0.000010
6	1.156305	-0.514249	-0.000402
6	0.688069	-1.855143	-0.000025
1	-1.327431	-2.728350	0.000216
1	1.325111	-2.729518	-0.000223
14	-1.761222	1.128318	-0.000080
14	1.762235	1.126995	0.000131

Ge2C5H2

6	-0.690878	2.317602	-0.000061
6	-1.156922	0.976000	-0.000108
6	0.000027	0.090515	0.000198
6	1.156918	0.976021	0.000062
6	0.690858	2.317620	0.000138
1	-1.324639	3.194159	-0.000187
1	1.324594	3.194194	0.000157
32	-1.858111	-0.725859	-0.000073
32	1.858112	-0.725856	0.000031

C6Li6

6	0.362010	1.371763	0.000000
6	1.369640	0.372527	0.000000
6	-1.007000	0.999367	0.000000
6	1.006732	-0.999196	0.000000
6	-1.369841	-0.372395	0.000000
6	-0.362040	-1.371732	0.000000

3	-0.787384	2.893413	0.000000
3	-2.902036	0.766766	0.000000
3	-2.112084	-2.129707	0.000000
3	0.787310	-2.896173	0.000000
3	2.901317	-0.765248	0.000000
3	2.113876	2.130281	0.000000

C2B8

6	0.752528	0.000005	0.001449
6	-0.752413	-0.000035	0.001509
5	0.802776	-1.700228	0.000282
5	-2.060159	0.809928	-0.000658
5	-0.803876	-1.699696	0.000494
5	-0.802731	1.699948	0.000465
5	2.060165	-0.809892	-0.000895
5	0.803802	1.699899	-0.000065
5	2.060613	0.808958	-0.001311
5	-2.060727	-0.808882	-0.001864

TS1

6	-1.062165	-1.162438	-1.072778
6	-1.605476	-0.980710	0.187434
6	-0.507387	0.958677	-0.470459
6	-0.391329	0.016112	-1.469538
6	-1.656659	0.518499	0.434453
6	0.103473	-1.206932	1.486747
6	0.813733	-0.033734	1.282462
1	-2.319917	-1.652187	0.645360
1	-0.161822	1.983647	-0.531143
1	0.205344	0.119510	-2.366216
1	-1.060240	-2.092805	-1.624996
1	-0.513161	-1.327274	2.373013
5	1.913715	0.155081	0.220422
1	0.593732	0.793822	1.955727
6	2.406137	-1.070223	-0.650656
1	1.641349	-1.827562	-0.841293
1	2.847737	-0.773096	-1.605723
1	3.201931	-1.571423	-0.082375
6	2.667992	1.538269	0.075746
1	3.731459	1.403618	0.306334
1	2.638932	1.893835	-0.960530
1	2.284576	2.331852	0.722090
8	-2.910078	0.983578	-0.053118
1	-2.898119	1.942893	-0.018197

1	-1.540852	0.800887	1.480475
1	0.451191	-2.134863	1.049846

TS2

6	-2.689830	-0.316123	-0.018768
6	-1.631811	-0.825946	0.727126
6	-1.017133	1.223425	-0.153823
6	-2.301277	0.915574	-0.572096
6	-0.743686	0.356194	1.043530
1	-1.171405	0.841971	1.932439
6	-0.338273	-1.467333	-0.921891
1	-1.093042	-1.847265	-1.602411
6	0.369637	-0.304825	-1.171895
1	0.211648	0.197914	-2.121505
1	-1.697524	-1.689846	1.378353
1	-0.517209	2.164256	-0.329362
1	-2.871354	1.482939	-1.294663
1	-3.597640	-0.854399	-0.252811
5	1.580017	0.048678	-0.165613
7	0.692567	0.074449	1.285161
1	1.096438	0.786036	1.890928
1	0.796745	-0.815125	1.770962
6	2.691199	-1.115517	0.025080
1	3.384546	-0.899074	0.848602
1	2.271946	-2.113570	0.201919
1	3.303439	-1.195954	-0.878325
6	2.267334	1.503727	-0.333437
1	3.007945	1.704039	0.451802
1	2.819546	1.526419	-1.279027
1	1.582088	2.356944	-0.358533
1	0.088830	-2.224874	-0.269386

TS3

6	2.631286	-0.038806	0.417059
6	1.802734	-0.956654	-0.218599
6	0.887582	1.165323	-0.412197
6	2.056037	1.243057	0.322910
6	0.929408	-0.137295	-1.148740
1	1.551674	0.046352	-2.042653
6	0.233050	-1.164840	1.273426
1	0.919392	-1.368516	2.085921
6	-0.460906	0.028863	1.187111
1	-0.196682	0.811800	1.893987
1	2.074797	-1.985905	-0.423057

1	0.276192	1.998260	-0.730755
1	2.422046	2.128907	0.823553
1	3.511427	-0.287459	0.994538
8	-0.332566	-0.608950	-1.542138
1	-0.228669	-1.429491	-2.030329
5	-1.800758	0.180565	0.394677
6	-2.749409	-1.048409	0.115131
1	-2.255922	-2.021993	0.120912
1	-3.505575	-1.070092	0.911625
1	-3.298598	-0.934056	-0.824108
6	-2.334083	1.614693	0.001201
1	-2.177342	1.733204	-1.079519
1	-3.412024	1.716259	0.157902
1	-1.822382	2.441959	0.499773
1	-0.168200	-2.046042	0.782119

TS4

6	-0.796436	-0.749268	0.802095
6	-0.419611	0.252831	-1.272345
6	0.313669	1.750068	0.309061
6	-0.469708	0.331102	1.617535
1	-1.275551	0.910284	2.053627
1	0.425062	0.287818	2.226832
6	0.865152	0.716249	-0.646454
1	1.374477	1.306403	-1.437619
6	-1.349960	1.284675	-1.176036
6	-0.892814	2.212246	-0.238003
1	-0.495513	-0.585272	-1.953398
1	0.950546	2.361979	0.937143
5	1.944868	-0.350375	-0.202162
6	2.831165	-0.140510	1.076968
1	3.879001	-0.386896	0.879826
1	2.776498	0.846657	1.539317
1	2.502378	-0.876743	1.824229
6	2.210075	-1.598306	-1.119546
1	2.734104	-2.408953	-0.608756
1	1.320144	-2.001893	-1.607048
1	2.875276	-1.260731	-1.927769
1	-1.450388	3.067287	0.121831
1	-2.319952	1.297115	-1.654604
6	-2.190686	-1.070169	0.487163
8	-2.578816	-2.117070	0.030214
1	-0.094373	-1.562164	0.633211
1	-2.900602	-0.239955	0.699644

TS5

6	-1.026422	-1.168265	-1.079597
6	-1.580967	-0.998808	0.182748
6	-0.518785	0.954694	-0.455647
6	-0.373469	0.017261	-1.460859
6	-1.666801	0.500124	0.432519
6	0.115059	-1.219106	1.465905
6	0.820858	-0.037997	1.275055
1	-2.283945	-1.694488	0.625945
1	-0.188048	1.984735	-0.509542
1	0.234348	0.137949	-2.347750
1	-1.005452	-2.097121	-1.634069
1	-0.493481	-1.351511	2.356180
5	1.929113	0.167771	0.227943
1	0.591438	0.782187	1.953830
6	2.444097	-1.043668	-0.650422
1	1.694164	-1.815070	-0.842947
1	2.876641	-0.732345	-1.605275
1	3.252465	-1.530457	-0.087426
6	2.665955	1.562084	0.094784
1	3.733924	1.440357	0.310764
1	2.618980	1.929469	-0.936933
1	2.277610	2.342530	0.754042
1	-1.538490	0.767564	1.482492
1	0.478207	-2.142213	1.030752
7	-2.929889	1.010630	-0.129566
1	-3.705314	0.647510	0.415449
1	-2.956534	2.019724	-0.025196

TS6

6	-0.320354	-1.506681	-0.702617
6	-0.771264	-1.186122	0.609349
6	-0.346141	0.742659	-0.530577
6	0.006904	-0.333408	-1.358988
6	-1.184056	0.241960	0.544146
6	0.866930	-0.999218	1.600984
6	1.520495	0.206039	1.237599
1	-1.345057	-1.907072	1.181688
1	-0.233579	1.791156	-0.774302
1	0.497844	-0.254128	-2.319871
1	-0.156087	-2.508662	-1.078372
1	0.404993	-1.042319	2.586015
5	2.511719	0.368330	0.121955

1	1.194501	1.094548	1.778670
6	3.095631	-0.874955	-0.695000
1	2.495000	-1.784727	-0.610366
1	3.215366	-0.648441	-1.761005
1	4.100573	-1.111132	-0.318394
6	3.107122	1.803389	-0.253437
1	4.202621	1.810580	-0.183648
1	2.874421	2.053429	-1.296524
1	2.722635	2.611498	0.375594
1	-1.203473	0.816887	1.463457
6	-2.810591	0.431073	-0.064390
8	-3.240653	-0.537823	-0.661199
8	-3.218874	1.540604	0.245984
1	1.359807	-1.933945	1.346596

TS7

6	-2.807288	-0.879081	0.220460
6	-4.199794	-0.815834	0.198848
6	-2.187634	-2.052508	-0.231641
8	-0.802076	-2.166415	-0.185176
6	-4.945968	-1.896004	-0.259174
6	-2.914360	-3.125872	-0.703555
1	-6.026705	-1.841021	-0.261098
1	-2.392541	-4.005811	-1.056723
6	-4.305160	-3.043851	-0.709175
1	-4.885189	-3.883536	-1.070213
6	-0.091270	-1.024331	-0.351890
1	-0.437918	-0.353986	-1.139180
6	-2.912127	2.339686	-0.504993
6	-1.987966	1.575358	0.247030
6	-0.779541	2.176333	0.704786
6	-0.500634	3.534334	0.476143
6	-1.440838	4.252361	-0.225027
6	-2.634464	3.663187	-0.721777
6	-1.944667	0.222228	0.639032
6	-0.674919	0.008168	1.236918
7	-0.016821	1.230073	1.313576
1	-3.813808	1.883104	-0.894070
1	0.408528	3.995953	0.839482
1	-1.265024	5.304495	-0.414099
1	-3.325825	4.277585	-1.283474
1	-0.432432	-0.767336	1.950327
6	2.247221	1.090445	-1.204355
6	2.306871	-0.173957	-0.605081

6	3.557589	-0.712318	-0.249068
6	4.756742	-0.035300	-0.471043
6	4.672552	1.211948	-1.063483
6	3.432645	1.767433	-1.428219
6	1.323684	-1.151567	-0.208476
6	2.016197	-2.212715	0.356343
7	3.341289	-1.957765	0.327847
1	1.297877	1.532766	-1.488920
1	5.712887	-0.464204	-0.197234
1	5.579624	1.770423	-1.256415
1	3.411376	2.741781	-1.900154
1	1.633296	-3.142899	0.749078
6	1.232839	1.464676	2.021053
1	1.721549	0.505098	2.185984
1	1.892574	2.082654	1.411350
1	1.044078	1.949986	2.980632
6	4.400826	-2.849923	0.771157
1	5.036142	-3.121660	-0.072929
1	5.003041	-2.359358	1.536958
1	3.953574	-3.749230	1.188771
1	-4.692963	0.072993	0.574515

TS8

6	-2.880669	-0.142241	0.169322
6	-4.102236	0.462408	0.436323
6	-2.864091	-1.379871	-0.471625
8	-1.599318	-1.905911	-0.672435
6	-5.276759	-0.184961	0.059579
6	-4.012492	-2.043771	-0.850501
1	-6.233485	0.279135	0.261167
1	-3.953717	-3.000421	-1.352503
6	-5.229463	-1.425228	-0.571064
1	-6.150318	-1.916456	-0.859109
6	-0.681920	-0.906753	-0.779360
1	-0.867857	-0.210381	-1.597766
6	-1.216218	2.564054	-0.884900
6	-0.940318	1.654616	0.132237
6	0.159248	1.865676	0.972841
6	1.016833	2.948301	0.841812
6	0.726032	3.848658	-0.174832
6	-0.374575	3.661669	-1.022205
6	-1.527485	0.368558	0.509318
6	-0.809008	-0.017403	1.673989
7	0.208796	0.797953	1.888384

1	-2.069481	2.425202	-1.539042
1	1.874838	3.086293	1.487939
1	1.360234	4.715107	-0.312552
1	-0.572970	4.392203	-1.796443
1	-0.946221	-0.913350	2.264736
6	2.111821	0.755905	-1.392289
6	1.863158	-0.488120	-0.796795
6	2.949507	-1.254307	-0.327674
6	4.273849	-0.821782	-0.421820
6	4.489787	0.412412	-1.006120
6	3.420376	1.189923	-1.488598
6	0.677441	-1.265366	-0.520852
6	1.101730	-2.439153	0.082003
7	2.448206	-2.437761	0.194422
1	1.299598	1.368787	-1.768789
1	5.097548	-1.427306	-0.063758
1	5.501834	0.784268	-1.104010
1	3.631102	2.146152	-1.951271
1	0.514453	-3.286126	0.404848
6	1.303467	0.600090	2.829825
1	2.229599	0.456621	2.268615
1	1.391237	1.474127	3.474939
1	1.095202	-0.279722	3.434516
6	3.271850	-3.526958	0.693582
1	3.894476	-3.176335	1.517798
1	2.624324	-4.325872	1.048351
1	3.909701	-3.908568	-0.105005
1	-4.133756	1.424456	0.934010

TS9

6	-4.117293	-1.120048	0.109594
6	-4.382718	0.262437	-0.146827
6	-3.353590	1.106789	-0.434836
6	-2.018130	0.618462	-0.527251
6	-1.724119	-0.772798	-0.219478
6	-2.854083	-1.621991	0.095513
1	-4.951805	-1.776266	0.332852
1	-5.402355	0.624735	-0.113520
1	-3.539928	2.157770	-0.633520
6	-0.912455	1.441171	-0.753801
8	-0.539087	-1.158899	-0.162529
6	3.545061	-1.545747	-0.184760
6	2.347372	-1.198033	0.419711
6	1.989560	0.149313	0.573098

6	2.866084	1.135703	0.100534
6	4.064220	0.784694	-0.505705
6	4.407254	-0.556001	-0.649383
1	3.804283	-2.590698	-0.304337
1	1.645649	-1.958242	0.739772
1	2.629243	2.184272	0.236373
1	4.736508	1.557869	-0.857634
1	5.343700	-0.828450	-1.121324
6	0.716275	0.473392	1.206897
6	0.048812	1.666398	1.036170
1	0.291562	-0.288097	1.847566
1	0.589663	2.526331	0.656514
1	-2.646667	-2.663693	0.308515
1	-0.795848	1.893574	1.673539
1	-0.034391	0.999067	-1.210961
1	-1.090423	2.490574	-0.970455

TS10

6	-2.280686	0.508696	-0.155493
8	-2.279793	-0.671476	0.242895
15	0.690315	0.081853	-0.058080
6	-0.385265	1.190654	-0.832327
1	-2.728816	0.775520	-1.126456
6	0.309873	0.009344	1.710410
6	0.406934	-1.561833	-0.751375
6	2.496418	0.362880	-0.150428
1	-2.318291	1.338720	0.573751
1	-0.348055	1.106110	-1.917339
1	1.009716	-0.646366	2.229987
1	-0.711655	-0.371779	1.788729
1	0.370051	1.013675	2.133265
1	1.004630	-2.309313	-0.228123
1	0.675098	-1.554773	-1.809124
1	-0.660994	-1.764979	-0.632899
1	3.038886	-0.427564	0.373827
1	2.735607	1.326189	0.302570
1	2.804566	0.382375	-1.196515
1	-0.270770	2.217757	-0.488348

TS11

6	2.898676	-1.226926	-0.790284
6	2.658110	0.141199	-0.207877
6	2.399315	0.120554	1.254288
1	2.787307	-1.209353	-1.876329

1	2.478836	1.061241	1.785353
6	1.036635	-0.196837	0.698274
8	1.959856	-2.164871	-0.252673
6	0.842812	-1.612918	0.289287
8	-0.151876	-2.262299	0.432087
6	2.563298	1.289474	-0.993844
6	2.208781	2.508411	-0.436512
1	2.615879	2.795528	0.523143
6	0.080720	0.780293	0.401239
6	0.323414	2.122511	0.656321
1	-0.376082	2.840865	0.245433
1	0.807727	2.401963	1.579952
8	-0.873029	0.440029	-0.508220
14	-2.478306	0.038732	-0.145231
6	-2.606803	-0.373054	1.669794
1	-3.636155	-0.634827	1.928796
1	-2.308378	0.474988	2.291541
1	-1.961948	-1.221467	1.906127
6	-2.911842	-1.396755	-1.245944
1	-3.956308	-1.691157	-1.115022
1	-2.274914	-2.249914	-1.004665
1	-2.762912	-1.139760	-2.297327
6	-3.521595	1.540451	-0.548015
1	-4.582864	1.335810	-0.382775
1	-3.395128	1.838006	-1.591632
1	-3.244666	2.389802	0.082243
1	2.864032	-0.694993	1.802549
1	3.891825	-1.604037	-0.535543
1	2.464875	1.145401	-2.065613
1	1.976432	3.338377	-1.092892

TS12

6	-2.106337	-1.759170	0.903819
6	-1.926420	-0.644879	-0.111696
6	-1.446929	-1.370673	-1.327742
6	-1.966352	-2.817941	-1.245749
6	-2.762100	-2.864136	0.079029
1	-2.645978	-1.467012	1.802074
1	-1.542985	-0.897533	-2.298830
1	-1.138558	-3.529916	-1.240249
1	-2.595152	-3.054462	-2.103428
1	-2.713289	-3.827922	0.585382
1	-3.809558	-2.606697	-0.095356
6	-0.132019	-1.081906	-0.631776

8	-0.821525	-2.255186	1.334161
6	0.227874	-1.931103	0.542205
8	1.332024	-2.302002	0.822910
6	-2.077565	0.722009	0.068791
6	-1.930569	3.070603	-0.932991
6	-1.601669	2.722042	1.527492
6	-2.329026	3.544839	0.467008
6	-2.097091	1.277123	1.483272
6	-1.855786	1.553220	-1.044044
1	-0.964646	3.512166	-1.193696
1	-0.523775	2.738907	1.331012
1	-3.409324	3.424091	0.605024
1	-3.119511	1.239791	1.880084
1	-2.643093	3.445003	-1.673148
1	-1.760615	3.139064	2.524324
1	-2.108480	4.609385	0.572734
1	-1.478825	0.650046	2.131539
1	-2.216164	1.158722	-1.986163
6	0.582271	0.093923	-0.856690
6	0.111445	1.054012	-1.750934
1	0.626166	2.008207	-1.750162
1	-0.272323	0.732076	-2.708438
8	1.449354	0.498034	0.117755
14	3.130923	0.309773	0.068240
6	3.571755	-0.981575	-1.204676
1	4.656433	-1.106818	-1.260519
1	3.214225	-0.695740	-2.197346
1	3.122372	-1.939059	-0.935765
6	3.653112	-0.156088	1.791946
1	4.740367	-0.242367	1.864067
1	3.205364	-1.113390	2.064650
1	3.325754	0.596707	2.513040
6	3.844840	1.971076	-0.424053
1	4.937872	1.944489	-0.429777
1	3.531638	2.753270	0.271773
1	3.513732	2.257158	-1.426070

TS13

6	1.192500	2.612052	-1.076032
6	0.240004	2.950011	-0.166227
6	-0.373574	1.949904	0.648611
6	0.013823	0.621057	0.540190
6	0.984279	0.245981	-0.433791
6	1.665405	1.266573	-1.179391

1	1.624427	3.375054	-1.714576
1	-0.096088	3.977253	-0.072942
8	1.379606	-0.970314	-0.566232
7	-1.341359	2.322355	1.554235
6	-0.680841	-0.420215	1.375631
1	-0.524872	-0.216445	2.439844
1	-0.265156	-1.403575	1.146321
8	-2.096975	-0.421385	1.179113
14	-2.782030	-0.788840	-0.311699
6	-1.874411	-2.240795	-1.061808
1	-0.815085	-2.013492	-1.213993
1	-2.306757	-2.499013	-2.032319
1	-1.943919	-3.122817	-0.419532
6	-2.707194	0.689427	-1.464418
1	-1.693535	0.864002	-1.833167
1	-3.038625	1.598523	-0.954481
1	-3.361655	0.532701	-2.326673
6	-4.561357	-1.200539	0.077099
1	-5.063356	-0.353779	0.551297
1	-4.623671	-2.052016	0.757993
1	-5.113773	-1.450631	-0.832297
6	3.388837	1.178656	-0.154127
1	3.756809	2.185504	-0.167418
6	3.622858	0.003588	0.211249
6	3.061735	-1.257937	0.263704
6	2.575266	-1.744728	1.606228
1	2.065583	-0.941420	2.140975
1	1.895858	-2.586787	1.469946
6	3.565929	-2.313613	-0.683387
1	3.811317	-1.875555	-1.649707
1	4.460025	-2.785416	-0.267267
1	3.427086	-2.072941	2.207797
1	2.150288	0.950574	-2.094757
1	2.795143	-3.073139	-0.817051
1	-2.009936	1.604065	1.800838
1	-1.732785	3.243677	1.441066

TS14

6	1.879527	0.444453	0.263073
6	0.775649	1.061217	1.051762
8	0.538550	2.277464	0.950751
6	2.817809	-0.007177	-0.340707
6	-0.672817	0.016127	0.271924
6	3.959605	-0.537381	-1.081922

7	-0.953197	-1.286595	0.294080
7	-1.721303	0.548844	-0.391908
7	-2.127531	-1.613462	-0.317422
6	-0.139679	-2.330952	0.890902
6	-2.574488	-0.468761	-0.728653
6	-1.891751	1.967147	-0.717421
1	0.684262	0.556136	2.034391
1	-3.495518	-0.326422	-1.270789
1	-1.016998	2.492485	-0.335537
1	-2.794401	2.342127	-0.236163
1	-1.970343	2.078290	-1.798376
1	3.629041	-1.167736	-1.909755
1	4.557421	0.277666	-1.493721
1	4.602029	-1.135275	-0.432883
1	-0.641626	-2.733407	1.770173
1	0.818411	-1.891419	1.161697
1	0.010401	-3.121693	0.157952

TS15

6	-1.240403	2.335647	0.616691
6	-0.048225	1.930259	0.087076
6	0.291683	0.555803	0.157839
8	-0.701335	0.099708	-1.497948
8	-0.280670	-0.218839	1.048523
6	1.609337	0.100846	-0.373843
6	-1.922655	0.206885	-1.120140
7	1.883613	-1.065329	-0.974867
7	2.744493	0.791597	-0.358168
6	-2.596166	1.400242	-1.139245
6	-2.534323	-1.013552	-0.465089
8	-3.606327	-0.721611	0.281598
6	-4.210806	-1.843782	0.928662
6	3.211088	-1.029865	-1.267870
6	1.044544	-2.269132	-1.028301
7	3.756863	0.093948	-0.914601
6	3.047760	2.036746	0.340281
6	-1.726732	3.752181	0.543860
1	-1.710509	1.681534	1.343825
1	0.476110	2.551697	-0.630898
1	0.460540	-0.774092	1.540274
1	-2.206218	2.202652	-1.751095
1	-3.614552	1.466392	-0.779840
8	-2.116933	-2.129360	-0.618342
1	-5.052013	-1.445078	1.488661

1	-4.547550	-2.570652	0.189269
1	-3.492917	-2.320463	1.596295
1	3.732749	-1.846411	-1.738287
1	0.012802	-1.982581	-1.204955
1	1.416218	-2.887991	-1.842733
1	1.149238	-2.779487	-0.069931
1	2.397132	2.114664	1.208230
1	4.084540	1.962058	0.656079
1	2.913804	2.888502	-0.325150
1	-1.291862	4.282121	-0.305240
1	-2.813389	3.796641	0.467604
1	-1.443263	4.280638	1.459093
17	2.054462	-1.327912	2.178946

TS16

6	2.031210	-1.359839	1.082375
6	3.208151	-1.457692	0.317583
6	3.696234	-0.267906	-0.185424
1	4.655396	-0.133115	-0.668932
6	2.705084	0.772965	-0.284530
8	2.871337	1.950448	-0.580172
6	1.319176	0.231020	-0.012618
6	0.100737	0.423792	-0.209686
6	-1.280500	0.212550	-0.125550
6	-1.932615	-0.757071	-0.930283
6	-2.100641	0.967858	0.751563
6	-3.300430	-0.954446	-0.851121
1	-1.330378	-1.346139	-1.611889
6	-3.466783	0.757170	0.817725
1	-1.630636	1.720660	1.373379
6	-4.090745	-0.204012	0.020541
1	-3.761401	-1.709822	-1.480592
1	-4.059589	1.353863	1.504576
1	-5.161440	-0.361005	0.074791
1	3.611044	-2.422793	0.005584
1	1.362030	-2.210196	1.175611
1	2.011002	-0.681370	1.925392

TS17

6	0.441907	1.045286	-0.653739
6	0.157227	2.067288	0.431576
6	-1.244122	2.639930	0.181545
6	-1.664376	3.610700	1.283730
6	-2.190515	1.478328	0.071530

6	1.939485	-0.082391	0.206919
7	3.188773	-0.122598	-0.257385
7	1.850262	-1.233753	0.920897
7	3.897173	-1.224310	0.121101
6	3.823431	0.876795	-1.102230
6	3.048119	-1.889561	0.838828
6	0.646283	-1.721813	1.583693
6	-1.757081	0.255979	-0.249173
6	-2.722356	-0.885171	-0.279650
8	-2.112360	-2.066342	-0.453660
6	-2.994637	-3.187911	-0.512708
1	-1.228294	3.175518	-0.775893
8	0.829345	1.346847	-1.759681
1	4.560700	1.431426	-0.522187
1	3.040647	1.531648	-1.479089
1	4.314542	0.366660	-1.928596
1	3.252289	-2.836081	1.312945
1	0.154617	-0.888339	2.082460
1	0.935847	-2.466970	2.323772
1	-0.037038	-2.144966	0.849094
1	-1.685232	3.103296	2.251979
1	-2.661641	4.011887	1.090463
1	-0.966369	4.448072	1.349403
1	-3.249213	1.599926	0.265647
8	-0.479274	-0.078206	-0.556724
8	-3.910455	-0.769913	-0.145097
1	-2.360501	-4.054317	-0.679563
1	-3.549409	-3.285705	0.421048
1	-3.703314	-3.066916	-1.331935
1	0.184526	1.596542	1.417958
1	0.926142	2.839124	0.379571

TS18

6	-1.039328	1.243732	-0.812586
6	0.360800	1.229779	-0.620543
6	1.020279	0.009480	-0.740033
6	2.486070	-0.097665	-0.463790
7	3.122929	-1.251974	-0.274953
7	3.443728	0.851970	-0.478521
7	4.446250	-1.065291	-0.083028
6	2.547395	-2.558821	0.043557
6	4.616856	0.211915	-0.203961
6	3.275227	2.299313	-0.476941
6	-1.793491	2.542529	-0.714399

6	-1.714999	0.189143	0.768582
6	-2.451702	-0.745180	0.059836
8	-1.934628	-1.653286	-0.700068
6	-3.961955	-0.709082	-0.010184
8	-4.449316	0.436706	0.480317
6	-5.877645	0.530756	0.476213
1	-1.388505	0.566881	-1.588212
1	0.819148	2.033566	-0.066346
8	0.474741	-1.094268	-1.018292
1	1.859721	-2.415244	0.878161
1	3.386467	-3.183590	0.335535
1	2.027158	-2.958440	-0.820228
1	5.561426	0.721719	-0.113666
1	2.857897	2.591092	0.488832
1	2.617610	2.594570	-1.291329
1	4.257366	2.746591	-0.615526
1	-0.919031	-1.486092	-0.795892
1	-1.463268	3.117690	0.152148
1	-2.867653	2.373222	-0.637890
1	-1.600329	3.134197	-1.614132
1	-2.270258	0.890735	1.375838
1	-0.737738	-0.098941	1.152449
8	-4.627020	-1.599354	-0.448305
1	-6.109988	1.503845	0.898427
1	-6.256623	0.446923	-0.542371
1	-6.305293	-0.267265	1.082906
17	1.701547	0.255989	2.190182

TS19

6	-0.965576	-1.369916	0.804184
6	-0.051350	-0.906386	-0.167373
6	0.342773	0.455041	0.192416
6	-0.205090	0.670562	1.555071
7	-1.032831	-0.438491	1.823286
6	0.224113	-1.706365	-1.266825
1	0.935743	-1.371458	-2.014818
6	-1.645264	-2.567841	0.667131
1	-2.369549	-2.887884	1.407739
6	-1.370926	-3.347142	-0.461741
1	-1.889096	-4.289939	-0.596043
6	-0.437234	-2.930024	-1.406277
1	-0.227029	-3.557402	-2.265175
6	-1.909638	-0.510413	2.958162
1	-2.955890	-0.549147	2.633811

1	-1.693748	-1.392607	3.569786
1	-1.740409	0.390025	3.548692
8	-0.058279	1.593033	2.332300
6	1.695078	0.976265	-0.121502
6	1.925706	2.276639	-0.361258
1	2.942672	2.640547	-0.473688
6	0.872551	3.326673	-0.499066
8	1.166839	4.487942	-0.286222
6	-0.451670	2.875728	-0.947915
6	-0.885830	1.692541	-0.714751
6	-2.168757	0.984431	-0.813644
6	-3.126090	1.146195	0.191975
6	-2.437195	0.095014	-1.857614
6	-4.313625	0.423154	0.163577
1	-2.910306	1.837018	1.000482
6	-3.623458	-0.627536	-1.887188
1	-1.694642	-0.035780	-2.634868
6	-4.562901	-0.471938	-0.872864
1	-5.045997	0.559492	0.952468
1	-3.806000	-1.326681	-2.695543
1	-5.483908	-1.044049	-0.890024
6	2.837719	0.020798	-0.082633
6	2.890141	-1.000250	0.872280
6	3.888396	0.122541	-1.000093
6	3.966955	-1.875701	0.919944
1	2.076182	-1.098252	1.582159
6	4.964663	-0.755872	-0.956559
1	3.841509	0.890202	-1.764238
6	5.010060	-1.758701	0.005846
1	3.990097	-2.655929	1.672365
1	5.764215	-0.663446	-1.683387
1	5.846179	-2.448041	0.038959

TS20

6	-0.732637	-0.195237	-1.356571
6	-1.157379	-0.431562	0.007251
6	-0.315877	0.474916	0.800657
7	0.618280	0.949764	-0.136372
8	-0.357735	0.760168	1.986109
6	-2.567796	-0.699168	0.380097
6	-2.778817	-1.871311	0.994856
1	-3.724763	-2.218171	1.391629
6	-1.596373	-2.754062	1.078847
8	-1.626398	-3.861158	1.570639

6	-0.392371	-2.129195	0.471431
6	0.824207	-2.455138	0.317411
6	2.120440	-2.010509	-0.034417
6	2.736532	-2.350083	-1.258987
6	2.874817	-1.242828	0.883479
6	4.020835	-1.919785	-1.551307
1	2.180826	-2.944063	-1.975478
6	4.160283	-0.827875	0.578890
1	2.411258	-0.952278	1.820043
6	4.751599	-1.159859	-0.638862
1	4.460322	-2.183051	-2.508480
1	4.693968	-0.204700	1.289598
1	5.752348	-0.819620	-0.877460
6	-3.623547	0.290277	0.068059
6	-3.293160	1.632531	-0.145556
6	-4.967002	-0.090886	-0.037765
6	-4.280019	2.568002	-0.433514
1	-2.256713	1.941306	-0.072972
6	-5.951127	0.842840	-0.328791
1	-5.233388	-1.133816	0.088901
6	-5.611422	2.178861	-0.525203
1	-4.004873	3.604937	-0.587236
1	-6.984837	0.527129	-0.413284
1	-6.379301	2.908479	-0.755472
6	1.801061	1.659650	0.099607
6	2.096030	2.182651	1.365855
6	2.720557	1.818911	-0.943727
6	3.302239	2.841732	1.568962
1	1.387361	2.049149	2.168977
6	3.914988	2.485142	-0.718806
1	2.493267	1.380408	-1.904472
6	4.220671	3.001561	0.536805
1	3.522451	3.234498	2.555801
1	4.624269	2.581129	-1.533563
1	5.160135	3.513939	0.708748
7	0.335164	0.530470	-1.429316
6	-1.344086	-0.820656	-2.562911
1	-0.800841	-0.510773	-3.455252
1	-1.302952	-1.909978	-2.471772
1	-2.395461	-0.531754	-2.657153

TS21

6	3.601458	-0.829319	0.443273
6	3.167230	0.452087	0.785029

6	2.770194	-1.612892	-0.357974
1	3.792722	1.082459	1.410325
1	3.078744	-2.616533	-0.635438
6	1.950617	0.943257	0.341183
6	1.551066	-1.134247	-0.807606
1	1.635951	1.945453	0.614205
1	0.918462	-1.763025	-1.426910
6	1.096292	0.168149	-0.482911
1	4.554851	-1.206655	0.793477
6	-0.192080	0.617026	-0.900695
1	-0.753407	0.034074	-1.618561
6	-0.628418	1.928144	-0.662988
7	-1.011459	2.996762	-0.413353
6	-2.771906	0.001197	0.967360
1	-3.103944	0.917760	1.441466
6	-1.459651	-0.345850	0.955347
1	-0.725021	0.174869	1.557375
1	-1.161452	-1.299536	0.534186
6	-3.754654	-0.779092	0.245525
8	-3.542500	-1.787629	-0.406212
1	-4.797586	-0.395923	0.319776

TS22

8	-1.576060	-1.400737	0.675535
6	-1.846117	-0.681746	-0.299852
15	1.085982	-0.044178	-0.085742
6	-0.286670	0.850541	-0.635871
1	-1.634435	-1.052317	-1.322448
1	-0.283557	0.952311	-1.722370
6	1.105979	-1.697491	-0.825075
1	2.031906	-2.215302	-0.571216
1	0.242904	-2.232468	-0.422542
1	1.024500	-1.611903	-1.909861
6	2.763548	0.634303	-0.387639
1	3.528670	0.015968	0.087818
1	2.948375	0.677289	-1.462088
1	2.817849	1.646365	0.017078
6	0.989454	-0.245015	1.710364
1	1.754900	-0.945302	2.047859
1	1.145595	0.720131	2.194319
1	-0.006460	-0.632535	1.935913
6	-3.016057	0.278787	-0.242347
1	-3.038772	0.953865	-1.099577
1	-3.931540	-0.321180	-0.237966

1	-2.988942	0.852649	0.685321
6	-0.581617	2.134061	0.125536
1	-1.466827	2.615394	-0.295786
1	-0.817020	1.920638	1.174007
1	0.220475	2.884328	0.112694

Acetylenebromide dimer

6	2.234330	-1.076852	0.000000
6	1.052165	-1.275802	0.000000
1	0.000000	-1.438746	0.000000
6	-2.234334	1.076876	0.000000
6	-1.052170	1.275832	0.000000
1	-0.000006	1.438782	0.000000
35	-4.005765	0.794239	0.000000
35	4.005766	-0.794249	0.000000

Acetonitrile dimer

6	-2.243256	-0.673107	0.000004
6	-1.512529	0.588303	0.000121
7	-0.926190	1.575633	0.000214
1	-1.523511	-1.492464	-0.000181
1	-2.870938	-0.734933	-0.888483
1	-2.870770	-0.735196	0.888592
7	0.926162	-1.575603	-0.000171
6	1.512449	-0.588249	-0.000059
6	2.243340	0.673058	-0.000069
1	2.871059	0.734921	0.888389
1	1.523544	1.492364	0.000107
1	2.870782	0.735071	-0.888713

Acetylene dimer

6	2.238958	1.091393	0.000000
6	1.055682	1.271289	0.000000
1	3.292465	0.940322	0.000000
1	0.000000	1.414903	0.000000
6	-2.238957	-1.091389	0.000000
6	-1.055682	-1.271286	0.000000
1	-3.292471	-0.940363	0.000000
1	-0.000001	-1.414908	0.000000

Vinylchloride dimer

6	1.343396	0.670955	-0.468083
1	0.715472	0.449450	-1.319601
6	1.394725	1.840235	0.141867

1	2.036559	2.014913	0.995740
1	0.774787	2.651086	-0.219416
6	-1.343396	-0.670954	0.468085
1	-0.715475	-0.449447	1.319604
6	-1.394724	-1.840235	-0.141864
1	-0.774787	-2.651085	0.219422
1	-2.036556	-2.014915	-0.995738
17	2.286023	-0.702143	0.043023
17	-2.286023	0.702143	-0.043025

Diyne dimer

6	0.000000	1.703616	0.000000
6	1.369454	1.847434	0.000000
6	2.565284	1.974659	0.000000
6	0.000000	-1.703625	0.000000
6	-1.369603	-1.846106	0.000000
6	-2.565481	-1.973015	0.000000
6	1.194361	-1.569602	0.000000
1	2.249649	-1.435538	0.000000
6	-1.194088	1.567230	0.000000
1	-2.248940	1.429818	0.000000
1	-3.622004	-2.097784	0.000000
1	3.621735	2.099957	0.000000

Diyneflouride dimer

6	0.055044	1.632763	0.000000
6	-1.320826	1.590779	0.000000
6	-2.521849	1.538418	0.000000
6	-0.055044	-1.632763	0.000000
6	1.320826	-1.590779	0.000000
6	2.521849	-1.538418	0.000000
6	-1.250761	-1.635903	0.000000
9	-2.521849	-1.649757	0.000000
6	1.250761	1.635903	0.000000
9	2.521849	1.649757	0.000000
1	3.584889	-1.498192	0.000000
1	-3.584889	1.498192	0.000000

Diynecyanide dimer

6	-1.267552	1.551415	-0.508537
6	-0.062479	1.619283	-0.491538
6	1.305670	1.662215	-0.461825
6	1.267552	-1.551415	0.508537
6	0.062479	-1.619283	0.491538

6	-1.305670	-1.662215	0.461825
6	2.636813	-1.435683	0.515689
7	3.783312	-1.313160	0.514090
6	-2.636813	1.435683	-0.515689
7	-3.783312	1.313160	-0.514090
6	-2.508230	-1.670033	0.426468
6	2.508230	1.670033	-0.426468
1	-3.573346	-1.654608	0.388181
1	3.573346	1.654608	-0.388181

C12 dimer

6	2.434274	-0.830109	-1.603109
6	2.334596	0.398712	-1.602791
6	1.923767	1.696944	-1.611361
6	0.500247	-2.534748	-1.589113
6	-0.829332	-2.240769	-1.578177
6	-1.943096	-1.712096	-1.579183
6	0.810359	2.226118	-1.603881
6	1.515124	-1.834742	-1.590763
6	-2.353541	-0.413643	-1.576685
6	-0.519330	2.520200	-1.603185
6	-1.533914	1.819892	-1.590114
6	-2.453024	0.815149	-1.585917
6	2.029077	1.611278	1.579780
6	2.353105	0.421705	1.577125
6	2.407909	-0.938863	1.587424
6	-0.369593	2.556268	1.587501
6	-1.520693	1.828840	1.590520
6	-2.389174	0.953860	1.603492
6	1.539571	-1.814063	1.589121
6	0.822803	2.243241	1.577768
6	-2.333982	-0.406801	1.603552
6	0.388599	-2.541650	1.602987
6	-0.803784	-2.228387	1.602920
6	-2.009969	-1.596336	1.612090

diyne_CN_NMe_2_dimer

6	-0.651322	1.843069	-0.000400
6	0.540818	1.613029	-0.000343
6	1.864986	1.333619	-0.000099
6	0.651331	-1.843005	-0.000088
6	-0.540827	-1.613059	-0.000198
6	-1.865009	-1.333714	-0.000145
6	2.004257	-2.045202	-0.000141

7	3.149259	-2.204507	-0.000169
6	-2.004238	2.045321	-0.000250
7	-3.149247	2.204581	-0.000160
6	-3.040672	-1.014973	-0.000043
6	3.040633	1.014822	0.000090
7	4.313927	0.704758	0.000150
7	-4.313936	-0.704779	0.000204
6	4.945630	0.258067	1.241377
1	4.418336	0.693807	2.087578
1	4.913830	-0.832777	1.308525
1	5.981949	0.600901	1.249662
6	4.945728	0.257847	-1.240957
1	4.914255	-0.833028	-1.307704
1	4.418231	0.693103	-2.087279
1	5.981933	0.601023	-1.249425
6	-4.945942	-0.258064	-1.240864
1	-4.418858	-0.693799	-2.087198
1	-5.982258	-0.600909	-1.248888
1	-4.914176	0.832782	-1.308019
6	-4.945388	-0.257831	1.241474
1	-4.913854	0.833044	1.308252
1	-5.981611	-0.600943	1.250197
1	-4.417712	-0.693139	2.087658

Dimethylcynamide dimer

6	1.061084	1.118757	-0.000336
7	0.100408	1.764215	-0.000611
7	2.194820	0.427882	0.000042
6	2.542981	-0.274711	-1.237203
1	2.026187	-1.236484	-1.294946
1	2.268991	0.344856	-2.089642
1	3.622996	-0.428643	-1.247673
6	2.542083	-0.274874	1.237446
1	2.025258	-1.236665	1.294706
1	3.622089	-0.428811	1.248679
1	2.267486	0.344584	2.089770
6	-1.061096	-1.118783	-0.000286
7	-0.100407	-1.764222	-0.000729
7	-2.194818	-0.427879	0.000272
6	-2.543145	0.274826	-1.236863
1	-2.026395	1.236626	-1.294577
1	-2.269242	-0.344646	-2.089399
1	-3.623165	0.428729	-1.247190
6	-2.541912	0.274778	1.237781

1	-2.025039	1.236540	1.295059
1	-3.621911	0.428756	1.249150
1	-2.267239	-0.344768	2.090016

Thioacetone dimer

6	-1.672258	-0.532285	0.000002
16	-2.454996	0.893983	-0.000009
6	-1.287005	-1.242954	-1.265226
6	-1.286995	-1.242931	1.265239
1	-1.592155	-0.685887	-2.147773
1	-1.592117	-0.685837	2.147778
1	-1.750293	-2.234990	-1.281422
1	-0.203486	-1.403488	-1.282376
1	-0.203479	-1.403490	1.282373
1	-1.750307	-2.234956	1.281468
6	1.672257	0.532285	0.000002
16	2.454996	-0.893983	-0.000009
6	1.286995	1.242931	1.265239
6	1.287005	1.242954	-1.265226
1	1.592116	0.685837	2.147778
1	1.592154	0.685887	-2.147773
1	0.203479	1.403491	1.282373
1	1.750307	2.234955	1.281468
1	1.750294	2.234990	-1.281422
1	0.203486	1.403489	-1.282376

Vinylfluoride dimer

6	-1.462293	-0.088764	0.442986
1	-0.909498	-0.021000	1.371389
6	-2.124490	0.891159	-0.137239
1	-2.645887	0.732828	-1.071934
1	-2.144321	1.866617	0.325906
6	1.462293	0.088763	-0.442986
1	0.909498	0.020996	-1.371389
6	2.124493	-0.891157	0.137240
1	2.144326	-1.866616	-0.325902
1	2.645890	-0.732823	1.071935
9	-1.394669	-1.314791	-0.099361
9	1.394666	1.314791	0.099359

diyneCF_3 dimer

6	-1.905559	-0.912110	-0.000176
6	-0.842863	-1.472286	-0.001702
6	0.380299	-2.098552	-0.003408

6	1.905742	0.912462	-0.000244
6	0.842887	1.472331	-0.001729
6	-0.380418	2.098309	-0.003445
6	-1.451737	2.642355	-0.004996
6	1.451372	-2.643091	-0.004919
1	-2.410352	3.105938	-0.006540
1	2.409856	-3.106960	-0.006329
6	-3.216179	-0.259406	0.001530
9	-4.201778	-1.156659	0.002322
9	-3.373386	0.515618	1.078897
9	-3.375760	0.516287	-1.075077
6	3.216303	0.259630	0.001666
9	3.376364	-0.515235	-1.075425
9	4.202074	1.156655	0.003791
9	3.372645	-0.516314	1.078538

C2@endoC60

6	-3.364549	0.913720	0.689595
6	-3.350516	0.905777	-0.762909
6	-3.307377	-0.478504	-1.203192
6	-3.295847	-1.326584	-0.023954
6	-3.330168	-0.465720	1.145728
6	-2.594055	-0.803353	2.272346
6	-1.861285	0.219079	2.996034
6	-1.893291	1.533416	2.561012
6	-2.660334	1.889089	1.381527
6	-1.913788	2.901982	0.658325
6	-1.900419	2.894243	-0.725853
6	-2.633148	1.873395	-1.451996
6	-1.843885	1.504954	-2.612638
6	-1.803814	0.186143	-3.033013
6	-2.550087	-0.828280	-2.311929
6	-1.750272	-2.039269	-2.296524
6	-1.738877	-2.847180	-1.172496
6	-2.527410	-2.482202	-0.010359
6	-1.761260	-2.834477	1.170408
6	-1.794159	-2.014407	2.285261
6	-0.570995	-1.740124	3.016107
6	-0.612806	-0.360222	3.455719
6	0.546844	0.397908	3.462625
6	0.513597	1.772867	3.007072
6	-0.677772	2.326048	2.566432
6	-0.690111	3.171746	1.390390
6	0.490154	3.423798	0.710153
6	0.504013	3.416051	-0.738050

6	-0.663123	3.156127	-1.437562
6	-0.628490	2.297601	-2.603707
6	0.571037	1.740169	-3.016000
6	0.612837	0.360252	-3.455629
6	-0.546828	-0.397875	-3.462631
6	-0.513569	-1.772835	-3.007059
6	0.677820	-2.325934	-2.566348
6	0.690142	-3.171637	-1.390333
6	-0.490128	-3.423853	-0.710144
6	-0.503972	-3.416074	0.738120
6	0.663159	-3.156096	1.437628
6	0.628545	-2.297518	2.603745
6	1.843933	-1.504850	2.612664
6	1.803867	-0.186081	3.033074
6	2.550070	0.828305	2.311870
6	1.750310	2.039237	2.296526
6	1.738904	2.847061	1.172466
6	2.527514	2.482186	0.010417
6	1.761317	2.834424	-1.170313
6	1.794224	2.014442	-2.285203
6	2.594089	0.803430	-2.272236
6	1.861329	-0.219005	-2.995969
6	1.893321	-1.533285	-2.560862
6	2.660576	-1.889029	-1.381451
6	1.913762	-2.901683	-0.658239
6	1.900454	-2.894095	0.725933
6	2.633238	-1.873289	1.452038
6	3.350527	-0.905625	0.762934
6	3.307520	0.478578	1.203279
6	3.295919	1.326572	0.023999
6	3.330347	0.465840	-1.145717
6	3.364670	-0.913586	-0.689536
6	0.649575	-0.001366	0.000006
6	-0.651278	-0.000403	-0.001583

quinazoline

6	-1.213670	1.401323	0.000012
6	0.019919	0.707765	0.000003
6	-2.386475	0.696254	0.000009
1	-3.336322	1.216471	0.000008
6	0.040555	-0.705171	0.000008
6	-2.368497	-0.721403	-0.000008
1	-3.308201	-1.260800	-0.000016
6	-1.186829	-1.412694	-0.000013
1	-1.147950	-2.494663	-0.000023

1	-1.211809	2.485962	0.000010
6	1.286073	1.343067	-0.000022
7	1.217000	-1.391003	0.000002
7	2.412881	0.681732	-0.000012
6	2.309009	-0.675701	0.000047
1	1.342803	2.430469	-0.000017
1	3.251804	-1.213182	-0.000096

trizole

6	1.113818	0.024326	-0.000025
7	0.432630	-1.101388	0.000026
7	0.360536	1.156674	0.000014
7	-0.837508	-0.660149	-0.000022
6	-0.864617	0.685368	0.000005
1	-1.600266	-1.317905	0.000016
1	-1.776510	1.261411	-0.000006
1	2.191969	0.032373	-0.000016

tetrazole

7	-1.141450	0.241598	-0.000399
7	-0.158668	1.172909	0.000334
7	-0.660239	-0.942339	0.000300
6	0.964621	0.505392	-0.000119
7	0.672153	-0.805127	-0.000135
1	1.959983	0.915489	-0.000187
1	1.269712	-1.617128	0.000200

TS_{C-N}

6	1.548657	-0.068525	0.103476
6	1.809747	-0.855079	1.362822
1	0.893322	-1.213750	1.826922
1	2.435196	-1.708012	1.099635
1	2.364656	-0.208626	2.046927
8	2.333361	0.543226	-0.540679
16	0.036817	-1.229103	-0.951440
6	-0.915976	-0.154017	-0.039362
7	0.023344	0.869086	0.441235
1	-0.180012	1.111728	1.412257
16	-2.495908	-0.118332	0.354025
6	0.033760	2.085367	-0.393431
1	-0.934446	2.581936	-0.331475
1	0.833904	2.734767	-0.041961
1	0.245415	1.785035	-1.417906

NNDMAacetylCl

6	2.122154	-0.392810	-0.118190
8	1.046439	0.178971	-0.159757
7	3.300885	0.286536	-0.004062
6	3.277750	1.728775	0.166037
1	3.941939	2.200468	-0.562808
1	2.261538	2.081087	0.016613
1	3.612487	2.002101	1.172178
6	2.199228	-1.905787	-0.206079
1	1.180050	-2.278157	-0.262490
1	2.746032	-2.222445	-1.096382
1	2.693319	-2.333690	0.668020
6	4.597714	-0.338896	0.164925
1	5.342260	0.222748	-0.404153
1	4.904948	-0.343644	1.217160
1	4.596369	-1.360799	-0.204198
6	-1.820629	0.582716	-0.112038
1	-1.497763	-0.068024	-0.923713
1	-1.425378	1.585147	-0.257279
1	-1.425632	0.152894	0.807570
6	-3.311994	0.637111	-0.057711
8	-4.028287	1.562570	-0.153079
17	-4.033348	-1.026025	0.196408

benzoyl isothiocyanate

16	-3.812024	-0.604982	-0.000012
7	-1.473146	0.871482	0.000347
6	0.965115	0.580127	-0.000090
6	-0.219122	1.530392	-0.000254
6	2.244654	1.135314	0.000045
6	0.816980	-0.800905	-0.000143
6	3.364760	0.316497	0.000110
6	1.942138	-1.621681	-0.000057
6	3.215041	-1.067816	0.000063
6	-2.463295	0.245222	0.000121
1	-0.171881	2.177039	0.880991
1	-0.172281	2.176207	-0.882138
1	2.363249	2.214572	0.000095
1	-0.172449	-1.241914	-0.000222
1	4.354411	0.757098	0.000217
1	1.817625	-2.697736	-0.000082
1	4.088092	-1.708816	0.000130

lenthionine

16	1.114038	-1.507228	-0.605093
16	1.888346	-0.098734	0.688714
16	-1.916228	-0.920645	-0.177692
16	-0.197426	1.819452	-0.706584
16	-1.450102	0.918119	0.669975
6	-0.457178	-1.914314	0.233745
6	1.479600	1.505761	-0.058204
1	-0.707056	-2.927792	-0.088122
1	-0.289019	-1.916116	1.308660
1	1.719767	2.217371	0.733062
1	2.123734	1.702411	-0.915955

terthienyl

6	-0.134088	-5.131602	0.000000
6	-1.390009	-4.608269	0.000000
6	-1.388566	-3.186168	0.000000
6	-0.128609	-2.649030	0.000000
16	1.072227	-3.902650	0.000000
6	0.259761	-1.249858	0.000000
6	1.517139	-0.708685	0.000000
6	1.517139	0.708686	0.000000
6	0.259761	1.249858	0.000000
16	-0.946890	0.000000	0.000000
6	-0.128608	2.649030	0.000000
6	-1.388566	3.186168	0.000000
6	-1.390009	4.608268	0.000000
6	-0.134087	5.131602	0.000000
16	1.072227	3.902650	0.000000
1	0.161133	-6.169018	0.000000
1	-2.286163	-5.212507	0.000000
1	-2.285553	-2.580797	0.000000
1	2.416295	-1.310757	0.000000
1	2.416296	1.310757	0.000000
1	-2.285553	2.580798	0.000000
1	-2.286163	5.212506	0.000000
1	0.161134	6.169017	0.000000

$TS_{C\text{-}S}$

6	0.882446	-0.012742	-0.006065
8	1.548701	-0.955431	-0.002308
1	-1.476874	-0.305326	1.254042
8	0.802078	1.226019	0.015359

16	-1.387744	-0.183311	-0.081307
1	-0.420125	1.150042	-0.021150

CO_2….H_2S complex

6	-0.043331	1.501608	0.000000
8	-0.042775	1.512691	1.154642
8	-0.042775	1.512691	-1.154642
1	0.814398	-2.151172	0.972099
1	0.814398	-2.151172	-0.972099
16	-0.042775	-1.806897	0.000000

N_2

7	0.000000	0.000000	0.545007
7	0.000000	0.000000	-0.545007

N_2F_4

7	0.314994	0.678044	0.000000
9	-0.314994	1.240161	1.062910
9	-0.314994	1.240161	-1.062910
7	-0.314994	-0.678044	0.000000
9	0.314994	-1.240161	1.062910
9	0.314994	-1.240161	-1.062910

N_2O_4

7	0.000182	0.847675	0.000000
8	-0.000182	1.301991	1.087503
8	-0.000182	1.301991	-1.087503
7	-0.000182	-0.847675	0.000000
8	0.000182	-1.301991	1.087503
8	0.000182	-1.301991	-1.087503

N_3CH_3_dimer

6	-2.700042	0.578264	0.064365
1	-2.212596	1.262221	-0.634394
1	-3.465831	-0.001702	-0.457492
1	-3.169807	1.151721	0.858108
7	-1.714954	-0.303435	0.714191
7	-1.063967	-0.996355	-0.056306
7	-0.406506	-1.666523	-0.679454
6	2.699733	-0.578587	0.064336
1	2.211205	-1.264007	-0.632221
1	3.464411	0.000603	-0.460006
1	3.171061	-1.150359	0.858366
7	1.715435	0.304010	0.714173

7	1.064099	0.996478	-0.056447
7	0.406380	1.666320	-0.679668

N_3H

7	0.000000	0.000000	0.112070
7	0.000000	0.000000	-1.061688
7	0.000000	0.000000	1.242646
1	0.000000	0.000000	-2.051192

hydrazine

7	0.000000	0.735632	0.000000
1	-0.586552	0.983336	0.794022
1	-0.586552	0.983336	-0.794022
7	0.000000	-0.735632	0.000000
1	0.586552	-0.983336	0.794022
1	0.586552	-0.983336	-0.794022

Aminimide_1

6	-0.546933	2.106343	-0.637232
1	-1.337208	1.600074	-1.187558
1	-0.949074	2.957243	-0.082801
6	0.580061	2.558675	-1.546704
1	0.962773	1.701919	-2.109988
1	0.197329	3.310392	-2.236881
6	2.175601	2.226378	0.093057
1	2.972167	2.731683	0.639613
1	2.604855	1.386586	-0.461198
6	1.134929	1.741714	1.089631
1	1.528996	1.000183	1.782495
1	0.743440	2.592630	1.652430
6	-1.152803	0.870910	1.405027
1	-0.690358	0.284528	2.196640
1	-1.449355	1.851893	1.782631
6	-2.308241	0.141162	0.806989
1	-2.115254	-0.880195	0.499439
6	-3.518877	0.688617	0.693011
1	-3.665488	1.710430	1.041480
6	-4.721157	0.031859	0.154544
6	-5.970735	0.617128	0.375300
1	-6.030156	1.544090	0.936087
6	-7.131921	0.023535	-0.104332
1	-8.092494	0.488927	0.081209
6	-7.058173	-1.164261	-0.821398
1	-7.960507	-1.629568	-1.199253

6	-5.817132	-1.750718	-1.058790
1	-5.752393	-2.671313	-1.626183
6	-4.658534	-1.159176	-0.578738
1	-3.698700	-1.616905	-0.787532
6	2.727008	-1.120269	0.105823
6	3.225170	-1.174039	-1.194160
1	2.552153	-1.391767	-2.015634
6	4.573967	-0.946720	-1.411177
1	4.969358	-0.985793	-2.420952
6	5.441079	-0.669772	-0.346683
6	4.921507	-0.639894	0.944605
1	5.583337	-0.444309	1.781457
6	3.566031	-0.865809	1.178411
1	3.157801	-0.861459	2.182504
6	6.906767	-0.438637	-0.605575
1	7.418885	-0.097641	0.294433
1	7.052258	0.309531	-1.387622
1	7.387981	-1.361435	-0.939262
7	0.252342	-0.056611	-0.413088
7	-0.044811	1.116465	0.382941
8	0.575638	-2.483600	-0.395274
8	0.765213	-1.260169	1.807392
8	1.610316	3.167557	-0.795434
16	0.958871	-1.300073	0.350773

Aminimide_2

16	-0.138629	-1.472077	-0.483708
8	-0.463696	-2.186851	0.759344
8	-0.064212	-2.201986	-1.733733
7	-1.133536	-0.227385	-0.775266
7	-1.698471	0.423705	0.395676
6	-2.827415	-0.397623	0.999658
1	-2.343928	-1.290171	1.396189
1	-3.253427	0.194162	1.814276
6	-3.867888	-0.763904	-0.009218
1	-3.514597	-1.327987	-0.865665
6	-5.151589	-0.466711	0.145961
1	-5.506810	0.097340	1.003276
1	-5.895017	-0.790860	-0.571796
6	-2.276638	1.700073	-0.167490
1	-2.936985	1.375850	-0.971236
1	-2.866291	2.166405	0.625813
6	-1.222066	2.624059	-0.686073
1	-0.576748	2.209647	-1.452737

6	-1.101874	3.879119	-0.274073
1	-1.750082	4.291370	0.493331
1	-0.359293	4.543091	-0.699095
6	-0.728498	0.766397	1.483414
1	-0.421738	-0.155155	1.971420
1	-1.224841	1.431778	2.190673
1	0.127235	1.263763	1.033925
6	1.499294	-0.783310	-0.208073
6	2.217259	-1.104962	0.935780
1	1.785052	-1.789257	1.656362
6	3.476517	-0.548059	1.125773
1	4.044726	-0.798969	2.015701
6	4.027884	0.323573	0.185454
6	3.289035	0.623149	-0.961178
1	3.709704	1.289801	-1.706224
6	2.030150	0.073582	-1.164638
1	1.458326	0.297924	-2.058147
6	5.393517	0.919175	0.410482
1	5.705221	1.526488	-0.439549
1	6.138672	0.134634	0.559416
1	5.400063	1.552484	1.300982

CH_3COO_dimer

8	2.249164	-0.250069	-0.359209
6	1.482702	0.599200	0.332186
8	0.764926	0.265368	1.239530
6	1.616100	1.996186	-0.203233
1	0.973763	2.062169	-1.085248
1	2.641082	2.197084	-0.509720
1	1.286102	2.711077	0.547198
6	2.076153	-1.633185	-0.055651
1	1.108286	-1.962793	-0.434169
1	2.879715	-2.153411	-0.570063
1	2.133090	-1.800546	1.019894
8	-2.253940	0.260789	0.346908
6	-1.479449	-0.603240	-0.317322
8	-0.769763	-0.290766	-1.238626
6	-1.589822	-1.981575	0.268497
1	-2.602218	-2.175143	0.617951
1	-0.914230	-2.013787	1.127355
1	-1.283066	-2.720930	-0.468125
6	-2.097449	1.632955	-0.008791
1	-2.893159	2.166155	0.504487
1	-1.124014	1.983345	0.335556

1	-2.177868	1.762150	-1.088055

CrO_5

24	0.000056	0.214414	-0.115345
8	1.265980	-0.857861	0.573059
8	-1.586959	-0.264727	-0.626899
8	0.002181	1.600381	0.452449
8	-1.267685	-0.855189	0.573901
8	1.586316	-0.265845	-0.626474

$H_2S_2O_8$

8	-0.475351	0.016806	-0.894338
8	0.481076	-0.845040	-0.302850
16	-1.797840	0.125673	0.083998
16	1.807892	0.045341	0.159501
8	2.390928	0.433466	-1.261989
1	2.776192	-0.344009	-1.692351
8	-2.362606	-1.328574	-0.247017
1	-3.285895	-1.399919	0.034236
8	2.616179	-0.956841	0.767009
8	1.384013	1.254325	0.763897
8	-1.391812	0.183942	1.445267
8	-2.598819	1.117881	-0.549714

O_2

8	0.000000	0.000000	0.594027
8	0.000000	0.000000	-0.594027

O_2F_2

8	-0.525270	0.531885	0.379202
8	0.524875	0.532642	-0.378916
9	1.392636	-0.473123	0.126928
9	-1.392284	-0.473123	-0.127182

O_2H_2

8	-0.702228	0.141001	-0.000070
8	0.702372	-0.141053	-0.000070
1	1.045761	0.757469	0.000562
1	-1.046907	-0.757052	0.000562

O_3

8	0.000000	0.000000	0.421993
8	0.000000	1.057757	-0.210996
8	0.000000	-1.057757	-0.210996

cyclopentanone_dimer

6	-2.868671	-0.633333	-0.720663
6	-3.214901	0.754546	-0.148539
6	-1.932364	-1.236243	0.330521
6	-1.886238	1.234671	0.442848
6	-1.201112	-0.037771	0.919568
1	-2.319549	-0.515056	-1.657214
1	-2.494529	-1.704582	1.146995
1	-3.962492	0.654230	0.644313
1	-1.953802	1.970102	1.244418
1	-3.616242	1.431728	-0.902016
1	-1.244232	1.639619	-0.348903
1	-1.220062	-1.966191	-0.053595
1	-3.751496	-1.243871	-0.909692
8	-0.226961	-0.085258	1.628216
6	2.868062	-0.626746	0.726652
6	3.214292	0.756287	0.142977
6	1.933507	-1.239124	-0.320586
6	1.885985	1.230755	-0.453879
6	1.201399	-0.046100	-0.919535
1	2.317114	-0.500665	1.661103
1	2.497075	-1.712952	-1.132929
1	3.962753	0.649453	-0.648200
1	1.954202	1.958685	-1.262222
1	3.614541	1.440151	0.890980
1	1.243471	1.643214	0.333516
1	1.221948	-1.967153	0.068554
1	3.750872	-1.235185	0.922350
8	0.227045	-0.100141	-1.627422

S_2Cl_2

16	-0.813618	0.758325	-0.565475
16	0.813583	0.758382	0.565454
17	-2.073461	-0.713746	0.208838
17	2.073494	-0.713744	-0.208818

$[(CH_3)_3P^+\text{-}SCH_3...CH_3S^-$
$...H_2O$

16	-2.515914	-0.291375	-0.269425
16	-0.622229	-1.048631	-0.642609
6	-2.124593	1.227061	0.649154
1	-1.631509	0.992034	1.591820
1	-1.496650	1.879950	0.045172

1	-3.086440	1.701846	0.843252
6	-0.262970	-1.877433	0.933832
1	-0.219023	-1.156536	1.750665
1	-1.017787	-2.634135	1.137201
1	0.716130	-2.341378	0.815476
15	2.781480	-0.150426	-0.053367
6	4.550849	0.224927	0.349707
1	5.199959	-0.233874	-0.398203
1	4.744108	1.300794	0.374845
1	4.804727	-0.203652	1.320891
6	2.595147	0.924954	-1.546970
1	2.933042	1.947062	-1.355307
1	1.545790	0.941707	-1.845834
1	3.175057	0.508321	-2.372422
6	1.969703	0.956961	1.191724
1	2.384892	1.968231	1.166725
1	0.900405	1.008432	0.976180
1	2.100390	0.546285	2.195104
1	-5.080227	0.869123	-0.898701
8	-5.305977	0.973936	0.029582
1	-5.405769	0.071970	0.344843

$H_2S_2O_3$

16	-0.219003	-0.006984	0.132271
8	-0.916990	-1.042338	-0.901931
1	-0.784966	-1.944950	-0.578494
8	-0.847989	-0.198599	1.415991
16	1.664741	0.010794	-0.049372
8	-0.807767	1.307755	-0.556888
1	-1.764872	1.349445	-0.405263

$H_2S_2O_6$

16	-1.091657	0.171607	0.011064
16	1.086181	0.078204	-0.139563
8	-1.295741	-1.411973	0.206942
1	-1.335024	-1.845525	-0.659951
8	1.419289	-0.453061	1.325805
1	1.276582	-1.410413	1.377981
8	-1.456463	0.790790	1.242516
8	1.613860	1.397932	-0.238929
8	1.326602	-0.970754	-1.092679
8	-1.589292	0.554437	-1.276410

DHS_{red}

6	1.055461	0.756373	0.212881
6	1.071125	-0.712470	-0.209313
6	-0.109607	-1.526016	0.314633
16	-1.684144	-0.976438	-0.409779
16	-1.709313	0.938103	0.406735
6	-0.147959	1.531930	-0.305101
1	1.057673	0.785486	1.311900
1	1.087140	-0.746450	-1.306175
1	0.002349	-2.575067	0.026834
1	-0.163505	-1.464364	1.402604
1	-0.047596	2.576701	-0.004920
1	-0.196828	1.481837	-1.393716
8	2.196366	1.400570	-0.308566
1	2.945646	0.834986	-0.092552
8	2.291350	-1.216074	0.323933
1	2.494589	-2.054642	-0.096804

$C_4H_{10}S_2O_2$

16	0.538953	0.881758	-1.096618
16	-0.538953	-0.881758	-1.096618
6	-0.302515	1.801038	0.238131
1	-1.365118	1.861165	-0.004930
1	-0.182856	1.271802	1.183989
6	0.302515	3.195743	0.359913
1	0.183973	3.741243	-0.583870
1	1.370143	3.122840	0.572529
8	-0.267297	3.899128	1.444004
1	-1.189307	4.070398	1.237869
6	0.302515	-1.801038	0.238131
1	1.365118	-1.861165	-0.004930
1	0.182856	-1.271802	1.183989
6	-0.302515	-3.195743	0.359913
1	-0.183973	-3.741243	-0.583870
1	-1.370143	-3.122840	0.572529
8	0.267297	-3.899128	1.444004
1	1.189307	-4.070398	1.237869

$H_2O...(CH_3)_3P...CH_3SSCH_3...H2O$

16	-2.933356	-0.120828	-0.280888
16	-1.195168	-1.188943	-0.649029
6	-2.291416	1.313513	0.631678
1	-1.841404	1.002200	1.573714
1	-1.564250	1.849773	0.024261
1	-3.159544	1.943442	0.826291

6	-0.982598	-2.059681	0.931396
1	-0.818531	-1.352449	1.744765
1	-1.854023	-2.678134	1.136020
1	-0.094535	-2.680897	0.816239
15	2.313378	-0.914855	-0.048357
6	4.121587	-0.842625	0.353151
1	4.688105	-1.373554	-0.414330
1	4.467752	0.192018	0.418017
1	4.304746	-1.339563	1.307523
6	2.319508	0.191564	-1.534100
1	2.838260	1.125278	-1.306933
1	1.290685	0.403171	-1.830048
1	2.817406	-0.308325	-2.366855
6	1.713765	0.319627	1.198603
1	2.332671	1.220488	1.182997
1	0.677954	0.581212	0.971028
1	1.747080	-0.117375	2.198887
1	-5.299800	1.415560	-0.878726
8	-5.486031	1.572015	0.051039
1	-5.695482	0.698806	0.392641
8	4.131396	2.763026	0.102107
1	3.386411	3.268585	-0.232058
1	4.684220	2.614207	-0.668941

$TS_{S\text{-}S}$

16	-2.854363	0.241278	0.117339
16	-0.489463	0.094438	0.297623
6	-3.272547	0.712765	1.823419
1	-3.088493	-0.114569	2.509533
1	-2.671475	1.569960	2.125246
1	-4.328383	0.977984	1.866068
6	-0.517615	-1.408781	1.355675
1	-1.556566	-1.697941	1.498193
1	0.014497	-2.214359	0.853331
1	-0.070120	-1.190170	2.324069
15	2.005980	-0.055052	0.377120
6	2.859654	-1.583040	0.923904
1	2.519575	-2.399907	0.288317
1	3.943591	-1.470003	0.838116
1	2.604956	-1.801758	1.962301
6	2.627419	0.216544	-1.312610
1	3.720167	0.222813	-1.329543
1	2.246138	1.181400	-1.647983
1	2.243997	-0.590159	-1.938722

6	2.781545	1.257566	1.385091
1	3.866215	1.266332	1.249911
1	2.353038	2.208011	1.066473
1	2.550929	1.088924	2.438450
1	-2.066373	2.082279	-1.132256
8	-1.398773	2.454700	-1.731510
1	-1.193590	1.719397	-2.316088
8	-1.994988	-2.579426	-1.202859
1	-2.448506	-1.897487	-0.680866
1	-2.551570	-2.700399	-1.975381
8	0.809244	-2.477282	-1.437315
1	-0.138501	-2.261611	-1.400382
1	0.812178	-3.425287	-1.588896
8	1.117204	2.984882	-0.675301
1	1.330522	3.835597	-1.063550
1	0.187053	2.831953	-0.919521

Table 39. Sample input file for each calculation

Step 1. Optimization of the molecule and vibrational frequency analysis

```
%nproc=8
%mem=8gb
%chk=benzene.chk
#T m062x/6-311G** opt freq

benzene

0 1
6       1.204328000     0.695319000     0.000000000
6       0.000000000     1.390637000     0.000000000
6       1.204327000    -0.695318000     0.000000000
1       0.000000000     2.474103000     0.000000000
1       2.142636000    -1.237052000     0.000000000
6      -1.204328000     0.695319000     0.000000000
6       0.000000000    -1.390639000     0.000000000
1      -2.142638000     1.237052000     0.000000000
1       0.000000000    -2.474105000     0.000000000
6      -1.204327000    -0.695318000     0.000000000
1      -2.142636000    -1.237052000     0.000000000
1       2.142638000     1.237052000     0.000000000
```

Step 2. Generation of wave function file wfx

```
%nproc=8
%mem=8gb
```

%chk=benzene.chk
#T m062x/6-311G** out=wfx

benzene

0 1

benzene.wfx

Step 3. Generate fchk file using formchk utility of gaussian

Step 4. Run DAMQT program for topology calculation of MESP with input fchk file.

Step 5. Run AIMALL program for topology calculation of MED with input wfx file