

Optimized geometries at the B3LYP/6-31+G\*\* computational level.

**A/5, p-WC**

N	-0.200	0.000	0.396
C	-0.161	0.000	1.743
N	0.901	0.000	2.546
C	2.045	0.000	1.842
C	2.170	0.000	0.451
C	0.968	0.000	-0.297
N	3.340	0.000	2.309
C	4.162	0.000	1.199
N	3.500	0.000	0.066
N	0.951	0.000	-1.639
H	-1.130	0.000	2.236
H	3.619	0.000	3.279
H	5.239	0.000	1.292
H	0.070	0.000	-2.168
H	1.833	0.000	-2.128
C	-3.980	0.000	-0.308
O	-5.102	0.000	-0.784
N	-2.807	0.000	-1.033
H	-3.795	0.000	0.780
H	-1.901	0.000	-0.527
C	-2.789	0.000	-2.411
N	-1.681	0.000	-3.057
H	-3.784	0.000	-2.861
H	-1.849	0.000	-4.061

**A/5, p-H**

N	-3.206	0.000	0.783
C	-3.252	0.000	2.121
N	-2.234	0.000	2.991
C	-1.058	0.000	2.353
C	-0.840	0.000	0.971
C	-2.005	0.000	0.159
N	0.204	0.000	2.913
C	1.103	0.000	1.876
N	0.523	0.000	0.695
N	-1.991	0.000	-1.185
H	-4.249	0.000	2.555
H	0.409	0.000	3.902
H	2.171	0.000	2.047
H	-2.889	0.000	-1.646
H	-1.141	0.000	-1.757
C	3.496	0.000	-1.654
O	4.317	0.000	-2.555
N	2.129	0.000	-1.819
H	3.784	0.000	-0.588
H	1.525	0.000	-0.979
C	1.532	0.000	-3.063
N	0.256	0.000	-3.180
H	2.245	0.000	-3.888
H	-0.012	0.000	-4.163

**5/A/5**

N	-1.557	0.000	1.150
C	-1.549	0.000	2.493
N	-0.503	0.000	3.319
C	0.650	0.000	2.634
C	0.813	0.000	1.246
C	-0.379	0.000	0.464

N	1.929	0.000	3.146
C	2.789	0.000	2.075
N	2.163	0.000	0.918
N	-0.403	0.000	-0.870
H	-2.528	0.000	2.967
H	2.171	0.000	4.126
H	3.862	0.000	2.206
H	-1.304	0.000	-1.359
H	0.450	0.000	-1.435
C	5.106	0.000	-1.506
O	5.900	0.000	-2.430
N	3.735	0.000	-1.630
H	5.426	0.000	-0.449
H	3.154	0.000	-0.776
C	3.096	0.000	-2.853
N	1.817	0.000	-2.920
H	3.779	0.000	-3.704
H	1.507	0.000	-3.891
C	-5.354	0.000	0.506
O	-6.485	0.000	0.050
N	-4.196	0.000	-0.238
H	-5.151	0.000	1.591
H	-3.280	0.000	0.248
C	-4.197	0.000	-1.618
N	-3.096	0.000	-2.274
H	-5.198	0.000	-2.053
H	-3.275	0.000	-3.276

**A/6, p-WC**

C	0.042	0.000	-4.205
C	0.101	0.000	-2.798
N	1.266	0.000	-2.124
C	2.408	0.000	-2.826
C	2.457	0.000	-4.217
C	1.242	0.000	-4.908
H	-0.918	0.000	-4.701
H	3.324	0.000	-2.240
H	3.410	0.000	-4.736
H	1.225	0.000	-5.994
N	-1.033	0.000	-1.980
C	-2.348	0.000	-2.363
O	-2.785	0.000	-3.505
H	-3.015	0.000	-1.482
H	-0.865	0.000	-0.963
N	-0.796	0.000	1.036
C	-1.905	0.000	1.801
N	-2.000	0.000	3.130
C	-0.788	0.000	3.706
C	0.448	0.000	3.054
C	0.417	0.000	1.640
N	-0.474	0.000	5.047
C	0.905	0.000	5.132
N	1.495	0.000	3.960
N	1.531	0.000	0.887
H	-2.847	0.000	1.257
H	-1.135	0.000	5.810
H	1.414	0.000	6.087
H	1.468	0.000	-0.136

H	2.427	0.000	1.350
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**A/6, p-H**

C	3.113	2.511	-0.035
C	2.036	1.606	-0.012
N	2.206	0.278	0.114
C	3.455	-0.192	0.235
C	4.588	0.617	0.229
C	4.399	1.995	0.088
H	2.924	3.569	-0.147
H	3.547	-1.271	0.341
H	5.577	0.183	0.330
H	5.250	2.670	0.074
N	0.698	2.002	-0.114
C	0.202	3.264	-0.303
O	0.841	4.300	-0.420
H	-0.902	3.250	-0.344
H	-0.006	1.257	-0.021
N	-1.430	-3.559	-0.251
C	-2.755	-3.736	-0.144
N	-3.705	-2.815	0.056
C	-3.178	-1.588	0.141
C	-1.826	-1.239	0.043
C	-0.921	-2.312	-0.156
N	-3.838	-0.393	0.337
C	-2.884	0.596	0.345
N	-1.665	0.135	0.171
N	0.412	-2.152	-0.262
H	-3.097	-4.764	-0.229
H	-4.836	-0.282	0.449
H	-3.144	1.637	0.483
H	0.962	-2.989	-0.388
H	0.881	-1.254	-0.129

**A/7, p-WC**

N	0.312	0.000	2.849
C	0.352	0.000	4.196
N	1.415	0.000	5.000
C	2.558	0.000	4.295
C	2.683	0.000	2.904
C	1.480	0.000	2.158
N	3.854	0.000	4.762
C	4.676	0.000	3.652
N	4.013	0.000	2.519
N	1.458	0.000	0.816
H	-0.617	0.000	4.691
H	4.134	0.000	5.732
H	5.753	0.000	3.744
H	0.575	0.000	0.298
H	2.333	0.000	0.316
C	-2.419	0.000	0.070
N	-1.238	0.000	-0.538
C	-1.195	0.000	-1.894
C	-2.382	0.000	-2.688
C	-3.625	0.000	-2.005
C	-3.663	0.000	-0.633
N	0.042	0.000	-2.453

C	-2.232	0.000	-4.095
H	-4.549	0.000	-2.577
H	-4.589	0.000	-0.076
C	-0.978	0.000	-4.659
C	0.136	0.000	-3.773
H	-3.116	0.000	-4.728
H	-0.818	0.000	-5.728
N	1.461	0.000	-4.238
N	-2.350	0.000	1.462
H	-1.398	0.000	1.868
H	2.144	0.000	-3.489
C	-3.382	0.000	2.368
O	-4.579	0.000	2.125
H	-2.995	0.000	3.402
C	1.943	0.000	-5.525
O	1.280	0.000	-6.548
H	3.048	0.000	-5.536

**A/7, p-H**

N	0.015	4.129	0.000
C	-0.810	5.186	0.000
N	-2.148	5.202	0.000
C	-2.645	3.959	0.000
C	-1.925	2.761	0.000
C	-0.511	2.883	0.000
N	-3.971	3.575	0.000
C	-3.990	2.201	0.000
N	-2.786	1.671	0.000
N	0.319	1.828	0.000
H	-0.322	6.158	0.000
H	-4.765	4.198	0.000
H	-4.919	1.646	0.000
H	1.312	1.995	0.000
H	0.000	0.860	0.000
C	3.384	-1.436	0.000
N	2.163	-0.927	0.000
C	1.107	-1.781	0.000
C	1.286	-3.199	0.000
C	2.611	-3.696	0.000
C	3.677	-2.829	0.000
N	-0.127	-1.214	0.000
C	0.122	-4.007	0.000
H	2.779	-4.770	0.000
H	4.705	-3.163	0.000
C	-1.123	-3.429	0.000
C	-1.195	-2.003	0.000
H	0.223	-5.089	0.000
H	-2.035	-4.007	0.000
N	-2.416	-1.325	0.000
N	4.398	-0.465	0.000
H	4.041	0.484	0.000
H	-2.367	-0.296	0.000
C	5.765	-0.615	0.000
O	6.377	-1.669	0.000
H	6.272	0.366	0.000
C	-3.684	-1.846	0.000
O	-4.004	-3.025	0.000
H	-4.436	-1.038	0.000