SUPPORTING INFORMATION

Analytic Gradients for Complete Active Space Pair-Density Functional Theory

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Table S1: Computed equilibrium geometries for selected molecules in the SE47 database.[54] Bond lengths are given an Angstroms and bond angles are given in degrees.

		cc-pVDZ					cc-pVTZ				
	Ref.[54]	tPBE	CASSCF	CASPT2	PBE	ftPBE	tPBE	CASSCF	CASPT2	PBE	ftPBE
NH_3											
r(N-H)	1.011	1.032	1.032	1.027	1.033	1.033	1.022	1.022	1.014	1.023	1.024
a(H-N-H)	106.9	104.0	103.4	103.6	103.2	104.0	106.0	105.1	105.6	105.4	106.0
HCN											
r(H-C)	1.065	1.084	1.087	1.083	1.085	1.085	1.074	1.076	1.068	1.075	1.075
a(C-N)	1.154	1.170	1.173	1.175	1.170	1.169	1.159	1.163	1.160	1.159	1.158
CO_2H											
r(C-O)	1.205	1.214	1.209	1.215	1.213	1.214	1.209	1.205	1.209	1.208	1.208
r(C-H)	1.100	1.130	1.128	1.123	1.131	1.133	1.119	1.116	1.107	1.119	1.122
a(H C O)	121.6	122.4	122.9	122.5	122.6	122.5	122.2	122.6	122.0	122.2	122.2
HCCH											
r(C-C)	1.204	1.221	1.228	1.229	1.220	1.221	1.208	1.216	1.210	1.207	1.208
r(C-H)	1.061	1.079	1.085	1.080	1.079	1.081	1.070	1.074	1.065	1.070	1.071
oxirane											
r(C-C)	1.462	1.476	1.451	1.476	1.476	1.478	1.469	1.449	1.465	1.469	1.473
r(C-O)	1.428	1.433	1.444	1.435	1.437	1.429	1.432	1.440	1.428	1.435	1.427
r(C-H)	1.081	1.104	1.088	1.098	1.106	1.102	1.092	1.076	1.081	1.094	1.091
a(C-O-C)	61.6	62.0	60.3	61.9	61.8	62.3	61.7	60.4	61.7	61.6	62.1
a(H-C-H)	116.3	115.6	114.9	115.7	115.3	115.5	115.8	115.3	116.2	115.6	115.7
a(H-C-O)	114.8	115.6	115.3	115.4	115.7	115.9	115.5	114.9	115.2	115.4	115.7
acrolein											
r(C1-C2)	1.473	1.493	1.486	1.492	1.489	1.491	1.489	1.485	1.481	1.485	1.488
r(C2-C3)	1.336	1.343	1.344	1.353	1.349	1.344	1.334	1.337	1.339	1.340	1.335
r(C1-O)	1.211	1.217	1.205	1.221	1.225	1.216	1.211	1.200	1.214	1.219	1.211
r(C1-H)	1.104	1.126	1.099	1.116	1.130	1.125	1.116	1.090	1.101	1.119	1.115
r(C2-H)	1.082	1.100	1.084	1.095	1.103	1.099	1.091	1.075	1.081	1.093	1.090
r(C3-H_{cis})	1.083	1.100	1.082	1.094	1.102	1.099	1.090	1.073	1.080	1.092	1.089

r(C3-H_{trans})	1.079	1.098	1.082	1.093	1.100	1.097	1.088	1.073	1.079	1.090	1.087
a(C1-C2-C3)	120.2	120.6	122.3	120.8	121.2	121.1	121.3	122.8	121.2	121.8	121.7
a(O-C1-C2)	124.0	124.4	123.8	123.9	124.4	124.3	124.7	124.1	124.0	124.6	124.6
a(C2-C1-H)	115.1	114.8	116.1	117.6	114.8	115.0	114.9	116.0	115.7	114.9	115.0
a(C3-C2-H)	122.9	121.7	121.0	121.6	121.6	121.7	121.6	120.9	121.5	121.4	121.5
a(C2-C3-H_{cis})	120.4	119.3	120.7	121.8	119.3	119.6	119.8	120.9	119.8	119.8	120.0
a(C2-C3-H_{trans})	122.1	122.2	121.4	119.6	122.1	122.0	122.1	121.3	121.7	122.1	121.9
butadiene											
r(C1-C2)	1.339	1.346	1.347	1.356	1.352	1.338	1.338	1.339	1.342	1.344	1.338
r(C2-C3)	1.454	1.463	1.466	1.464	1.456	1.457	1.458	1.462	1.453	1.451	1.457
r(C1-H_{cis})	1.082	1.100	1.084	1.095	1.102	1.089	1.090	1.075	1.081	1.092	1.089
r(C1-H_{trans})	1.079	1.098	1.082	1.093	1.099	1.087	1.088	1.073	1.079	1.090	1.087
r(C2-H)	1.084	1.102	1.085	1.097	1.105	1.092	1.093	1.076	1.083	1.095	1.092
a(C1-C2-C3)	123.5	124.2	124.1	123.6	124.4	124.2	124.2	124.1	123.5	124.3	124.2
a(C1-C2-H)	119.8	119.4	119.3	119.6	119.3	119.5	119.5	119.3	119.7	119.3	119.5
a(C2-C1-H_{cis})	120.9	121.2	121.5	121.1	121.2	121.3	121.3	121.6	121.0	121.2	121.3
a(C2-C1-H_{trans})	121.4	121.6	121.4	121.5	121.6	121.7	121.7	121.4	121.5	121.7	121.7
pyrrole											
r(C-N)	1.377	1.373	1.368	1.377	1.379	1.373	1.369	1.364	1.370	1.375	1.369
r(C2-C3)	1.379	1.388	1.374	1.391	1.391	1.387	1.380	1.367	1.378	1.383	1.379
r(C3-C4)	1.428	1.425	1.432	1.431	1.429	1.425	1.419	1.427	1.420	1.424	1.420
r(N-H)	0.994	1.016	0.995	1.012	1.017	1.014	1.009	0.988	1.003	1.011	1.008
r(C2-H)	1.074	1.092	1.077	1.088	1.094	1.092	1.083	1.068	1.075	1.084	1.082
r(C3-H)	1.075	1.093	1.078	1.089	1.095	1.092	1.083	1.068	1.075	1.085	1.082
a(H-N-C2)	125.2	124.9	125.2	124.9	124.9	124.9	124.9	125.2	125.0	125.0	125.0
a(C5-N-C2)	109.6	110.2	109.7	110.1	110.1	110.1	110.1	109.6	110.0	110.0	110.0
a(N-C2-C3)	107.9	107.6	108.1	107.7	107.5	107.6	107.6	108.1	107.6	107.5	107.6
a(C2-C3-C4)	107.3	107.3	107.0	107.3	107.4	107.3	107.4	107.1	107.4	107.5	107.4
a(N-C2-H)	121.9	121.2	121.2	121.2	121.1	121.2	121.2	121.3	121.2	121.2	121.3
a(C2-C3-H)	125.4	125.6	125.9	125.6	125.7	125.6	125.6	125.9	125.6	125.7	125.7
pyridine											

r(C2-C3)	1.391	1.399	1.397	1.405	1.404	1.400	1.392	1.391	1.393	1.397	1.392
r(C3-C4)	1.389	1.397	1.395	1.403	1.402	1.397	1.390	1.389	1.391	1.395	1.390
r(N-C2)	1.336	1.342	1.334	1.348	1.348	1.341	1.336	1.328	1.338	1.342	1.335
r(C2-H)	1.082	1.102	1.083	1.096	1.104	1.101	1.092	1.074	1.082	1.094	1.091
r(C3-H)	1.080	1.098	1.081	1.093	1.100	1.097	1.088	1.072	1.080	1.091	1.087
r(C4-H)	1.080	1.099	1.082	1.094	1.100	1.098	1.089	1.073	1.080	1.091	1.088
a(C6-N-C2)	116.9	116.5	117.5	116.3	116.5	116.6	116.9	117.8	116.7	116.9	117.0
a(N-C2-C3)	123.8	124.2	123.6	124.3	124.2	124.2	123.9	123.4	124.0	123.8	123.8
a(C2-C3-C4)	118.5	118.4	118.6	118.5	118.4	118.3	118.4	118.6	118.5	118.5	118.4
a(C3-C4-C5)	118.4	118.4	118.2	118.2	118.4	118.5	118.5	118.3	118.4	118.5	118.6
a(N-C2-H)	116.0	115.7	116.1	115.7	115.7	115.8	116.0	116.2	115.9	115.9	116.0
a(C3-C2-H)	120.3	120.1	120.3	120.0	120.1	120.0	120.2	120.4	120.2	120.2	120.1
a(C2-C3-H)	120.1	120.3	120.1	120.2	120.4	120.4	120.2	120.1	120.2	120.3	120.3
a(C3-C4-H)	120.8	120.8	120.9	120.9	120.8	120.8	120.7	120.8	120.8	120.8	120.7
maleic anhydride											
r(C1-C2)	1.332	1.341	1.341	1.349	1.347	1.341	1.333	1.333	1.336	1.338	1.332
r(C2-C3)	1.485	1.496	1.486	1.495	1.493	1.495	1.491	1.484	1.484	1.488	1.491
r(C3-O4)	1.385	1.389	1.361	1.392	1.405	1.388	1.388	1.359	1.387	1.403	1.387
r(C3-O7)	1.189	1.200	1.184	1.200	1.207	1.199	1.194	1.179	1.194	1.201	1.193
r(C1-H)	1.077	1.094	1.077	1.090	1.096	1.093	1.084	1.068	1.076	1.087	1.084
a(C1-C2-C3)	108.0	107.8	107.4	107.7	108.1	107.8	108.0	107.5	107.9	108.3	108.0
a(C2-C3-O7)	129.7	129.6	129.6	129.4	129.8	129.6	129.8	129.7	129.6	129.9	129.7
a(C1-C2-H)	129.9	130.1	129.8	129.9	122.1	122.2	129.8	129.8	122.3	129.7	129.8
a(C2-C3-O4)	107.8	107.9	107.7	108.0	108.0	107.9	107.7	107.5	107.9	107.7	107.7
a(C3-O4-C5)	108.5	108.5	109.9	108.6	108.0	108.5	108.6	110.0	108.4	108.1	108.6
a(O4-C5-O6)	122.6	122.5	122.8	122.6	122.3	122.4	122.6	122.8	122.5	122.4	122.6

Table S2: Cartesian coordinates for converged structures.

NH_3
cc-pVDZ
tPBE

N	0.00000000	-0.14766472	0.00159492
H	-0.81287007	0.28932101	0.46318920
H	0.81287007	0.28932101	0.46318920
H	0.00000000	0.26421428	-0.94458186

CASSCF

N	0.00000000	-0.16538529	0.00175373
H	-0.81002690	0.27779935	0.46296293
H	0.81002690	0.27779935	0.46296293
H	0.00000000	0.25718720	-0.93989149

CASPT2

N	0.00000000	-0.16239035	0.00111724
H	-0.80716704	0.27595633	0.46086712
H	0.80716704	0.27595633	0.46086712
H	0.00000000	0.25603528	-0.93715919

PBE

N	0.00000000	-0.16749308	0.00188547
H	-0.80987204	0.27917134	0.46276915
H	0.80987204	0.27917134	0.46276915
H	0.00000000	0.25792300	-0.93982945

cc-pVTZ
tPBE

N	0.00000000	-0.13613215	0.00029953
H	-0.81662591	0.25921817	0.47171729
H	0.81662591	0.25921817	0.47171729
H	0.00000000	0.25880922	-0.94279536

CASSCF

N	0.00000000	-0.14762469	0.00060721
H	-0.81081767	0.26625688	0.46425421
H	0.81081767	0.26625688	0.46425421
H	0.00000000	0.25096906	-0.94003624

CASPT2

N	0.00000000	-0.14053877	-0.00032342
H	-0.80791967	0.26175633	0.46224823
H	0.80791967	0.26175633	0.46224823
H	0.00000000	0.24838370	-0.93709963

PBE

N	0.00000000	-0.14428808	0.00088894
H	-0.81377613	0.26396783	0.46667652
H	0.81377613	0.26396783	0.46667652

H 0.00000000 0.24992151 -0.94274029

HCN
cc-pVDZ
tPBE
C 0.64514852 0.00000000 0.00000000
H 1.72910410 0.00000000 0.00000000
N -0.52473075 0.00000000 0.00000000
CASSCF
C 0.64334135 0.00000000 0.00000000
H 1.72991061 0.00000000 0.00000000
N -0.52976236 0.00000000 0.00000000
CASPT2
C 0.64501574 0.00000000 0.00000000
H 1.72840309 0.00000000 0.00000000
N -0.52992924 0.00000000 0.00000000
PBE
C 0.64280437 0.00000000 0.00000000
H 1.72762403 0.00000000 0.00000000
N -0.52693880 0.00000000 0.00000000
cc-pVTZ
tPBE
C 0.64435475 0.00000000 0.00000000
H 1.71827923 0.00000000 0.00000000
N -0.51427341 0.00000000 0.00000000
CASSCF
C 0.64351628 0.00000000 0.00000000
H 1.71926723 0.00000000 0.00000000
N -0.51929391 0.00000000 0.00000000
CASPT2
C 0.64524053 0.00000000 0.00000000
H 1.71322143 0.00000000 0.00000000
N -0.51497235 0.00000000 0.00000000
PBE
C 0.64246394 0.00000000 0.00000000
H 1.71710702 0.00000000 0.00000000
N -0.51608136 0.00000000 0.00000000

CH2O
cc-pVDZ
tPBE
C 0.00000000 0.00000000 0.07812042
O 0.00000000 0.00000000 1.29249167
H 0.95376854 0.00000000 -0.52785384

H -0.95376854 0.00000000 -0.52785384
CASSCF
C 0.00000000 0.00000000 0.08611615
O 0.00000000 0.00000000 1.29540759
H 0.94711555 0.00000000 -0.52602374
H -0.94711555 0.00000000 -0.52602374
CASPT2
C 0.00000000 0.00000000 0.08135830
O 0.00000000 0.00000000 1.29629416
H 0.94726985 0.00000000 -0.52215246
H -0.94726985 0.00000000 -0.52215246
PBE
C 0.00000000 0.00000000 0.08422637
O 0.00000000 0.00000000 1.29683382
H 0.95271204 0.00000000 -0.52556019
H -0.95271204 0.00000000 -0.52556019
cc-pVTZ
tPBE
C 0.00000000 0.00000000 0.10477625
O 0.00000000 0.00000000 1.31350639
H 0.94694717 0.00000000 -0.49065199
H -0.94694717 0.00000000 -0.49065199
CASSCF
C 0.00000000 0.00000000 0.08350455
O 0.00000000 0.00000000 1.28890579
H 0.94057748 0.00000000 -0.51691034
H -0.94057748 0.00000000 -0.51691034
CASPT2
C 0.00000000 0.00000000 0.07785862
O 0.00000000 0.00000000 1.28679783
H 0.93803561 0.00000000 -0.50915645
H -0.93803561 0.00000000 -0.50915645
PBE
C 0.00000000 0.00000000 0.08133352
O 0.00000000 0.00000000 1.28943199
H 0.94624806 0.00000000 -0.51526551
H -0.94624806 0.00000000 -0.51526551

HCCH
cc-pVDZ
tPBE
C 0.00000000 0.00000000 -0.61055259
C 0.00000000 0.00000000 0.61055259
H 0.00000000 0.00000000 -1.68990453
H 0.00000000 0.00000000 1.68990453
CASSCF

C 0.00000000 0.00000000 -0.61406016
C 0.00000000 0.00000000 0.61406016
H 0.00000000 0.00000000 -1.69865819
H 0.00000000 0.00000000 1.69865819

CASPT2
C 0.00000000 0.00000000 -0.61427712
C 0.00000000 0.00000000 0.61427712
H 0.00000000 0.00000000 -1.69434385
H 0.00000000 0.00000000 1.69434385
PBE
C 0.00000000 0.00000000 -0.60997953
C 0.00000000 0.00000000 0.60997953
H 0.00000000 0.00000000 -1.68930141
H 0.00000000 0.00000000 1.68930141
cc-pVTZ
tPBE
C 0.00000000 0.00000000 -0.60401869
C 0.00000000 0.00000000 0.60401869
H 0.00000000 0.00000000 -1.67445607
H 0.00000000 0.00000000 1.67445607
CASSCF
C 0.00000000 0.00000000 -0.60780492
C 0.00000000 0.00000000 0.60780492
H 0.00000000 0.00000000 -1.68167182
H 0.00000000 0.00000000 1.68167182
CASPT2
C 0.00000000 0.00000000 -0.60514462
C 0.00000000 0.00000000 0.60514462
H 0.00000000 0.00000000 -1.67012036
H 0.00000000 0.00000000 1.67012036
PBE
C 0.00000000 0.00000000 -0.60344121
C 0.00000000 0.00000000 0.60344121
H 0.00000000 0.00000000 -1.67360527
H 0.00000000 0.00000000 1.67360527

oxirane
cc-pVDZ
tPBE
O 0.00000000 0.00000000 -0.81734522
C -0.73783357 0.00000000 0.41113702
C 0.73783357 0.00000000 0.41113702
H 1.27815021 0.93449561 0.64327315
H -1.27815021 -0.93449561 0.64327315
H 1.27815021 -0.93449561 0.64327315

H -1.27815021 0.93449561 0.64327315
CASSCF
O 0.00000000 0.00000000 -0.82811357
C -0.72574515 0.00000000 0.42017196
C 0.72574515 0.00000000 0.42017196
H 1.26758491 0.91715215 0.64275809
H -1.26758491 -0.91715215 0.64275809
H 1.26758491 -0.91715215 0.64275809
H -1.26758491 0.91715215 0.64275809
CASPT2
O 0.00000000 0.00000000 -0.81782382
C -0.73781673 0.00000000 0.41260210
C 0.73781673 0.00000000 0.41260210
H 1.27553673 0.92940375 0.64003820
H -1.27553673 -0.92940375 0.64003820
H 1.27553673 -0.92940375 0.64003820
H -1.27553673 0.92940375 0.64003820
PBE
O 0.00000000 0.00000000 -0.82117360
C -0.73784297 0.00000000 0.41168325
C 0.73784297 0.00000000 0.41168325
H 1.28154719 0.93429615 0.64430683
H -1.28154719 -0.93429615 0.64430683
H 1.28154719 -0.93429615 0.64430683
H -1.28154719 0.93429615 0.64430683
cc-pVTZ
tPBE
O 0.00000000 0.00000000 -0.81691896
C -0.73452294 0.00000000 0.41196652
C 0.73452294 0.00000000 0.41196652
H 1.26837940 0.92506162 0.63976892
H -1.26837940 -0.92506162 0.63976892
H 1.26837940 -0.92506162 0.63976892
H -1.26837940 0.92506162 0.63976892
CASSCF
O 0.00000000 0.00000000 -0.81474618
C -0.72431157 0.00000000 0.42953481
C 0.72431157 0.00000000 0.42953481
H 1.25901820 0.90872413 0.64189098
H -1.25901820 -0.90872413 0.64189098
H 1.25901820 -0.90872413 0.64189098
H -1.25901820 0.90872413 0.64189098
CASPT2
O 0.00000000 0.00000000 -0.80524861
C -0.73246916 0.00000000 0.42022872
C 0.73246916 0.00000000 0.42022872

H	1.25973320	0.91788115	0.64169948
H	-1.25973320	-0.91788115	0.64169948
H	1.25973320	-0.91788115	0.64169948
H	-1.25973320	0.91788115	0.64169948

PBE

O	0.00000000	0.00000000	-0.81895999
C	-0.73465756	0.00000000	0.41415009
C	0.73465756	0.00000000	0.41415009
H	1.27244120	0.92609871	0.63962638
H	-1.27244120	-0.92609871	0.63962638
H	1.27244120	-0.92609871	0.63962638
H	-1.27244120	0.92609871	0.63962638

acrolein
cc-pVDZ
tPBE

C	1.52093858	-0.56658322	0.00000000
C	0.80606628	0.57004693	0.00000000
C	-0.68648113	0.52961617	0.00000000
O	-1.34600110	-0.49295815	0.00000000
H	-1.18571987	1.53926441	0.00000000
H	1.28999782	1.55826030	0.00000000
H	0.99509924	-1.53261517	0.00000000
H	2.61882538	-0.56728369	0.00000000

CASSCF

C	1.51401313	-0.55676318	0.00000000
C	0.79208620	0.57719454	0.00000000
C	-0.69428424	0.57280676	0.00000000
O	-1.36210404	-0.43050701	0.00000000
H	-1.18088205	1.55807084	0.00000000
H	1.27669408	1.54670165	0.00000000
H	1.02535388	-1.52211501	0.00000000
H	2.59582303	-0.53718860	0.00000000

CASPT2

C	1.51388797	-0.55521951	0.00000000
C	0.79948639	0.59341662	0.00000000
C	-0.69175917	0.56496920	0.00000000
O	-1.35281048	-0.46114803	0.00000000
H	-1.18982341	1.56393634	0.00000000
H	1.28866557	1.57330755	0.00000000
H	0.99233063	-1.51669482	0.00000000
H	2.60672249	-0.55436735	0.00000000

PBE

C	1.51707614	-0.55348446	0.00000000
C	0.79723327	0.58706290	0.00000000
C	-0.69154475	0.55933269	0.00000000
O	-1.36364591	-0.46439241	0.00000000
H	-1.18428702	1.57633753	0.00000000
H	1.28348303	1.57674656	0.00000000
H	0.99165525	-1.52199945	0.00000000
H	2.61672999	-0.55140336	0.00000000

cc-pVTZ

tPBE

C	1.75417334	-1.00410313	0.00000000
C	0.92551768	0.04097900	0.00000000
C	-0.55154603	-0.14326315	0.00000000
O	-1.11208781	-1.21708140	0.00000000
H	-1.14259312	0.80297013	0.00000000
H	1.29899213	1.06590434	0.00000000
H	1.34947899	-2.01600736	0.00000000
H	2.83553481	-0.88356451	0.00000000

CASSCF

C	1.51321520	-0.55462496	0.00000000
C	0.79160587	0.57032832	0.00000000
C	-0.69296918	0.57233716	0.00000000
O	-1.36730112	-0.42057873	0.00000000
H	-1.17002185	1.55281914	0.00000000
H	1.27052864	1.53261316	0.00000000
H	1.03598540	-1.51536666	0.00000000
H	2.58565704	-0.52932741	0.00000000

CASPT2

C	1.50789332	-0.54966544	0.00000000
C	0.79840014	0.58579861	0.00000000
C	-0.68249871	0.56470179	0.00000000
O	-1.34782085	-0.45109909	0.00000000
H	-1.17377428	1.55021072	0.00000000
H	1.28088284	1.55331895	0.00000000
H	0.99702406	-1.50127915	0.00000000
H	2.58659349	-0.54378638	0.00000000

PBE

C	1.51542385	-0.55107245	0.00000000
C	0.79523157	0.57890496	0.00000000
C	-0.68945898	0.56086865	0.00000000
O	-1.37012704	-0.45091396	0.00000000
H	-1.17310988	1.57007397	0.00000000
H	1.27589812	1.56066252	0.00000000
H	1.00762014	-1.51766327	0.00000000
H	2.60522221	-0.54266040	0.00000000

butadiene
cc-pVDZ
tPBE

C	0.63084227	0.37033097	0.00000000
C	-0.63084227	-0.37033097	0.00000000
C	-1.84767650	0.20581625	0.00000000
C	1.84767650	-0.20581625	0.00000000
H	1.95988403	-1.30030021	0.00000000
H	-1.95988403	1.30030021	0.00000000
H	-2.76777602	-0.39308344	0.00000000
H	2.76777602	0.39308344	0.00000000
H	-0.55185247	-1.46990328	0.00000000
H	0.55185247	1.46990328	0.00000000

CASSCF

C	0.63187848	0.37175526	0.00000000
C	-0.63187848	-0.37175526	0.00000000
C	-1.84818501	0.20663026	0.00000000
C	1.84818501	-0.20663026	0.00000000
H	1.96375925	-1.28437437	0.00000000
H	-1.96375925	1.28437437	0.00000000
H	-2.75393717	-0.38529961	0.00000000
H	2.75393717	0.38529961	0.00000000
H	-0.55905958	-1.45462480	0.00000000
H	0.55905958	1.45462480	0.00000000

CASPT2

C	0.62810328	0.37593687	0.00000000
C	-0.62810328	-0.37593687	0.00000000
C	-1.85226682	0.20718757	0.00000000
C	1.85226682	-0.20718757	0.00000000
H	1.95886671	-1.29689658	0.00000000
H	-1.95886671	1.29689658	0.00000000
H	-2.76847820	-0.38869778	0.00000000
H	2.76847820	0.38869778	0.00000000
H	-0.54903434	-1.47040547	0.00000000
H	0.54903434	1.47040547	0.00000000

PBE

C	0.62798026	0.36861504	0.00000000
C	-0.62798026	-0.36861504	0.00000000
C	-1.85126215	0.20784362	0.00000000
C	1.85126215	-0.20784362	0.00000000
H	1.96505899	-1.30380738	0.00000000
H	-1.96505899	1.30380738	0.00000000

H	-2.77159977	-0.39328274	0.00000000
H	2.77159977	0.39328274	0.00000000
H	-0.54909442	-1.47046131	0.00000000
H	0.54909442	1.47046131	0.00000000

cc-pVTZ

tPBE

C	0.62855399	0.36943172	0.00000000
C	-0.62855399	-0.36943172	0.00000000
C	-1.83726382	0.20320297	0.00000000
C	1.83726382	-0.20320297	0.00000000
H	1.94835782	-1.28799605	0.00000000
H	-1.94835782	1.28799605	0.00000000
H	-2.75074551	-0.38793206	0.00000000
H	2.75074551	0.38793206	0.00000000
H	-0.55098247	-1.45971076	0.00000000
H	0.55098247	1.45971076	0.00000000

CASSCF

C	0.63013476	0.37093000	0.00000000
C	-0.63013476	-0.37093000	0.00000000
C	-1.83909450	0.20482707	0.00000000
C	1.83909450	-0.20482707	0.00000000
H	1.95322976	-1.27344172	0.00000000
H	-1.95322976	1.27344172	0.00000000
H	-2.73796236	-0.38080052	0.00000000
H	2.73796236	0.38080052	0.00000000
H	-0.55749515	-1.44474596	0.00000000
H	0.55749515	1.44474596	0.00000000

CASPT2

C	0.62301634	0.37366637	0.00000000
C	-0.62301634	-0.37366637	0.00000000
C	-1.83461899	0.20423722	0.00000000
C	1.83461899	-0.20423722	0.00000000
H	1.93722986	-1.28028811	0.00000000
H	-1.93722986	1.28028811	0.00000000
H	-2.73990225	-0.38267610	0.00000000
H	2.73990225	0.38267610	0.00000000
H	-0.54402190	-1.45414065	0.00000000
H	0.54402190	1.45414065	0.00000000

PBE

C	0.62580374	0.36726388	0.00000000
C	-0.62580374	-0.36726388	0.00000000
C	-1.84131678	0.20588182	0.00000000
C	1.84131678	-0.20588182	0.00000000
H	1.95519166	-1.29196166	0.00000000
H	-1.95519166	1.29196166	0.00000000

H	-2.75475104	-0.38797631	0.00000000
H	2.75475104	0.38797631	0.00000000
H	-0.54768080	-1.45969065	0.00000000
H	0.54768080	1.45969065	0.00000000

pyrrole
cc-pVDZ
tPBE

C	0.71258300	0.00000000	0.99183549
C	-0.71258300	0.00000000	0.99183549
C	1.12608733	0.00000000	-0.33328432
C	-1.12608733	0.00000000	-0.33328432
N	0.00000000	0.00000000	-1.11859460
H	-2.12462137	0.00000000	-0.77611468
H	2.12462137	0.00000000	-0.77611468
H	0.00000000	0.00000000	-2.13409354
H	1.37104712	0.00000000	1.86399344
H	-1.37104712	0.00000000	1.86399344

CASSCF

C	0.71586309	0.00000000	0.96946670
C	-0.71586309	0.00000000	0.96946670
C	1.11854963	0.00000000	-0.34464328
C	-1.11854963	0.00000000	-0.34464328
N	0.00000000	0.00000000	-1.13260727
H	-2.10503520	0.00000000	-0.77609852
H	2.10503520	0.00000000	-0.77609852
H	0.00000000	0.00000000	-2.12755338
H	1.36546946	0.00000000	1.82943573
H	-1.36546946	0.00000000	1.82943573

CASPT2

C	0.71553242	0.00000000	0.98205686
C	-0.71553242	0.00000000	0.98205686
C	1.12899973	0.00000000	-0.34602696
C	-1.12899973	0.00000000	-0.34602696
N	0.00000000	0.00000000	-1.13501049
H	-2.12404599	0.00000000	-0.78672741
H	2.12404599	0.00000000	-0.78672741
H	0.00000000	0.00000000	-2.14721441
H	1.37218793	0.00000000	1.85092241
H	-1.37218793	0.00000000	1.85092241

PBE

C	0.71464395	0.00000000	0.98189460
C	-0.71464395	0.00000000	0.98189460
C	1.13060377	0.00000000	-0.34498614
C	-1.13060377	0.00000000	-0.34498614
N	0.00000000	0.00000000	-1.13475126

H	-2.13020278	0.00000000	-0.78884731
H	2.13020278	0.00000000	-0.78884731
H	0.00000000	0.00000000	-2.15213104
H	1.37239645	0.00000000	1.85682115
H	-1.37239645	0.00000000	1.85682115

cc-pVTZ

tPBE

C	0.70969707	0.00000000	0.97488371
C	-0.70969707	0.00000000	0.97488371
C	1.12216863	0.00000000	-0.34233420
C	-1.12216863	0.00000000	-0.34233420
N	0.00000000	0.00000000	-1.12639557
H	-2.11279323	0.00000000	-0.77969608
H	2.11279323	0.00000000	-0.77969608
H	0.00000000	0.00000000	-2.13583973
H	1.36164811	0.00000000	1.84012467
H	-1.36164811	0.00000000	1.84012467

CASSCF

C	0.71373284	0.00000000	0.96334574
C	-0.71373284	0.00000000	0.96334574
C	1.11489256	0.00000000	-0.34375249
C	-1.11489256	0.00000000	-0.34375249
N	0.00000000	0.00000000	-1.13012575
H	-2.09385910	0.00000000	-0.76983987
H	2.09385910	0.00000000	-0.76983987
H	0.00000000	0.00000000	-2.11827775
H	1.35680561	0.00000000	1.81665012
H	-1.35680561	0.00000000	1.81665012

CASPT2

C	0.71022498	0.00000000	0.97146645
C	-0.71022498	0.00000000	0.97146645
C	1.12182466	0.00000000	-0.34374446
C	-1.12182466	0.00000000	-0.34374446
N	0.00000000	0.00000000	-1.12986162
H	-2.10521670	0.00000000	-0.77673896
H	2.10521670	0.00000000	-0.77673896
H	0.00000000	0.00000000	-2.13302114
H	1.35755819	0.00000000	1.82989974
H	-1.35755819	0.00000000	1.82989974

PBE

C	0.71184593	0.00000000	0.97520343
C	-0.71184593	0.00000000	0.97520343
C	1.12670568	0.00000000	-0.34366297
C	-1.12670568	0.00000000	-0.34366297
N	0.00000000	0.00000000	-1.13223987
H	-2.11864310	0.00000000	-0.78116762

H 2.11864310 0.00000000 -0.78116762
H 0.00000000 0.00000000 -2.14340671
H 1.36269597 0.00000000 1.84327374
H -1.36269597 0.00000000 1.84327374

pyridine

cc-pVDZ

tPBE
C -0.71255550 0.00000000 -1.14107210
C -0.71255550 0.00000000 1.14107210
N -1.41920015 0.00000000 0.00000000
C 0.68527435 0.00000000 1.20038796
C 0.68527435 0.00000000 -1.20038796
C 1.40045691 0.00000000 0.00000000
H 1.19876901 0.00000000 -2.17047829
H 1.19876901 0.00000000 2.17047829
H 2.49900529 0.00000000 0.00000000
H -1.30425010 0.00000000 2.07049051
H -1.30425010 0.00000000 -2.07049051

CASSCF
C -0.71115649 0.00000000 -1.14026491
C -0.71115649 0.00000000 1.14026491
N -1.40314516 0.00000000 0.00000000
C 0.68468217 0.00000000 1.19724737
C 0.68468217 0.00000000 -1.19724737
C 1.40111761 0.00000000 0.00000000
H 1.18857782 0.00000000 -2.15392262
H 1.18857782 0.00000000 2.15392262
H 2.48296963 0.00000000 0.00000000
H -1.29554575 0.00000000 2.05190925
H -1.29554575 0.00000000 -2.05190925

CASPT2
C -0.71602932 0.00000000 -1.14460599
C -0.71602932 0.00000000 1.14460599
N -1.42778703 0.00000000 0.00000000
C 0.68766242 0.00000000 1.20379939
C 0.68766242 0.00000000 -1.20379939
C 1.40788910 0.00000000 0.00000000
H 1.19708021 0.00000000 -2.17136007
H 1.19708021 0.00000000 2.17136007
H 2.50203028 0.00000000 0.00000000
H -1.30334585 0.00000000 2.07001451
H -1.30334585 0.00000000 -2.07001451

PBE
C -0.71628588 0.00000000 -1.14597577
C -0.71628588 0.00000000 1.14597577
N -1.42597153 0.00000000 0.00000000

C	0.68676669	0.00000000	1.20437548
C	0.68676669	0.00000000	-1.20437548
C	1.40468181	0.00000000	0.00000000
H	1.20256506	0.00000000	-2.17582136
H	1.20256506	0.00000000	2.17582136
H	2.50493798	0.00000000	0.00000000
H	-1.30919432	0.00000000	2.07705246
H	-1.30919432	0.00000000	-2.07705246

cc-pVTZ

tPBE

C	-0.72174722	0.00000000	-1.13842659
C	-0.72174722	0.00000000	1.13842659
N	-1.42077081	0.00000000	0.00000000
C	0.66892506	0.00000000	1.19475225
C	0.66892506	0.00000000	-1.19475225
C	1.37931159	0.00000000	0.00000000
H	1.17861053	0.00000000	-2.15645891
H	1.17861053	0.00000000	2.15645891
H	2.46859891	0.00000000	0.00000000
H	-1.30815231	0.00000000	2.05958239
H	-1.30815231	0.00000000	-2.05958239

CASSCF

C	-0.70623964	0.00000000	-1.13723650
C	-0.70623964	0.00000000	1.13723650
N	-1.39255446	0.00000000	0.00000000
C	0.68353994	0.00000000	1.19248629
C	0.68353994	0.00000000	-1.19248629
C	1.39569514	0.00000000	0.00000000
H	1.18395292	0.00000000	-2.14096099
H	1.18395292	0.00000000	2.14096099
H	2.46872587	0.00000000	0.00000000
H	-1.28561994	0.00000000	2.04150078
H	-1.28561994	0.00000000	-2.04150078

CASPT2

C	-0.70622578	0.00000000	-1.13875850
C	-0.70622578	0.00000000	1.13875850
N	-1.40866346	0.00000000	0.00000000
C	0.68521612	0.00000000	1.19459877
C	0.68521612	0.00000000	-1.19459877
C	1.39708711	0.00000000	0.00000000
H	1.18967163	0.00000000	-2.14912166
H	1.18967163	0.00000000	2.14912166
H	2.47743228	0.00000000	0.00000000
H	-1.28701808	0.00000000	2.05181027
H	-1.28701808	0.00000000	-2.05181027

PBE

C	-0.71071149	0.00000000	-1.14319744
C	-0.71071149	0.00000000	1.14319744
N	-1.41306868	0.00000000	0.00000000
C	0.68505141	0.00000000	1.19854681
C	0.68505141	0.00000000	-1.19854681
C	1.39834159	0.00000000	0.00000000
H	1.19700388	0.00000000	-2.16151056
H	1.19700388	0.00000000	2.16151056
H	2.48929571	0.00000000	0.00000000
H	-1.29841261	0.00000000	2.06598589
H	-1.29841261	0.00000000	-2.06598589

Maleic anhydride
cc-pVDZ
tPBE

C	0.67042807	0.00000000	1.09180151
C	-0.67042807	0.00000000	1.09180151
C	1.12774297	0.00000000	-0.33270601
C	-1.12774297	0.00000000	-0.33270601
O	0.00000000	0.00000000	-1.14418670
O	-2.24210058	0.00000000	-0.77815708
O	2.24210058	0.00000000	-0.77815708
H	1.37481000	0.00000000	1.92931592
H	-1.37481000	0.00000000	1.92931592

CASSCF

C	0.67035141	0.00000000	1.08322278
C	-0.67035141	0.00000000	1.08322278
C	1.11436675	0.00000000	-0.33486586
C	-1.11436675	0.00000000	-0.33486586
O	0.00000000	0.00000000	-1.11689507
O	-2.21021661	0.00000000	-0.78185095
O	2.21021661	0.00000000	-0.78185095
H	1.36071000	0.00000000	1.91038909
H	-1.36071000	0.00000000	1.91038909

CASPT2

C	0.67464930	0.00000000	1.09026078
C	-0.67464930	0.00000000	1.09026078
C	1.13003189	0.00000000	-0.33402691
C	-1.13003189	0.00000000	-0.33402691
O	0.00000000	0.00000000	-1.14678626
O	-2.24585475	0.00000000	-0.77645323
O	2.24585475	0.00000000	-0.77645323
H	1.37321732	0.00000000	1.92700563
H	-1.37321732	0.00000000	1.92700563

PBE

C	0.67369062	0.00000000	1.08958250

C	-0.67369062	0.00000000	1.08958250
C	1.13680617	0.00000000	-0.32943976
C	-1.13680617	0.00000000	-0.32943976
O	0.00000000	0.00000000	-1.15561365
O	-2.25857041	0.00000000	-0.77608676
O	2.25857041	0.00000000	-0.77608676
H	1.37591615	0.00000000	1.93155766
H	-1.37591615	0.00000000	1.93155766

cc-pVTZ

tPBE

C	0.66631593	0.00000000	1.08125692
C	-0.66631593	0.00000000	1.08125692
C	1.12775827	0.00000000	-0.33660175
C	-1.12775827	0.00000000	-0.33660175
O	0.00000000	0.00000000	-1.14649514
O	-2.23665431	0.00000000	-0.77882501
O	2.23665431	0.00000000	-0.77882501
H	1.36103444	0.00000000	1.91398587
H	-1.36103444	0.00000000	1.91398587

CASSCF

C	0.66653199	0.00000000	1.08195442
C	-0.66653199	0.00000000	1.08195442
C	1.11253525	0.00000000	-0.33323148
C	-1.11253525	0.00000000	-0.33323148
O	0.00000000	0.00000000	-1.11285129
O	-2.20431871	0.00000000	-0.77865626
O	2.20431871	0.00000000	-0.77865626
H	1.35027927	0.00000000	1.90278461
H	-1.35027927	0.00000000	1.90278461

CASPT2

C	0.66816459	0.00000000	1.08401445
C	-0.66816459	0.00000000	1.08401445
C	1.12453099	0.00000000	-0.32774521
C	-1.12453099	0.00000000	-0.32774521
O	0.00000000	0.00000000	-1.13894456
O	-2.23393429	0.00000000	-0.76857364
O	2.23393429	0.00000000	-0.76857364
H	1.35605160	0.00000000	1.91124896
H	-1.35605160	0.00000000	1.91124896

PBE

C	0.66923577	0.00000000	1.08597448
C	-0.66923577	0.00000000	1.08597448
C	1.13588148	0.00000000	-0.32707521
C	-1.13588148	0.00000000	-0.32707521
O	0.00000000	0.00000000	-1.15136874
O	-2.25265774	0.00000000	-0.76976028

O 2.25265774 0.00000000 -0.76976028
H 1.36318804 0.00000000 1.92222975
H -1.36318804 0.00000000 1.92222975

Ozone

cc-pVDZ

tPBE

O -0.47645515 0.00000000 0.00000000
O 0.19162828 0.00000000 1.08847090
O 0.19162828 0.00000000 -1.08847090

CASSCF

O -0.48246976 0.00000000 0.00000000
O 0.19764290 0.00000000 1.09628368
O 0.19764290 0.00000000 -1.09628368

CASPT2

O -0.48244396 0.00000000 0.00000000
O 0.19761709 0.00000000 1.09649016
O 0.19761709 0.00000000 -1.09649016

PBE

O 0.19625261 0.00000000 1.08844311
O 0.19625261 0.00000000 -1.08844311
O -0.44243537 0.00000000 0.00000000

cc-pVTZ

tPBE

O -0.47437353 0.00000000 0.00000000
O 0.18954666 0.00000000 1.08694724
O 0.18954666 0.00000000 -1.08694724

CASSCF

O -0.47842751 0.00000000 0.00000000
O 0.19360064 0.00000000 1.09201944
O 0.19360064 0.00000000 -1.09201944

CASPT2

O -0.47885811 0.00000000 0.00000000
O 0.19403124 0.00000000 1.09113875
O 0.19403124 0.00000000 -1.09113875

PBE

O 0.000000 0.000000 -0.437636
O -1.094375 0.000000 0.218818
O 1.094375 -0.000000 0.218818

***o*-benzyne**

cc-pVDZ

tPBE

C -0.70434679 0.00000000 -1.07449812
C 0.70434679 0.00000000 -1.07449812
C -1.46477820 0.00000000 0.11970509
C 1.46477820 0.00000000 0.11970509
C -0.63379949 0.00000000 1.23122643

C	0.63379949	0.00000000	1.23122643
H	-1.23537601	0.00000000	-2.03695414
H	1.23537601	0.00000000	-2.03695414
H	2.56166110	0.00000000	0.11788758
H	-2.56166110	0.00000000	0.11788758

tBLYP

C	-0.70641145	0.00000000	-1.07865726
C	0.70641145	0.00000000	-1.07865726
C	-1.46549712	0.00000000	0.11940032
C	1.46549712	0.00000000	0.11940032
C	-0.63321883	0.00000000	1.23598878
C	0.63321883	0.00000000	1.23598878
H	-1.23782410	0.00000000	-2.03914569
H	1.23782410	0.00000000	-2.03914569
H	2.56064272	0.00000000	0.11978069
H	-2.56064272	0.00000000	0.11978069

CASSCF

C	-0.71174744	0.00000000	-1.07662456
C	0.71174744	0.00000000	-1.07662456
C	-1.45388115	0.00000000	0.10599867
C	1.45388115	0.00000000	0.10599867
C	-0.63107476	0.00000000	1.24320016
C	0.63107476	0.00000000	1.24320016
H	-1.22978245	0.00000000	-2.02741036
H	1.22978245	0.00000000	-2.02741036
H	2.53361168	0.00000000	0.11220294
H	-2.53361168	0.00000000	0.11220294

CASPT2

C	-0.70796716	0.00000000	-1.08015930
C	0.70796716	0.00000000	-1.08015930
C	-1.46808985	0.00000000	0.11754257
C	1.46808985	0.00000000	0.11754257
C	-0.64019625	0.00000000	1.24359707
C	0.64019625	0.00000000	1.24359707
H	-1.23713475	0.00000000	-2.03912301
H	1.23713475	0.00000000	-2.03912301
H	2.56071194	0.00000000	0.11550952
H	-2.56071194	0.00000000	0.11550952

PBE

C	-0.72347833	0.00000000	-1.14088589
C	0.72347833	0.00000000	-1.14088589
C	-1.42480158	0.00000000	0.11860283
C	1.42480158	0.00000000	0.11860283
C	-0.69304798	0.00000000	1.33940077
C	0.69304798	0.00000000	1.33940077
H	-1.26597506	0.00000000	-2.09561724

H 1.26597506 0.00000000 -2.09561724
H 2.52402991 0.00000000 0.13586637
H -2.52402991 0.00000000 0.13586637
BLYP
C -0.708002 0.0 -1.131831
C 0.708010 0.0 -1.131825
C -1.475055 0.0 0.071307
C 1.475058 0.0 0.071317
C -0.633563 0.0 1.185703
C 0.633553 0.0 1.185703
H -1.242001 0.0 -2.094620
H 1.242013 0.0 -2.094613
H 2.573229 0.0 0.069577
H -2.573227 0.0 0.069559
cc-pVTZ
tPBE
C -0.70081736 0.00000000 -1.07190031
C 0.70081736 0.00000000 -1.07190031
C -1.45665977 0.00000000 0.11751890
C 1.45665977 0.00000000 0.11751890
C -0.62719846 0.00000000 1.22005104
C 0.62719846 0.00000000 1.22005104
H -1.22792075 0.00000000 -2.02603246
H 1.22792075 0.00000000 -2.02603246
H 2.54390551 0.00000000 0.11772966
H -2.54390551 0.00000000 0.11772966
tBLYP
C -0.70228068 0.00000000 -1.07593979
C 0.70228068 0.00000000 -1.07593979
C -1.45540291 0.00000000 0.11662729
C 1.45540291 0.00000000 0.11662729
C -0.62577759 0.00000000 1.22316221
C 0.62577759 0.00000000 1.22316221
H -1.22904849 0.00000000 -2.02594382
H 1.22904849 0.00000000 -2.02594382
H 2.53871195 0.00000000 0.11946095
H -2.53871195 0.00000000 0.11946095
CASSCF
C -0.70949322 0.00000000 -1.07401976
C 0.70949322 0.00000000 -1.07401976
C -1.44742648 0.00000000 0.10329887
C 1.44742648 0.00000000 0.10329887
C -0.62508269 0.00000000 1.23365042
C 0.62508269 0.00000000 1.23365042
H -1.22305410 0.00000000 -2.01719136
H 1.22305410 0.00000000 -2.01719136

H 2.51786943 0.00000000 0.11162867
H -2.51786943 0.00000000 0.11162867
CASPT2
C -0.70179915 0.00000000 -1.07408782
C 0.70179915 0.00000000 -1.07408782
C -1.45600560 0.00000000 0.11427106
C 1.45600560 0.00000000 0.11427106
C -0.63073428 0.00000000 1.22474346
C 0.63073428 0.00000000 1.22474346
H -1.22394175 0.00000000 -2.02117357
H 1.22394175 0.00000000 -2.02117357
H 2.53448204 0.00000000 0.11361371
H -2.53448204 0.00000000 0.11361371
PBE
C -0.701954 0.0 -1.123706
C 0.701963 0.0 -1.123699
C -1.465315 0.0 0.068550
C 1.465316 0.0 0.068562
C -0.627003 0.0 1.167850
C 0.626993 0.0 1.167856
H -1.230444 0.0 -2.079596
H 1.230456 0.0 -2.079588
H 2.554508 0.0 0.067032
H -2.554507 0.0 0.067017
BLYP
C -0.704097 0.0 -1.129453
C 0.704105 0.0 -1.129448
C -1.464730 0.0 0.068218
C 1.464730 0.0 0.068227
C -0.626533 0.0 1.173495
C 0.626525 0.0 1.173498
H -1.233336 0.0 -2.081675
H 1.233350 0.0 -2.081667
H 2.550993 0.0 0.069549
H -2.550992 0.0 0.069532

***m*-benzyne**

cc-pVDZ

tPBE
C 1.52030567 0.00000000 0.00000000
C 0.72493717 0.00000000 -1.17315942
C 0.72493717 0.00000000 1.17315942
C -0.61133698 0.00000000 -0.79285095
C -0.61133698 0.00000000 0.79285095
C -1.71646153 0.00000000 0.00000000
H 1.09922657 0.00000000 -2.20229714
H 1.09922657 0.00000000 2.20229714

H 2.62151142 0.00000000 0.00000000
H -2.81625900 0.00000000 0.00000000
tBLYP
C 1.45353601 0.00000000 0.00000000
C 0.68382474 0.00000000 -1.18133200
C 0.68382474 0.00000000 1.18133200
C -0.68967556 0.00000000 -1.02007836
C -0.68967556 0.00000000 1.02007836
C -1.61128077 0.00000000 0.00000000
H 1.13656876 0.00000000 -2.17950954
H 1.13656876 0.00000000 2.17950954
H 2.55353132 0.00000000 0.00000000
H -2.70458118 0.00000000 0.00000000
CASSCF
C 1.40864780 0.00000000 0.00000000
C 0.66883057 0.00000000 -1.18941478
C 0.66883057 0.00000000 1.18941478
C -0.71340306 0.00000000 -1.09852175
C -0.71340306 0.00000000 1.09852175
C -1.55262029 0.00000000 0.00000000
H 1.14718177 0.00000000 -2.15904012
H 1.14718177 0.00000000 2.15904012
H 2.49211944 0.00000000 0.00000000
H -2.62883290 0.00000000 0.00000000
CASPT2
C 1.44150663 0.00000000 0.00000000
C 0.67865025 0.00000000 -1.18690753
C 0.67865025 0.00000000 1.18690753
C -0.70429849 0.00000000 -1.06312001
C -0.70429849 0.00000000 1.06312001
C -1.59362356 0.00000000 0.00000000
H 1.14395187 0.00000000 -2.17642321
H 1.14395187 0.00000000 2.17642321
H 2.53852540 0.00000000 0.00000000
H -2.68278879 0.00000000 0.00000000
PBE
C 1.511699 0.0 0.000011
C 0.713411 0.0 -1.172308
C 0.713396 0.0 1.172318
C -0.631478 0.0 -0.834975
C -0.631489 0.0 0.834968
C -1.707179 0.0 -0.000010
H 1.100973 0.0 -2.199470
H 1.100944 0.0 2.199485
H 2.615696 0.0 0.000016
H -2.808858 0.0 -0.000019

BLYP

C	1.468444	0.0	0.000010
C	0.686903	0.0	-1.181945
C	0.686889	0.0	1.181955
C	-0.686558	0.0	-1.010753
C	-0.686570	0.0	1.010744
C	-1.621833	0.0	-0.000010
H	1.137993	0.0	-2.184476
H	1.137965	0.0	2.184492
H	2.572423	0.0	0.000017
H	-2.718541	0.0	-0.000017

cc-pVTZ

tPBE

C	1.51327960	0.00000000	0.00000000
C	0.72084292	0.00000000	-1.16720780
C	0.72084292	0.00000000	1.16720780
C	-0.60787574	0.00000000	-0.78667520
C	-0.60787574	0.00000000	0.78667520
C	-1.70553820	0.00000000	0.00000000
H	1.09099575	0.00000000	-2.18779101
H	1.09099575	0.00000000	2.18779101
H	2.60514876	0.00000000	0.00000000
H	-2.79492975	0.00000000	0.00000000

tBLYP

C	1.44937374	0.00000000	0.00000000
C	0.68137549	0.00000000	-1.17287635
C	0.68137549	0.00000000	1.17287635
C	-0.68071396	0.00000000	-1.00190066
C	-0.68071396	0.00000000	1.00190066
C	-1.60498723	0.00000000	0.00000000
H	1.12524567	0.00000000	-2.16248958
H	1.12524567	0.00000000	2.16248958
H	2.53809335	0.00000000	0.00000000
H	-2.68646374	0.00000000	0.00000000

CASSCF

C	1.40573294	0.00000000	0.00000000
C	0.66714540	0.00000000	-1.18291290
C	0.66714540	0.00000000	1.18291290
C	-0.70720282	0.00000000	-1.08695888
C	-0.70720282	0.00000000	1.08695888
C	-1.54819055	0.00000000	0.00000000
H	1.13876619	0.00000000	-2.14587811
H	1.13876619	0.00000000	2.14587811
H	2.48045760	0.00000000	0.00000000
H	-2.61478544	0.00000000	0.00000000

CASPT2

C	1.43998355	0.00000000	0.00000000
C	0.67707309	0.00000000	-1.17283235
C	0.67707309	0.00000000	1.17283235
C	-0.68983884	0.00000000	-1.03150856
C	-0.68983884	0.00000000	1.03150856
C	-1.59032241	0.00000000	0.00000000
H	1.12685091	0.00000000	-2.15438361
H	1.12685091	0.00000000	2.15438361
H	2.52354379	0.00000000	0.00000000
H	-2.66536678	0.00000000	0.00000000

PBE

C	1.503992	0.0	0.000010
C	0.709061	0.0	-1.165710
C	0.709047	0.0	1.165720
C	-0.629347	0.0	-0.836361
C	-0.629357	0.0	0.836354
C	-1.691865	0.0	-0.000010
H	1.095057	0.0	-2.183504
H	1.095027	0.0	2.183519
H	2.598611	0.0	0.000017
H	-2.783111	0.0	-0.000017

BLYP

C	1.462321	0.0	0.000010
C	0.683892	0.0	-1.174459
C	0.683877	0.0	1.174468
C	-0.678764	0.0	-0.998513
C	-0.678777	0.0	0.998506
C	-1.611604	0.0	-0.000010
H	1.128898	0.0	-2.167233
H	1.128869	0.0	2.167248
H	2.554743	0.0	0.000017
H	-2.696339	0.0	-0.000016

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cc-pVDZ

tPBE

C	1.21165351	0.00000000	0.72091528
C	-1.21165351	0.00000000	0.72091528
C	1.21165351	0.00000000	-0.72091528
C	-1.21165351	0.00000000	-0.72091528
C	0.00000000	0.00000000	-1.35716940
C	0.00000000	0.00000000	1.35716940
H	-2.18196218	0.00000000	-1.23361409
H	2.18196218	0.00000000	-1.23361409
H	-2.18196218	0.00000000	1.23361409
H	2.18196218	0.00000000	1.23361409

tBLYP

C 1.21383819 0.00000000 0.72415052
C -1.21383819 0.00000000 0.72415052
C 1.21383819 0.00000000 -0.72415052
C -1.21383819 0.00000000 -0.72415052
C 0.00000000 0.00000000 -1.35962493
C 0.00000000 0.00000000 1.35962493
H -2.18306259 0.00000000 -1.23520104
H 2.18306259 0.00000000 -1.23520104
H -2.18306259 0.00000000 1.23520104
H 2.18306259 0.00000000 1.23520104
CASSCF
C 1.22286377 0.00000000 0.70675268
C -1.22286377 0.00000000 0.70675268
C 1.22286377 0.00000000 -0.70675268
C -1.22286377 0.00000000 -0.70675268
C 0.00000000 0.00000000 -1.35604553
C 0.00000000 0.00000000 1.35604553
H -2.15846083 0.00000000 -1.24887565
H 2.15846083 0.00000000 -1.24887565
H -2.15846083 0.00000000 1.24887565
H 2.15846083 0.00000000 1.24887565
CASPT2
C 1.21971733 0.00000000 0.72091728
C -1.21971733 0.00000000 0.72091728
C 1.21971733 0.00000000 -0.72091728
C -1.21971733 0.00000000 -0.72091728
C 0.00000000 0.00000000 -1.36706887
C 0.00000000 0.00000000 1.36706887
H -2.18109250 0.00000000 -1.24166800
H 2.18109250 0.00000000 -1.24166800
H -2.18109250 0.00000000 1.24166800
H 2.18109250 0.00000000 1.24166800
PBE
C 1.201005 0.0 0.740271
C -1.201004 0.0 0.740270
C 1.201006 0.0 -0.740271
C -1.201006 0.0 -0.740273
C -0.000000 0.0 -1.373070
C -0.000000 0.0 1.373071
H -2.196637 0.0 -1.204374
H 2.196635 0.0 -1.204376
H -2.196634 0.0 1.204376
H 2.196635 0.0 1.204376
BLYP
C 1.204664 0.0 0.744683
C -1.204664 0.0 0.744681

C 1.204665 0.0 -0.744682
C -1.204665 0.0 -0.744683
C -0.000001 0.0 -1.377801
C -0.000001 0.0 1.377802
H -2.198547 0.0 -1.210002
H 2.198547 0.0 -1.210003
H -2.198544 0.0 1.210003
H 2.198547 0.0 1.210003

cc-pVTZ

tPBE

C 1.20366753 0.00000000 0.71930672
C -1.20366753 0.00000000 0.71930672
C 1.20366753 0.00000000 -0.71930672
C -1.20366753 0.00000000 -0.71930672
C 0.00000000 0.00000000 -1.34784681
C 0.00000000 0.00000000 1.34784681
H -2.16788919 0.00000000 -1.22320308
H 2.16788919 0.00000000 -1.22320308
H -2.16788919 0.00000000 1.22320308
H 2.16788919 0.00000000 1.22320308

tBLYP

C 1.20444349 0.00000000 0.72215246
C -1.20444349 0.00000000 0.72215246
C 1.20444349 0.00000000 -0.72215246
C -1.20444349 0.00000000 -0.72215246
C 0.00000000 0.00000000 -1.34884302
C 0.00000000 0.00000000 1.34884302
H -2.16570623 0.00000000 -1.22327724
H 2.16570623 0.00000000 -1.22327724
H -2.16570623 0.00000000 1.22327724
H 2.16570623 0.00000000 1.22327724

CASSCF

C 1.21712000 0.00000000 0.70402776
C -1.21712000 0.00000000 0.70402776
C 1.21712000 0.00000000 -0.70402776
C -1.21712000 0.00000000 -0.70402776
C 0.00000000 0.00000000 -1.34822200
C 0.00000000 0.00000000 1.34822200
H -2.14481913 0.00000000 -1.24178996
H 2.14481913 0.00000000 -1.24178996
H -2.14481913 0.00000000 1.24178996
H 2.14481913 0.00000000 1.24178996

CASPT2

C 1.19966907 0.00000000 0.71673005
C -1.19966907 0.00000000 0.71673005
C 1.19966907 0.00000000 -0.71673005

C	-1.19966907	0.00000000	-0.71673005
C	0.00000000	0.00000000	-1.38169899
C	0.00000000	0.00000000	1.38169899
H	-2.15937430	0.00000000	-1.21393803
H	2.15937430	0.00000000	-1.21393803
H	-2.15937430	0.00000000	1.21393803
H	2.15937430	0.00000000	1.21393803

PBE

C	1.194208	0.0	0.738755
C	-1.194207	0.0	0.738754
C	1.194208	0.0	-0.738754
C	-1.194209	0.0	-0.738755
C	0.000000	0.0	-1.361666
C	-0.000000	0.0	1.361666
H	-2.182023	0.0	-1.197038
H	2.182022	0.0	-1.197039
H	-2.182022	0.0	1.197039
H	2.182023	0.0	1.197038

BLYP

C	1.197096	0.0	0.742752
C	-1.197096	0.0	0.742752
C	1.197097	0.0	-0.742752
C	-1.197097	0.0	-0.742753
C	0.000000	0.0	-1.364675
C	0.000000	0.0	1.364675
H	-2.180920	0.0	-1.202250
H	2.180919	0.0	-1.202251
H	-2.180919	0.0	1.202251
H	2.180919	0.0	1.202250

Table S3: Computed equilibrium geometries for ftPBE. Bond lengths are given an Angstroms and bond angles are given in degrees.

	ftPBE	
	cc-pVDZ	**cc-pVTZ**
NH3		
r(N-H)	1.033	1.024
a(H-N-H)	104	106
HCN		
r(H-C)	1.085	1.075
r(C-N)	1.169	1.158
CH2O		
r(C-O)	1.214	1.208
r(C-H)	1.133	1.122
a(H-C-O)	122.5	122.2

HCCH		
r(C-C)	1.221	1.208
r(C-H)	1.081	1.071
oxirane		
r(C-C)	1.478	1.473
r(C-O)	1.429	1.427
r(C-H)	1.102	1.091
a(C-O-C)	62.3	62.1
a(H-C-H)	115.5	115.7
a(H-C-O)	115.9	115.7
acrolein		
r(C1-C2)	1.491	1.488
r(C2-C3)	1.344	1.335
r(C1-O)	1.216	1.211
r(C1-H)	1.125	1.115
r(C2-H)	1.099	1.090
r(C3-H_{cis})	1.099	1.089
r(C3-H_{trans})	1.097	1.087
a(C1-C2-C3)	121.1	121.7
a(O-C1-C2)	124.3	124.6
a(C2-C1-H)	115.0	115.0
a(C3-C2-H)	121.7	121.5
a(C2-C3-H_{cis})	119.6	120.0
a(C2-C3-H_{trans})	122.0	121.9
butadiene		
r(C1-C2)	1.338	1.338
r(C2-C3)	1.457	1.457
r(C1-H_{cis})	1.089	1.089
r(C1-H_{trans})	1.087	1.087
r(C2-H)	1.092	1.092
a(C1-C2-C3)	124.2	124.2
a(C1-C2-H)	119.5	119.5
a(C2-C1-H_{cis})	121.3	121.3
a(C2-C1-H_{trans})	121.7	121.7
pyrrole		
r(C-N)	1.373	1.369
r(C2-C3)	1.387	1.379
r(C3-C4)	1.425	1.420
r(N-H)	1.014	1.008
r(C2-H)	1.092	1.082
r(C3-H)	1.092	1.082
a(H-N-C2)	124.9	125.0
a(C5-N-C2)	110.1	110.0

a(N-C2-C3)	107.6	107.6
a(C2-C3-C4)	107.3	107.4
a(N-C2-H)	121.2	121.3
a(C2-C3-H)	125.6	125.7
pyridine		
r(C2-C3)	1.400	1.392
r(C3-C4)	1.397	1.390
r(N-C2)	1.341	1.335
r(C2-H)	1.101	1.091
r(C3-H)	1.097	1.087
r(C4-H)	1.098	1.088
a(C6-N-C2)	116.6	117.0
a(N-C2-C3)	124.2	123.8
a(C2-C3-C4)	118.3	118.4
a(C3-C4-C5)	118.5	118.6
a(N-C2-H)	115.8	116.0
a(C3-C2-H)	120.0	120.1
a(C2-C3-H)	120.4	120.3
a(C3-C4-H)	120.8	120.7
maleic anhydride		
r(C1-C2)	1.341	1.332
r(C2-C3)	1.495	1.491
r(C3-O4)	1.388	1.387
r(C3-O7)	1.199	1.193
r(C1-H)	1.093	1.084
a(C1-C2-C3)	107.8	108.0
a(C2-C3-O7)	129.6	129.7
a(C1-C2-H)	122.2	129.8
a(C2-C3-O4)	107.9	107.7
a(C3-O4-C5)	108.5	108.6
a(O4-C5-O6)	122.4	122.6

Table S4: Approximate time needed for gradient calculation at each iterative step. A single processor was used for all calculations. Time is given in seconds.

	cc-PVDZ		cc-pVTZ	
molecule	CASPT2	tPBE	CASPT2	tPBE
NH3	16	7	32	14
HCN	9	4	17	10
CH2O	29	9	29	15
HCCH	20	6	20	11
oxirane	55	27	136	45
acrolein	87	39	1082	212
butadiene	558	177	3390	160
pyrrole	85	29	933	137
pyridine	183	32	2256	156
maleic anhydride	123	36	1148	218

Table S5: Computed equilibrium geometries for benzyne species. Bond lengths are given an Angstroms and bond angles are given in degrees.

		cc-pVDZ						cc-pVTZ					
	Ref.[a]	tPBE	tBLYP	CASSCF	CASPT2	PBE	BLYP	tPBE	tBLYP	CASSCF	CASPT2	PBE	BLYP
***o*-benzyne**													
r(C1-C2)	1.383	1.388	1.393	1.404	1.398	1.390	1.396	1.380	1.383	1.398	1.384	1.382	1.387
r(C2-C3)	1.403	1.416	1.418	1.396	1.419	1.423	1.427	1.409	1.410	1.389	1.407	1.416	1.419
r(C3-C4)	1.405	1.409	1.418	1.423	1.416	1.411	1.416	1.402	1.405	1.419	1.404	1.404	1.408
r(C1-C6)	1.255	1.268	1.266	1.262	1.280	1.267	1.267	1.254	1.252	1.250	1.261	1.254	1.253
r(C2-H)	1.080	1.097	1.095	1.080	1.093	1.099	1.098	1.087	1.083	1.070	1.078	1.089	1.086
r(C3-H)	1.082	1.099	1.098	1.083	1.095	1.102	1.101	1.090	1.086	1.074	1.081	1.092	1.089
a(C1-C2-C3)	111.0	110.7	110.9	112.0	111.3	110.1	110.4	110.6	110.9	111.9	111.0	110.0	110.4
a(C2-C3-C4)	122.4	122.5	122.4	122.1	122.4	122.7	112.5	112.4	122.3	122.1	122.4	122.6	122.4
a(C6-C1-C2)	126.7	126.8	126.7	125.9	126.3	127.2	127.1	127.0	126.9	126.0	126.6	127.3	127.2
a(C1-C2-H)	127.4	126.9	126.7	125.6	126.4	127.4	127.1	126.9	126.7	125.6	126.7	127.4	127.1
a(C2-C3-H)	118.9	118.6	118.7	119.3	118.7	118.4	118.5	118.6	118.7	119.4	118.7	118.4	118.5
***m*-benzyne**													
r(C1-C2)	1.383	1.360	1.375	1.382	1.386	1.362	1.377	1.350	1.363	1.374	1.369	1.352	1.366
r(C3-C4)	1.388	1.389	1.383	1.385	1.388	1.387	1.384	1.382	1.373	1.378	1.374	1.378	1.374
r(C4-C5)	1.409	1.417	1.410	1.401	1.411	1.418	1.417	1.411	1.402	1.395	1.399	1.411	1.409
r(C2-H)	1.093	1.100	1.093	1.076	1.089	1.102	1.097	1.089	1.081	1.067	1.075	1.091	1.085
r(C4-H)	1.090	1.095	1.096	1.081	1.093	1.098	1.099	1.086	1.085	1.072	1.080	1.089	1.088
r(C5-H)	1.102	1.101	1.100	1.083	1.094	1.104	1.104	1.092	1.089	1.075	1.084	1.095	1.092
a(C1-C2-C3)	99.3	71.3	95.8	105.2	100.2	75.6	94.4	71.3	94.6	104.5	97.8	76.4	93.9
a(C2-C3-C4)	135.6	160.2	138.8	131.1	135.0	156.3	139.9	160.4	139.8	131.7	137.0	155.6	140.4
a(C3-C4-C5)	117.8	108.3	116.4	118.1	117.6	110.2	116.4	108.2	116.1	118.0	117.1	110.5	116.2
a(C4-C5-C6)	113.9	111.7	113.8	116.2	114.5	111.5	113.1	111.7	113.6	116.0	113.9	111.4	112.9
a(C1-C2-H)	130.3	144.3	132.1	127.4	129.9	142.2	132.8	144.4	132.7	127.7	131.1	141.8	112.9
a(C3-C4-H)	120.0	125.9	121.1	120.0	120.3	124.8	121.3	125.9	121.3	120.1	120.5	124.6	121.5

[a] *o*-benzyne: Ref. 73 ; *m*-benzyne and *p*-benzyne: Ref. 69

a(C4-C5-H)	123.1	124.1	123.1	121.9	122.7	124.3	123.5	124.2	123.2	122.0	123.0	124.3	123.5
***p*-benzyne**													
r(C1-C2)	1.373	1.369	1.370	1.385	1.380	1.358	1.361	1.358	1.358	1.377	1.372	1.347	1.349
r(C2-C3)	1.433	1.442	1.448	1.414	1.442	1.481	1.489	1.439	1.443	1.408	1.433	1.478	1.486
r(C2-H)	1.433	1.097	1.096	1.081	1.093	1.098	1.097	1.088	1.084	1.072	1.081	1.089	1.086
a(C1-C2-C3)	118.0	117.7	117.6	118.0	117.9	117.8	117.7	117.6	117.5	117.9	119.0	117.5	117.5
a(C6-C1-C2)	124.0	124.6	124.7	124.1	124.2	124.4	124.6	124.9	125.0	124.2	122.0	124.9	125.1
a(C1-C2-H)	123.6	124.4	124.6	121.9	123.6	127.2	127.2	124.8	125.0	122.0	123.6	127.6	127.5