Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Tuning the UV spectrum of PAHs by means of different N-doping types taking pyrene as paradigmatic example: categorization via valence bond theory and high-level computational approaches

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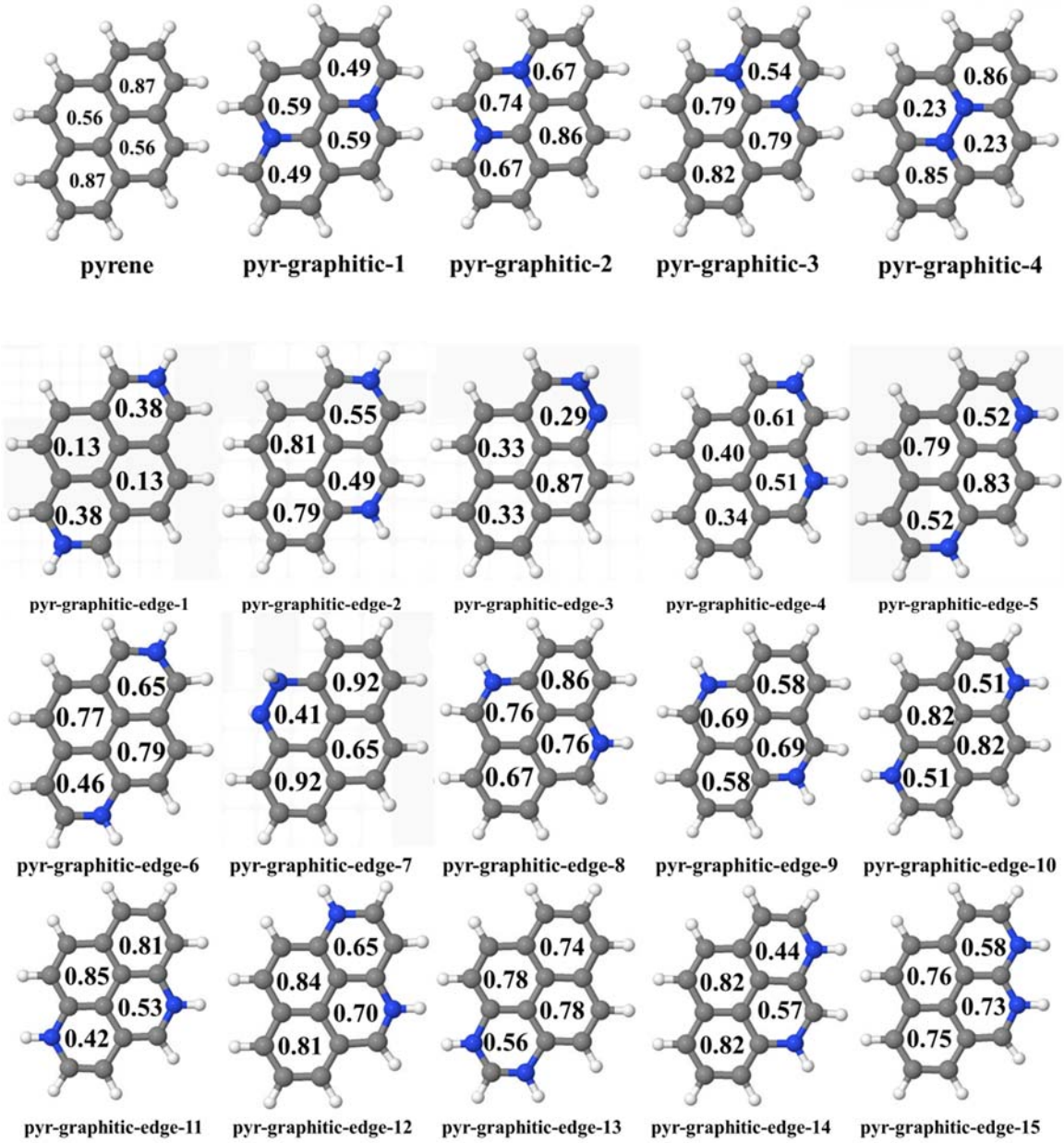
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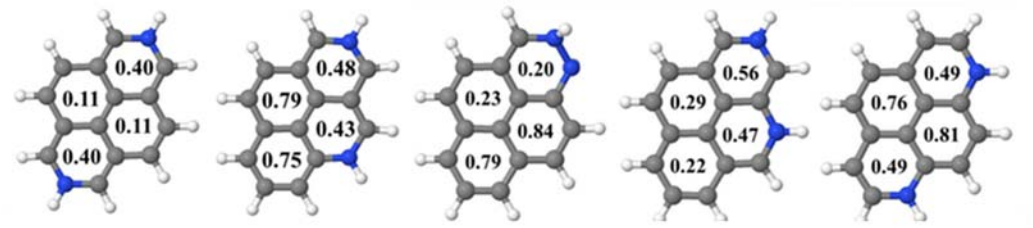

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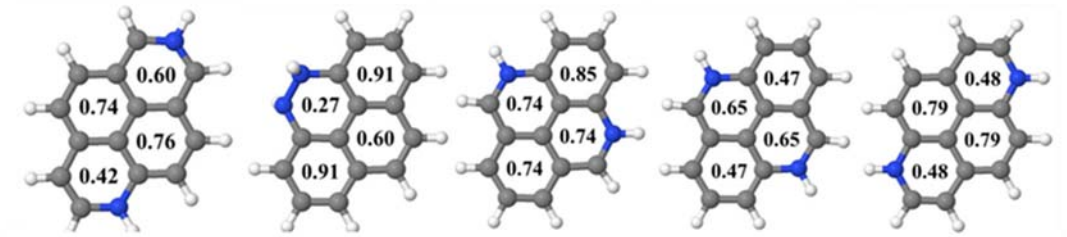

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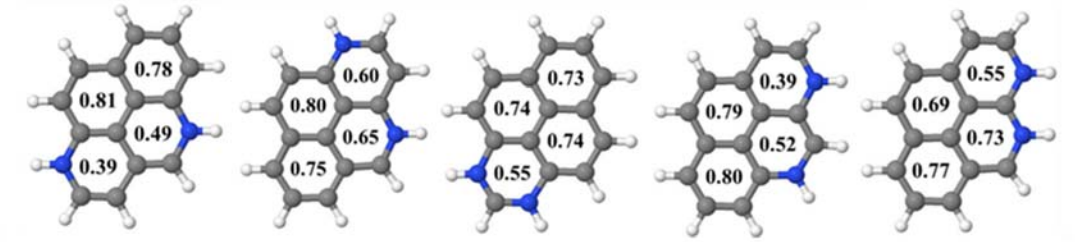

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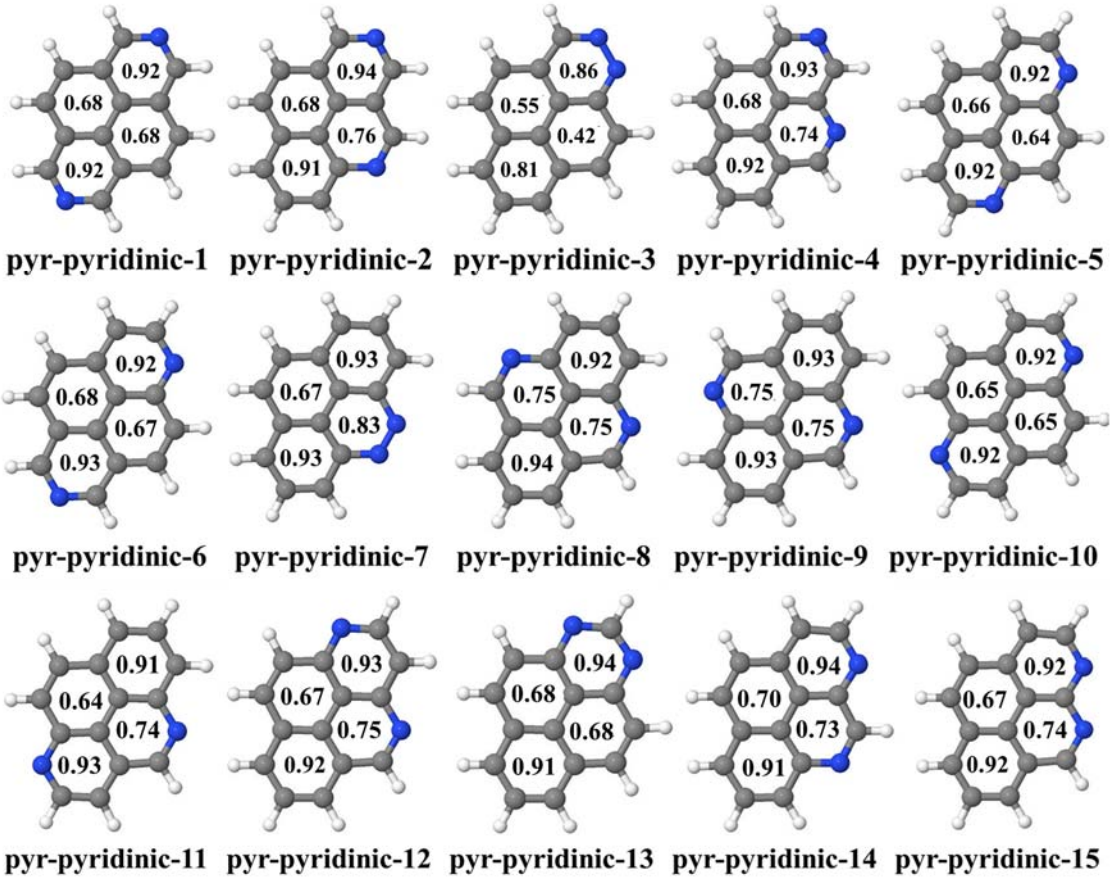


Figure S1. HOMA values for pyrene and doped isomers using the B3LYP method and the def2-TZVP basis set.

Table S1 Excited state properties of pristine pyrene and graphitic N-doping of pyrene calculated at five computational levels using the def2-TZVP basis.[a]

DFT/MRCI			SC-NEVPT2			ADC(2)			TD-B3LYP			TD-CAM-B3LYP		
	pyrene													
State	△E(eV)	f	State	△E	f	State	△E	f	State	△E	f	State	△E	f
1 A'	3.56	0.000	1 A'	3.90	0.000	1 A'	3.75	0.001	1 A'	3.67	0.254	1 A'	4.02	0.000
2 A'	3.78	0.514	2 A'	3.95	0.403	2 A'	4.03	0.261	2 A'	3.75	0.000	2 A'	4.05	0.308
3 A'	4.43	0.000	3 A'	4.77	0.348	3 A'	4.56	0.000	3 A'	4.30	0.000	3 A'	4.77	0.000
4 A'	4.70	0.530	4 A'	4.89	0.000	4 A'	4.84	0.284	4 A'	4.57	0.256	4 A'	5.09	0.394
5 A'	4.80	0.000	5 A'	4.97	0.000	5 A'	4.99	0.000	5 A'	4.62	0.000	5 A'	5.16	0.000
6 A'	4.81	0.000	6 A'	4.98	0.000	6 A'	5.09	0.000	6 A'	5.00	0.000	6 A'	5.60	0.000
7 A'	5.23	0.000	7 A'	5.53	1.329	7 A'	5.43	0.000	7 A'	5.16	0.000	7 A'	5.70	1.011
8 A'	5.39	0.000	8 A'	5.64	0.000	8 A'	5.60	0.893	8 A'	5.37	0.753	8 A'	5.80	0.000
9 A'	5.41	1.270	9 A'	5.71	0.000	9 A'	5.62	0.000	9 A'	5.61	0.000	9 A'	6.02	0.000

10 A'	5.69	0.000	10 A'	5.84	0.000	10 A'	6.25	0.000	10 A'	5.66	0.000	10 A'	6.11	0.000
pyr-graphitic-1														
1 A'	1.40	0.000	1 A'	1.35	0.000	1 A'	1.49	0.000	1 A'	1.30	0.000	1 A'	1.63	0.000
2 A'	1.97	0.009	2 A'	1.93	0.008	2 A'	2.10	0.019	2 A'	1.88	0.005	2 A'	2.29	0.004
3 A'	2.39	0.239	3 A'	2.33	0.180	3 A'	2.46	0.111	3 A'	2.35	0.149	3 A'	2.65	0.201
4 A'	2.75 D	0.000	4 A'	2.59 D	0.000	1 A"	4.41	0.001	1 A"	3.84	0.001	1 A"	4.47	0.002
5 A'	3.21 D	0.042	5 A'	3.18 D	0.035	4 A'	4.42	0.096	2 A"	4.02	0.000	2 A"	4.69	0.000
6 A'	3.60 D	0.000	6 A'	3.55 D	0.060	5 A'	4.63	0.000	4 A'	4.14	0.114	4 A'	4.69	0.157
7 A'	3.62 D	0.068	7 A'	3.70 D	0.000	2 A"	4.66	0.000	5 A'	4.25	0.000	3 A"	4.76	0.007
8 A'	3.84 D	0.000	8 A'	3.76 D	0.000	3 A"	4.67	0.000	6 A'	4.37	0.384	4 A"	4.82	0.000
1 A"	4.14	0.002	9 A'	4.44 D	0.000	6 A'	4.86	0.691	7 A'	4.39	0.000	5 A"	5.06	0.000
9 A'	4.30	0.342	10 A'	4.45	0.481	7 A'	4.88	0.000	3 A"	4.42	0.000	5 A'	5.19	0.660
pyr-graphitic-2														
State	△E(eV)	f	State	△E	f	State	△E	f	State	△E	f	State	△E	f
1 A'	0.61	0.012	1 A'	0.44	0.000	1 A'	0.73	0.005	1 A'	0.39	0.006	1 A'	0.37	0.009
2 A'	0.98 D	0.001	2 A'	0.80 D	0.000	2 A'	2.10	0.002	2 A'	1.40	0.009	2 A'	1.51	0.010
3 A'	1.50	0.009	3 A'	1.58	0.003	3 A'	2.31	0.005	3 A'	2.21	0.151	3 A'	2.32	0.197
4 A'	2.10 D	0.007	4 A'	1.72 D	0.001	1 A"	3.94	0.001	4 A'	3.36	0.007	1 A"	3.77	0.000
5 A'	2.35	0.168	5 A'	2.18	0.028	4 A'	3.95	0.022	1 A"	3.40	0.000	4 A'	3.85	0.085
6 A'	2.50 D	0.008	6 A'	2.34 D	0.007	2 A"	4.45	0.000	5 A'	3.78	0.091	5 A'	4.05	0.064
7 A'	3.37 D	0.000	7 A'	3.46 D	0.004	3 A"	4.49	0.000	2 A"	3.86	0.000	2 A"	4.18	0.000
8 A'	3.53	0.000	8 A'	3.62 D	0.022	5 A'	4.55	0.103	6 A'	4.06	0.047	3 A"	4.27	0.000
9 A'	3.61 D	0.003	9 A'	3.65 D	0.000	6 A'	4.60	0.023	3 A"	4.07	0.000	6 A'	4.55	0.001
10 A'	3.63	0.100	10 A'	4.19 D	0.002	7 A'	4.73	0.910	7 A'	4.09	0.000	4 A"	4.58	0.058
pyr-graphitic-3														
1 A'	0.43	0.000	1 A'	0.49	0.000	1 A'	0.32	0.001	1 A'	0.56	0.000	1 A'	0.78	0.001
2 A'	1.25	0.009	2 A'	1.50	0.001	2 A'	1.04	0.040	2 A'	1.32	0.006	2 A'	1.71	0.005
3 A'	1.49	0.197	3 A'	1.75	0.234	3 A'	1.32	0.173	3 A'	1.93	0.158	3 A'	2.18	0.170
4 A'	2.04 D	0.025	4 A'	2.19 D	0.061	4 A'	3.65	0.066	4 A'	3.56	0.031	1 A"	3.98	0.000
5 A'	2.49 D	0.004	5 A'	3.25 D	0.019	1 A"	3.77	0.000	1 A"	3.58	0.000	4 A'	4.09	0.121
6 A'	2.70 D	0.005	6 A'	3.33 D	0.015	5 A'	3.94	0.143	5 A'	3.90	0.002	2 A"	4.35	0.000
7 A'	3.50 D	0.009	7 A'	4.20	0.196	2 A"	3.98	0.000	2 A"	3.92	0.002	5 A'	4.44	0.006
8 A'	3.50 D	0.016	1 A"	4.40	0.002	6 A'	4.10	0.001	6 A'	4.06	0.149	3 A"	4.45	0.005
1 A"	3.64	0.00	8 A'	4.73 D	0.000	7 A'	4.20	0.002	3 A"	4.10	0.000	6 A'	4.67	0.147
9 A'	3.68	0.214	9 A'	4.97 D	0.004	3 A"	4.23	0.004	4 A"	4.21	0.000	4 A"	4.83	0.000
pyr-graphitic-4														
1 A'	0.75	0.017	1 A'	0.58	0.015	1 A'	0.53	0.028	1 A'	0.68	0.008	1 A'	1.41	0.013
2 A'	1.50	0.061	2 A'	1.13	0.029	2 A'	1.19	0.008	2 A'	1.32	0.027	2 A'	1.64	0.020
3 A'	2.00 D	0.000	3 A'	1.55 D	0.000	3 A'	2.26	0.000	3 A'	2.45	0.000	3 A'	3.24	0.024
4 A'	2.04 D	0.000	4 A'	1.63 D	0.000	4 A'	3.49	0.034	4 A'	3.52	0.063	4 A'	3.78	0.398
5 A'	2.77 D	0.000	5 A'	2.30 D	0.000	5 A'	3.49	0.007	5 A'	3.57	0.464	5 A'	3.84	0.106
6 A'	2.93	0.000	6 A'	2.64 D	0.002	6 A'	3.73	0.401	6 A"	3.72	0.001	6 A'	4.71	0.001

7 A'	3.18 D	0.000	7 A'	3.21 D	0.079	1 A"	3.82	0.000	7 A'	3.79	0.000	1 A"	4.79	0.031
8 A'	3.39	0.114	8 A'	3.21	0.129	2 A"	4.06	0.000	1 A"	3.82	0.000	8 A'	4.79	0.003
9 A'	3.57	0.780	9 A'	3.25	0.037	3 A"	4.46	0.000	2 A"	4.28	0.000	2 A"	5.20	0.000
10 A'	3.79 D	0.000	10 A'	3.52	0.566	4 A"	4.66	0.000	3 A"	4.55	0.000	3 A"	5.25	0.002

[a] States with dominating double excitations are labelled by D. Otherwise, states are classified as single excitations.

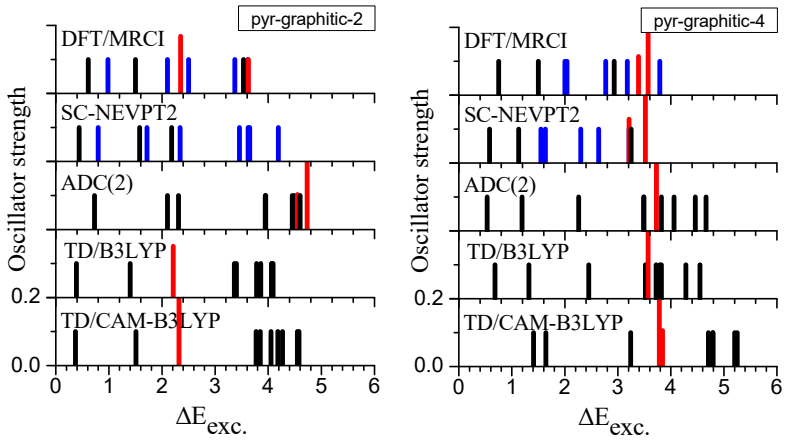


Figure S2 Excitation spectrum of pyr-graphitic-2 and pyr-graphitic-4, calculated at the DFT/MRCI, SC-NEVPT2, ADC(2), TD-B3LYP and CAM-TD-B3LYP levels. Bright singly excited states are highlighted in red, bright doubly excited states are highlighted in green, dark doubly excited states are in blue and the remaining dark singly excited states are in black.

Table S2 Excited state properties of pyr-graphitic-edge-y calculated at five computational levels.[a]

DFT/MRCI			SC-NEVPT2			ADC(2)			TD-B3LYP			TD-CAM-B3LYP		
pyr-graphitic-edge-1														
State	△E(eV)	f	State	△E	f	State	△E	f	State	△E	f	State	△E	f
1 A'	1.36	0.000	1 A'	1.38	0.000	1 A'	1.38	0.000	1 A'	1.02	0.000	1 A'	1.29	0.000
2 A'	2.33 D	0.000	2 A'	2.20 D	0.000	2 A'	2.76	0.065	2 A'	2.48	0.018	2 A'	2.78	0.053
3 A'	2.68	0.071	3 A'	2.66	0.023	3 A'	3.14	0.007	3 A'	2.94	0.003	3 A'	3.29	0.008
4 A'	2.83	0.000	1 A"	2.81	0.000	4 A'	3.47	0.220	4 A'	3.03	0.112	4 A'	3.67	0.252
5 A'	3.39	0.287	2 A"	3.40	0.196	1 A"	4.00	0.000	1 A"	3.24	0.000	1 A"	3.76	0.000
1 A"	3.58	0.001	3 A"	3.91 D	0.007	2 A"	4.00	0.003	2 A"	3.27	0.000	2 A"	3.77	0.000
2 A"	3.61	0.001	4 A"	4.51 D	0.786	5 A'	4.97	0.954	3 A"	4.26	0.000	3 A"	4.82	0.000
7 A'	3.82 D	0.000	4 A'	4.68	0.087	3 A"	5.08	0.000	4 A"	4.31	0.000	4 A"	4.92	0.000
8 A'	4.33 D	0.000	5 A'	4.73 D	0.002	4 A"	5.14	0.001	5 A'	4.63	1.057	5 A'	5.15	1.274
9 A'	4.42 D	0.043	6 A'	4.75	0.958	6 A'	5.16	0.000	6 A'	4.67	0.000	5 A"	5.25	0.000
pyr-graphitic-edge-2														
1 A'	1.24	0.006	1 A'	1.20	0.003	1 A'	1.26	0.014	1 A'	1.12	0.003	1 A'	1.35	0.007
2 A'	2.21	0.050	2 A'	2.30	0.041	2 A'	2.15	0.025	2 A'	2.15	0.029	2 A'	2.47	0.033
3 A'	2.51 D	0.007	3 A'	2.44 D	0.004	3 A'	3.04	0.144	1 A"	2.78	0.000	1 A"	3.24	0.000
4 A'	3.00	0.073	4 A'	2.97 D	0.004	1 A"	3.38	0.000	3 A'	3.01	0.087	3 A'	3.37	0.152
1 A"	3.10	0.000	1 A"	3.24	0.090	4 A'	3.79	0.067	4 A'	3.46	0.049	2 A"	3.93	0.000
5 A'	3.29 D	0.037	2 A"	3.39 D	0.002	5 A'	3.97	0.187	2 A"	3.47	0.000	4 A'	4.21	0.227
6 A'	3.38	0.095	5 A'	4.14	0.170	2 A"	4.08	0.001	5 A'	3.87	0.212	5 A'	4.30	0.121
2 A"	3.78	0.000	6 A'	4.29	0.131	6 A'	4.48	0.040	6 A'	4.21	0.041	6 A'	4.72	0.064
7 A'	3.81	0.394	7 A'	4.44 D	0.079	3 A"	4.92	0.000	3 A"	4.37	0.000	3 A"	4.83	0.001
8 A'	4.18	0.019	8 A	4.60 D	0.005	4 A"	4.98	0.001	4 A"	4.44	0.000	4 A"	5.08	0.000
pyr-graphitic-edge-3														
1 A'	2.92	0.330	1 A'	3.05	0.279	1 A'	3.04	0.135	1 A'	2.73	0.164	1 A'	3.07	0.206
2 A'	3.51	0.008	2 A'	3.88	0.002	2 A'	3.72	0.003	2 A'	3.52	0.011	2 A'	3.94	0.008
3 A'	3.88	0.004	3 A'	4.24 D	0.003	3 A'	4.13	0.012	3 A'	3.81	0.005	3 A'	4.35	0.003
4 A'	3.98 D	0.006	4 A'	4.27	0.033	4 A'	4.60	0.216	4 A'	4.32	0.194	4 A'	4.83	0.222
5 A'	4.57	0.344	5 A'	4.84	0.357	1 A"	4.72	0.027	5 A'	4.39	0.007	5 A'	5.10	0.007
6 A'	4.65	0.081	6 A'	4.87	0.048	5 A'	4.90	0.011	6 A'	4.48	0.014	6 A'	5.19	0.132
7 A'	4.97	0.485	7 A'	5.75	0.208	2 A"	5.11	0.284	7 A'	4.86	0.272	7 A'	5.31	0.324
1 A"	5.19	0.021	8 A'	5.83	0.005	3 A"	5.39	0.038	1 A"	5.03	0.029	1 A"	5.59	0.048
2 A"	5.35	0.053	1 A"	5.93 D	0.010	6 A'	5.55	0.023	2 A"	5.19	0.001	2 A"	5.79	0.019
8 A'	5.41	0.030	9 A'	5.97	0.110	4 A"	5.79	0.009	3 A"	5.33	0.018	3 A"	5.92	0.057
pyr-graphitic-edge-4														
1 A'	1.03	0.036	1 A'	0.98	0.020	1 A'	1.16	0.012	1 A'	0.99	0.017	1 A'	1.30	0.036
2 A'	2.13	0.039	2 A'	2.16 D	0.015	2 A'	2.19	0.023	2 A'	2.02	0.030	2 A'	2.38	0.035
3 A'	2.22 D	0.014	3 A'	2.20	0.015	3 A'	3.00	0.035	1 A"	2.81	0.000	3 A'	3.31	0.077

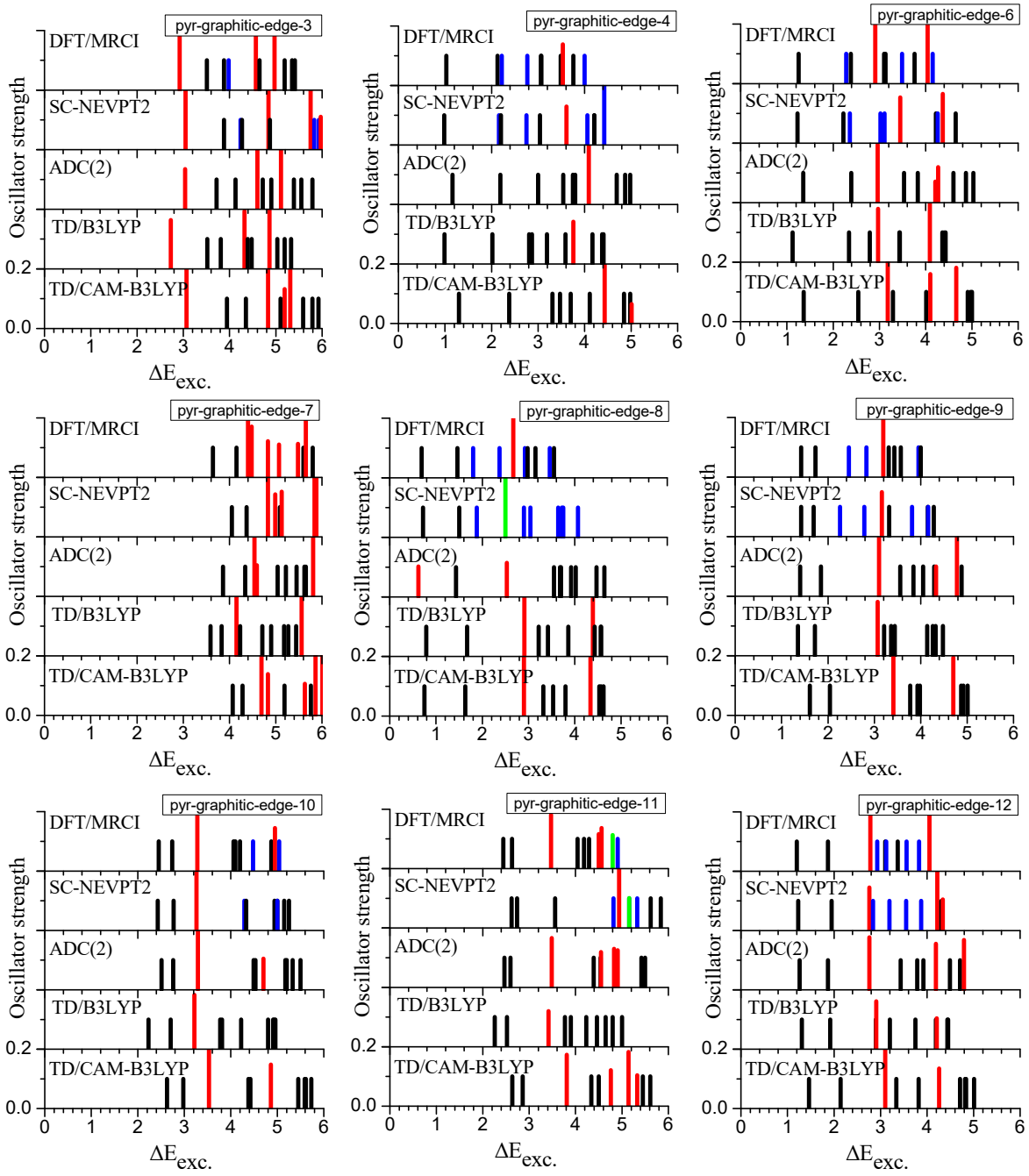
4 A'	2.77 D	0.026	4 A'	2.75 D	0.043	1 A"	3.54	0.002	3 A'	2.87	0.039	1 A"	3.47	0.000
1 A"	3.06	0.001	1 A"	3.04	0.004	4 A'	3.75	0.044	2 A"	3.19	0.001	4 A'	3.70	0.000
5 A'	3.07	0.017	5 A'	3.61	0.129	2 A"	3.80	0.000	4 A'	3.59	0.071	5 A'	4.11	0.096
2 A"	3.49	0.001	6 A'	4.06 D	0.010	5 A'	4.09	0.254	5 A'	3.76	0.142	6 A'	4.43	0.242
6 A'	3.53	0.138	7 A'	4.21 D	0.029	6 A'	4.69	0.087	3 A"	4.17	0.000	2 A"	4.85	0.001
7 A'	3.76	0.079	8 A'	4.21	0.010	3 A"	4.87	0.000	4 A"	4.38	0.000	3 A"	4.98	0.000
8 A'	4.00 D	0.083	9 A'	4.42	0.215	4 A"	4.98	0.000	6 A'	4.41	0.030	7 A'	5.01	0.065
pyr-graphitic-edge-5														
1 A'	2.35	0.054	1 A'	2.50	0.050	1 A'	2.41	0.011	1 A'	2.17	0.026	1 A'	2.56	0.036
2 A'	2.75	0.074	2 A'	3.09	0.092	2 A'	2.77	0.036	2 A'	2.73	0.042	2 A'	3.00	0.053
3 A'	3.38	0.248	3 A'	3.35	0.121	3 A'	3.37	0.205	3 A'	3.26	0.162	3 A'	3.57	0.200
4 A'	3.95	0.049	4 A'	5.01 D	0.044	1 A"	4.44	0.000	1 A"	3.73	0.000	1 A"	4.33	0.000
1 A"	4.02	0.000	5 A'	5.14 D	0.008	2 A"	4.50	0.002	2 A"	3.79	0.000	2 A"	4.40	0.000
2 A"	4.07	0.001	6 A'	5.38 D	0.050	4 A'	4.64	0.092	4 A'	4.16	0.047	4 A'	4.84	0.135
5 A'	4.63 D	0.039	7 A'	5.39 D	0.026	5 A'	4.96	0.070	5 A'	4.79	0.075	3 A"	5.46	0.000
6 A'	4.79	0.166	8 A'	5.58 D	0.277	6 A'	5.24	0.000	3 A"	4.80	0.000	5 A'	5.53	0.108
7 A'	4.89 D	0.035	9 A'	5.83 D	0.002	7 A'	5.26	0.039	4 A"	4.95	0.000	4 A"	5.58	0.000
8 A'	5.08	0.095	10 A'	6.01	0.130	3 A"	5.55	0.000	6 A'	4.99	0.000	6 A'	5.66	0.017
pyr-graphitic-edge-6														
1 A'	1.25	0.010	1 A'	1.23	0.006	1 A'	1.35	0.003	1 A'	1.12	0.005	1 A'	1.36	0.009
2 A'	2.28 D	0.001	2 A'	2.22	0.057	2 A'	2.39	0.029	2 A'	2.34	0.033	2 A'	2.54	0.045
3 A'	2.38	0.062	3 A'	2.36 D	0.001	3 A'	2.96	0.195	1 A"	2.79	0.000	3 A'	3.18	0.226
4 A'	2.91	0.247	1 A"	3.02 D	0.058	1 A"	3.53	0.000	3 A'	2.97	0.179	1 A"	3.29	0.000
1 A"	3.10	0.000	4 A'	3.11 D	0.049	4 A'	3.83	0.023	2 A"	3.43	0.009	2 A"	4.01	0.000
5 A'	3.13	0.018	2 A"	3.45	0.154	2 A"	4.21	0.071	4 A'	3.44	0.014	4 A'	4.10	0.160
6 A'	3.49 D	0.067	5 A'	4.22	0.063	3 A"	4.27	0.119	5 A'	4.09	0.230	5 A'	4.66	0.181
2 A"	3.76	0.000	6 A'	4.26 D	0.080	5 A'	4.60	0.019	3 A"	4.36	0.000	3 A"	4.91	0.000
7 A'	4.04	0.392	7 A'	4.37	0.165	6 A'	4.87	0.000	6 A'	4.40	0.006	4 A"	4.97	0.000
8 A'	4.15 D	0.054	8 A'	4.65	0.000	4 A"	5.03	0.000	4 A"	4.43	0.000	6 A'	5.00	0.004
pyr-graphitic-edge-7														
1 A'	3.64	0.001	1 A'	4.05	0.000	1 A'	3.86	0.000	1 A'	3.59	0.006	1 A'	4.07	0.002
2 A'	4.15	0.005	2 A'	4.37	0.054	2 A'	4.34	0.003	2 A'	3.83	0.001	2 A'	4.28	0.000
3 A'	4.40	0.527	3 A'	4.83	0.752	3 A'	4.54	0.240	3 A'	4.15	0.239	3 A'	4.69	0.397
4 A'	4.48	0.171	4 A'	4.99	0.143	4 A'	4.59	0.105	4 A'	4.23	0.068	4 A'	4.83	0.139
5 A'	4.83	0.122	5 A'	5.09	0.039	5 A'	5.04	0.060	5 A'	4.71	0.006	5 A'	5.19	0.006
6 A'	5.07	0.110	6 A'	5.13	0.152	6 A'	5.22	0.058	6 A'	4.90	0.055	6 A'	5.63	0.106
7 A'	5.48	0.113	7 A'	5.84	0.290	1 A"	5.45	0.007	1 A"	5.18	0.000	7 A'	5.76	0.030
1 A"	5.60	0.061	8 A'	5.88	0.948	7 A'	5.62	0.027	7 A'	5.27	0.011	1 A"	5.86	0.346
2 A"	5.65	1.166	9 A'	6.31	0.068	2 A"	5.65	0.022	2 A"	5.44	0.036	2 A"	6.01	0.649
3 A"	5.80	0.077	10 A'	6.51	0.000	8 A'	5.81	0.894	8 A'	5.56	0.995	3 A"	6.12	0.060
pyr-graphitic-edge-8														
1 A'	0.69	0.013	1 A'	0.72	0.010	1 A'	0.62	0.102	1 A'	0.79	0.014	1 A'	0.75	0.012

2 A'	1.46	0.020	2 A'	1.50	0.035	2 A'	1.43	0.002	2 A'	1.67	0.018	2 A'	1.63	0.016
3 A'	1.80 D	0.002	3 A'	1.88 D	0.007	3 A'	2.53	0.114	3 A'	2.91	0.276	3 A'	2.90	0.281
4 A'	2.37 D	0.057	4 A'	2.50 S/D	0.291	4 A'	3.55	0.004	1 A"	3.22	0.000	1 A"	3.32	0.000
5 A'	2.67	0.289	5 A'	2.90 D	0.026	1 A"	3.68	0.000	2 A"	3.42	0.001	2 A"	3.53	0.001
6 A'	2.92 D	0.007	6 A'	3.04 D/S	0.012	5 A'	3.70	0.060	4 A'	3.86	0.017	4 A'	3.80	0.016
1 A"	2.98	0.000	7 A'	3.64 D/S	0.019	2 A"	3.92	0.000	5 A'	4.39	0.195	5 A'	4.34	0.196
2 A"	3.15	0.001	8 A'	3.72 D	0.130	6 A'	4.02	0.088	3 A"	4.43	0.000	3 A"	4.53	0.000
7 A'	3.46 D	0.002	9 A'	3.75 D	0.000	7 A'	4.47	0.002	4 A"	4.56	0.000	6 A'	4.57	0.053
8 A'	3.55	0.068	10 A'	4.07 D	0.007	8 A'	4.64	0.002	6 A'	4.57	0.061	4 A"	4.62	0.000
pyr-graphitic-edge-9														
1 A'	1.42	0.093	1 A'	1.42	0.085	1 A'	1.40	0.011	1 A'	1.35	0.049	1 A'	1.61	0.075
2 A'	1.73	0.000	2 A'	1.69	0.004	2 A'	1.85	0.000	2 A'	1.72	0.000	2 A'	2.04	0.000
3 A'	2.45 D	0.000	3 A'	2.26 D	0.001	3 A'	3.10	0.210	3 A'	3.07	0.181	3 A'	3.41	0.226
4 A'	2.83 D	0.038	4 A'	2.78 D	0.016	4 A'	3.56	0.000	1 A"	3.21	0.001	1 A"	3.77	0.001
5 A'	3.19	0.271	1 A"	3.16	0.150	1 A"	3.84	0.000	2 A"	3.36	0.000	2 A"	3.93	0.000
6 A'	3.31	0.000	2 A"	3.32	0.062	2 A"	4.05	0.000	4 A'	3.44	0.000	4 A'	3.98	0.000
1 A"	3.43	0.002	5 A'	3.81 D	0.003	5 A'	4.29	0.000	5 A'	4.14	0.086	5 A'	4.70	0.194
2 A"	3.57	0.000	3 A"	4.15	0.096	6 A'	4.33	0.100	6 A'	4.26	0.000	6 A'	4.87	0.000
7 A'	3.95 D	0.000	4 A"	4.16 D	0.015	7 A'	4.78	0.263	3 A"	4.32	0.000	3 A"	4.92	0.000
8 A'	4.00	0.069	6 A'	4.28	0.001	8 A'	4.88	0.000	4 A"	4.48	0.001	4 A"	5.01	0.003
pyr-graphitic-edge-10														
1 A'	2.45	0.000	1 A'	2.43	0.000	1 A'	2.51	0.000	1 A'	2.23	0.000	1 A'	2.63	0.000
2 A'	2.74	0.096	2 A'	2.77	0.084	2 A'	2.76	0.043	2 A'	2.71	0.060	2 A'	2.98	0.071
3 A'	3.28	0.309	3 A'	3.26	0.199	3 A'	3.29	0.223	3 A'	3.22	0.183	3 A'	3.53	0.233
1 A"	4.06	0.001	4 A'	4.29 D	0.000	1 A"	4.49	0.001	1 A"	3.77	0.000	1 A"	4.38	0.000
2 A"	4.10	0.000	1 A"	4.33	0.062	2 A"	4.53	0.000	2 A"	3.81	0.000	2 A"	4.42	0.000
4 A'	4.20	0.094	5 A'	4.94	0.079	4 A'	4.70	0.105	4 A'	4.22	0.057	4 A'	4.86	0.148
5 A'	4.48 D	0.000	6 A'	5.00	0.000	5 A'	5.17	0.000	3 A"	4.80	0.000	3 A"	5.45	0.000
6 A'	4.87	0.000	7 A'	5.00 D	0.055	6 A'	5.20	0.087	5 A'	4.91	0.088	4 A"	5.59	0.000
7 A'	4.95	0.145	8 A'	5.15	0.000	7 A'	5.33	0.000	6 A'	4.93	0.000	5 A'	5.61	0.000
8 A'	5.04 D	0.048	9 A'	5.25	0.000	8 A'	5.50	0.000	4 A"	4.96	0.000	6 A'	5.73	0.000
pyr-graphitic-edge-11														
1 A'	2.44	0.012	1 A'	2.62	0.002	1 A'	2.47	0.008	1 A'	2.26	0.004	1 A'	2.64	0.003
2 A'	2.63	0.078	2 A'	2.74	0.091	2 A'	2.60	0.035	2 A'	2.52	0.043	2 A'	2.86	0.054
3 A'	3.47	0.181	3 A'	3.56	0.081	3 A'	3.49	0.166	3 A'	3.42	0.120	3 A'	3.81	0.173
1 A"	4.04	0.000	4 A'	4.82 D	0.011	1 A"	4.39	0.000	1 A"	3.77	0.000	1 A"	4.34	0.000
2 A"	4.18	0.000	5 A'	4.94	0.215	2 A"	4.54	0.003	2 A"	3.90	0.000	2 A"	4.50	0.000
4 A'	4.29	0.073	6 A'	5.16 D	0.096	4 A'	4.55	0.119	4 A'	4.23	0.040	4 A'	4.76	0.121
5 A'	4.50	0.116	7 A'	5.16 D	0.101	5 A'	4.83	0.130	5 A'	4.46	0.089	5 A'	5.14	0.182
6 A'	4.56	0.137	8 A'	5.33 D	0.046	6 A'	4.91	0.125	6 A'	4.65	0.092	6 A'	5.33	0.104
7 A'	4.80 D	0.113	9 A'	5.62	0.023	7 A'	5.42	0.054	3 A"	4.80	0.000	3 A"	5.45	0.000
8 A'	4.91 D	0.080	10 A'	5.84	0.076	3 A"	5.50	0.000	4 A"	5.00	0.000	4 A"	5.61	0.000

pyr-graphitic-edge-12														
1 A'	1.20	0.043	1 A'	1.23	0.048	1 A'	1.26	0.018	1 A'	1.31	0.021	1 A'	1.46	0.031
2 A'	1.87	0.047	2 A'	1.95	0.037	2 A'	1.87	0.012	2 A'	1.92	0.027	2 A'	2.14	0.037
3 A'	2.78	0.225	3 A'	2.76	0.145	3 A'	2.76	0.177	1 A"	2.90	0.000	3 A'	3.10	0.218
4 A'	2.93 D	0.004	4 A'	2.84 D	0.037	1 A"	3.43	0.000	3 A'	2.91	0.161	1 A"	3.34	0.001
1 A"	3.10	0.001	5 A'	3.19 D	0.031	2 A"	3.79	0.002	2 A"	3.20	0.000	2 A"	3.82	0.000
5 A'	3.12 D	0.050	6 A'	3.55 D	0.004	4 A'	3.92	0.044	4 A'	3.75	0.040	4 A'	4.26	0.135
2 A"	3.37	0.000	7 A'	3.87 D	0.001	5 A'	4.19	0.155	3 A"	4.19	0.000	5 A'	4.71	0.082
6 A'	3.56 D	0.002	8 A'	4.22	0.230	6 A'	4.49	0.009	5 A'	4.21	0.104	3 A"	4.82	0.000
7 A'	3.83 D	0.035	9 A'	4.31	0.008	3 A"	4.71	0.000	4 A"	4.44	0.000	4 A"	4.84	0.002
8 A'	4.05	0.204	10 A'	4.34	0.105	7 A'	4.79	0.168	6 A'	4.45	0.004	6 A'	5.01	0.007
pyr-graphitic-edge-13														
1 A'	0.44	0.000	1 A'	0.72	0.000	1 A'	0.62	0.002	1 A'	0.39	0.000	1 A'	0.83	0.001
2 A'	2.05 D	0.000	2 A'	2.23	0.008	2 A'	2.18	0.015	1 A"	1.97	0.000	2 A'	2.45	0.014
3 A'	2.21	0.018	3 A'	2.75 D	0.048	1 A"	2.57	0.000	2 A'	2.27	0.010	1 A"	2.64	0.000
1 A"	2.22	0.000	1 A"	3.06	0.110	3 A'	2.96	0.161	2 A"	2.75	0.000	3 A'	3.30	0.195
4 A'	2.83 D	0.000	2 A"	3.25 D	0.001	2 A"	3.37	0.003	3 A'	3.07	0.093	2 A"	3.40	0.000
5 A'	2.94	0.205	4 A'	3.29 D	0.001	4 A'	3.57	0.189	4 A'	3.39	0.019	4 A'	3.86	0.194
6 A'	2.97 D	0.002	5 A'	3.49	0.199	5 A'	3.87	0.020	5 A'	3.62	0.137	3 A"	4.34	0.000
2 A"	2.97	0.000	6 A'	4.32	0.000	3 A"	4.21	0.000	3 A"	3.71	0.000	5 A'	4.50	0.014
7 A'	3.46	0.263	7 A'	4.50	0.432	6 A'	4.41	0.403	6 A'	3.92	0.008	4 A"	4.64	0.000
3 A"	3.73 D	0.000	8 A'	4.82	0.455	7 A'	4.47	0.043	7 A'	4.08	0.423	5 A"	4.79	0.000
pyr-graphitic-edge-14														
1 A'	2.34	0.032	1 A'	2.29	0.039	1 A'	2.35	0.014	1 A'	2.21	0.016	1 A'	2.59	0.024
2 A'	2.63	0.065	2 A'	2.59	0.076	2 A'	2.61	0.022	2 A'	2.53	0.035	2 A'	2.89	0.039
3 A'	3.38	0.164	1 A"	3.37	0.079	3 A'	3.41	0.173	3 A'	3.34	0.122	3 A'	3.75	0.178
1 A"	3.85	0.001	3 A'	4.18	0.052	1 A"	4.19	0.001	1 A"	3.58	0.001	1 A"	4.08	0.001
2 A"	4.09	0.000	4 A'	4.59	0.158	2 A"	4.43	0.000	2 A"	3.82	0.000	2 A"	4.36	0.000
4 A'	4.19	0.137	5 A'	4.59 D	0.087	4 A'	4.44	0.126	4 A'	4.26	0.101	4 A'	4.72	0.179
5 A'	4.36	0.112	6 A'	4.81	0.057	5 A'	4.81	0.135	5 A'	4.37	0.035	5 A'	5.16	0.175
6 A'	4.49 D	0.140	7 A'	4.97	0.133	6 A'	4.94	0.011	6 A'	4.70	0.111	6 A'	5.33	0.044
7 A'	4.71	0.072	8 A'	5.26	0.053	7 A'	5.34	0.114	3 A"	4.82	0.000	3 A"	5.50	0.001
8 A'	4.77 D	0.052	9 A'	5.51	0.069	3 A"	5.48	0.000	4 A"	5.00	0.000	4 A"	5.58	0.005
pyr-graphitic-edge-15														
1 A'	1.40	0.009	1 A'	1.47	0.006	1 A'	1.33	0.022	1 A'	1.49	0.005	1 A'	1.67	0.014
2 A'	1.80	0.109	2 A'	1.82	0.113	2 A'	1.79	0.031	2 A'	1.86	0.062	2 A'	2.09	0.077
1 A"	2.51	0.000	1 A"	3.09 S/D	0.060	3 A'	2.74	0.199	1 A"	2.31	0.000	1 A"	2.79	0.000
3 A'	2.78	0.227	2 A"	3.24	0.062	1 A"	2.87	0.001	3 A'	2.97	0.168	3 A'	3.17	0.220
4 A'	3.24 D	0.035	3 A'	3.44 D	0.025	2 A"	4.01	0.000	2 A"	3.43	0.001	2 A"	4.00	0.001
5 A'	3.34 D	0.024	4 A'	3.54 D	0.062	4 A'	4.08	0.089	4 A'	3.95	0.069	4 A'	4.45	0.170
2 A"	3.62	0.001	5 A'	3.84 D	0.185	5 A'	4.22	0.069	5 A'	4.14	0.058	5 A'	4.65	0.081
6 A'	3.64 D	0.006	3 A"	4.38 D	0.010	6 A'	4.51	0.003	3 A"	4.29	0.000	3 A"	4.77	0.000

7 A'	3.89	0.089	4 A"	4.52	0.209	3 A"	4.64	0.000	6 A'	4.51	0.064	4 A"	5.04	0.000
8 A'	4.00	0.148	6 A'	4.56	0.021	7 A'	4.69	0.035	4 A"	4.60	0.000	6 A'	5.16	0.037

[a] States with dominating double excitations are labelled by D. Otherwise, states are classified as single excitations.



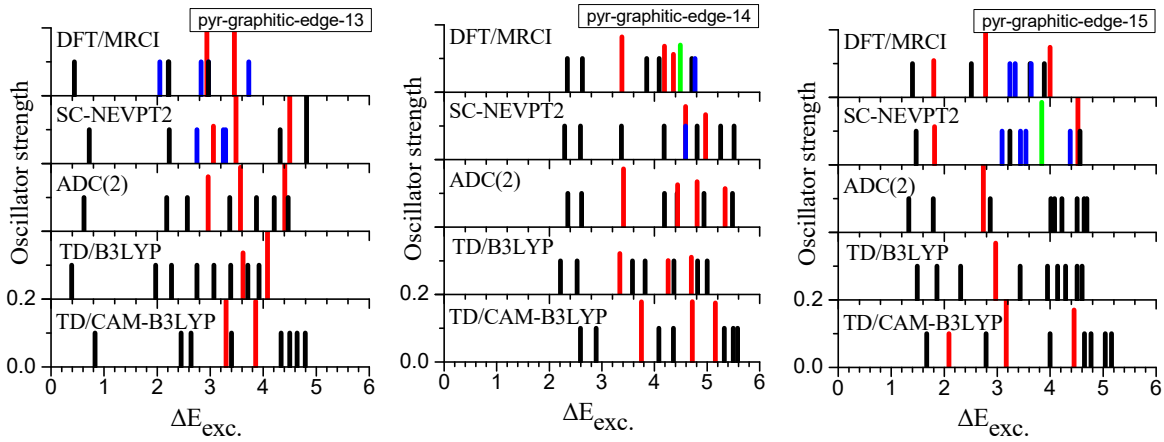


Figure S3 Excitation spectrum of pyr-graphitic-edge-y, calculated at the DFT/MRCI, SC-NEVPT2, ADC(2), TD-B3LYP and CAM-TD-B3LYP levels. Bright singly excited states are highlighted in red, bright doubly excited states, strongly mixed with singly-excited configurations, are highlighted in green, dark doubly excited states are in blue and the remaining dark singly excited states are in black.

Table S3 Excited state properties of Pyridinic N-doping of pyrene structure calculated at five computational levels.[a]

DFT/MRCI[b,c,d]			SC-NEVPT2[c,d]			ADC(2)			TD-B3LYP			TD-CAM-B3LYP		
pyr-pyridinic-1														
State	△E(eV)	f	State	△E	f	State	△E	f	State	△E	f	State	△E	f
1 A'	3.50	0.093	1 A'	3.55	0.076	1 A'	3.67	0.029	1 A'	3.67	0.059	1 A'	3.96	0.071
2 A'	3.83	0.535	2 A'	3.68	0.001	2 A'	4.10	0.269	2 A'	3.72	0.280	2 A'	4.11	0.351
3 A'	4.45	0.000	3 A'	3.70	0.000	1 A"	4.41	0.000	1 A"	4.02	0.000	1 A"	4.70	0.000
1 A"	4.53	0.000	4 A'	4.00	0.441	2 A"	4.56	0.000	2 A"	4.17	0.000	3 A'	4.77	0.000
2 A"	4.64	0.008	5 A'	4.80	0.000	3 A'	4.59	0.000	3 A'	4.32	0.000	2 A"	4.85	0.000
3 A"	4.65	0.000	6 A'	4.96	0.424	3 A"	4.67	0.002	3 A"	4.42	0.003	3 A"	4.90	0.004
4 A"	4.73	0.000	7 A'	5.24	0.000	4 A"	4.81	0.000	4 A"	4.54	0.000	4 A"	5.02	0.000
4 A'	4.84	0.000	8 A'	5.32	0.000	4 A'	5.13	0.000	4 A'	4.70	0.000	4 A'	5.32	0.000
5 A'	4.90	0.000	9 A'	5.39	0.000	5 A'	5.16	0.000	5 A'	4.92	0.174	5 A'	5.45	0.297
6 A'	5.03	0.399	10 A'	5.55	1.513	6 A'	5.17	0.228	6 A'	5.04	0.000	6 A'	5.62	0.000
pyr-pyridinic-2														
1 A'	3.59	0.031	1 A'	3.31	0.000	1 A'	3.77	0.009	1 A'	3.66	0.225	1 A'	4.05	0.168
2 A'	3.75	0.418	2 A'	3.82	0.069	2 A'	3.98	0.218	1 A"	3.76	0.000	2 A'	4.10	0.134
1 A"	4.10	0.002	3 A'	3.95	0.000	1 A"	4.05	0.000	2 A'	3.79	0.010	1 A"	4.30	0.001
3 A'	4.45	0.059	4 A'	3.96	0.208	3 A'	4.60	0.027	2 A"	4.30	0.000	3 A'	4.82	0.008
4 A'	4.66	0.347	5 A'	4.53	0.021	2 A"	4.63	0.000	3 A'	4.34	0.024	2 A"	4.84	0.001
2 A"	4.69	0.001	6 A'	4.85	0.212	3 A"	4.71	0.000	3 A"	4.48	0.001	3 A"	5.01	0.002
3 A"	4.75	0.003	7 A'	4.92	0.048	4 A'	4.81	0.198	4 A'	4.55	0.167	4 A'	5.08	0.274
5 A'	4.86	0.008	8 A'	5.46	1.176	5 A'	5.15	0.046	5 A'	4.92	0.016	5 A'	5.51	0.096

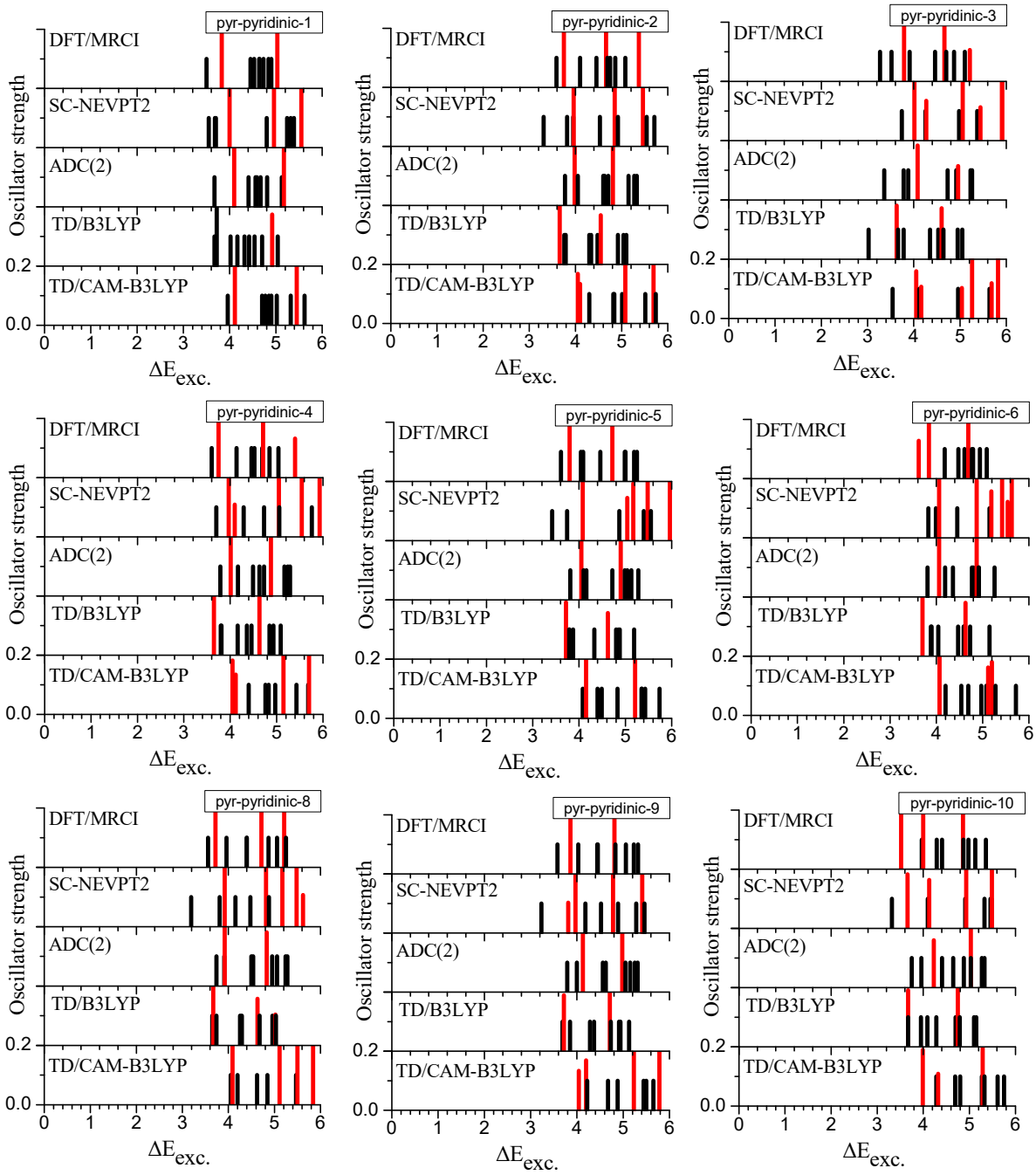
6 A'	5.08	0.058	9 A'	5.54	0.699	6 A'	5.27	0.036	4 A"	5.04	0.001	6 A'	5.69	0.271
7 A'	5.37	0.582	10 A'	5.71	0.054	4 A"	5.33	0.001	6 A'	5.10	0.037	4 A"	5.74	0.001
pyr-pyridinic-3														
1 A"	3.27	0.004	1 A'	3.74	0.007	1 A"	3.36	0.000	1 A"	3.02	0.001	1 A"	3.54	0.002
1 A'	3.52	0.070	2 A'	4.01	0.293	1 A'	3.78	0.023	1 A'	3.63	0.181	1 A'	4.05	0.159
2 A'	3.79	0.338	3 A'	4.25	0.000	2 A"	3.88	0.001	2 A"	3.66	0.001	2 A"	4.12	0.001
2 A"	3.91	0.003	4 A'	4.27	0.135	2 A'	4.08	0.184	2 A'	3.78	0.025	2 A'	4.16	0.107
3 A'	4.46	0.092	5 A	4.98	0.012	3 A'	4.73	0.084	3 A'	4.35	0.046	3 A'	4.96	0.051
4 A'	4.66	0.338	1 A"	5.06	0.281	4 A'	4.92	0.089	4 A'	4.53	0.024	4 A'	5.04	0.103
5 A'	4.70	0.043	6 A'	5.37	0.000	3 A"	4.93	0.000	5 A'	4.60	0.172	5 A'	5.26	0.236
6 A'	4.87	0.028	7 A'	5.44	0.113	5 A'	4.96	0.114	3 A"	4.64	0.000	3 A"	5.64	0.000
3 A"	5.10	0.000	2 A"	5.91	0.377	6 A'	5.23	0.015	4 A"	4.95	0.000	6 A'	5.68	0.119
7 A'	5.21	0.106	8 A'	5.91	0.772	4 A"	5.26	0.000	6 A'	5.05	0.007	7 A'	5.82	0.735
pyr-pyridinic-4														
1 A'	3.60	0.051	1 A'	3.70	0.000	1 A'	3.79	0.012	1 A'	3.65	0.228	1 A'	4.05	0.182
2 A'	3.75	0.414	2 A'	3.97	0.399	2 A'	4.01	0.220	1 A"	3.80	0.000	2 A'	4.12	0.135
1 A"	4.14	0.002	3 A'	4.10	0.109	1 A"	4.17	0.000	2 A'	3.81	0.018	1 A"	4.40	0.001
3 A'	4.46	0.028	4 A'	4.29	0.000	2 A"	4.49	0.000	2 A"	4.16	0.000	2 A"	4.76	0.001
2 A"	4.52	0.001	5 A'	4.73	0.008	3 A'	4.63	0.016	3 A'	4.36	0.015	3 A'	4.83	0.007
3 A"	4.69	0.004	6 A'	5.05	0.306	3 A"	4.73	0.001	3 A"	4.46	0.001	3 A"	4.97	0.002
4 A'	4.71	0.437	7 A'	5.06	0.022	4 A'	4.88	0.229	4 A'	4.63	0.210	4 A'	5.15	0.333
5 A'	4.85	0.002	8 A'	5.54	0.401	5 A'	5.17	0.001	5 A'	4.85	0.001	5 A'	5.43	0.003
6 A'	5.04	0.002	9 A'	5.76	0.047	4 A"	5.24	0.000	4 A"	4.93	0.001	4 A"	5.68	0.000
7 A'	5.40	0.132	10 A'	5.93	0.573	6 A'	5.29	0.001	6 A'	5.09	0.016	6 A'	5.70	0.209
pyr-pyridinic-5														
1 A'	3.61	0.032	1 A'	3.42	0.002	1 A'	3.81	0.008	1 A'	3.72	0.192	1 A'	4.08	0.028
2 A'	3.80	0.415	2 A'	3.74	0.071	2 A'	4.05	0.204	2 A'	3.79	0.025	2 A'	4.15	0.254
1 A"	4.04	0.005	3 A'	4.08	0.266	1 A"	4.10	0.001	1 A"	3.79	0.001	1 A"	4.40	0.002
2 A"	4.09	0.000	4 A'	4.87	0.007	2 A"	4.16	0.000	2 A"	3.87	0.000	2 A"	4.49	0.000
3 A'	4.46	0.020	5 A'	5.04	0.144	3 A'	4.72	0.013	3 A'	4.33	0.013	3 A'	4.83	0.003
4 A'	4.72	0.312	6 A'	5.17	0.193	4 A'	4.90	0.198	4 A'	4.62	0.156	4 A'	5.21	0.286
5 A'	4.99	0.009	7 A'	5.40	0.099	3 A"	4.99	0.000	3 A"	4.80	0.000	5 A'	5.35	0.045
6 A'	5.00	0.021	8 A'	5.48	1.082	4 A"	5.04	0.000	5 A'	4.85	0.000	3 A"	5.36	0.000
3 A"	5.19	0.000	9 A'	5.55	0.091	5 A'	5.13	0.002	4 A"	4.88	0.001	4 A"	5.43	0.001
4 A"	5.25	0.002	10 A'	5.96	0.315	6 A'	5.28	0.000	6 A'	5.19	0.000	6 A'	5.74	0.013
pyr-pyridinic-6														
1 A'	3.62	0.128	1 A'	3.83	0.005	1 A'	3.81	0.039	1 A'	3.70	0.229	1 A'	4.07	0.220
2 A'	3.84	0.354	2 A'	3.99	0.000	2 A'	4.06	0.201	2 A'	3.88	0.020	2 A'	4.20	0.094
1 A"	4.18	0.003	3 A'	4.06	0.326	1 A"	4.19	0.000	1 A"	3.90	0.000	1 A"	4.54	0.001
2 A"	4.48	0.000	4 A'	4.45	0.002	2 A"	4.36	0.000	2 A"	4.04	0.000	2 A"	4.69	0.000
3 A'	4.61	0.011	5 A'	4.87	0.193	3 A"	4.77	0.001	3 A'	4.47	0.003	3 A'	4.97	0.000
4 A'	4.69	0.380	6 A'	5.15	0.032	3 A'	4.80	0.010	4 A'	4.59	0.030	3 A"	5.08	0.003

5 A'	4.77	0.002	7 A'	5.19	0.157	4 A'	4.87	0.228	3 A"	4.60	0.002	4 A'	5.12	0.162
3 A"	4.79	0.005	8 A'	5.42	0.366	4 A"	4.92	0.001	5 A'	4.63	0.180	5 A'	5.20	0.180
6 A'	4.94	0.046	9 A'	5.54	0.122	5 A'	4.92	0.002	4 A"	4.73	0.000	4 A"	5.28	0.000
4 A"	5.09	0.000	10 A'	5.63	1.181	6 A'	5.26	0.017	6 A'	5.15	0.005	6 A'	5.72	0.002
pyr-pyridinic-7														
1 A"	2.80	0.005	1 A'	2.79	0.005	1 A"	3.06	0.001	1 A"	2.67	0.001	1 A"	2.94	0.002
1 A'	3.50	0.022	2 A'	3.80	0.340	1 A'	3.69	0.009	1 A'	3.44	0.191	1 A'	3.88	0.264
2 A'	3.50	0.358	1 A"	3.83	0.010	2 A'	3.72	0.177	2 A'	3.71	0.012	2 A'	4.00	0.011
3 A'	4.40	0.095	3 A'	4.13	0.000	2 A"	4.40	0.000	2 A"	3.99	0.000	3 A'	4.74	0.020
2 A"	4.43	0.000	4 A'	4.48	0.002	3 A'	4.58	0.053	3 A"	4.19	0.001	2 A"	4.77	0.000
4 A'	4.54	0.304	5 A'	4.68	0.068	3 A"	4.61	0.001	3 A'	4.30	0.040	4 A'	4.99	0.274
3 A"	4.70	0.003	6 A'	4.82	0.448	4 A'	4.68	0.168	4 A'	4.46	0.151	3 A"	5.16	0.001
5 A'	4.72	0.028	7 A'	4.94D	0.000	5 A'	5.04	0.001	5 A'	4.82	0.001	5 A'	5.33	0.010
6 A'	4.91	0.000	8 A'	5.21	0.125	6 A'	5.12	0.000	4 A"	5.01	0.000	6 A'	5.62	0.009
4 A"	5.13 D	0.000	2 A"	5.22	0.022	4 A"	5.43	0.000	6 A'	5.02	0.014	4 A"	5.73	0.000
pyr-pyridinic-8														
1 A'	3.56	0.020	1 A'	3.19	0.001	1 A'	3.74	0.008	1 A"	3.65	0.001	1 A'	4.05	0.014
2 A'	3.72	0.433	2 A'	3.81	0.012	1 A"	3.91	0.001	1 A'	3.67	0.211	2 A'	4.09	0.268
1 A"	3.96	0.004	3 A'	3.92	0.270	2 A'	3.92	0.227	2 A'	3.74	0.014	1 A"	4.20	0.002
3 A'	4.40	0.034	4 A'	4.15	0.000	2 A"	4.50	0.000	2 A"	4.25	0.000	2 A"	4.62	0.000
2 A"	4.40	0.000	5 A'	4.48	0.002	3 A'	4.54	0.021	3 A'	4.29	0.020	3 A'	4.85	0.017
4 A'	4.72	0.349	6 A'	4.82	0.231	4 A'	4.83	0.181	4 A'	4.63	0.157	4 A'	5.11	0.280
5 A'	4.87	0.028	1 A"	4.88	0.004	3 A"	4.95	0.000	3 A"	4.68	0.000	5 A'	5.47	0.009
6 A'	5.06	0.013	7 A'	5.17	0.636	5 A'	5.06	0.075	4 A"	4.96	0.000	3 A"	5.49	0.000
7 A'	5.21	0.296	8 A'	5.48	1.211	6 A'	5.24	0.001	5 A'	5.02	0.104	6 A'	5.50	0.400
3 A"	5.25	0.000	9 A'	5.62	0.107	4 A"	5.28	0.000	6 A'	5.03	0.031	7 A'	5.84	0.408
pyr-pyridinic-9														
1 A'	3.58	0.086	1 A"	3.23	0.001	1 A'	3.79	0.023	1 A"	3.69	0.001	1 A'	4.04	0.133
2 A'	3.86	0.421	1 A'	3.81	0.103	1 A"	4.00	0.001	1 A'	3.72	0.189	2 A'	4.20	0.169
1 A"	4.03	0.004	2 A'	3.97	0.238	2 A'	4.13	0.244	2 A'	3.85	0.069	1 A"	4.22	0.002
2 A"	4.44	0.000	2 A"	4.18	0.000	2 A"	4.56	0.000	2 A"	4.28	0.000	2 A"	4.67	0.000
3 A'	4.45	0.000	3 A'	4.52	0.000	3 A'	4.62	0.000	3 A'	4.37	0.000	3 A'	4.88	0.000
4 A'	4.81	0.496	4 A'	4.78	0.354	4 A'	4.98	0.272	4 A'	4.71	0.237	4 A'	5.23	0.378
5 A'	4.83	0.000	5 A'	4.89	0.000	3 A"	5.05	0.000	3 A"	4.73	0.000	5 A'	5.44	0.000
6 A'	5.06	0.000	6 A'	5.28	0.000	5 A'	5.15	0.000	5 A'	4.91	0.000	3 A"	5.50	0.000
7 A'	5.23	0.000	7 A'	5.41	1.757	6 A'	5.25	0.000	4 A"	4.94	0.000	6 A'	5.65	0.000
3 A"	5.32	0.000	8 A'	5.46	0.000	4 A"	5.31	0.000	6 A'	5.13	0.000	7 A'	5.78	1.080
pyr-pyridinic-10														
1 A'	3.52	0.222	1 A'	3.32	0.002	1 A'	3.75	0.079	1 A'	3.67	0.191	1 A'	3.99	0.190
1 A"	3.97	0.005	2 A'	3.66	0.183	1 A"	3.96	0.001	1 A"	3.67	0.001	1 A"	4.28	0.002
2 A'	4.00	0.262	3 A'	4.10	0.000	2 A'	4.23	0.160	2 A'	3.95	0.056	2 A'	4.32	0.109
2 A"	4.29	0.000	4 A'	4.13	0.164	2 A"	4.41	0.000	2 A"	4.09	0.000	2 A"	4.69	0.000

3 A'	4.41	0.000	5 A'	4.91	0.000	3 A'	4.65	0.000	3 A'	4.28	0.000	3 A'	4.80	0.000
4 A'	4.86	0.498	6 A'	4.93	0.377	3 A"	4.88	0.000	3 A"	4.70	0.000	3 A"	5.27	0.001
5 A'	4.87	0.000	7 A'	5.33	0.000	4 A'	5.03	0.280	4 A'	4.75	0.232	4 A'	5.29	0.371
6 A'	4.98	0.000	8 A'	5.46	0.000	5 A'	5.03	0.000	5 A'	4.79	0.000	5 A'	5.33	0.000
3 A"	5.13	0.001	9 A'	5.48	0.000	4 A"	5.27	0.000	4 A"	5.10	0.000	4 A"	5.61	0.000
7 A'	5.36	0.000	10 A'	5.49	1.585	6 A'	5.33	0.000	6 A'	5.15	0.000	6 A'	5.75	0.000
pyr-pyridinic-11														
1 A'	3.50	0.192	1 A"	3.22	0.000	1 A'	3.71	0.065	1 A'	3.57	0.208	1 A'	3.95	0.215
2 A'	3.70	0.233	1 A'	3.80	0.278	2 A'	3.92	0.137	1 A"	3.63	0.000	2 A'	4.10	0.072
1 A"	3.90	0.000	2 A'	4.02	0.085	1 A"	3.93	0.000	2 A'	3.75	0.016	1 A"	4.13	0.000
2 A"	4.33	0.007	2 A"	4.45	0.000	2 A"	4.49	0.002	2 A"	4.17	0.002	2 A"	4.67	0.003
3 A'	4.56	0.193	3 A'	4.86	0.178	3 A'	4.73	0.133	3 A'	4.45	0.087	3 A'	5.01	0.172
4 A'	4.70	0.142	4 A'	5.14	0.006	4 A'	4.84	0.053	4 A'	4.61	0.029	4 A'	5.04	0.016
5 A'	4.71	0.022	5 A'	5.15	0.202	3 A"	4.94	0.000	5 A'	4.67	0.058	5 A'	5.21	0.095
6 A'	5.01	0.033	6 A'	5.67	0.180	5 A'	4.95	0.014	3 A"	4.71	0.000	3 A"	5.30	0.000
3 A"	5.16	0.000	7 A'	5.67	0.146	6 A'	5.27	0.052	6 A'	5.14	0.073	6 A'	5.65	0.330
7 A'	5.36	0.078	8 A'	5.73	1.232	4 A"	5.51	0.000	4 A"	5.21	0.000	7 A'	5.87	0.470
pyr-pyridinic-12														
1 A'	3.58	0.087	1 A'	3.74	0.065	1 A'	3.78	0.029	1 A'	3.65	0.186	1 A'	4.06	0.133
2 A'	3.76	0.335	2 A'	3.87	0.001	2 A'	4.00	0.190	1 A"	3.79	0.000	2 A'	4.13	0.138
1 A"	4.04	0.000	3 A'	3.96	0.271	1 A"	4.05	0.000	2 A'	3.80	0.024	1 A"	4.31	0.000
2 A"	4.22	0.005	4 A'	4.94	0.260	2 A"	4.28	0.001	2 A"	3.99	0.001	2 A"	4.61	0.002
3 A'	4.67	0.310	5 A'	4.97	0.029	3 A'	4.84	0.203	3 A'	4.58	0.151	3 A'	5.10	0.051
4 A'	4.74	0.036	6 A'	5.15	0.001	4 A'	4.91	0.012	4 A'	4.65	0.022	4 A'	5.15	0.248
5 A'	4.85	0.012	7 A'	5.28	0.001	3 A"	4.91	0.000	5 A'	4.73	0.001	5 A'	5.24	0.017
6 A'	4.93	0.045	8 A'	5.39	0.365	5 A'	5.06	0.002	3 A"	4.78	0.000	3 A"	5.37	0.000
3 A"	5.19	0.001	9 A'	5.40	0.153	6 A'	5.23	0.027	4 A"	5.07	0.000	6 A'	5.72	0.217
7 A'	5.36	0.344	10 A'	5.58	1.304	4 A"	5.39	0.000	6 A'	5.14	0.035	4 A"	5.80	0.000
pyr-pyridinic-13														
1 A'	3.64	0.030	1 A"	3.06	0.002	1 A"	3.66	0.001	1 A"	3.48	0.001	1 A"	4.09	0.002
1 A"	3.73	0.004	1 A'	3.92	0.067	1 A'	3.82	0.008	1 A'	3.77	0.209	1 A'	4.10	0.026
2 A'	3.83	0.436	2 A'	4.07	0.244	2 A'	4.04	0.236	2 A'	3.81	0.022	2 A'	4.17	0.259
3 A'	4.43	0.000	2 A"	4.15	0.000	2 A"	4.54	0.000	3 A'	4.30	0.000	3 A'	4.81	0.000
4 A'	4.82	0.389	3 A'	4.93	0.042	3 A'	4.65	0.002	2 A"	4.47	0.000	2 A"	4.98	0.000
2 A"	4.82	0.000	4 A'	5.02	0.223	4 A'	4.96	0.212	4 A'	4.69	0.125	4 A'	5.24	0.236
5 A'	5.00	0.079	5 A'	5.39	0.048	3 A"	5.05	0.000	3 A"	4.71	0.000	3 A"	5.37	0.000
3 A"	5.05	0.000	6 A'	5.54	0.427	5 A'	5.10	0.050	5 A'	4.89	0.111	5 A'	5.37	0.112
6 A'	5.06	0.000	7 A'	5.68	1.126	6 A'	5.33	0.002	6 A'	5.22	0.010	6 A'	5.72	0.237
7 A'	5.36	0.001	8 A'	5.74	0.019	4 A"	5.36	0.000	4 A"	5.22	0.000	7 A'	5.81	0.537
pyr-pyridinic-14														
1 A'	3.56	0.078	1 A'	3.75	0.001	1 A'	3.77	0.027	1 A"	3.61	0.000	1 A'	4.04	0.120
2 A'	3.77	0.391	2 A'	3.87	0.149	1 A"	3.94	0.000	1 A'	3.67	0.204	1 A"	4.11	0.000

1 A"	3.90	0.000	3 A'	4.06	0.194	2 A'	4.00	0.208	2 A'	3.78	0.036	2 A'	4.13	0.175
2 A"	4.38	0.006	4 A'	4.95	0.117	2 A"	4.49	0.001	2 A"	4.17	0.002	2 A"	4.71	0.003
3 A'	4.56	0.098	5 A'	5.06	0.001	3 A'	4.72	0.054	3 A'	4.44	0.046	3 A'	5.05	0.058
4 A'	4.77	0.193	6 A'	5.14	0.009	4 A'	4.93	0.147	4 A'	4.67	0.029	4 A'	5.09	0.116
5 A'	4.86	0.105	7 A'	5.19	0.260	3 A"	4.96	0.000	3 A"	4.69	0.000	5 A'	5.30	0.154
6 A'	4.94	0.053	8 A'	5.50	0.303	5 A'	5.06	0.028	5 A'	4.79	0.154	3 A"	5.34	0.000
3 A"	5.16	0.001	9 A'	5.56	0.338	6 A'	5.21	0.040	4 A"	5.10	0.001	6 A'	5.61	0.400
7 A'	5.25	0.290	10 A'	5.75	0.970	4 A"	5.42	0.000	6 A'	5.11	0.038	7 A'	5.83	0.367
pyr-pyridinic-15														
1 A'	3.56	0.163	1 A'	3.77	0.202	1 A"	3.76	0.000	1 A"	3.49	0.000	1 A'	4.02	0.158
1 A"	3.76	0.000	2 A'	3.96	0.002	1 A'	3.76	0.050	1 A'	3.69	0.184	1 A"	4.05	0.000
2 A'	3.91	0.318	3 A'	4.16	0.126	2 A'	4.15	0.198	2 A'	3.89	0.059	2 A'	4.25	0.132
2 A"	4.33	0.006	4 A'	4.80	0.031	2 A"	4.41	0.002	2 A"	4.15	0.002	2 A"	4.72	0.003
3 A'	4.63	0.032	5 A'	5.02	0.425	3 A"	4.70	0.000	3 A"	4.52	0.000	3 A'	5.09	0.008
4 A'	4.72	0.137	6 A'	5.03	0.048	3 A'	4.80	0.005	3 A'	4.56	0.020	3 A"	5.15	0.000
5 A'	4.88	0.332	7 A'	5.39	0.002	4 A'	4.92	0.166	4 A'	4.64	0.058	4 A'	5.17	0.109
3 A"	4.97	0.000	8 A'	5.42	0.117	5 A'	5.04	0.115	5 A'	4.77	0.161	5 A'	5.27	0.253
6 A'	5.02	0.022	9 A'	5.48	0.000	4 A"	5.18	0.000	4 A"	4.94	0.001	6 A'	5.69	0.425
7 A'	5.32	0.255	10 A'	5.51	1.089	6 A'	5.29	0.037	6 A'	5.17	0.018	7 A'	5.82	0.481

[a] States with dominating double excitations are labelled by D. Otherwise, states are classified as single excitations.


pyr-pyridinic-1
pyr-pyridinic-2
pyr-pyridinic-3
pyr-pyridinic-4
pyr-pyridinic-5
pyr-pyridinic-6
pyr-pyridinic-8
pyr-pyridinic-9
pyr-pyridinic-10
DFT/MRCI
SC-NEVPT2
ADC(2)
TD/B3LYP
TD/CAM-B3LYP
Oscillator strength
0.0
0.2
0 1 2 3 4 5 6
ΔE exc.

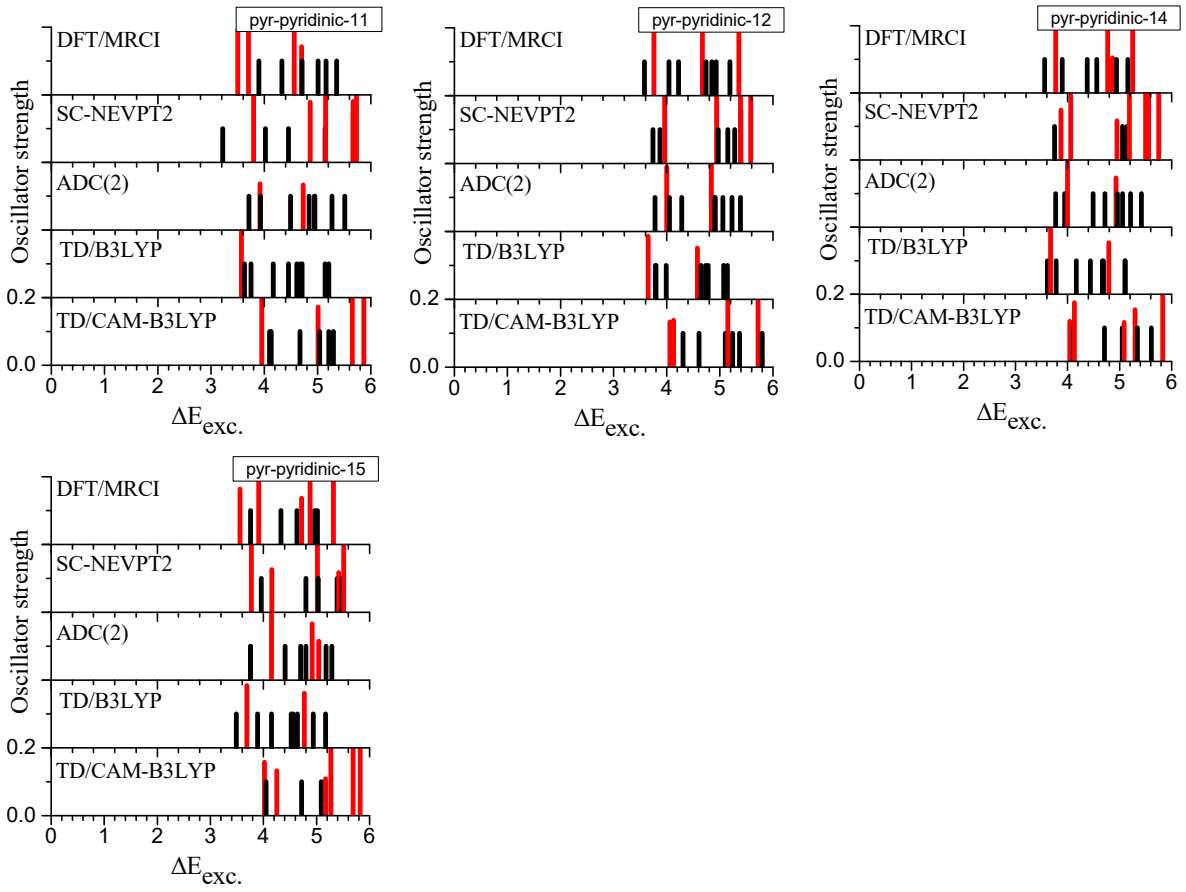


Figure S4 Excitation spectrum of pyr-pyridinic-z, calculated at the DFT/MRCI, SC-NEVPT2, ADC(2), TD-B3LYP and CAM-TD-B3LYP levels. Bright singly excited states are highlighted in red, dark singly excited states are in black.

Cartesian Coordinates (Å) for SOS-MP2 and total energies (a.u.) for SOS-MP2, B3LYP and CAM-B3LYP

Pyrene

SOS-MP2: E = -614.30991a.u.
B3LYP: E = -615.61841 a.u.
CAM-B3LYP: E = -615.64240 a.u.

Coordinates SOS-MP2:
Coordinates...

C	-1.7406304	-3.0595361	0.0000000
C	-0.3465163	-3.0570803	0.0000000
C	0.3656593	-1.8488873	0.0000000
C	-0.3532316	-0.6209001	0.0000000
C	-1.7761425	-0.6303786	0.0000000
C	-2.4508331	-1.8598939	0.0000000
C	1.8058087	-1.8101997	0.0000000
C	0.3532309	0.6209005	0.0000000
C	1.7761426	0.6303788	0.0000000
C	2.4787453	-0.6273406	0.0000000
C	2.4508323	1.8598940	0.0000000
C	1.7406315	3.0595354	0.0000000
C	0.3465159	3.0570810	0.0000000
C	-0.3656596	1.8488871	0.0000000
C	-1.8058082	1.8102017	0.0000000
C	-2.4787467	0.6273392	0.0000000
H	3.5371550	1.8692363	0.0000000
H	-3.5652212	0.6132558	0.0000000
H	-2.3488752	2.7513187	0.0000000
H	2.3488747	-2.7513191	0.0000000
H	-2.2774118	-4.0030443	0.0000000
H	0.2004929	-3.9956706	0.0000000
H	-3.5371546	-1.8692372	0.0000000
H	3.5652215	-0.6132556	0.0000000
H	2.2774126	4.0030440	0.0000000
H	-0.2004919	3.9956710	0.0000000

Pyr-graphitic-1

SOS-MP2: E = -647.47513 a.u.
B3LYP: E = -648.81927 a.u.
CAM-B3LYP: E = -648.85199 a.u.

Coordinates SOS-MP2:
Coordinates..

C	-1.7852231	-3.0290419	0.0000000
C	-0.3353162	-3.0558613	0.0000000

```
C     0.3574194   -1.8751770    0.0000000
C    -0.3327902   -0.6064561    0.0000000
C    -2.4405675   -1.8538204    0.0000000
C     1.8045968   -1.7677787    0.0000000
C     0.3327897    0.6064532    0.0000000
C     2.4284188   -0.5668032    0.0000000
C     2.4405682    1.8538227    0.0000000
C     1.7852210    3.0290436    0.0000000
C     0.3353131    3.0558601    0.0000000
C    -0.3574201    1.8751739    0.0000000
C    -1.8045962    1.7677808    0.0000000
C    -2.4284169    0.5668002    0.0000000
N     1.7466144    0.6276595    0.0000000
N    -1.7466124   -0.6276606    0.0000000
H     3.5189452    1.7611883    0.0000000
H    -3.5086501    0.4801023    0.0000000
H    -2.4055254    2.6696775    0.0000000
H     2.4055266   -2.6696781    0.0000000
H    -2.3583915   -3.9480384    0.0000000
H     0.1956848   -4.0010215    0.0000000
H    -3.5189434   -1.7611816    0.0000000
H     3.5086564   -0.4801051    0.0000000
H     2.3583880    3.9480420    0.0000000
H    -0.1956892    4.0010199    0.0000000
```

Pyr-graphitic-2

SOS-MP2: E = -647.45638 a.u.
B3LYP: E = -648.79117 a.u.
CAM-B3LYP: E = -648.81258 a.u.

Coordinates SOS-MP2:
Coordinates...

```
C    -1.7910078   -3.0267355    0.0000000
C    -0.3392655   -3.0416968    0.0000000
C     0.3684074   -1.8722654    0.0000000
C    -0.3259928   -0.5979858    0.0000000
C    -2.4333215   -1.8341356    0.0000000
C     1.8170302   -1.8136673    0.0000000
C     0.3473916    0.5857049    0.0000000
C     1.7976028    0.6399053    0.0000000
C     2.4874690   -0.6352943    0.0000000
C     2.4412865    1.8457474    0.0000000
C     1.6866979    3.0861150    0.0000000
C     0.3333377    3.0289077    0.0000000
C    -1.7573029    1.7695704    0.0000000
C    -2.4189429    0.6064831    0.0000000
N    -0.3469453    1.8313943    0.0000000
N    -1.7515210   -0.6374775    0.0000000
```

```
H     3.5266114    1.8727768    0.0000000
H    -3.4997856    0.5739186    0.0000000
H    -2.2817704    2.7152697    0.0000000
H     2.3625525   -2.7531890    0.0000000
H    -2.3632151   -3.9444116    0.0000000
H     0.1921272   -3.9884583    0.0000000
H    -3.5139067   -1.7459663    0.0000000
H     3.5738343   -0.6241873    0.0000000
H     2.1831478    4.0469237    0.0000000
H    -0.2945187    3.9127540    0.0000000
```

Pyr-graphitic-3

SOS-MP2: E = -647.44602 a.u.
B3LYP: E = -648.80258 a.u.
CAM-B3LYP: E = -648.83271 a.u.

Coordinates SOS-MP2:

Coordinates...

```
C    -1.7427890   -3.0633883    0.0000000
C    -0.3506120   -3.0700372    0.0000000
C     0.3654263   -1.8609548    0.0000000
C    -0.3584773   -0.6301154    0.0000000
C    -1.7863893   -0.6367549    0.0000000
C    -2.4598815   -1.8700458    0.0000000
C     1.7861771   -1.7827032    0.0000000
C     0.3473861    0.6106193    0.0000000
C     2.3949519   -0.5627144    0.0000000
C     2.4613200    1.8706091    0.0000000
C     1.7238690    3.0300864    0.0000000
C     0.3503218    3.0715830    0.0000000
C    -1.7074275    1.7712169    0.0000000
C    -2.4451044    0.6244828    0.0000000
N    -0.3417823    1.7875838    0.0000000
N     1.7112656    0.6195922    0.0000000
H     3.5312703    1.7657058    0.0000000
H    -3.5264384    0.6862037    0.0000000
H    -2.1613889    2.7534569    0.0000000
H     2.3917479   -2.6807172    0.0000000
H    -2.2797419   -4.0071903    0.0000000
H     0.1960680   -4.0074393    0.0000000
H    -3.5449945   -1.8790911    0.0000000
H     3.4712795   -0.4510150    0.0000000
H     2.2604718    3.9733313    0.0000000
H    -0.2865284    3.9376958    0.0000000
```

Pyr-graphitic-4

SOS-MP2: E = -647.41511 a.u.
B3LYP: E = -648.76981 a.u.
CAM-B3LYP: E = -648.79825 a.u.

Coordinates SOS-MP2:

Coordinates...

C	-1.7307473	-3.0421921	-0.0002511
C	-0.3376735	-3.0281074	-0.0001808
C	0.3783825	-1.8305742	-0.0001143
C	-1.7668679	-0.6101059	-0.0002231
C	-2.4303819	-1.8374815	-0.0003340
C	1.7739849	-1.8119844	-0.0001649
C	1.7668777	0.6100895	0.0001079
C	2.4640118	-0.5990947	-0.0000351
C	2.4304159	1.8375013	0.0002457
C	1.7307269	3.0421937	0.0004148
C	0.3376683	3.0280873	0.0004162
C	-0.3783506	1.8305717	0.0002531
C	-1.7740144	1.8119855	0.0001097
C	-2.4640022	0.5990986	-0.0002114
N	0.3649517	0.6415109	-0.0001700
N	-0.3649555	-0.6415138	0.0003495
H	3.5143777	1.8141196	0.0002424
H	-3.5461539	0.5549510	-0.0003568
H	-2.2889946	2.7647574	0.0001707
H	2.2890015	-2.7647684	-0.0002416
H	-2.2671969	-3.9850815	-0.0003256
H	0.2362860	-3.9479583	-0.0002139
H	-3.5143914	-1.8140952	-0.0004685
H	3.5461653	-0.5549524	-0.0000910
H	2.2671940	3.9850890	0.0005530
H	-0.2363144	3.9479542	0.0005191

Pyr-graphitic-edge-1

SOS-MP2: E = -647.49520 a.u.
B3LYP: E = -648.83550 a.u.
CAM-B3LYP: E =-648.86716 a.u.

Coordinates SOS-MP2:

Coordinates...

C	-0.3363802	-3.0283205	-0.0288373
C	0.3695225	-1.8672787	-0.0135062
C	-0.3376171	-0.5934239	-0.0288116
C	-1.7939440	-0.6364502	-0.0134798

```
C    -2.4313245   -1.8364755   -0.0287933
C     1.8257099   -1.8180917    0.0110642
C     0.3376865    0.5935452   -0.0283566
C     1.7939680    0.6364938   -0.0123504
C     2.4956709   -0.6404092    0.0121156
C     2.4312578    1.8364682   -0.0280409
C     0.3364302    3.0283229   -0.0280448
C    -0.3695220    1.8672710   -0.0123348
C    -1.8256723    1.8180600    0.0121468
C    -2.4956997    0.6404354    0.0111213
N     1.7302176    3.0412070   -0.1224532
N    -1.7303394   -3.0414120   -0.1225674
H     3.5123040    1.9231178   -0.0156105
H    -3.5827695    0.6350363    0.0262370
H    -2.3764803    2.7551842    0.0284881
H     2.3765035   -2.7552746    0.0261474
H     0.1415937   -4.0018564   -0.0168244
H    -3.5124146   -1.9230536   -0.0167207
H     3.5826681   -0.6350625    0.0284522
H    -0.1414761    4.0017815   -0.0156453
H     2.2044605    3.8748237    0.1875928
H    -2.2043534   -3.8746382    0.1890121
```

Pyr-graphitic-edge-2

SOS-MP2: E = -647.49803 a.u.
B3LYP: E = -648.84352 a.u.
CAM-B3LYP: E = -648.87311 a.u.

Coordinates SOS-MP2:
Coordinates...

```
C    -1.7722750   -3.0404179   -0.0808090
C    -0.3547941   -3.0491048   -0.0662866
C     0.3484775   -1.8558623   -0.0353606
C    -0.3638303   -0.6125468   -0.0173033
C    -1.7836774   -0.6194847   -0.0328962
C    -2.4811261   -1.8657712   -0.0649307
C     0.3512073    0.6234300    0.0152273
C     1.8178537    0.5849132    0.0336808
C     2.4576289   -0.6156049    0.0143731
C     2.4825928    1.8639465    0.0746503
C     0.3927947    3.0738728    0.0620232
C    -0.3455662    1.8400526    0.0295593
C    -1.7646066    1.8185901    0.0131433
C    -2.4581051    0.6304736   -0.0162960
N     1.7434244    2.9859745    0.0840001
N     1.7298884   -1.8126482   -0.0219481
H     3.5568654    1.9862817    0.0981074
H    -3.5443987    0.6377304   -0.0273762
```

```
H    -2.3048879    2.7614532    0.0249526
H    -2.2984077   -3.9899475   -0.1049793
H     0.1821156   -3.9934475   -0.0801111
H    -3.5664611   -1.8674766   -0.0767525
H     3.5354657   -0.7188395    0.0265629
H    -0.0472332    4.0592913    0.0744429
H     2.2553182    3.8594992    0.1112439
H     2.2317369   -2.6843572   -0.0369178
```

Pyr-graphitic-edge-3

SOS-MP2: E = -647.49852 a.u.
B3LYP: E = -648.84148 a.u.
CAM-B3LYP: E = -648.87589 a.u.

Coordinates SOS-MP2:
Coordinates...

```
C    -1.7172041   -3.0226688    0.0501447
C    -0.3404777   -3.0442211    0.0927554
C     0.3994147   -1.8297824    0.0518399
C    -0.3124026   -0.6008556   -0.0104222
C    -1.7414280   -0.5906436   -0.0663916
C    -2.4203795   -1.7978912   -0.0354242
C     1.8201519   -1.7962436    0.0678227
C     0.4038919    0.6225907   -0.0662046
C     1.7900520    0.6161326   -0.0800299
C     2.5020811   -0.5971709    0.0090406
C     0.4179981    3.0137903    0.1969416
C    -0.3071265    1.8962198   -0.0678201
C    -1.7548133    1.8682227   -0.1759973
C    -2.4282785    0.6933552   -0.1641779
N     1.8181821    2.9939837    0.2760879
N     2.5017770    1.8556538   -0.2447352
H    -3.5131729    0.6858507   -0.2218775
H    -2.2929315    2.8104219   -0.2318996
H     2.3686176   -2.7322921    0.1232073
H    -2.2734553   -3.9543644    0.0781033
H     0.1945095   -3.9878127    0.1522536
H    -3.5059384   -1.8033683   -0.0823159
H     3.5871755   -0.5699465    0.0157149
H    -0.0395509    3.9813184    0.3872951
H     2.1951399    3.2532077    1.1819838
H     2.6481678    2.0365139   -1.2358948
```

Pyr-graphitic-edge-4

SOS-MP2: E = -647.48806 a.u.
B3LYP: E = -648.83427 a.u.

CAM-B3LYP: E = -648.86487 a.u.

Coordinates SOS-MP2:
Coordinates...

C	-1.6770460	-3.0976594	-0.0788831
C	-0.3189069	-3.1109610	-0.0651343
C	0.4263642	-1.8653120	-0.0359921
C	-0.3287792	-0.6112430	-0.0197651
C	-1.7762788	-0.6490748	-0.0361040
C	-2.4250904	-1.8579752	-0.0651771
C	1.7836656	-1.7971624	-0.0234261
C	0.3409800	0.5965987	0.0139063
C	1.7816179	0.6576333	0.0313764
C	2.4324492	1.8584531	0.0721519
C	0.3314665	3.0378374	0.0721429
C	-0.3726489	1.8626217	0.0343645
C	-1.8163451	1.8137989	0.0138543
C	-2.4740950	0.6273282	-0.0197522
N	1.6880390	3.0582084	0.0924439
N	2.4452642	-0.5696788	0.0014017
H	3.5092495	1.9624856	0.0878011
H	-3.5608289	0.6122786	-0.0344139
H	-2.3711826	2.7484888	0.0261861
H	2.4258181	-2.6697999	-0.0350652
H	-2.2228040	-4.0362580	-0.1005141
H	0.2272068	-4.0502290	-0.0758488
H	-3.5105077	-1.8888518	-0.0773195
H	-0.1651160	4.0025674	0.0882052
H	2.1755621	3.9367208	0.1187602
H	3.4519466	-0.5708159	0.0148012

Pyr-graphitic-edge-5

SOS-MP2: E = -647.53979 a.u.
B3LYP: E = -648.88481 a.u.
CAM-B3LYP: E = -648.92009 a.u.

Coordinates SOS-MP2:
Coordinates...

C	-1.7289432	-3.0478691	0.0000000
C	0.3736980	-1.8336788	0.0000000
C	-0.3608536	-0.6121569	0.0000000
C	-1.7936833	-0.6156066	0.0000000
C	-2.4592203	-1.9125759	0.0000000
C	1.7570527	-1.8111990	0.0000000
C	0.3418467	0.6229701	0.0000000
C	1.7671562	0.6157122	0.0000000
C	2.4547172	-0.5849207	0.0000000

```
C     1.7364568    3.0435437    0.0000000
C     0.3875589    3.0911909    0.0000000
C    -0.3873360    1.8564079    0.0000000
C    -1.7720307    1.8200494    0.0000000
C    -2.4699684    0.5932721    0.0000000
N    -0.3497119   -3.0303568    0.0000000
N     2.4262637    1.8490057    0.0000000
H    -3.5565047    0.5942293    0.0000000
H    -2.3280246    2.7535608    0.0000000
H     2.3156287   -2.7431954    0.0000000
H    -2.1803319   -4.0330180    0.0000000
H    -3.5408414   -1.9696791    0.0000000
H     3.5412578   -0.5888513    0.0000000
H     2.3527404    3.9349478    0.0000000
H    -0.1161016    4.0501534    0.0000000
H     0.1570289   -3.8993879    0.0000000
H     3.4321455    1.8574523    0.0000000
```

Pyr-graphitic-edge-6

SOS-MP2: E = -647.50576 a.u.
B3LYP: E = -648.84980 a.u.
CAM-B3LYP: E = -648.87928 a.u.

Coordinates SOS-MP2:
Coordinates...

```
C    -1.7130037   -3.0564796   -0.0873530
C     0.3861710   -1.8319304   -0.0814487
C    -0.3561655   -0.6146566   -0.0485023
C    -1.7888517   -0.6238822   -0.0538465
C    -2.4480074   -1.9287395   -0.0464691
C     1.7697020   -1.8095195   -0.0370882
C     0.3474470    0.6188240    0.0050629
C     1.7853969    0.6246756    0.0390703
C     2.4687788   -0.5888447    0.0263620
C     2.4463074    1.8960025    0.0846755
C     0.3476905    3.0727633    0.0702746
C    -0.3971657    1.8487203    0.0256606
C    -1.7902261    1.8099504    0.0021443
C    -2.4737525    0.5794085   -0.0318555
N     1.6932085    3.0153771    0.0958572
N    -0.3279477   -3.0368514   -0.1986556
H     3.5195169    2.0217567    0.1058373
H    -3.5606136    0.5713061   -0.0323927
H    -2.3511181    2.7401282    0.0164759
H     2.3238954   -2.7443536   -0.0628497
H    -2.1591790   -4.0442228   -0.0754617
H    -3.5286566   -1.9912587   -0.0021006
H     3.5543211   -0.5947220    0.0584178
```

```
H    -0.1058814    4.0537659    0.0851974
H     2.1879782    3.8986016    0.1260677
H     0.1701554   -3.8858191    0.0169201
```

Pyr-graphitic-edge-7

SOS-MP2: E = -647.52191 a.u.
B3LYP: E = -648.86500 a.u.
CAM-B3LYP: E = -648.90194 a.u.

Coordinates SOS-MP2:
Coordinates...

```
C    -1.7852641   -3.0168933    0.0740814
C    -0.4022869   -3.0394899    0.1162320
C     0.3269974   -1.8297080    0.0835957
C    -0.3799932   -0.6088683    0.0276487
C    -1.7899409   -0.6019589   -0.0343705
C    -2.4873589   -1.7970846    0.0013198
C     1.7659271   -1.7871589    0.0504598
C     0.3292199    0.6377561   -0.0274423
C     1.7399080    0.6538334   -0.0835155
C     2.4385704   -0.6048021   -0.0503483
C     2.4071795    1.8988841   -0.1163753
C     1.6811068    3.0761519   -0.0743593
C     0.2738048    3.0563811   -0.0014265
C    -0.3971438    1.8462232    0.0345319
N    -1.8171883    1.8219612    0.1989135
N    -2.4946836    0.6311119   -0.1985430
H     3.4919309    1.9225144   -0.1630111
H     2.3131476   -2.7251036    0.0872677
H    -2.3418468   -3.9481999    0.0994601
H     0.1316621   -3.9840210    0.1627647
H    -3.5720394   -1.7827620   -0.0344766
H     3.5244520   -0.5959294   -0.0871419
H     2.1972299    4.0304605   -0.0999928
H    -0.2927326    3.9814612    0.0342931
H    -2.0709383    2.0141099    1.1628483
H    -2.7897197    0.7511310   -1.1624134
```

Pyr-graphitic-edge-8

SOS-MP2: E = -647.48492 a.u.
B3LYP: E = -648.84035 a.u.
CAM-B3LYP: E = -648.86681 a.u.

Coordinates SOS-MP2:
Coordinates...

```
C    -1.7440334   -3.0655549    0.0000000
```

```
C    -0.3525472   -3.0946968    0.0000000
C     0.3664265   -1.8711233    0.0000000
C    -0.3621054   -0.6364904    0.0000000
C    -1.7956594   -0.6411018    0.0000000
C    -2.4800863   -1.8843087    0.0000000
C     1.7721672   -1.7846834    0.0000000
C     0.3441142    0.6048626    0.0000000
C     1.7663941    0.6374691    0.0000000
C     2.4633769    1.8637675    0.0000000
C     1.7348505    3.0494201    0.0000000
C     0.3434186    3.0698404    0.0000000
C    -0.3545852    1.8441129    0.0000000
C    -2.4396270    0.6114609    0.0000000
N     2.4033118   -0.5665277    0.0000000
N    -1.7149859    1.7764109    0.0000000
H     3.5482927    1.8751982    0.0000000
H    -3.5163965    0.7203779    0.0000000
H     2.4159777   -2.6546240    0.0000000
H    -2.2817687   -4.0107707    0.0000000
H     0.1862935   -4.0356572    0.0000000
H    -3.5642707   -1.9019120    0.0000000
H     2.2718330    3.9932989    0.0000000
H    -0.2010992    4.0082778    0.0000000
H     3.4141981   -0.5571856    0.0000000
H    -2.2234897    2.6501393    0.0000000
```

Pyr-graphitic-edge-9

SOS-MP2: E = -647.50143 a.u.
B3LYP: E = -648.85054 a.u.
CAM-B3LYP: E = -648.88054 a.u.

Coordinates SOS-MP2:
Coordinates...

```
C    -1.8155338   -3.0197182    0.0000000
C    -0.3816215   -3.0512113    0.0000000
C     0.3197205   -1.8626127    0.0000000
C    -0.3626960   -0.5996630    0.0000000
C    -1.8110679   -0.5901072    0.0000000
C    -2.5183151   -1.8527567    0.0000000
C     0.3626855    0.5996763    0.0000000
C     1.8110538    0.5901031    0.0000000
C     2.4339360   -0.6318482    0.0000000
C     2.5183014    1.8527475    0.0000000
C     1.8155570    3.0196943    0.0000000
C     0.3816384    3.0512322    0.0000000
C    -0.3197217    1.8626190    0.0000000
C    -2.4339534    0.6318524    0.0000000
N     1.7071258   -1.8004248    0.0000000
```

```
N    -1.7071322    1.8004441    0.0000000
H     3.6035885    1.8520632    0.0000000
H    -3.5114052    0.7453132    0.0000000
H    -2.3510735   -3.9644573    0.0000000
H     0.1444664   -4.0004615    0.0000000
H    -3.6035954   -1.8521184    0.0000000
H     3.5113835   -0.7452908    0.0000000
H     2.3511076    3.9644379    0.0000000
H    -0.1444266    4.0004840    0.0000000
H     2.2097200   -2.6754837    0.0000000
H    -2.2097420    2.6754869    0.0000000
```

Pyr-graphitic-edge-10

SOS-MP2: E = -647.54095 a.u.
B3LYP: E = -648.88577 a.u.
CAM-B3LYP: E = -648.92114 a.u.

Coordinates SOS-MP2:
Coordinates...

```
C    -1.7681846   -3.0265444    0.0000000
C    -0.4211126   -3.0882746    0.0000000
C     0.3644908   -1.8595517    0.0000000
C    -0.3491051   -0.6185766    0.0000000
C    -1.7757689   -0.5951736    0.0000000
C     1.7487449   -1.8312190    0.0000000
C     0.3491071    0.6185756    0.0000000
C     1.7757702    0.5951736    0.0000000
C     2.4566344   -0.6115080    0.0000000
C     1.7681805    3.0265455    0.0000000
C     0.4211135    3.0882734    0.0000000
C    -0.3644901    1.8595503    0.0000000
C    -1.7487444    1.8312178    0.0000000
C    -2.4566325    0.6115077    0.0000000
N     2.4434130    1.8192370    0.0000000
N    -2.4434112   -1.8192356    0.0000000
H    -3.5434052    0.6174485    0.0000000
H    -2.3027594    2.7656893    0.0000000
H     2.3027611   -2.7656897    0.0000000
H    -2.3966252   -3.9090451    0.0000000
H     0.0733507   -4.0520816    0.0000000
H     3.5434065   -0.6174505    0.0000000
H     2.3966223    3.9090479    0.0000000
H    -0.0733553    4.0520797    0.0000000
H     3.4495637    1.8163378    0.0000000
H    -3.4495640   -1.8163336    0.0000000
```

Pyr-graphitic-edge-11

SOS-MP2: E = -647.53744 a.u.
B3LYP: E = -648.88254 a.u.
CAM-B3LYP: E = -648.91788 a.u.

Coordinates SOS-MP2:
Coordinates...

C	-1.7149303	-3.0521913	0.0000000
C	-0.3666649	-3.1016849	0.0000000
C	0.4130016	-1.8679566	0.0000000
C	-0.3508491	-0.6229118	0.0000000
C	-1.7424058	-0.6324042	0.0000000
C	1.7662449	-1.8036629	0.0000000
C	0.3436310	0.6229739	0.0000000
C	1.7735905	0.6383796	0.0000000
C	2.4499286	1.8479445	0.0000000
C	1.7271774	3.0641939	0.0000000
C	0.3523753	3.0799623	0.0000000
C	-0.3698867	1.8514255	0.0000000
C	-1.7891853	1.7928200	0.0000000
C	-2.4564935	0.5871905	0.0000000
N	2.4338004	-0.5800573	0.0000000
N	-2.4157237	-1.8563992	0.0000000
H	3.5362247	1.8615471	0.0000000
H	-3.5436156	0.5684603	0.0000000
H	-2.3537522	2.7207403	0.0000000
H	2.3995137	-2.6827515	0.0000000
H	-2.3260527	-3.9469610	0.0000000
H	0.1292911	-4.0651931	0.0000000
H	2.2787267	3.9994212	0.0000000
H	-0.1934456	4.0182619	0.0000000
H	3.4400953	-0.5756959	0.0000000
H	-3.4205961	-1.8654514	0.0000000

Pyr-graphitic-edge-12

SOS-MP2: E = -647.50613 a.u.
B3LYP: E = -648.85504 a.u.
CAM-B3LYP: E = -648.88403 a.u.

Coordinates SOS-MP2:
Coordinates...

C	-1.7018981	-3.0894939	0.0000000
C	-0.2912181	-3.0749632	0.0000000
C	0.3965603	-1.8611062	0.0000000
C	-0.3563361	-0.6374735	0.0000000
C	-1.7784853	-0.6597864	0.0000000
C	-2.4387192	-1.9259027	0.0000000

```
C     1.8245367   -1.7612789    0.0000000
C     0.3335430    0.6202202    0.0000000
C     1.7597150    0.6451775    0.0000000
C     2.4433366    1.9204030    0.0000000
C     1.7054161    3.0543929    0.0000000
C    -0.3906438    1.8193302    0.0000000
C    -1.7921378    1.7875910    0.0000000
C    -2.4713312    0.5803680    0.0000000
N     2.4062842   -0.5380648    0.0000000
N     0.3260089    3.0359148    0.0000000
H     3.5256261    1.9828160    0.0000000
H    -3.5572600    0.5753349    0.0000000
H    -2.3483205    2.7220807    0.0000000
H     2.4860092   -2.6159143    0.0000000
H    -2.2161681   -4.0466189    0.0000000
H     0.2623513   -4.0091000    0.0000000
H    -3.5239067   -1.9558740    0.0000000
H     2.1616470    4.0370630    0.0000000
H     3.4193145   -0.5075622    0.0000000
H    -0.1839243    3.9024468    0.0000000
```

Pyr-graphitic-edge-13

SOS-MP2: E = -647.48501 a.u.
B3LYP: E = -648.83604 a.u.
CAM-B3LYP: E = -648.86779 a.u.

Coordinates SOS-MP2:
Coordinates...

```
C    -1.7144183   -3.0136232    0.0000000
C     0.3871875   -1.8153951    0.0000000
C    -0.3489436   -0.6134054    0.0000000
C    -1.7583327   -0.5947813    0.0000000
C     1.7762903   -1.8330547    0.0000000
C     0.3561379    0.6259754    0.0000000
C     1.7945128    0.6179749    0.0000000
C     2.4785506   -0.6342067    0.0000000
C     2.4617418    1.8627018    0.0000000
C     1.7361304    3.0516582    0.0000000
C     0.3433098    3.0678731    0.0000000
C    -0.3856863    1.8583187    0.0000000
C    -1.8116011    1.8065086    0.0000000
C    -2.4833073    0.5902868    0.0000000
N    -0.3993597   -3.0300492    0.0000000
N    -2.4006772   -1.8914135    0.0000000
H     3.5475322    1.8824457    0.0000000
H    -3.5715598    0.5667391    0.0000000
H    -2.3736815    2.7344766    0.0000000
H     2.3121383   -2.7805515    0.0000000
```

```
H    -2.2501047   -3.9550098    0.0000000
H     3.5634447   -0.6432291    0.0000000
H     2.2736792    3.9965718    0.0000000
H    -0.1945279    4.0112975    0.0000000
H     0.0703584   -3.9237736    0.0000000
H    -3.4088137   -1.9443351    0.0000000
```

Pyr-graphitic-edge-14

SOS-MP2: E = -647.53161 a.u.
B3LYP: E = -648.87758 a.u.
CAM-B3LYP: E = -648.91305 a.u.

Coordinates SOS-MP2:
Coordinates...

```
C    -1.7819918   -3.0314738    0.0000000
C    -0.3713801   -3.0484548    0.0000000
C     0.3368953   -1.8536509    0.0000000
C    -0.3678021   -0.6101542    0.0000000
C    -1.7902476   -0.6088142    0.0000000
C    -2.4872767   -1.8483128    0.0000000
C     0.3452939    0.6267448    0.0000000
C     1.7990871    0.5783223    0.0000000
C     2.4399939   -0.6153069    0.0000000
C     1.7866846    3.0177142    0.0000000
C     0.4399604    3.0828874    0.0000000
C    -0.3367672    1.8441444    0.0000000
C    -1.7530201    1.8305265    0.0000000
C    -2.4575730    0.6475875    0.0000000
N     2.4659918    1.8138573    0.0000000
N     1.7155073   -1.8126512    0.0000000
H    -3.5437635    0.6606886    0.0000000
H    -2.2862456    2.7775437    0.0000000
H    -2.3150738   -3.9773337    0.0000000
H     0.1627340   -3.9943401    0.0000000
H    -3.5725465   -1.8483170    0.0000000
H     3.5185066   -0.7145171    0.0000000
H     2.4168050    3.8993551    0.0000000
H    -0.0567327    4.0447761    0.0000000
H     3.4718407    1.8214575    0.0000000
H     2.2211203   -2.6822787    0.0000000
```

Pyr-graphitic-edge-15

SOS-MP2: E = -647.49869 a.u.
B3LYP: E = -648.84807 a.u.
CAM-B3LYP: E = -648.87809 a.u.

Coordinates SOS-MP2:
Coordinates...

C	-1.7210853	-3.0737497	0.0000000
C	-0.3305286	-3.0837230	0.0000000
C	0.3863555	-1.8634481	0.0000000
C	-0.3590141	-0.6356831	0.0000000
C	-1.7885345	-0.6469040	0.0000000
C	-2.4558078	-1.8886966	0.0000000
C	1.7913028	-1.7860152	0.0000000
C	0.3222048	0.6274351	0.0000000
C	1.7338474	0.6228508	0.0000000
C	1.7439680	3.0475202	0.0000000
C	0.3991841	3.0866998	0.0000000
C	-0.3780795	1.8557209	0.0000000
C	-1.7876667	1.8113657	0.0000000
C	-2.4697198	0.6143167	0.0000000
N	2.3903454	-0.5434345	0.0000000
N	2.4297466	1.8200546	0.0000000
H	-3.5560845	0.6116992	0.0000000
H	-2.3419648	2.7466558	0.0000000
H	2.4573677	-2.6360409	0.0000000
H	-2.2507835	-4.0227678	0.0000000
H	0.2132687	-4.0234732	0.0000000
H	-3.5407834	-1.9121387	0.0000000
H	2.3765126	3.9251318	0.0000000
H	-0.1027299	4.0473523	0.0000000
H	3.4024296	-0.5225517	0.0000000
H	3.4362493	1.8218235	0.0000000

Pyr- pyridinic-1

SOS-MP2: E = -646.36334 a.u.
B3LYP: E = -647.69745 a.u.
CAM-B3LYP: E = -647.72825 a.u.

Coordinates SOS-MP2:

Coordinates...

C	-0.3963913	-3.0200418	0.0000000
C	0.3603786	-1.8398125	0.0000000
C	-0.3512379	-0.6174038	0.0000000
C	-1.7656541	-0.6302773	0.0000000
C	-2.3935080	-1.8838455	0.0000000
C	1.8024476	-1.8095425	0.0000000
C	0.3512378	0.6174039	0.0000000
C	1.7656541	0.6302773	0.0000000
C	2.4764603	-0.6247884	0.0000000
C	2.3935080	1.8838453	0.0000000

```
C     0.3963914    3.0200418    0.0000000
C    -0.3603786    1.8398128    0.0000000
C    -1.8024477    1.8095426    0.0000000
C    -2.4764605    0.6247883    0.0000000
N     1.7360118    3.0514131    0.0000000
N    -1.7360116   -3.0514131    0.0000000
H     3.4796745    1.9472687    0.0000000
H    -3.5624659    0.6090000    0.0000000
H    -2.3438013    2.7511279    0.0000000
H     2.3438008   -2.7511280    0.0000000
H     0.1040360   -3.9861315    0.0000000
H    -3.4796744   -1.9472692    0.0000000
H     3.5624658   -0.6090000    0.0000000
H    -0.1040355    3.9861319    0.0000000
```

Pyr- pyridinic-2

SOS-MP2: E = -646.36435 a.u.
B3LYP: E = -647.69894 a.u.
CAM-B3LYP: E = -647.72990 a.u.

Coordinates SOS-MP2:

Coordinates...

```
C    -1.5029648   -2.9994618    0.0000000
C    -0.1063814   -2.9785523    0.0000000
C     0.5761535   -1.7576959    0.0000000
C    -0.1775998   -0.5588856    0.0000000
C    -1.5957525   -0.5734748    0.0000000
C    -2.2445959   -1.8162759    0.0000000
C     0.5145701    0.6779223    0.0000000
C     1.9223664    0.6727372    0.0000000
C     2.5850462   -0.6119995    0.0000000
C     2.5807408    1.9078393    0.0000000
C     0.5984481    3.0735734    0.0000000
C    -0.1806141    1.9074676    0.0000000
C    -1.6217488    1.8810631    0.0000000
C    -2.2915117    0.6926733    0.0000000
N     1.9394905    3.0846497    0.0000000
N     1.9717707   -1.7610249    0.0000000
H     3.6675560    1.9519742    0.0000000
H    -3.3779378    0.6825757    0.0000000
H    -2.1664919    2.8205655    0.0000000
H    -2.0208149   -3.9531226    0.0000000
H     0.4707836   -3.8970382    0.0000000
H    -3.3302458   -1.8558230    0.0000000
H     3.6743080   -0.6381898    0.0000000
H     0.1154257    4.0485029    0.0000000
```

Pyr- pyridinic-3

SOS-MP2: E = -646.33513 a.u.
B3LYP: E = -647.66878 a.u.
CAM-B3LYP: E = -647.69890 a.u.

Coordinates SOS-MP2:

Coordinates...

C	-1.4947137	-2.8156243	0.0000000
C	-0.0960825	-2.8071329	0.0000000
C	0.6061302	-1.5969063	0.0000000
C	-0.1351551	-0.3861543	0.0000000
C	-1.5543489	-0.3899802	0.0000000
C	-2.2207452	-1.6269142	0.0000000
C	2.0513452	-1.5246153	0.0000000
C	0.5535177	0.8559366	0.0000000
C	1.9704958	0.9087275	0.0000000
C	2.7076797	-0.3326391	0.0000000
C	0.6578769	3.2302670	0.0000000
C	-0.1434723	2.0741840	0.0000000
C	-1.5795410	2.0612423	0.0000000
C	-2.2506068	0.8721728	0.0000000
N	1.9910233	3.2255260	0.0000000
N	2.6608171	2.0598914	0.0000000
H	-3.3369691	0.8600812	0.0000000
H	-2.1205635	3.0028453	0.0000000
H	2.6117325	-2.4554557	0.0000000
H	-2.0217417	-3.7642375	0.0000000
H	0.4524674	-3.7446728	0.0000000
H	-3.3066033	-1.6511261	0.0000000
H	3.7907773	-0.2744422	0.0000000
H	0.2066799	4.2190270	0.0000000

Pyr- pyridinic-4

SOS-MP2: E = -646.36498 a.u.
B3LYP: E = -647.69873 a.u.
CAM-B3LYP: E = -647.72967 a.u.

Coordinates SOS-MP2:

Coordinates...

C	-1.4810805	-2.9205831	0.0000000
C	-0.0850432	-2.9082205	0.0000000

```
C     0.5972835   -1.6849620    0.0000000
C    -0.1476751   -0.4839688    0.0000000
C    -1.5651309   -0.4894371    0.0000000
C    -2.2159567   -1.7317415    0.0000000
C     2.0403829   -1.5722555    0.0000000
C     0.5638861    0.7417554    0.0000000
C     1.9742579    0.7262649    0.0000000
C     2.6349308    1.9612750    0.0000000
C     0.6592134    3.1398693    0.0000000
C    -0.1229788    1.9769717    0.0000000
C    -1.5652581    1.9597691    0.0000000
C    -2.2519360    0.7812902    0.0000000
N     1.9999882    3.1416764    0.0000000
N     2.7112098   -0.4538069    0.0000000
H     3.7211418    1.9807252    0.0000000
H    -3.3382170    0.7830891    0.0000000
H    -2.1002531    2.9051513    0.0000000
H     2.6271689   -2.4907519    0.0000000
H    -2.0067445   -3.8698920    0.0000000
H     0.4717816   -3.8407277    0.0000000
H    -3.3017230   -1.7685837    0.0000000
H     0.1807519    4.1170928    0.0000000
```

Pyr- pyridinic-5

SOS-MP2: E = -646.36874 a.u.
B3LYP: E = -647.70198 a.u.
CAM-B3LYP: E =-647.73321 a.u.

Coordinates SOS-MP2:

Coordinates...

```
C    -1.4821779   -3.1033385    0.0000000
C     0.4770701   -1.9124506    0.0000000
C    -0.2334783   -0.6847456    0.0000000
C    -1.6491333   -0.7000122    0.0000000
C    -2.2720319   -1.9529056    0.0000000
C     1.9184651   -1.8752334    0.0000000
C     0.4693162    0.5505762    0.0000000
C     1.8877185    0.5670832    0.0000000
C     2.5922133   -0.6909700    0.0000000
C     1.9103257    2.8597607    0.0000000
C     0.5178253    2.9509043    0.0000000
C    -0.2408978    1.7752836    0.0000000
C    -1.6833035    1.7414770    0.0000000
C    -2.3570770    0.5571637    0.0000000
N     2.6008362    1.7109104    0.0000000
N    -0.1417985   -3.1098968    0.0000000
H    -3.4433733    0.5434902    0.0000000
```

```
H    -2.2265975    2.6822516    0.0000000
H     2.4407780   -2.8260590    0.0000000
H    -1.9544501   -4.0822223    0.0000000
H    -3.3542091   -2.0368934    0.0000000
H     3.6764297   -0.6541344    0.0000000
H     2.5104708    3.7658943    0.0000000
H     0.0370795    3.9240667    0.0000000
```

Pyr- pyridinic-6

SOS-MP2: E = -646.36576 a.u.
B3LYP: E = -647.70047 a.u.
CAM-B3LYP: E = -647.73159 a.u.

Coordinates SOS-MP2:

Coordinates...

```
C    -0.3308886   -3.0927966    0.0000000
C     0.4150119   -1.9053003    0.0000000
C    -0.3045281   -0.6890002    0.0000000
C    -1.7178665   -0.7181743    0.0000000
C    -2.3367928   -1.9757099    0.0000000
C     1.8561870   -1.8633438    0.0000000
C     0.3849194    0.5548009    0.0000000
C     1.8022162    0.5815834    0.0000000
C     2.5175745   -0.6722025    0.0000000
C     1.8046276    2.8731581    0.0000000
C     0.4113988    2.9518832    0.0000000
C    -0.3385134    1.7710061    0.0000000
C    -1.7812949    1.7210004    0.0000000
C    -2.4417921    0.5294287    0.0000000
N     2.5052869    1.7303785    0.0000000
N    -1.6694739   -3.1373757    0.0000000
H    -3.5276125    0.5027196    0.0000000
H    -2.3347000    2.6556266    0.0000000
H     2.4071903   -2.7991952    0.0000000
H     0.1801157   -4.0532617    0.0000000
H    -3.4224158   -2.0470937    0.0000000
H     3.6013591   -0.6246446    0.0000000
H     2.3961999    3.7849083    0.0000000
H    -0.0762087    3.9216046    0.0000000
```

Pyr- pyridinic-7

SOS-MP2: E = -646.33134 a.u.
B3LYP: E = -647.66622 a.u.

CAM-B3LYP: E = -647.69562 a.u.

Coordinates SOS-MP2:

Coordinates...

C	-1.4280659	-3.1863257	0.0000000
C	-0.0347169	-3.1465720	0.0000000
C	0.6159382	-1.9053358	0.0000000
C	-0.1522689	-0.7238708	0.0000000
C	-1.5694173	-0.7573993	0.0000000
C	-2.1916313	-2.0117640	0.0000000
C	0.5444403	0.5007631	0.0000000
C	1.9525567	0.4440982	0.0000000
C	2.6870681	1.6376272	0.0000000
C	2.0092880	2.8556632	0.0000000
C	0.6094794	2.9118672	0.0000000
C	-0.1508486	1.7360761	0.0000000
C	-1.5939865	1.6919260	0.0000000
C	-2.2688602	0.5056824	0.0000000
N	2.6502972	-0.7664004	0.0000000
N	2.0130086	-1.8865941	0.0000000
H	3.7708010	1.5883197	0.0000000
H	-3.3552975	0.4978522	0.0000000
H	-2.1423875	2.6298251	0.0000000
H	-1.9340021	-4.1463887	0.0000000
H	0.5614080	-4.0529629	0.0000000
H	-3.2763675	-2.0726134	0.0000000
H	2.5760393	3.7811261	0.0000000
H	0.1075253	3.8754005	0.0000000

Pyr- pyridinic-8

SOS-MP2: E = -646.36629 a.u.
B3LYP: E = -647.70048 a.u.
CAM-B3LYP: E = -647.73139 a.u.

Coordinates SOS-MP2:

Coordinates...

C	-1.6807118	-2.9542441	0.0000000
C	-0.2829176	-2.9617084	0.0000000
C	0.4213074	-1.7510201	0.0000000
C	-0.3093481	-0.5437489	0.0000000
C	-1.7204599	-0.5325342	0.0000000
C	-2.4013405	-1.7565034	0.0000000
C	1.8644334	-1.6397282	0.0000000

```
C     0.3895893    0.6847949    0.0000000
C     1.8043418    0.6730102    0.0000000
C     2.4815536    1.8972318    0.0000000
C     1.7601648    3.0938945    0.0000000
C     0.3629064    3.1025629    0.0000000
C    -0.3434173    1.8949025    0.0000000
C    -2.3621704    0.7648534    0.0000000
N     2.5290180   -0.5181852    0.0000000
N    -1.7376563    1.9091928    0.0000000
H     3.5664278    1.8940808    0.0000000
H    -3.4513973    0.8040856    0.0000000
H     2.4547050   -2.5559875    0.0000000
H    -2.2172745   -3.8973799    0.0000000
H     0.2571410   -3.9043108    0.0000000
H    -3.4875544   -1.7739015    0.0000000
H     2.2967861    4.0371249    0.0000000
H    -0.1941262    4.0335179    0.0000000
```

Pyr- pyridinic-9

SOS-MP2: E = -646.36759 a.u.
B3LYP: E = -647.70134 a.u.
CAM-B3LYP: E = -647.73233 a.u.

Coordinates SOS-MP2:

Coordinates...

```
C    -1.7382350   -3.0133252    0.0000000
C    -0.3415797   -3.0305991    0.0000000
C     0.3656454   -1.8214504    0.0000000
C    -0.3583623   -0.6087989    0.0000000
C    -1.7722111   -0.5873974    0.0000000
C    -2.4520596   -1.8107652    0.0000000
C     1.8083609   -1.7201318    0.0000000
C     0.3583623    0.6087989    0.0000000
C     1.7722110    0.5873973    0.0000000
C     2.4520597    1.8107652    0.0000000
C     1.7382349    3.0133251    0.0000000
C     0.3415799    3.0305992    0.0000000
C    -0.3656454    1.8214504    0.0000000
C    -1.8083609    1.7201317    0.0000000
N     2.4894180   -0.6069392    0.0000000
N    -2.4894180    0.6069393    0.0000000
H     3.5371009    1.8040812    0.0000000
H    -2.3896551    2.6422980    0.0000000
H     2.3896551   -2.6422980    0.0000000
H    -2.2825398   -3.9521229    0.0000000
H     0.1954339   -3.9747958    0.0000000
```

```
H    -3.5371009   -1.8040813    0.0000000
H     2.2825400    3.9521229    0.0000000
H    -0.1954338    3.9747959    0.0000000
```

Pyr- pyridinic-10

SOS-MP2: E = -646.36936 a.u.
B3LYP: E = -647.70257 a.u.
CAM-B3LYP: E = -647.73380 a.u.

Coordinates SOS-MP2:

Coordinates...

```
C    -1.7394590   -2.9583147    0.0000000
C    -0.3458106   -3.0245886    0.0000000
C     0.3946107   -1.8369642    0.0000000
C    -0.3378681   -0.6252000   -0.0000000
C    -1.7553721   -0.6674009    0.0000000
C     1.8350177   -1.7764787   -0.0000000
C     0.3378681    0.6252000    0.0000000
C     1.7553721    0.6674009    0.0000000
C     2.4835867   -0.5781378    0.0000000
C     1.7394590    2.9583147    0.0000000
C     0.3458106    3.0245886    0.0000000
C    -0.3946107    1.8369642    0.0000000
C    -1.8350177    1.7764787    0.0000000
C    -2.4835867    0.5781378    0.0000000
N     2.4507453    1.8214790   -0.0000000
N    -2.4507453   -1.8214790   -0.0000000
H    -3.5669988    0.5197796    0.0000000
H    -2.3966825    2.7061072    0.0000000
H     2.3966825   -2.7061072    0.0000000
H    -2.3231110   -3.8752115    0.0000000
H     0.1516401   -3.9894078   -0.0000000
H     3.5669988   -0.5197796    0.0000000
H     2.3231110    3.8752115    0.0000000
H    -0.1516401    3.9894078    0.0000000
```

Pyr- pyridinic-11

SOS-MP2: E = -646.36692 a.u.
B3LYP: E = -647.70043 a.u.
CAM-B3LYP: E = -647.73135 a.u.

Coordinates SOS-MP2:
Coordinates...

```
C    -1.7312453   -3.0660313    0.0000000
C    -0.3368105   -3.1265857    0.0000000
C     0.3826879   -1.9273899    0.0000000
C    -0.3520256   -0.7250227    0.0000000
C    -1.7690599   -0.7696208    0.0000000
C     1.8247292   -1.8221519    0.0000000
C     0.3442396    0.5091284    0.0000000
C     1.7607879    0.4893064    0.0000000
C     2.4526106    1.7061648    0.0000000
C     1.7457184    2.9099091    0.0000000
C     0.3489960    2.9296303    0.0000000
C    -0.3768900    1.7301304    0.0000000
C    -1.8193003    1.6693671    0.0000000
C    -2.4869045    0.4799499    0.0000000
N     2.4876968   -0.6996111    0.0000000
N    -2.4498547   -1.9317524    0.0000000
H     3.5372242    1.6882220    0.0000000
H    -3.5709446    0.4377054    0.0000000
H    -2.3746930    2.6031464    0.0000000
H     2.4148726   -2.7382754    0.0000000
H    -2.3112261   -3.9850645    0.0000000
H     0.1692596   -4.0867904    0.0000000
H     2.2915573    3.8479551    0.0000000
H    -0.1814255    3.8776808    0.0000000
```

Pyr- pyridinic-12

SOS-MP2: E = -646.36785 a.u.
B3LYP: E = -647.70204 a.u.
CAM-B3LYP: E = -647.73326 a.u.

Coordinates SOS-MP2:

Coordinates...

```
C    -1.5860094   -2.9077440    0.0000000
C    -0.1898509   -2.9074165    0.0000000
C     0.5002659   -1.6889133    0.0000000
C    -0.2315917   -0.4805786    0.0000000
C    -1.6484768   -0.4757205    0.0000000
C    -2.3099992   -1.7127502    0.0000000
C     1.9442599   -1.5910581    0.0000000
C     0.4935217    0.7379455    0.0000000
C     1.9045818    0.7099666    0.0000000
C     2.5671139    1.9383201    0.0000000
C     1.8097160    3.1118691    0.0000000
C    -0.1832912    1.9822146    0.0000000
C    -1.6260378    1.9703622    0.0000000
C    -2.3248076    0.7993175    0.0000000
N     0.4691655    3.1600019    0.0000000
```

```
N     2.6274106   -0.4817740    0.0000000
H     3.6508219    1.9705319    0.0000000
H    -3.4110385    0.8112672    0.0000000
H    -2.1325287    2.9298661    0.0000000
H     2.5209753   -2.5161718    0.0000000
H    -2.1202309   -3.8523647    0.0000000
H     0.3602912   -3.8439188    0.0000000
H    -3.3961101   -1.7388783    0.0000000
H     2.3118490    4.0756263    0.0000000
```

Pyr- pyridinic-13

SOS-MP2: E = -646.37317 a.u.
B3LYP: E = -646.99573 a.u.
CAM-B3LYP: E = -647.73884 a.u.

Coordinates SOS-MP2:

Coordinates...

```
C    -1.5937563   -2.8014038    0.0000000
C    -0.1981699   -2.8056038    0.0000000
C     0.5132279   -1.5970257    0.0000000
C    -0.2165967   -0.3807253    0.0000000
C    -1.6350464   -0.3748431    0.0000000
C    -2.3104523   -1.6038976    0.0000000
C     1.9558502   -1.5376144    0.0000000
C     0.4861214    0.8544746    0.0000000
C     1.8977810    0.8943823    0.0000000
C     2.6238700   -0.3495633    0.0000000
C     1.8024403    3.1682247    0.0000000
C    -0.2008739    2.0883347    0.0000000
C    -1.6411776    2.0768767    0.0000000
C    -2.3210970    0.8955989    0.0000000
N     2.5611333    2.0657505    0.0000000
N     0.4670874    3.2570806    0.0000000
H    -3.4076619    0.8930831    0.0000000
H    -2.1558662    3.0317587    0.0000000
H     2.5088814   -2.4729130    0.0000000
H    -2.1303258   -3.7445588    0.0000000
H     0.3439799   -3.7468759    0.0000000
H    -3.3965920   -1.6188108    0.0000000
H     3.7076762   -0.3040859    0.0000000
H     2.3395669    4.1123566    0.0000000
```

Pyr- pyridinic-14

SOS-MP2: E = -646.36751 a.u.

B3LYP: E = -647.70089 a.u.
CAM-B3LYP: E = -647.73192 a.u.

Coordinates SOS-MP2:

Coordinates...

C	-1.4365554	-3.0837003	0.0000000
C	-0.0410380	-3.0494074	0.0000000
C	0.6312424	-1.8214859	0.0000000
C	-0.1321127	-0.6290121	0.0000000
C	-1.5503835	-0.6598385	0.0000000
C	-2.1897696	-1.9073771	0.0000000
C	0.5454270	0.6159162	0.0000000
C	1.9554677	0.6237537	0.0000000
C	2.6268279	-0.6579713	0.0000000
C	2.0054910	2.9052229	0.0000000
C	0.6109061	3.0067696	0.0000000
C	-0.1632543	1.8413001	0.0000000
C	-1.6037046	1.7945594	0.0000000
C	-2.2592473	0.5980184	0.0000000
N	2.6895666	1.7521828	0.0000000
N	2.0242240	-1.8142640	0.0000000
H	-3.3457363	0.5763885	0.0000000
H	-2.1609118	2.7268070	0.0000000
H	-1.9450679	-4.0424417	0.0000000
H	0.5461432	-3.9615798	0.0000000
H	-3.2750293	-1.9557792	0.0000000
H	3.7151168	-0.6529575	0.0000000
H	2.6096378	3.8085012	0.0000000
H	0.1427602	3.9863949	0.0000000

Pyr- pyridinic-15

SOS-MP2: E = -646.36584 a.u.
B3LYP: E = -645.15857 a.u.
CAM-B3LYP: E = -647.73147 a.u.

Coordinates SOS-MP2:
Coordinates...

C	-1.4178215	-3.0045423	0.0000000
C	-0.0223669	-2.9795715	0.0000000
C	0.6481548	-1.7503925	0.0000000
C	-0.0997896	-0.5536930	0.0000000
C	-1.5175273	-0.5750505	0.0000000
C	-2.1607392	-1.8212507	0.0000000
C	2.0891754	-1.6259097	0.0000000
C	0.6034509	0.6790823	0.0000000

```
C     2.0211056    0.6802340    0.0000000
C     2.0561902    2.9682042    0.0000000
C     0.6653679    3.0747976    0.0000000
C    -0.1017829    1.9057423    0.0000000
C    -1.5439932    1.8701824    0.0000000
C    -2.2190960    0.6858856    0.0000000
N     2.7373622    1.8130834    0.0000000
N     2.7510480   -0.5053942    0.0000000
H    -3.3054802    0.6761208    0.0000000
H    -2.0884260    2.8100117    0.0000000
H     2.6825566   -2.5405430    0.0000000
H    -1.9357988   -3.9581465    0.0000000
H     0.5446702   -3.9058860    0.0000000
H    -3.2462975   -1.8639914    0.0000000
H     2.6655482    3.8681443    0.0000000
H     0.1944891    4.0528828    0.0000000
```