

Local Chemical Environment Along Graphene Edges

Supporting Information

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Table S1. Values of relative energies (E_{rel} , kcal/mol) of oxyradicals and HOMO-LUMO gaps (HL, eV) of substrates and oxyradicals at GGA PBE and PM6 levels of theory

Molecule	E_{rel} , kcal/mol (PBE)	E_{rel} , kcal/mol (PM6)	HL, eV (PBE)	HL, eV (PM6)	Molecule	E_{rel} , kcal/mol (PBE)	E_{rel} , kcal/mol (PM6)	HL, eV (PBE)	HL, eV (PM6)
0-5Z2Z	0.00	0.00	0.89	5.29					
I-5Z2Z	26.92	26.86	1.04	3.12					
II-5Z2Z	9.32	9.04	1.10	3.13					
III-5Z2Z	0.00	0.38	1.36	3.45					
IV-5Z2Z	0.16	0.00	1.29	3.44					
V-5Z2Z	5.87	6.23	1.04	3.10					
VI-5Z2Z	19.39	19.31	1.01	2.97					
VII-5Z2Z	19.26	19.11	1.04	3.00					
VIII-5Z2Z	8.89	9.51	1.14	3.10					
0-5Z3Z	-	-	0.62	4.53	0-5Z3A	-	-	0.52	4.65
I-5Z3Z	32.51	50.75	0.83	2.29	I-5Z3A	32.28	33.19	0.73	2.72
II-5Z3Z	6.43	5.48	1.04	2.89	II-5Z3A	12.43	12.90	0.84	2.81
III-5Z3Z	0.00	0.00	1.21	3.13	III-5Z3A	0.84	1.95	1.10	3.07
IV-5Z3Z	2.20	3.24	0.93	2.84	IV-5Z3A	0.00	0.00	1.19	3.32
V-5Z3Z	9.21	12.33	0.80	2.56	V-5Z3A	5.66	6.48	0.87	2.94
VI-5Z3Z	22.91	28.11	0.80	2.49	VI-5Z3A	21.49	23.06	0.71	2.66
VII-5Z3Z	22.22	27.33	0.80	2.52	VII-5Z3A	25.13	27.49	0.74	2.64
VIII-5Z3Z	8.53	10.89	0.86	2.65	VIII-5Z3A	21.70	23.99	0.75	2.70
IX-5Z3Z	5.92	5.71	1.06	2.85	IX-5Z3A	10.17	14.10	0.75	2.67
0-5Z4Z	-	-	0.41	3.90	0-5Z4A	-	-	0.33	4.16
I-5Z4Z	33.82	48.72	0.89	2.04	I-5Z4A	35.81	51.65	0.36	2.13
II-5Z4Z	4.34	2.76	0.91	2.61	II-5Z4A	10.94	10.34	0.80	2.72
III-5Z4Z	0.00	0.00	0.87	2.65	III-5Z4A	0.00	0.41	1.07	2.98
IV-5Z4Z	3.01	5.52	0.73	2.40	IV-5Z4A	0.00	0.00	1.03	2.96
V-5Z4Z	10.13	17.25	0.76	2.15	V-5Z4A	6.57	7.71	0.73	2.64
VI-5Z4Z	26.05	36.36	0.44	2.09	VI-5Z4A	23.28	26.00	0.62	2.38
VII-5Z4Z	25.76	35.80	0.46	2.10	VII-5Z4A	26.78	33.15	0.67	2.32
VIII-5Z4Z	9.31	15.55	0.75	2.22	VIII-5Z4A	25.04	26.86	0.64	2.39
IX-5Z4Z	2.82	4.50	0.79	2.47	IX-5Z4A	21.61	27.67	0.46	2.28
X-5Z4Z	4.01	2.84	0.94	2.60	X-5Z4A	8.68	11.48	0.77	2.64
0-5Z5Z	-	-	0.26	3.34	0-5Z5A	-	-	0.22	3.77
I-5Z5Z	34.73	46.65	0.43	1.90	I-5Z5A	37.93	51.66	0.15	1.92
II-5Z5Z	3.30	0.54	0.76	2.32	II-5Z5A	11.74	11.81	0.69	2.55
III-5Z5Z	0.00	0.00	0.74	2.27	III-5Z5A	0.44	1.29	0.96	2.77
IV-5Z5Z	2.70	7.48	0.73	2.06	IV-5Z5A	0.00	0.00	0.99	2.91
V-5Z5Z	9.63	21.41	0.75	1.83	V-5Z5A	6.24	7.18	0.69	2.61
VI-5Z5Z	23.35	50.28	0.79	1.20	VI-5Z5A	23.42	25.07	0.55	2.33
					VII-5Z5A	31.83	51.46	0.42	1.87
					VIII-5Z5A	29.22	35.48	0.32	2.10
					IX-5Z5A	21.23	26.80	0.47	2.25
					X-5Z5A	9.43	13.09	0.67	2.46
					XI-5Z5A	25.53	31.97	0.39	2.00

Legend

“DFT”, “PM6_rohf”	Tables of HOMA values of individual rings at the respective levels of theory
“diff_DFT”, “diff_PM6”	Tables of difference between HOMA of a substrate (designated as 0) and oxyradicals (designated by Roman numbers)
	Arabic numbers on blue background enumerate rings
	Yellow fields mark the rings interacting with oxygen
HOMAtot	Cumulative HOMA calculated according to Eq. 1.

HOMA 5z2z

DFT	1	2	3	4	5	6	7	8	9	10
0	0.766	0.694	0.665	0.649	0.570	0.569	0.652	0.666	0.692	0.766
I	0.540	0.666	0.696	0.687	0.593	0.504	0.614	0.656	0.704	0.796
II	0.252	0.673	0.700	0.697	0.599	0.763	0.692	0.654	0.695	0.812
III	0.885	0.208	0.727	0.738	0.629	0.646	0.740	0.656	0.686	0.820
IV	0.834	0.732	0.193	0.789	0.688	0.607	0.734	0.670	0.663	0.814
V	0.800	0.714	0.668	0.237	0.807	0.586	0.688	0.720	0.639	0.778
VI	0.780	0.703	0.666	0.656	0.352	0.575	0.663	0.681	0.713	0.711
VII	0.787	0.707	0.661	0.608	0.354	0.563	0.641	0.656	0.700	0.784
VIII	0.814	0.694	0.654	0.701	0.788	0.604	0.711	0.707	0.631	0.252

Etot, eV	Erel, kcal/mol	HOMAtot
-5536.373819		
-5954.487730	26.924256	5.915
-5955.251155	9.319676	6.284
-5955.655304	0.000000	6.527
-5955.648548	0.155793	6.531
-5955.400703	5.871099	6.400
-5954.814300	19.393552	6.148
-5954.820174	19.258098	6.107
-5955.269957	8.886102	6.304

PM6_rohf	1	2	3	4	5	6	7	8	9	10
0	0.576	0.753	0.488	0.222	-0.009	-0.005	0.221	0.491	0.755	0.576
I	-0.296	0.520	0.753	0.364	0.037	-0.278	-0.002	0.322	0.720	0.678
II	-0.445	0.231	0.667	0.675	0.177	0.807	0.544	0.340	0.521	0.834
III	0.852	-0.342	0.530	0.783	0.272	0.453	0.727	0.382	0.478	0.849
IV	0.848	0.517	-0.341	0.769	0.492	0.217	0.728	0.534	0.428	0.817
V	0.750	0.652	0.275	-0.321	0.784	0.096	0.503	0.779	0.411	0.686
VI	0.626	0.745	0.409	0.150	-0.339	0.011	0.280	0.636	0.734	0.368
VII	0.683	0.716	0.309	0.180	-0.301	-0.012	0.223	0.571	0.757	0.458
VIII	0.834	0.523	0.333	0.518	0.833	0.168	0.664	0.683	0.195	-0.540

Heat of formation, kcal
146.0234
136.51914
118.70009
110.04471
109.6616
115.89058
128.97459
128.77157
119.16938

diff_DFT	1	2	3	4	5	6	7	8	9	10
0										
I	-0.226	-0.028	0.031	0.038	0.023	-0.065	-0.038	-0.010	0.012	0.030
II	-0.514	-0.021	0.035	0.048	0.029	0.194	0.040	-0.012	0.003	0.046
III	0.119	-0.486	0.062	0.089	0.059	0.077	0.088	-0.010	-0.006	0.054
IV	0.068	0.038	-0.472	0.140	0.118	0.038	0.082	0.004	-0.029	0.048
V	0.034	0.020	0.003	-0.412	0.237	0.017	0.036	0.054	-0.053	0.012
VI	0.014	0.009	0.001	0.007	-0.218	0.006	0.011	0.015	0.021	-0.055
VII	0.021	0.013	-0.004	-0.041	-0.216	-0.006	-0.011	-0.010	0.008	0.018
VIII	0.048	0.000	-0.011	0.052	0.218	0.035	0.059	0.041	-0.061	-0.514

diff_PM6	1	2	3	4	5	6	7	8	9	10
0										
I	-0.872	-0.233	0.264	0.142	0.045	-0.273	-0.223	-0.169	-0.035	0.102
II	-1.021	-0.523	0.179	0.453	0.186	0.812	0.323	-0.152	-0.233	0.258
III	0.276	-1.095	0.041	0.561	0.281	0.458	0.506	-0.109	-0.277	0.273
IV	0.272	-0.236	-0.829	0.546	0.501	0.222	0.507	0.043	-0.327	0.241
V	0.174	-0.101	-0.213	-0.544	0.793	0.101	0.282	0.288	-0.344	0.110
VI	0.050	-0.008	-0.079	-0.073	-0.331	0.016	0.059	0.145	-0.021	-0.208
VII	0.107	-0.037	-0.179	-0.042	-0.293	-0.007	0.002	0.080	0.002	-0.118
VIII	0.258	-0.231	-0.155	0.296	0.841	0.173	0.443	0.191	-0.560	-1.115

HOMA 5z3a

DFT	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	Etot, eV	Erel, kcal/mol	HOMAtot
0	0.775	0.682	0.662	0.673	0.621	0.456	0.677	0.709	0.719	0.787	0.775	0.683	0.660	0.671	0.620	-7433.554424		
I	0.591	0.657	0.684	0.714	0.657	0.408	0.661	0.700	0.712	0.791	0.788	0.687	0.662	0.685	0.639	-7851.692675	32.282386	9.446
II	0.284	0.656	0.696	0.723	0.659	0.627	0.731	0.706	0.706	0.790	0.784	0.675	0.681	0.725	0.667	-7852.553383	12.434459	9.828
III	0.898	0.203	0.709	0.748	0.678	0.487	0.746	0.705	0.701	0.787	0.822	0.642	0.673	0.734	0.680	-7853.056347	0.836109	10.009
IV	0.832	0.714	0.176	0.788	0.725	0.475	0.724	0.704	0.683	0.772	0.819	0.674	0.630	0.732	0.699	-7853.092605	0.000000	9.972
V	0.800	0.702	0.659	0.205	0.831	0.471	0.705	0.754	0.644	0.723	0.812	0.684	0.646	0.695	0.729	-7852.847255	5.657771	9.855
VI	0.788	0.690	0.665	0.673	0.330	0.469	0.698	0.734	0.737	0.617	0.801	0.686	0.657	0.694	0.715	-7852.160682	21.490144	9.625
VII	0.799	0.685	0.655	0.638	0.423	0.466	0.679	0.697	0.722	0.828	0.778	0.682	0.668	0.685	0.614	-7852.002865	25.129404	9.596
VIII	0.808	0.681	0.648	0.693	0.790	0.469	0.704	0.743	0.703	0.396	0.796	0.697	0.653	0.608	0.494	-7852.151434	21.703403	9.486
IX	0.182	0.586	0.700	0.727	0.660	0.613	0.727	0.705	0.706	0.790	0.785	0.674	0.685	0.727	0.668	-7852.651659	10.168215	9.752

PM6_rohf	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	Heat of formation, kcal
0	0.456	0.729	0.615	0.341	0.087	0.069	0.338	0.438	0.658	0.771	0.456	0.728	0.614	0.338	0.086	186.6575
I	-0.347	0.347	0.776	0.523	0.138	-0.148	0.155	0.326	0.597	0.813	0.353	0.701	0.663	0.334	0.071	176.55253
II	-0.421	0.124	0.531	0.776	0.346	0.546	0.683	0.381	0.416	0.813	0.780	0.409	0.518	0.782	0.369	156.26548
III	0.895	-0.352	0.435	0.802	0.422	0.265	0.773	0.412	0.387	0.776	0.847	0.411	0.446	0.788	0.440	145.31273
IV	0.821	0.548	-0.363	0.737	0.584	0.164	0.677	0.521	0.331	0.682	0.812	0.530	0.345	0.706	0.569	143.36246
V	0.740	0.643	0.228	-0.354	0.812	0.131	0.558	0.744	0.258	0.501	0.760	0.607	0.361	0.555	0.703	149.83806
VI	0.674	0.709	0.310	0.066	-0.396	0.106	0.467	0.783	0.456	-0.054	0.699	0.677	0.379	0.465	0.807	166.42542
VII	0.571	0.770	0.402	0.192	-0.266	0.052	0.280	0.420	0.728	0.692	0.471	0.750	0.573	0.253	0.003	170.85455
VIII	0.709	0.670	0.361	0.431	0.832	0.098	0.450	0.780	0.472	-0.390	0.667	0.714	0.315	0.000	-0.255	167.35324
IX	-0.604	0.073	0.563	0.764	0.329	0.567	0.647	0.373	0.426	0.819	0.749	0.411	0.541	0.777	0.351	157.46044

diff_DFT	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0															
I	-0.184	-0.024	0.022	0.042	0.036	-0.048	-0.016	-0.009	-0.006	0.004	0.013	0.003	0.002	0.014	0.018
II	-0.491	-0.025	0.035	0.051	0.038	0.171	0.054	-0.003	-0.012	0.004	0.009	-0.008	0.021	0.054	0.047
III	0.122	-0.479	0.047	0.075	0.056	0.031	0.069	-0.005	-0.018	0.001	0.047	-0.041	0.013	0.063	0.059
IV	0.057	0.033	-0.486	0.115	0.104	0.019	0.048	-0.005	-0.036	-0.014	0.044	-0.010	-0.030	0.061	0.079
V	0.025	0.020	-0.003	-0.468	0.209	0.015	0.028	0.045	-0.075	-0.064	0.037	0.001	-0.013	0.024	0.109
VI	0.013	0.008	0.003	0.000	-0.292	0.013	0.021	0.025	0.019	-0.169	0.026	0.003	-0.002	0.023	0.094
VII	0.023	0.003	-0.007	-0.034	-0.198	0.010	0.002	-0.012	0.003	0.042	0.003	-0.002	0.008	0.014	-0.006
VIII	0.032	0.000	-0.014	0.020	0.169	0.013	0.027	0.034	-0.015	-0.390	0.021	0.014	-0.007	-0.063	-0.127
IX	-0.593	-0.095	0.038	0.055	0.038	0.157	0.050	-0.005	-0.012	0.004	0.010	-0.009	0.025	0.056	0.048

diff_PM6	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0															
I	-0.803	-0.382	0.161	0.183	0.051	-0.217	-0.183	-0.112	-0.061	0.042	-0.103	-0.027	0.049	-0.005	-0.014
II	-0.877	-0.605	-0.084	0.436	0.259	0.477	0.345	-0.056	-0.241	0.042	0.323	-0.319	-0.096	0.444	0.283
III	0.438	-1.081	-0.180	0.462	0.335	0.196	0.435	-0.026	-0.271	0.005	0.390	-0.318	-0.168	0.450	0.354
IV	0.365	-0.181	-0.978	0.396	0.497	0.095	0.340	0.084	-0.327	-0.089	0.355	-0.199	-0.268	0.368	0.483
V	0.284	-0.086	-0.387	-0.695	0.725	0.062	0.221	0.307	-0.400	-0.270	0.304	-0.121	-0.253	0.217	0.618
VI	0.217	-0.020	-0.305	-0.275	-0.483	0.037	0.129	0.345	-0.201	-0.825	0.243	-0.051	-0.235	0.126	0.722
VII	0.114	0.041	-0.213	-0.149	-0.352	-0.017	-0.058	-0.017	0.070	-0.079	0.015	0.022	-0.041	-0.086	-0.083
VIII	0.253	-0.059	-0.254	0.091	0.745	0.029	0.112	0.342	-0.185	-1.161	0.210	-0.014	-0.299	-0.338	-0.341
IX	-1.061	-0.656	-0.052	0.423	0.242	0.498	0.310	-0.064	-0.232	0.048	0.293	-0.318	-0.072	0.438	0.265

HOMA 5z3z

DFT	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	Etot, eV	Erel, kcal/mol	HOMAtot
0	0.787	0.701	0.670	0.642	0.536	0.681	0.718	0.715	0.718	0.681	0.536	0.642	0.670	0.701	0.788	-7433.373614		
I	0.600	0.672	0.695	0.676	0.557	0.656	0.694	0.706	0.729	0.706	0.551	0.656	0.675	0.699	0.797	-7851.421617	32.514854	9.468
II	0.195	0.715	0.721	0.680	0.554	0.783	0.709	0.703	0.735	0.716	0.655	0.720	0.680	0.681	0.797	-7852.552915	6.427122	9.849
III	0.857	0.193	0.756	0.728	0.584	0.712	0.732	0.694	0.729	0.736	0.544	0.720	0.703	0.682	0.786	-7852.831628	0.000000	9.963
IV	0.822	0.723	0.199	0.801	0.653	0.694	0.752	0.685	0.701	0.747	0.546	0.663	0.718	0.690	0.769	-7852.736364	2.196788	9.965
V	0.799	0.713	0.680	0.256	0.787	0.690	0.733	0.740	0.659	0.718	0.546	0.659	0.688	0.711	0.758	-7852.432386	9.206521	9.881
VI	0.789	0.702	0.682	0.668	0.341	0.696	0.722	0.717	0.731	0.644	0.552	0.663	0.681	0.699	0.775	-7851.838181	22.908888	9.722
VII	0.796	0.700	0.665	0.611	0.332	0.692	0.713	0.705	0.730	0.706	0.552	0.659	0.672	0.700	0.799	-7851.867855	22.224605	9.701
VIII	0.806	0.692	0.657	0.698	0.783	0.692	0.736	0.719	0.657	0.271	0.533	0.626	0.647	0.714	0.812	-7852.461665	8.531347	9.773
IX	0.795	0.680	0.681	0.720	0.636	0.719	0.734	0.700	0.711	0.803	0.558	0.690	0.730	0.684	0.209	-7852.574703	5.924690	9.840
PM6_rohf	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15			Heat of formation, kcal
0	0.754	0.649	0.315	0.090	-0.144	0.201	0.565	0.742	0.565	0.202	-0.143	0.090	0.314	0.649	0.753	-5874.770190		195.99333
I	0.398	0.519	0.739	0.520	0.046	0.653	0.563	0.408	0.647	0.620	0.170	0.707	0.612	0.447	0.758	-6150.760540	50.753676	200.9116
II	-0.474	0.386	0.775	0.521	0.033	0.809	0.429	0.374	0.674	0.594	0.343	0.781	0.521	0.407	0.772	-6152.723640	5.484590	155.6415
III	0.775	-0.336	0.653	0.697	0.127	0.613	0.577	0.351	0.572	0.684	0.061	0.649	0.668	0.435	0.727	-6152.961480	0.000000	150.15678
IV	0.855	0.398	-0.343	0.827	0.361	0.426	0.775	0.385	0.428	0.767	-0.027	0.387	0.772	0.525	0.656	-6152.821110	3.236932	153.39392
V	0.831	0.524	0.188	-0.350	0.745	0.300	0.731	0.620	0.277	0.625	-0.094	0.211	0.609	0.693	0.586	-6152.426960	12.326031	162.48314
VI	0.771	0.630	0.264	0.042	-0.408	0.202	0.594	0.760	0.455	0.183	-0.147	0.088	0.338	0.735	0.614	-6151.742410	28.111754	178.26917
VII	0.827	0.531	0.250	0.113	-0.369	0.196	0.609	0.744	0.453	0.180	-0.155	0.070	0.326	0.694	0.711	-6151.776290	27.330481	177.48784
VIII	0.845	0.432	0.350	0.644	0.737	0.387	0.792	0.510	0.270	-0.285	-0.086	0.183	0.524	0.764	0.526	-6152.489150	10.891930	161.04893
IX	0.776	0.407	0.509	0.785	0.365	0.587	0.682	0.376	0.415	0.814	0.026	0.507	0.781	0.365	-0.530	-6152.713940	5.708272	155.86529
diff_DFT	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15			
0																		
I	-0.187	-0.030	0.025	0.034	0.021	-0.025	-0.024	-0.009	0.011	0.025	0.015	0.014	0.005	-0.003	0.009			
II	-0.592	0.013	0.051	0.038	0.018	0.102	-0.009	-0.012	0.018	0.036	0.119	0.077	0.010	-0.020	0.009			
III	0.070	-0.508	0.086	0.087	0.048	0.031	0.014	-0.022	0.011	0.055	0.008	0.078	0.034	-0.019	-0.002			
IV	0.035	0.022	-0.471	0.159	0.117	0.014	0.034	-0.031	-0.016	0.067	0.010	0.021	0.048	-0.011	-0.019			
V	0.012	0.012	0.010	-0.386	0.251	0.009	0.015	0.024	-0.058	0.038	0.010	0.017	0.018	0.010	-0.030			
VI	0.002	0.000	0.012	0.027	-0.195	0.016	0.005	0.002	0.014	-0.037	0.016	0.020	0.011	-0.002	-0.013			
VII	0.009	-0.001	-0.005	-0.030	-0.204	0.011	-0.005	-0.010	0.013	0.025	0.016	0.017	0.002	-0.002	0.012			
VIII	0.018	-0.009	-0.013	0.056	0.247	0.012	0.019	0.004	-0.061	-0.410	-0.003	-0.017	-0.022	0.013	0.024			
IX	0.008	-0.022	0.011	0.078	0.100	0.039	0.016	-0.015	-0.007	0.122	0.023	0.048	0.060	-0.018	-0.579			
diff_PM6	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15			
0																		
I	-0.356	-0.129	0.424	0.431	0.190	0.452	-0.002	-0.334	0.082	0.418	0.313	0.617	0.297	-0.202	0.004			
II	-1.228	-0.263	0.460	0.431	0.177	0.608	-0.136	-0.368	0.109	0.392	0.486	0.691	0.206	-0.242	0.019			
III	0.020	-0.985	0.338	0.607	0.271	0.412	0.012	-0.391	0.007	0.482	0.204	0.559	0.353	-0.214	-0.026			
IV	0.101	-0.251	-0.658	0.737	0.506	0.225	0.210	-0.356	-0.137	0.565	0.116	0.297	0.458	-0.124	-0.098			
V	0.077	-0.125	-0.127	-0.440	0.889	0.099	0.166	-0.121	-0.287	0.423	0.049	0.122	0.295	0.044	-0.168			
VI	0.017	-0.019	-0.052	-0.048	-0.264	0.001	0.029	0.018	-0.110	-0.019	-0.004	-0.002	0.024	0.086	-0.139			
VII	0.073	-0.117	-0.065	0.023	-0.224	-0.005	0.044	0.003	-0.112	-0.022	-0.012	-0.020	0.011	0.044	-0.042			
VIII	0.091	-0.217	0.035	0.554	0.881	0.186	0.227	-0.232	-0.295	-0.487	0.057	0.093	0.209	0.114	-0.227			
IX	0.022	-0.242	0.194	0.695	0.509	0.386	0.117	-0.366	-0.149	0.612	0.169	0.418	0.466	-0.284	-1.283			

HOMA 5z4a

DFT	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	Etot, eV	Erel, kcal/mol	HOMAtot
O	0.780	0.677	0.672	0.690	0.626	0.512	0.695	0.693	0.683	0.789	0.792	0.686	0.693	0.693	0.510	0.628	0.689	0.671	0.678	0.782	-9330.798		
I	0.560	0.653	0.707	0.715	0.636	0.490	0.678	0.684	0.681	0.795	0.791	0.686	0.700	0.701	0.514	0.645	0.700	0.673	0.680	0.791	-9748.892	35.806	12.920
II	0.239	0.643	0.701	0.723	0.644	0.662	0.729	0.689	0.673	0.795	0.741	0.678	0.714	0.725	0.527	0.702	0.722	0.658	0.667	0.815	-9749.970	10.936	13.207
III	0.889	0.193	0.717	0.749	0.661	0.532	0.741	0.685	0.668	0.796	0.793	0.633	0.705	0.733	0.535	0.679	0.729	0.660	0.663	0.816	-9750.444	0.004	13.384
IV	0.833	0.709	0.179	0.796	0.710	0.525	0.736	0.677	0.646	0.787	0.799	0.667	0.659	0.735	0.551	0.666	0.735	0.664	0.656	0.816	-9750.444	0.000	13.366
V	0.804	0.696	0.664	0.222	0.822	0.522	0.724	0.735	0.597	0.740	0.799	0.678	0.683	0.704	0.580	0.658	0.728	0.682	0.649	0.807	-9750.159	6.574	13.272
VI	0.796	0.683	0.677	0.691	0.357	0.528	0.720	0.720	0.701	0.638	0.796	0.679	0.695	0.718	0.586	0.657	0.722	0.680	0.675	0.792	-9749.435	23.277	13.154
VII	0.807	0.677	0.670	0.664	0.444	0.530	0.701	0.673	0.678	0.831	0.791	0.672	0.694	0.710	0.507	0.654	0.708	0.667	0.679	0.806	-9749.283	26.776	13.118
VIII	0.810	0.678	0.664	0.706	0.779	0.523	0.711	0.717	0.683	0.463	0.797	0.684	0.683	0.650	0.407	0.629	0.684	0.665	0.690	0.790	-9749.359	25.040	12.950
IX	0.799	0.692	0.660	0.610	0.501	0.519	0.717	0.721	0.628	0.326	0.798	0.679	0.682	0.702	0.616	0.650	0.723	0.691	0.672	0.777	-9749.507	21.608	12.839
X	0.814	0.670	0.664	0.725	0.700	0.530	0.730	0.717	0.674	0.736	0.798	0.678	0.690	0.725	0.645	0.648	0.730	0.711	0.596	0.165	-9750.068	8.675	13.181
PM6_rohf	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	Heat of formation, kcal		
O	0.523	0.740	0.565	0.306	0.061	0.127	0.369	0.491	0.694	0.700	0.702	0.694	0.489	0.370	0.124	0.064	0.306	0.566	0.741	0.524	-7371.710760		228.67014
I	0.272	0.436	0.610	0.723	0.287	0.379	0.719	0.409	0.415	0.829	0.749	0.329	0.474	0.782	0.284	0.503	0.755	0.400	0.468	0.832	-7647.797820	51.646790	10.381
II	-0.417	0.166	0.581	0.746	0.284	0.632	0.637	0.344	0.422	0.839	0.621	0.320	0.554	0.747	0.236	0.586	0.702	0.377	0.496	0.832	-7649.589200	10.337567	10.121
III	0.873	-0.342	0.498	0.792	0.348	0.356	0.728	0.360	0.390	0.826	0.756	0.291	0.478	0.780	0.272	0.487	0.757	0.403	0.474	0.839	-7650.019770	0.408623	10.709
IV	0.842	0.504	-0.339	0.773	0.522	0.239	0.741	0.450	0.306	0.755	0.831	0.392	0.340	0.762	0.366	0.356	0.788	0.483	0.430	0.834	-7650.037490	0.000000	10.715
V	0.782	0.589	0.202	-0.334	0.770	0.199	0.649	0.661	0.186	0.583	0.842	0.455	0.343	0.626	0.481	0.284	0.750	0.571	0.400	0.799	-7649.703300	7.706421	10.172
VI	0.745	0.638	0.242	0.044	-0.365	0.176	0.592	0.745	0.301	-0.016	0.836	0.495	0.360	0.557	0.654	0.237	0.695	0.643	0.428	0.719	-7648.909980	26.000381	9.092
VII	0.632	0.740	0.354	0.192	-0.256	0.098	0.303	0.507	0.746	0.593	0.700	0.698	0.445	0.305	0.066	0.042	0.274	0.570	0.750	0.486	-7648.599980	33.148981	8.502
VIII	0.766	0.609	0.354	0.473	0.842	0.150	0.532	0.769	0.373	-0.330	0.796	0.593	0.339	0.212	-0.073	0.075	0.359	0.668	0.701	0.396	-7648.872870	26.856137	8.933
IX	0.730	0.658	0.265	-0.022	-0.251	0.168	0.559	0.758	0.305	-0.422	0.832	0.515	0.357	0.511	0.672	0.220	0.674	0.670	0.434	0.674	-7648.837760	27.665774	8.731
X	0.829	0.500	0.378	0.695	0.603	0.232	0.739	0.566	0.313	0.590	0.840	0.429	0.336	0.605	0.639	0.276	0.738	0.604	0.115	-0.594	-7649.539630	11.480652	10.029
diff_DFT	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20			
O																							
I	-0.220	-0.024	0.035	0.025	0.010	-0.023	-0.017	-0.009	-0.002	0.006	-0.001	0.000	0.007	0.008	0.003	0.017	0.011	0.002	0.002	0.009			
II	-0.541	-0.035	0.028	0.033	0.017	0.150	0.033	-0.004	-0.010	0.006	-0.051	-0.008	0.022	0.032	0.017	0.073	0.033	-0.013	-0.011	0.033			
III	0.109	-0.484	0.045	0.059	0.035	0.019	0.046	-0.008	-0.015	0.007	0.001	-0.054	0.012	0.040	0.024	0.051	0.040	-0.011	-0.015	0.034			
IV	0.053	0.032	-0.493	0.106	0.083	0.012	0.040	-0.016	-0.037	-0.002	0.007	-0.019	-0.034	0.042	0.041	0.037	0.046	-0.007	-0.022	0.034			
V	0.024	0.019	-0.008	-0.468	0.195	0.010	0.028	0.042	-0.086	-0.049	0.006	-0.008	-0.010	0.011	0.070	0.030	0.039	0.011	-0.029	0.025			
VI	0.016	0.006	0.005	0.001	-0.269	0.016	0.025	0.027	0.018	-0.151	0.004	-0.008	0.003	0.024	0.076	0.029	0.033	0.009	-0.003	0.010			
VII	0.027	0.000	-0.002	-0.026	-0.182	0.018	0.005	-0.020	-0.005	0.042	-0.001	-0.014	0.001	0.017	-0.004	0.026	0.019	-0.004	0.001	0.024			
VIII	0.030	0.001	-0.009	0.016	0.152	0.011	0.016	0.024	-0.001	-0.326	0.005	-0.002	-0.009	-0.043	-0.103	0.001	-0.005	-0.006	0.012	0.008			
IX	0.019	0.015	-0.012	-0.080	-0.125	0.007	0.022	0.029	-0.055	-0.463	0.006	-0.007	-0.010	0.008	0.105	0.022	0.034	0.019	-0.006	-0.005			
X	0.034	-0.007	-0.009	0.035	0.073	0.018	0.035	0.024	-0.009	-0.053	0.006	-0.009	-0.002	0.032	0.135	0.020	0.041	0.039	-0.082	-0.617			
diff_PM6	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20			
O																							
I	-0.251	-0.305	0.045	0.417	0.227	0.252	0.350	-0.083	-0.279	0.129	0.046	-0.366	-0.015	0.412	0.160	0.439	0.449	-0.166	-0.273	0.309			
II	-0.940	-0.575	0.016	0.441	0.223	0.505	0.268	-0.148	-0.272	0.139	-0.081	-0.375	0.065	0.377	0.112	0.523	0.396	-0.189	-0.245	0.308			
III	0.350	-1.083	-0.067	0.487	0.287	0.229	0.360	-0.131	-0.304	0.126	0.054	-0.403	-0.011	0.410	0.148	0.423	0.450	-0.162	-0.267	0.315			
IV	0.319	-0.237	-0.904	0.468	0.461	0.112	0.373	-0.042	-0.388	0.055	0.129	-0.303	-0.149	0.392	0.242	0.293	0.482	-0.082	-0.311	0.310			
V	0.259	-0.151	-0.363	-0.640	0.709	0.072	0.280	0.170	-0.508	-0.118	0.140	-0.240	-0.146	0.256	0.357	0.221	0.444	0.005	-0.341	0.275			
VI	0.222	-0.102	-0.324	-0.262	-0.426	0.049	0.223	0.254	-0.394	-0.716	0.134	-0.199	-0.129	0.188	0.530	0.173	0.389	0.077	-0.313	0.195			
VII	0.109	-0.001	-0.211	-0.114	-0.317	-0.029	-0.065	0.016	0.052	-0.107	-0.002	0.004	-0.044	-0.065	-0.058	-0.021	-0.032	0.004	0.009	-0.037			
VIII	0.242	-0.132	-0.211	0.167	0.782	0.023	0.164	0.277	-0.322	-1.031	0.094	-0.101	-0.150	-0.158	-0.197	0.011	0.053	0.103	-0.040	-0.127			
IX	0.207	-0.082	-0.300	-0.327	-0.311	0.041	0.190	0.267	-0.390	-1.123	0.130	-0.180	-0.132	0.141	0.548	0.157	0.368	0.105	-0.307	0.150			
X	0.306	-0.240	-0.188	0.389	0.542	0.105	0.370	0.075	-0.381	-0.110	0.138	-0.265	-0.153	0.235	0.515	0.213	0.432	0.039	-0.626	-1.118			

HOMA 5z4z

DFT	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	Etot, eV	Erel, kcal/mol	HOMAtot	
0	0.783	0.699	0.667	0.638	0.529	0.700	0.723	0.720	0.710	0.647	0.646	0.710	0.719	0.723	0.699	0.528	0.638	0.669	0.698	0.782	-9330.321497			
I	0.598	0.667	0.697	0.676	0.557	0.686	0.695	0.713	0.728	0.681	0.684	0.718	0.712	0.720	0.719	0.562	0.674	0.691	0.697	0.773	-9748.426276	33.824523	13.049	
II	0.195	0.739	0.715	0.667	0.545	0.750	0.713	0.724	0.737	0.679	0.732	0.736	0.710	0.718	0.725	0.577	0.697	0.702	0.689	0.766	-9749.704973	4.337770	13.321	
III	0.839	0.184	0.758	0.716	0.571	0.711	0.713	0.703	0.735	0.704	0.629	0.746	0.720	0.707	0.720	0.527	0.666	0.707	0.700	0.758	-9749.893081	0.000000	13.331	
IV	0.809	0.725	0.190	0.796	0.645	0.702	0.742	0.685	0.706	0.726	0.653	0.704	0.734	0.707	0.704	0.541	0.648	0.694	0.711	0.758	-9749.762499	3.011221	13.391	
V	0.781	0.717	0.691	0.243	0.785	0.705	0.725	0.743	0.661	0.700	0.674	0.718	0.708	0.723	0.687	0.555	0.669	0.678	0.704	0.770	-9749.453661	10.133025	13.397	
VI	0.781	0.703	0.671	0.649	0.320	0.702	0.723	0.728	0.725	0.605	0.653	0.712	0.719	0.725	0.694	0.535	0.645	0.670	0.691	0.789	-9748.763220	26.054595	13.122	
VII	0.783	0.707	0.661	0.593	0.314	0.700	0.717	0.721	0.725	0.662	0.658	0.711	0.718	0.731	0.707	0.537	0.646	0.671	0.696	0.785	-9748.775801	25.764477	13.131	
VIII	0.784	0.693	0.665	0.699	0.784	0.711	0.728	0.721	0.660	0.254	0.671	0.703	0.703	0.744	0.724	0.554	0.663	0.674	0.693	0.802	-9749.489141	9.314856	13.376	
IX	0.780	0.684	0.686	0.723	0.643	0.721	0.730	0.706	0.710	0.801	0.660	0.725	0.739	0.693	0.213	0.534	0.627	0.641	0.704	0.820	-9749.770609	2.824204	13.327	
X	0.767	0.691	0.703	0.694	0.568	0.726	0.716	0.711	0.739	0.719	0.682	0.736	0.722	0.715	0.777	0.546	0.674	0.728	0.706	0.193	-9749.719030	4.013616	13.322	
PM6_rohf	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20			Heat of formation, kcal	
0	0.822	0.536	0.217	0.015	-0.188	0.346	0.708	0.652	0.380	0.040	0.039	0.383	0.652	0.708	0.348	-0.189	0.013	0.215	0.537	0.822	-7370.805350			249.54932
I	0.430	0.610	0.712	0.337	-0.049	0.707	0.469	0.495	0.773	0.397	0.460	0.735	0.434	0.453	0.761	0.000	0.469	0.763	0.503	0.642	-7647.266950	48.722321	9.669	243.60027
II	-0.505	0.519	0.774	0.371	-0.043	0.692	0.379	0.479	0.780	0.383	0.603	0.698	0.405	0.457	0.763	0.049	0.519	0.752	0.482	0.646	-7649.260250	2.756823	9.706	197.63375
III	0.713	-0.331	0.729	0.610	0.063	0.689	0.481	0.380	0.675	0.561	0.243	0.784	0.512	0.401	0.722	-0.085	0.305	0.733	0.596	0.610	-7649.379800	0.000000	9.722	194.87686
IV	0.823	0.325	-0.343	0.832	0.267	0.542	0.691	0.316	0.490	0.729	0.148	0.647	0.653	0.392	0.609	-0.139	0.159	0.595	0.707	0.600	-7649.140560	5.516874	9.387	200.39392
V	0.845	0.429	0.137	-0.357	0.686	0.433	0.759	0.475	0.227	0.686	0.084	0.495	0.759	0.469	0.418	-0.173	0.068	0.361	0.759	0.647	-7648.631830	17.248188	8.565	212.12546
VI	0.834	0.506	0.152	-0.024	-0.416	0.344	0.734	0.618	0.259	0.053	0.025	0.372	0.691	0.657	0.287	-0.198	-0.006	0.201	0.591	0.752	-7647.802970	36.361700	6.848	231.23932
VII	0.857	0.406	0.215	0.049	-0.376	0.359	0.761	0.564	0.276	0.037	0.021	0.369	0.693	0.680	0.290	-0.199	-0.005	0.204	0.563	0.812	-7647.827210	35.802725	6.952	230.68051
VIII	0.787	0.387	0.388	0.731	0.642	0.555	0.718	0.404	0.242	-0.325	0.102	0.531	0.751	0.538	0.245	-0.172	0.061	0.304	0.660	0.749	-7648.705640	15.546130	8.622	210.42328
IX	0.713	0.414	0.613	0.722	0.264	0.694	0.575	0.368	0.497	0.833	0.208	0.717	0.654	0.347	-0.298	-0.133	0.126	0.435	0.757	0.600	-7649.184520	4.503157	9.403	199.38015
X	0.649	0.477	0.748	0.530	0.059	0.762	0.462	0.401	0.689	0.619	0.372	0.781	0.485	0.375	0.697	-0.049	0.357	0.768	0.507	-0.523	-7649.256690	2.838917	9.690	197.71589
~																								
diff_DFT	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20				
0																								
I	-0.185	-0.032	0.030	0.038	0.028	-0.015	-0.029	-0.006	0.017	0.034	0.038	0.008	-0.007	-0.003	0.020	0.033	0.037	0.022	-0.001	-0.008				
II	-0.588	0.041	0.048	0.029	0.016	0.050	-0.010	0.005	0.027	0.032	0.085	0.025	-0.009	-0.005	0.026	0.049	0.059	0.033	-0.009	-0.015				
III	0.056	-0.514	0.091	0.078	0.042	0.011	-0.010	-0.017	0.024	0.057	-0.018	0.036	0.001	-0.016	0.021	-0.001	0.029	0.038	0.002	-0.024				
IV	0.027	0.026	-0.478	0.159	0.116	0.001	0.019	-0.035	-0.004	0.079	0.006	-0.006	0.015	-0.017	0.005	0.013	0.011	0.026	0.013	-0.024				
V	-0.002	0.018	0.024	-0.395	0.256	0.005	0.002	0.023	-0.049	0.053	0.028	0.008	-0.011	0.000	-0.012	0.027	0.032	0.009	0.007	-0.011				
VI	-0.001	0.004	0.004	0.012	-0.209	0.001	0.000	0.009	0.015	-0.042	0.007	0.002	-0.001	0.002	-0.005	0.007	0.007	0.001	-0.006	0.008				
VII	0.001	0.008	-0.006	-0.045	-0.215	0.000	-0.006	0.002	0.014	0.015	0.011	0.001	-0.001	0.008	0.008	0.009	0.009	0.003	-0.002	0.003				
VIII	0.001	-0.006	-0.002	0.061	0.255	0.010	0.005	0.001	-0.050	-0.393	0.024	-0.007	-0.016	0.020	0.025	0.025	0.026	0.005	-0.005	0.020				
IX	-0.002	-0.015	0.019	0.085	0.114	0.021	0.007	-0.014	-0.001	0.154	0.013	0.015	0.020	-0.031	-0.486	0.006	-0.011	-0.028	0.006	0.038				
X	-0.016	-0.007	0.036	0.056	0.039	0.026	-0.007	-0.008	0.028	0.072	0.035	0.026	0.003	-0.008	0.078	0.018	0.037	0.059	0.009	-0.588				
diff_PM6	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20				
0																								
I	-0.391	0.074	0.495	0.322	0.139	0.361	-0.239	-0.157	0.393	0.357	0.420	0.352	-0.218	-0.255	0.413	0.189	0.456	0.548	-0.035	-0.180				
II	-1.327	-0.018	0.557	0.355	0.145	0.345	-0.329	-0.173	0.400	0.343	0.564	0.315	-0.247	-0.251	0.415	0.239	0.506	0.537	-0.055	-0.177				
III	-0.109	-0.868	0.512	0.594	0.251	0.342	-0.226	-0.272	0.295	0.522	0.204	0.401	-0.139	-0.307	0.374	0.104	0.292	0.518	0.059	-0.213				
IV	0.001	-0.211	-0.560	0.817	0.455	0.196	-0.016	-0.335	0.110	0.689	0.108	0.264	0.002	-0.316	0.261	0.050	0.146	0.380	0.170	-0.222				

HOMA 5z5a

DFT	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
0	0.797	0.678	0.669	0.700	0.648	0.519	0.701	0.698	0.678	0.784	0.792	0.644	0.669	0.704	0.565	0.517	0.702	0.699	0.676	0.783	0.798	0.679	0.671	0.699	0.647
I	0.586	0.627	0.696	0.729	0.660	0.530	0.699	0.689	0.672	0.787	0.794	0.635	0.675	0.719	0.573	0.536	0.720	0.696	0.668	0.784	0.816	0.672	0.672	0.725	0.672
II	0.260	0.650	0.704	0.730	0.659	0.653	0.733	0.696	0.673	0.786	0.754	0.640	0.694	0.731	0.574	0.559	0.726	0.692	0.664	0.782	0.816	0.662	0.669	0.731	0.676
III	0.900	0.215	0.713	0.752	0.676	0.523	0.742	0.691	0.670	0.788	0.798	0.596	0.681	0.735	0.582	0.538	0.726	0.693	0.664	0.783	0.825	0.661	0.669	0.736	0.683
IV	0.840	0.715	0.211	0.795	0.721	0.518	0.731	0.685	0.652	0.778	0.801	0.632	0.638	0.734	0.597	0.529	0.729	0.693	0.657	0.778	0.825	0.669	0.663	0.735	0.690
V	0.813	0.701	0.672	0.242	0.826	0.518	0.720	0.742	0.601	0.730	0.798	0.646	0.666	0.704	0.624	0.527	0.726	0.715	0.650	0.767	0.823	0.673	0.664	0.730	0.703
VI	0.805	0.686	0.677	0.686	0.329	0.523	0.714	0.721	0.691	0.590	0.796	0.638	0.667	0.712	0.626	0.528	0.716	0.706	0.669	0.744	0.820	0.671	0.661	0.723	0.701
VII	0.805	0.673	0.697	0.687	0.439	0.539	0.711	0.677	0.680	0.825	0.792	0.629	0.672	0.720	0.556	0.535	0.718	0.692	0.671	0.790	0.815	0.670	0.672	0.726	0.668
VIII	0.825	0.677	0.648	0.706	0.785	0.518	0.716	0.714	0.661	0.497	0.797	0.639	0.653	0.672	0.501	0.514	0.702	0.696	0.678	0.795	0.805	0.681	0.677	0.715	0.657
IX	0.811	0.698	0.665	0.609	0.497	0.514	0.710	0.722	0.628	0.294	0.797	0.640	0.658	0.694	0.643	0.522	0.720	0.713	0.670	0.726	0.823	0.676	0.663	0.723	0.707
X	0.165	0.590	0.704	0.730	0.659	0.634	0.723	0.691	0.670	0.786	0.753	0.636	0.690	0.729	0.578	0.559	0.723	0.691	0.665	0.784	0.819	0.664	0.669	0.733	0.680
XI	0.787	0.679	0.687	0.728	0.672	0.599	0.697	0.691	0.674	0.788	0.383	0.605	0.687	0.714	0.573	0.423	0.642	0.691	0.681	0.790	0.804	0.696	0.670	0.689	0.641

Etot, eV	Erel, kcal/mol	HOMAtot
-11228.098449		
-11646.212798	37.93	16.448
-11647.348480	11.74	16.653
-11647.838610	0.44	16.822
-11647.857526	0.00	16.806
-11647.586943	6.24	16.739
-11646.841714	23.42	16.469
-11646.476998	31.83	16.620
-11646.590232	29.22	16.429
-11646.936984	21.23	16.230
-11647.448723	9.43	16.561
-11646.750458	25.53	16.307

PM6_rohf	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
0	0.516	0.735	0.591	0.337	0.085	0.130	0.371	0.476	0.667	0.739	0.628	0.701	0.553	0.421	0.186	0.131	0.372	0.477	0.667	0.739	0.516	0.736	0.593	0.338	0.084
I	0.257	0.465	0.580	0.739	0.348	0.308	0.725	0.466	0.401	0.797	0.819	0.339	0.395	0.770	0.393	0.290	0.787	0.442	0.340	0.765	0.847	0.447	0.410	0.772	0.470
II	-0.414	0.144	0.530	0.772	0.345	0.558	0.691	0.382	0.399	0.813	0.713	0.296	0.468	0.783	0.348	0.360	0.769	0.406	0.370	0.797	0.836	0.430	0.456	0.787	0.412
III	0.887	-0.328	0.453	0.796	0.405	0.303	0.757	0.406	0.374	0.792	0.816	0.287	0.401	0.780	0.385	0.297	0.784	0.431	0.350	0.776	0.845	0.449	0.428	0.779	0.451
IV	0.838	0.529	-0.328	0.754	0.556	0.209	0.704	0.490	0.312	0.723	0.844	0.396	0.283	0.718	0.459	0.234	0.752	0.494	0.309	0.724	0.838	0.490	0.385	0.738	0.523
V	0.777	0.605	0.216	-0.323	0.783	0.177	0.618	0.677	0.209	0.564	0.836	0.455	0.295	0.593	0.555	0.205	0.709	0.564	0.285	0.660	0.827	0.516	0.372	0.693	0.581
VI	0.746	0.644	0.248	0.055	-0.356	0.159	0.572	0.744	0.316	-0.005	0.828	0.481	0.310	0.540	0.695	0.191	0.679	0.616	0.311	0.552	0.818	0.531	0.362	0.651	0.644
VII	0.758	0.632	0.399	0.390	-0.256	0.223	0.681	0.568	0.394	0.814	0.841	0.400	0.335	0.713	0.444	0.239	0.767	0.483	0.294	0.709	0.844	0.466	0.363	0.730	0.545
VIII	0.756	0.629	0.360	0.461	0.842	0.143	0.494	0.769	0.409	-0.304	0.742	0.631	0.353	0.220	-0.015	0.109	0.332	0.506	0.717	0.667	0.549	0.750	0.536	0.266	0.033
IX	0.736	0.659	0.269	-0.005	-0.237	0.157	0.549	0.748	0.310	-0.407	0.822	0.497	0.308	0.498	0.695	0.188	0.664	0.632	0.310	0.507	0.813	0.540	0.367	0.641	0.668
X	-0.608	0.085	0.553	0.768	0.334	0.562	0.662	0.373	0.405	0.817	0.687	0.285	0.475	0.780	0.340	0.376	0.766	0.404	0.374	0.801	0.837	0.432	0.462	0.789	0.404
XI	0.708	0.421	0.615	0.727	0.275	0.631	0.564	0.358	0.474	0.838	-0.347	0.221	0.690	0.638	0.233	-0.040	0.207	0.333	0.550	0.821	0.399	0.682	0.689	0.404	0.106

Heat of formation, kcal
-8868.278580
269.94257
-9144.669000
51.66
13.115
265.63505
-9146.397150
11.81
12.865
225.7831
-9146.853340
1.29
13.432
215.26296
-9146.909150
0.00
13.301
213.97609
-9146.597670
7.18
12.771
221.15884
-9145.822200
25.07
11.686
239.04172
-9144.677630
51.46
13.029
265.43598
-9145.370610
35.48
11.258
249.45547
-9145.747060
26.80
11.339
240.77435
-9146.341630
13.09
12.770
227.06332
-9145.522600
31.97
11.544
245.95064

diff_DFT	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
0																									
I	-0.212	-0.050	0.027	0.029	0.013	0.012	-0.002	-0.009	-0.005	0.004	0.001	-0.009	0.007	0.015	0.008	0.019	0.018	-0.003	-0.008	0.001	0.018	-0.007	0.002	0.025	0.024
II	-0.537	-0.028	0.034	0.030	0.012	0.134	0.032	-0.002	-0.004	0.003	-0.039	-0.004	0.026	0.027	0.009	0.042	0.024	-0.007	-0.012	-0.001	0.018	-0.017	-0.002	0.032	0.028
III	0.103	-0.463	0.044	0.052	0.028	0.004	0.041	-0.007	-0.008	0.004	0.006	-0.048	0.013	0.032	0.017	0.021	0.023	-0.005	-0.012999e-05	0.027	-0.018	-0.002	0.037	0.036	
IV	0.043	0.037	-0.458	0.095	0.074	-0.001	0.030	-0.013	-0.026	-0.006	0.009	-0.011	-0.031	0.030	0.032	0.012	0.027	-0.005	-0.019	-0.004	0.027	-0.011	-0.008	0.036	0.043
V	0.015	0.023	0.003	-0.458	0.179	-0.001	0.019	0.044	-0.076	-0.054	0.006	0.002	-0.003	0.000	0.059	0.010	0.023	0.017	-0.026	-0.015	0.025	-0.006	-0.007	0.031	0.056
VI	0.008	0.008	0.007	-0.014	-0.318	0.004	0.013	0.023	0.014	-0.194	0.004	-0.006	-0.001	0.008	0.061	0.011	0.014	0.007	-0.007	-0.039	0.022	-0.008	-0.009	0.024	0.054
VII	0.008	-0.005	0.027	-0.013	-0.208	0.021	0.009	-0.022	0.002	0.042	-0.001	-0.015	0.004	0.016	-0.009	0.018	0.016	-0.007	-0.005	0.008	0.017	-0.009	0.001	0.027	0.021
VIII	0.027	-0.001	-0.021	0.006	0.137	-0.001	0.015	0.016	-0.017	-0.287	0.004	-0.005	-0.015	-0.032	-0.063	-0.003	-0.001	-0.002	0.002	0.012	0.007	0.002	0.006	0.016	0.009
IX	0.014	0.021	-0.005	-0.091	-0.151	-0.005	0.009	0.024	-0.049	-0.490	0.005	-0.003	-0.011	-0.009	0.078	0.005	0.017	0.014	-0.006	-0.056	0.025	-0.003	-0.007	0.024	0.060
X	-0.633	-0.088	0.035	0.030	0.011	0.116	0.022	-0.007	-0.008	0.003	-0.039	-0.008	0.021	0.025	0.013	0.042	0.021	-0.008	-0.011	0.002	0.021	-0.015	-0.002	0.034	0.032
XI	-0.011	0.001	0.017	0.028	0.025	0.080	-0.004	-0.008	-0.004	0.004	-0.410	-0.039	0.019	0.010	0.008	-0.094	-0.060	-0.007	0.005	0.007	0.006	0.017	-0.001	-0.011	-0.007

diff_PM6	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
0																									
I	-0.258	-0.270	-0.011	0.402	0.263	0.177	0.355	-0.010	-0.266	0.059	0.191	-0.361	-0.158	0.349	0.207	0.159	0.415	-0.035	-0.327	0.026	0.330	-0.289	-0.182	0.434	0.386
II	-0.929	-0.591	-0.061	0.436	0.260	0.428	0.320	-0.094	-0.268	0.075	0.085	-0.405	-0.085	0.362	0.162	0.229	0.398	-0.071	-0.298	0.058	0.320	-0.305	-0.137	0.448	0.328
III	0.371	-1.063	-0.137	0.460	0.320	0.173	0.387	-0.071	-0.294	0.053	0.189	-0.414	-0.152	0.359	0.199	0.166	0.412	-0.046	-0.318	0.038	0.329	-0.286	-0.165	0.440	0.367
IV	0.323	-0.206	-0.919	0.417	0.471	0.078	0.333	0.014	-0.355	-0.016	0.216	-0.305	-0.270	0.296	0.273	0.103	0.380	0.017	-0.358	-0.015	0.321	-0.245	-0.207	0.400	0.438
V	0.261	-0.130	-0.375	-0.659	0.698	0.047	0.247	0.201	-0.458	-0.174	0.209	-0.246	-0.258	0.171	0.369	0.074	0.337	0.087	-0.383	-0.079	0.310	-0.219	-0.221	0.354	0.497
VI	0.231	-0.090	-0.343	-0.281	-0.441	0.028	0.201	0.268	-0.352	-0.744	0.200	-0.219	-0.243	0.119	0.509	0.060	0.307	0.139	-0.357	-0.186	0.302	-0.204	-0.231	0.312	0.560
VII	0.242	-0.103	-0.192	0.053	-0.341	0.092	0.310	0.092	-0.274	0.075	0.213	-0.301	-0.218	0.291	0.258	0.108	0.395	0.006	-0.373	-0.030	0.328	-0.269	-0.229	0.392	0.461
VIII	0.240	-0.106	-0.231	0.124	0.758	0.013	0.124	0.293	-0.258	-1.043	0.114	-0.069	-0.200	-0.201	-0.201	-0.022	-0.040	0.029	0.049	-0.072	0.033	0.015	-0.057	-0.073	-0.051
IX	0.221	-0.076	-0.322	-0.342	-0.322	0.026	0.179	0.272	-0.357	-1.145	0.195	-0.204	-0.245	0.077	0.509	0.057	0.293	0.155	-0.357	-0.231	0.297	-0.195	-0.225	0.303	0.584
X	-1.124	-0.650	-0.038	0.431	0.250	0.431	0.291	-0.104	-0.263	0.078	0.059	-0.415	-0.078	0.359	0.154	0.245	0.394	-0.073	-0.293	0.062	0.320	-0.304	-0.130	0.451	0.320
XI	0.193	-0.314	0.024	0.390	0.190	0.500	0.194	-0.118	-0.193	0.100	-0.974	-0.479	0.137	0.216	0.047	-0.171	-0.165	-0.144	-0.117	0.082	-0.118	-0.054	0.096	0.065	0.022

HOMA 5z5z

DFT	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	Etot, eV	Erel, kcal/mol	HOMAtot
0	0.778	0.698	0.670	0.640	0.528	0.698	0.721	0.719	0.706	0.640	0.670	0.719	0.726	0.718	0.669	0.640	0.706	0.718	0.719	0.696	0.528	0.640	0.669	0.696	0.777	-11227.248338		
I	0.510	0.705	0.713	0.663	0.540	0.689	0.696	0.722	0.728	0.665	0.703	0.717	0.717	0.721	0.699	0.664	0.724	0.718	0.710	0.704	0.545	0.667	0.696	0.702	0.759	-11645.410075	34.734609	0.510
II	0.187	0.755	0.717	0.665	0.544	0.721	0.717	0.732	0.731	0.669	0.724	0.729	0.722	0.725	0.699	0.673	0.732	0.724	0.712	0.703	0.548	0.673	0.701	0.703	0.760	-11646.773040	3.304636	2.119
III	0.833	0.193	0.766	0.717	0.572	0.698	0.713	0.711	0.735	0.699	0.643	0.743	0.728	0.714	0.703	0.644	0.719	0.733	0.717	0.693	0.548	0.661	0.691	0.708	0.765	-11646.916346	0.000000	2.316
IV	0.804	0.732	0.183	0.794	0.646	0.687	0.734	0.687	0.701	0.723	0.678	0.695	0.737	0.708	0.686	0.676	0.704	0.718	0.726	0.688	0.561	0.678	0.685	0.700	0.773	-11646.799204	2.701295	2.162
V	0.772	0.724	0.695	0.230	0.784	0.692	0.719	0.744	0.656	0.700	0.694	0.715	0.712	0.725	0.669	0.678	0.722	0.704	0.725	0.698	0.559	0.681	0.694	0.695	0.778	-11646.498673	9.631539	1.485
VI	0.767	0.709	0.702	0.685	0.331	0.703	0.721	0.732	0.735	0.614	0.695	0.725	0.727	0.718	0.674	0.674	0.723	0.720	0.709	0.702	0.555	0.674	0.695	0.697	0.772	-11645.903870	23.347697	0.614
PM6_rohf	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25			
0	0.835	0.457	0.166	-0.014	-0.199	0.455	0.731	0.546	0.298	-0.016	0.167	0.545	0.714	0.545	0.167	-0.014	0.299	0.545	0.731	0.456	-0.198	-0.012	0.168	0.457	0.834	-8866.749710		Heat of formation, kcal
I	0.430	0.670	0.620	0.221	-0.105	0.668	0.447	0.599	0.743	0.240	0.620	0.599	0.410	0.581	0.674	0.222	0.742	0.580	0.393	0.652	-0.106	0.239	0.674	0.652	0.588	-9143.641520	46.648305	0.430
II	-0.525	0.601	0.724	0.276	-0.089	0.594	0.368	0.567	0.757	0.256	0.713	0.574	0.392	0.570	0.681	0.265	0.754	0.575	0.390	0.647	-0.092	0.249	0.675	0.653	0.587	-9145.641150	0.536837	1.572
III	0.651	-0.320	0.786	0.510	0.005	0.735	0.407	0.421	0.754	0.417	0.367	0.731	0.424	0.458	0.761	0.088	0.616	0.702	0.413	0.543	-0.155	0.132	0.535	0.739	0.604	-9145.664430	0.000000	1.947
IV	0.785	0.285	-0.337	0.806	0.197	0.612	0.610	0.291	0.564	0.639	0.255	0.725	0.523	0.373	0.697	0.028	0.436	0.767	0.488	0.437	-0.187	0.052	0.363	0.757	0.653	-9145.340130	7.478358	1.642
V	0.826	0.358	0.112	-0.339	0.580	0.530	0.712	0.377	0.217	0.762	0.199	0.645	0.656	0.350	0.441	-0.005	0.340	0.689	0.618	0.369	-0.197	0.002	0.231	0.658	0.725	-9144.735800	21.414208	1.342
VI	0.552	0.656	0.671	0.271	-0.280	0.610	0.374	0.597	0.717	0.283	0.719	0.551	0.429	0.613	0.539	0.272	0.757	0.605	0.514	0.595	-0.078	0.280	0.583	0.694	0.696	-9143.484030	50.280024	0.283
diff_DFT	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25			
0																												
I	-0.268	0.006	0.044	0.023	0.011	-0.009	-0.025	0.003	0.023	0.025	0.033	-0.001	-0.009	0.003	0.030	0.023	0.018	0.000	-0.008	0.008	0.016	0.026	0.027	0.005	-0.018			
II	-0.590	0.056	0.048	0.025	0.016	0.023	-0.004	0.013	0.025	0.029	0.055	0.011	-0.003	0.007	0.030	0.033	0.026	0.006	-0.006	0.007	0.019	0.033	0.032	0.006	-0.017			
III	0.055	-0.505	0.096	0.077	0.044	-0.001	-0.008	-0.008	0.029	0.059	-0.026	0.024	0.002	-0.004	0.034	0.004	0.013	0.015	-0.002	-0.004	0.019	0.021	0.022	0.012	-0.012			
IV	0.027	0.034	-0.487	0.154	0.117	-0.012	0.014	-0.032	-0.005	0.083	0.008	-0.024	0.012	-0.010	0.017	0.035	-0.002	0.000	0.007	-0.008	0.033	0.038	0.016	0.004	-0.003			
V	-0.005	0.025	0.025	-0.410	0.256	-0.006	-0.001	0.025	-0.050	0.060	0.025	-0.004	-0.013	0.007	0.000	0.038	0.016	-0.014	0.006	0.001	0.030	0.041	0.026	-0.001	0.001			
VI	-0.011	0.011	0.032	0.044	-0.198	0.005	0.000	0.014	0.029	-0.026	0.026	0.007	0.001	0.000	0.005	0.033	0.017	0.002	-0.010	0.006	0.026	0.034	0.026	0.001	-0.004			
diff_PM6	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25			
0																												
I	-0.405	0.213	0.453	0.235	0.094	0.213	-0.284	0.053	0.445	0.256	0.453	0.053	-0.304	0.036	0.507	0.236	0.444	0.035	-0.338	0.196	0.092	0.252	0.506	0.195	-0.246			
II	-1.360	0.145	0.558	0.290	0.110	0.138	-0.363	0.021	0.460	0.271	0.546	0.029	-0.322	0.024	0.513	0.279	0.455	0.030	-0.342	0.191	0.106	0.262	0.507	0.196	-0.246			
III	-0.184	-0.777	0.620	0.525	0.203	0.279	-0.324	-0.126	0.457	0.433	0.200	0.186	-0.290	-0.088	0.593	0.102	0.317	0.157	-0.318	0.087	0.043	0.144	0.367	0.282	-0.230			
IV	-0.050	-0.171	-0.503	0.820	0.396	0.157	-0.121	-0.255	0.267	0.655	0.088	0.179	-0.191	-0.172	0.530	0.042	0.137	0.222	-0.243	-0.019	0.011	0.065	0.195	0.300	-0.180			
V	-0.009	-0.098	-0.055	-0.325	0.779	0.075	-0.019	-0.169	-0.081	0.778	0.032	0.100	-0.058	-0.196	0.274	0.009	0.041	0.143	-0.113	-0.087	0.001	0.015	0.063	0.201	-0.109			
VI	-0.282	0.199	0.505	0.285	-0.082	0.155	-0.357	0.051	0.420	0.299	0.552	0.005	-0.285	0.067	0.372	0.286	0.458	0.060	-0.217	0.138	0.120	0.293	0.415	0.237	-0.138			