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

- Supporting Information -

Gauging Stability and Reactivity of Carbonyl *O*-Oxide Criegee Intermediates

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1. Optimized Geometries of Singlet Criegee Intermediates

Table S1. Optimized XYZ coordinates of singlet Criegee intermediates in Å at the B3LYP/CBSB7 level of theory and their CBS-QB3 energies in E_h

$^1CH_2OO$

C	1.071798000	-0.206395000	0.000000000
H	1.020586000	-1.290118000	0.000000000
H	1.979812000	0.382104000	0.000000000
O	0.000000000	0.455948000	0.000000000
O	-1.178898000	-0.187650000	0.000000000

CBS-QB3 (0 K)= -189.343104

CH_2O_2

C	0.730767000	0.000000000	0.000000000
H	1.304220000	-0.000001000	-0.927331000
H	1.304222000	0.000000000	0.927331000
O	-0.437065000	0.750013000	0.000000000
O	-0.437066000	-0.750013000	0.000000000

CBS-QB3 (0 K)= -189.383664

^{1}1

6	-1.153107000	-0.152076000	0.000000000
6	-0.736841000	1.141412000	0.000000000
6	1.091226000	-0.174959000	0.000000000
7	0.000000000	-0.948556000	0.000000000
7	0.674586000	1.115396000	0.000000000
6	-1.483325000	2.430452000	0.000000000
1	-1.249084000	3.032075000	0.884714000
1	-1.249084000	3.032075000	-0.884714000
1	-2.557780000	2.247141000	0.000000000
6	-2.514918000	-0.754951000	0.000000000
1	-2.670050000	-1.382455000	-0.883313000
1	-2.670050000	-1.382455000	0.883313000
1	-3.281613000	0.019991000	0.000000000
1	1.293794000	1.908896000	0.000000000
1	0.207258000	-1.950291000	0.000000000
8	2.289867000	-0.606880000	0.000000000
8	2.239669000	-2.097135000	0.000000000

CBS-QB3 (0 K)= -454.478507

^{1}2

C	0.000000000	0.676595000	-0.937874000
C	0.000000000	-0.676595000	-0.937874000
H	0.000000000	2.003549000	0.724185000

H	0.000000000	1.379586000	-1.753380000
H	0.000000000	-1.379586000	-1.753380000
H	0.000000000	-2.003549000	0.724185000
C	0.000000000	0.000000000	1.278115000
N	0.000000000	1.050008000	0.403156000
N	0.000000000	-1.050008000	0.403156000

CBS-QB3 (0 K)= -225.798462

^{1}3

C	0.000000000	0.677082000	-1.216280000
C	0.000000000	-0.677082000	-1.216280000
H	0.000000000	1.377916000	-2.034909000
H	0.000000000	-1.377916000	-2.034909000
C	0.000000000	0.000000000	0.980175000
N	0.000000000	1.062400000	0.119722000
N	0.000000000	-1.062400000	0.119722000
C	0.000000000	2.443002000	0.574850000
H	0.890168000	2.970622000	0.221207000
H	-0.890168000	2.970622000	0.221207000
H	0.000000000	2.425564000	1.662497000
C	0.000000000	-2.443002000	0.574850000
H	-0.890168000	-2.970622000	0.221207000
H	0.890168000	-2.970622000	0.221207000
H	0.000000000	-2.425564000	1.662497000

CBS-QB3 (0 K)= -304.242945

^{1}4

C	0.000000000	0.680708000	-0.639511000
C	0.000000000	-0.680708000	-0.639511000
C	0.000000000	0.000000000	1.567697000
N	0.000000000	1.060584000	0.708105000
N	0.000000000	-1.060584000	0.708105000
C	0.000000000	2.435172000	1.177597000
H	0.889032000	2.972492000	0.834340000
H	-0.889032000	2.972492000	0.834340000
H	0.000000000	2.400430000	2.264839000
C	0.000000000	-2.435172000	1.177597000
H	-0.889032000	-2.972492000	0.834340000
H	0.889032000	-2.972492000	0.834340000
H	0.000000000	-2.400430000	2.264839000
C	0.000000000	-1.658003000	-1.767247000
H	0.882251000	-2.307046000	-1.746357000
H	-0.882251000	-2.307046000	-1.746357000
H	0.000000000	-1.136339000	-2.725667000
C	0.000000000	1.658003000	-1.767247000
H	-0.882251000	2.307046000	-1.746357000

H	0.882251000	2.307046000	-1.746357000
H	0.000000000	1.136339000	-2.725667000

CBS-QB3 (0 K)= -382.708557

[1]5

C	0.000000000	-0.762819000	0.000000000
C	0.974206000	0.255714000	0.000000000
C	2.329092000	-0.037253000	0.000000000
C	2.690569000	-1.386348000	0.000000000
C	1.726032000	-2.397662000	0.000000000
C	0.361515000	-2.101336000	0.000000000
C	-1.058114000	1.206539000	0.000000000
H	3.078330000	0.745051000	0.000000000
H	-0.386449000	-2.884173000	0.000000000
H	-2.220685000	-0.409154000	0.000000000
H	0.666449000	2.401111000	0.000000000
N	-1.238874000	-0.124548000	0.000000000
N	0.279038000	1.471912000	0.000000000
H	3.740918000	-1.650946000	0.000000000
H	2.041247000	-3.433952000	0.000000000
O	-1.997715000	2.056624000	0.000000000
O	-3.294879000	1.335814000	0.000000000

CBS-QB3 (0 K)= -529.383490

[1]6

C	-1.938635000	-0.377642000	0.151742000
C	-1.459573000	1.067123000	-0.131139000
C	0.348892000	-0.333642000	-0.009035000
H	-2.226276000	-0.493023000	1.203157000
H	-2.774407000	-0.673041000	-0.482275000
H	-1.922171000	1.795336000	0.534953000
H	-1.660228000	1.354728000	-1.169185000
N	-0.026061000	0.939161000	0.114579000
N	-0.729615000	-1.157450000	-0.161461000
H	0.748331000	1.592628000	-0.013184000
H	-0.642399000	-2.122667000	0.118805000
O	1.554805000	-0.716172000	-0.025405000
O	2.453042000	0.458551000	0.033716000

CBS-QB3 (0 K)= -377.200560

[1]7

N	0.088481000	1.306599000	0.046998000
H	-0.956702000	1.322940000	-0.025539000
H	0.717194000	2.035141000	-0.243740000
C	0.419083000	0.025214000	0.005970000

N	1.695882000	-0.437395000	-0.079314000
H	1.787147000	-1.436955000	0.033164000
H	2.419904000	0.111607000	0.357773000
O	-0.530558000	-0.839263000	0.023778000
O	-1.841015000	-0.194292000	-0.015187000

CBS-QB3 (0 K)= -299.953303

[1]8

C	-1.618482000	1.170146000	0.172651000
C	-0.284067000	1.898314000	-0.023514000
C	0.075956000	-0.366059000	-0.062993000
H	-1.934800000	1.192694000	1.225519000
H	-2.422572000	1.577638000	-0.442424000
H	-0.111392000	2.682890000	0.715353000
H	-0.207819000	2.339386000	-1.026106000
N	0.695480000	0.818125000	0.123844000
N	-1.275223000	-0.191643000	-0.233615000
C	2.114616000	1.099210000	-0.093456000
H	2.632790000	0.141350000	-0.046445000
H	2.256427000	1.571446000	-1.073489000
H	2.465286000	1.780281000	0.685948000
C	-2.207945000	-1.283713000	-0.005041000
H	-2.423662000	-1.421094000	1.063043000
H	-3.139938000	-1.071785000	-0.531982000
H	-1.780376000	-2.203803000	-0.397580000
O	0.550304000	-1.542103000	-0.086136000
O	1.980170000	-1.718117000	0.169971000

CBS-QB3 (0 K)= -455.635328

[1]9

C	1.226491000	-0.715206000	0.196019000
C	-0.118047000	-0.053001000	0.075071000
H	1.192097000	-1.654501000	-0.368986000
H	1.366321000	-0.982659000	1.248699000
N	-0.269561000	1.250220000	0.135930000
H	-1.264699000	1.500734000	0.050830000
H	0.537473000	1.850055000	0.195806000
N	2.284650000	0.220599000	-0.188185000
H	3.169090000	-0.048505000	0.225303000
H	2.410936000	0.232090000	-1.194914000
O	-1.151242000	-0.793207000	-0.063877000
O	-2.369696000	-0.029756000	-0.113310000

CBS-QB3 (0 K)= -339.166979

[1]10

C	0.815398000	1.257333000	0.123646000
C	-0.371275000	0.346408000	0.015705000
C	1.428866000	-1.119268000	0.116659000
C	1.983804000	0.292878000	-0.199391000
H	0.742561000	2.107610000	-0.554791000
H	0.873018000	1.650836000	1.143926000
H	-0.801719000	-1.573789000	0.001622000
H	1.679255000	-1.441611000	1.133140000
H	1.787719000	-1.877873000	-0.580610000
H	2.886104000	0.516886000	0.369143000
H	2.229843000	0.357968000	-1.261050000
N	-0.011555000	-0.923876000	-0.017908000
O	-1.587337000	0.704078000	-0.007387000
O	-2.469745000	-0.446203000	-0.050830000

CBS-QB3 (0 K)= -361.155786

[1]11

C	-2.507449000	0.001654000	-0.060688000
H	-3.336297000	-0.696186000	0.019921000
H	-2.524151000	0.724004000	0.755175000
H	-2.532474000	0.524214000	-1.016635000
C	-0.152964000	-0.214426000	0.043439000
C	2.183949000	-0.770685000	-0.209803000
H	2.841886000	-1.160772000	0.562162000
H	2.288455000	-1.347645000	-1.128677000
H	2.304434000	0.302106000	-0.351642000
O	-1.321561000	-0.824521000	0.025384000
O	0.823774000	-1.028373000	0.288673000
O	-0.126693000	1.032519000	-0.145036000
O	1.101596000	1.764753000	0.146230000

CBS-QB3 (0 K)= -418.093553

[1]12

C	1.394882000	0.434650000	0.000000000
N	2.519200000	0.695436000	0.000000000
C	0.000000000	0.147018000	0.000000000
N	-0.935822000	1.079396000	0.000000000
H	-0.736983000	2.065142000	0.000000000
H	-1.868900000	0.644055000	0.000000000
O	-0.357231000	-1.090528000	0.000000000
O	-1.748651000	-1.237351000	0.000000000

CBS-QB3 (0 K)= -336.767918

[1]13

C	0.000000000	0.624055000	0.000000000
C	0.052917000	-1.892340000	0.000000000
C	1.340570000	-1.526526000	0.000000000
H	-0.283444000	-2.920368000	0.000000000
H	2.195317000	-2.188339000	0.000000000
S	-1.184029000	-0.630816000	0.000000000
S	1.680619000	0.195799000	0.000000000
O	-0.426748000	1.818420000	0.000000000
O	-1.850533000	1.786311000	0.000000000

CBS-QB3 (0 K)= -1060.947039

^{1}14

C	-2.097481000	0.970105000	0.000000000
C	-2.355577000	-0.368831000	0.000002000
C	-1.426203000	-1.455503000	0.000000000
C	-0.823213000	1.626201000	0.000000000
C	-0.062258000	-1.421737000	-0.000001000
C	0.429040000	1.095877000	-0.000001000
C	0.804409000	-0.290206000	-0.000001000
H	-2.958790000	1.630353000	-0.000002000
H	-3.401863000	-0.658579000	0.000001000
H	-1.872583000	-2.444502000	-0.000001000
H	-0.870590000	2.711350000	0.000000000
H	1.296628000	1.745575000	-0.000001000
H	0.467809000	-2.369418000	-0.000002000
O	2.069898000	-0.604352000	0.000000000
O	2.995988000	0.410575000	0.000001000

CBS-QB3 (0 K)= -419.945796

^{1}15

C	0.504669000	-0.424717000	-0.029162000
C	-2.009142000	0.022910000	0.370764000
C	-1.422011000	1.291790000	-0.231464000
H	-3.013461000	-0.184104000	-0.001730000
H	-1.819081000	2.179915000	0.262836000
S	-0.943536000	-1.396799000	-0.124660000
S	0.418555000	1.297243000	0.006024000
H	-1.626824000	1.358024000	-1.301262000
H	-2.029318000	0.065489000	1.460446000
O	1.654216000	-0.948039000	0.023338000
O	2.651694000	0.052250000	0.078794000

CBS-QB3 (0 K)= -1062.144010

^{1}16

C	0.342683000	-0.266181000	0.016205000

C	-1.497691000	0.996815000	0.116771000
C	-1.883405000	-0.460305000	-0.146168000
H	-1.696317000	1.312402000	1.142257000
H	-2.170212000	-0.643572000	-1.183535000
O	-0.061044000	0.986481000	-0.077442000
O	-0.643026000	-1.160807000	0.114334000
H	-2.641037000	-0.850856000	0.529343000
H	-1.926985000	1.706561000	-0.586447000
O	1.522071000	-0.640787000	0.019207000
O	2.515127000	0.421799000	-0.033907000

CBS-QB3 (0 K)= -416.905966

^{1}17

C	0.190310000	-0.184033000	0.000000000
C	2.638955000	0.309131000	-0.000001000
C	1.602426000	-0.537203000	0.000001000
H	1.780676000	-1.607810000	0.000002000
H	2.526114000	1.386287000	-0.000002000
H	3.653396000	-0.069117000	0.000000000
C	-0.296084000	1.170466000	0.000000000
H	0.488183000	1.919089000	0.000001000
C	-1.577217000	1.584963000	0.000000000
H	-2.393012000	0.881465000	-0.000001000
H	-1.785573000	2.650041000	0.000000000
O	-0.552574000	-1.246879000	0.000000000
O	-1.899941000	-1.155608000	0.000000000

CBS-QB3 (0 K)= -343.858105

^{1}18

C	0.000000000	0.381994000	0.000000000
C	0.403094000	-1.750521000	0.000000000
C	1.572469000	-1.122916000	0.000000000
H	0.102388000	-2.781685000	0.000000000
H	2.598682000	-1.440471000	0.000000000
O	-0.613273000	-0.798871000	0.000000000
O	1.335645000	0.247618000	0.000000000
O	-0.541101000	1.493257000	0.000000000
O	-2.000577000	1.454348000	0.000000000

CBS-QB3 (0 K)= -415.696595

^{1}19

C	-0.395558000	-0.285298000	0.065137000
C	0.065528000	1.121939000	-0.010485000
C	0.729863000	-1.269148000	0.160999000
C	1.594432000	1.013783000	0.166753000

C	1.938966000	-0.421400000	-0.295348000
H	0.848584000	-1.580223000	1.207913000
H	-0.468023000	1.735098000	0.722110000
H	1.852452000	1.135843000	1.223074000
H	-0.244164000	1.522674000	-0.986080000
H	2.140032000	1.775822000	-0.391005000
H	2.883766000	-0.785449000	0.110689000
H	2.014017000	-0.453165000	-1.386545000
H	0.548434000	-2.170992000	-0.426503000
O	-1.601963000	-0.637757000	0.017000000
O	-2.544847000	0.370400000	-0.091498000

CBS-QB3 (0 K)= -345.085703

^{1}20

C	-0.929595000	0.239143000	0.000001000
C	-0.071200000	1.392762000	0.000001000
C	-0.406382000	-1.097872000	0.000001000
H	-0.541212000	2.369154000	0.000001000
H	-1.119393000	-1.910607000	0.000002000
C	1.266913000	1.225246000	0.000000000
C	0.931184000	-1.271082000	0.000000000
H	1.954074000	2.062275000	0.000000000
H	1.382954000	-2.255972000	0.000000000
C	1.870106000	-0.123553000	0.000000000
O	3.081284000	-0.291656000	-0.000001000
O	-2.203794000	0.494996000	-0.000001000
O	-3.082813000	-0.509929000	-0.000001000

CBS-QB3 (0 K)= -455.879873

^{1}21

C	1.760840000	-0.531389000	0.000000000
C	0.381796000	0.028336000	0.000000000
H	1.730068000	-1.620550000	0.000001000
H	2.313068000	-0.184450000	-0.880153000
H	2.313068000	-0.184450000	0.880154000
C	0.054935000	1.467482000	0.000000000
H	-0.582799000	1.681685000	0.865479000
H	0.948747000	2.089884000	-0.000002000
H	-0.582802000	1.681684000	-0.865477000
O	-0.563954000	-0.818181000	0.000000000
O	-1.851643000	-0.338116000	0.000000000

CBS-QB3 (0 K)= -267.824432

^{1}22

C	2.104905000	-0.935904000	-0.606167000

C	1.184658000	-0.749430000	0.621199000
H	3.065202000	-1.346225000	-0.287483000
H	1.665624000	-1.623937000	-1.333031000
H	2.275801000	0.030980000	-1.077955000
C	-0.106600000	-0.119082000	0.246617000
H	0.993394000	-1.705301000	1.115047000
H	1.674633000	-0.059501000	1.316273000
C	-1.395177000	-0.874009000	0.160497000
H	-1.225580000	-1.730318000	-0.506998000
H	-1.574270000	-1.322255000	1.147782000
C	-2.610844000	-0.066128000	-0.294286000
H	-2.458194000	0.351966000	-1.290775000
H	-3.494051000	-0.707374000	-0.322655000
H	-2.811077000	0.764187000	0.384788000
O	-0.154861000	1.117550000	-0.027131000
O	1.008219000	1.859337000	0.038111000

CBS-QB3 (0 K)= -346.274829

^{1}23

C	-0.161698000	-2.530054000	0.000000000
C	0.000000000	-1.155401000	0.000000000
C	-1.140690000	-0.307916000	0.000000000
C	-2.433171000	-0.829282000	0.000000000
C	-2.578531000	-2.219863000	0.000000000
C	-1.462068000	-3.054541000	0.000000000
C	1.212273000	-0.313039000	0.000000000
C	0.807025000	1.042007000	0.000000000
C	-0.653026000	1.057756000	0.000000000
H	0.693879000	-3.195705000	0.000000000
H	-3.277624000	-0.156755000	0.000000000
H	-3.571715000	-2.653102000	0.000000000
H	-1.599877000	-4.130012000	0.000000000
C	1.733397000	2.077478000	0.000000000
H	1.408796000	3.111017000	0.000000000
C	3.090432000	1.747377000	0.000000000
H	3.834447000	2.535078000	0.000000000
C	2.562479000	-0.629829000	0.000000000
H	2.896307000	-1.661173000	0.000000000
C	3.497463000	0.412137000	0.000000000
H	4.555781000	0.177625000	0.000000000
O	-1.306035000	2.155469000	0.000000000
O	-2.666878000	2.118537000	0.000000000

CBS-QB3 (0 K)= -649.433613

^{1}24

C	-3.883293000	-0.991606000	-0.131394000

C	-3.695733000	0.225023000	0.524811000
C	-2.437000000	0.809135000	0.570551000
C	-1.337845000	0.177331000	-0.036587000
C	-1.537656000	-1.044555000	-0.699419000
C	-2.802514000	-1.620669000	-0.745768000
H	-4.867326000	-1.444933000	-0.165564000
H	-4.533053000	0.717402000	1.005654000
H	-2.289302000	1.752324000	1.080376000
H	-2.944935000	-2.558724000	-1.269748000
C	-0.015977000	0.827606000	-0.018291000
C	1.248403000	0.096030000	0.030906000
C	2.432447000	0.612591000	-0.531806000
C	3.605619000	-0.130889000	-0.485022000
C	3.635051000	-1.371381000	0.149208000
C	2.475340000	-1.881125000	0.732719000
C	1.290604000	-1.161134000	0.666912000
H	2.411407000	1.592885000	-0.980592000
H	4.507299000	0.270639000	-0.932775000
H	4.559822000	-1.935349000	0.198371000
H	2.495603000	-2.837743000	1.241714000
H	0.397277000	-1.558446000	1.131063000
H	-0.707430000	-1.528204000	-1.198193000
O	-0.105204000	2.112403000	-0.042876000
O	0.993449000	2.919098000	0.008972000

CBS-QB3 (0 K)= -650.603111

^{1}25

C	2.189132000	0.845579000	0.000000000
C	0.813334000	0.974041000	0.000000000
C	-0.009896000	-0.183173000	0.000000000
C	0.532146000	-1.459992000	0.000000000
C	1.931825000	-1.577467000	0.000000000
C	2.742358000	-0.448023000	0.000000000
C	-0.059793000	2.160715000	0.000000000
C	-1.355998000	1.767771000	0.000000000
C	-1.375658000	0.312563000	0.000000000
H	2.834261000	1.717064000	0.000000000
H	-0.118697000	-2.321728000	0.000000000
H	2.383402000	-2.562413000	0.000000000
H	3.820330000	-0.563444000	0.000001000
H	0.294831000	3.182385000	-0.000001000
H	-2.242325000	2.383421000	0.000001000
O	-2.479217000	-0.335633000	0.000001000
O	-2.447846000	-1.687788000	-0.000001000

CBS-QB3 (0 K)= -496.054631

^{1}26

C	-0.495515000	1.093401000	-0.000001000
C	0.119555000	-0.256587000	-0.000001000
C	-1.169674000	-1.024829000	0.000000000
C	-1.887194000	0.372479000	0.000001000
H	-0.238957000	1.688921000	0.881488000
H	-0.238960000	1.688920000	-0.881491000
H	-1.332783000	-1.643559000	0.886746000
H	-1.332785000	-1.643558000	-0.886747000
H	-2.488801000	0.560717000	0.887871000
H	-2.488804000	0.560717000	-0.887867000
O	1.309700000	-0.639545000	0.000000000
O	2.280058000	0.349676000	0.000001000

CBS-QB3 (0 K)= -305.821926

^{1}27

C	-1.307970000	-0.652069000	0.000000000
O	-2.352839000	-0.043232000	0.000000000
H	-1.249415000	-1.755761000	-0.000001000
C	0.002603000	0.028327000	0.000001000
C	0.207383000	1.482885000	0.000000000
H	0.810341000	1.762389000	0.871437000
H	0.810344000	1.762386000	-0.871437000
H	-0.751526000	1.996406000	-0.000002000
O	0.991506000	-0.787254000	0.000000000
O	2.232354000	-0.284549000	0.000000000

CBS-QB3 (0 K)= -341.769521

^{1}28

P	-1.079784000	1.211627000	-0.110794000
C	0.149496000	-0.119896000	-0.000101000
P	1.975826000	-0.000277000	0.124752000
H	2.271420000	-0.974850000	-0.860565000
H	2.093056000	1.108461000	-0.747246000
H	-1.771764000	0.951250000	1.091453000
H	-0.203339000	2.216177000	0.388416000
O	-0.356186000	-1.290135000	-0.009106000
O	-1.734686000	-1.303853000	-0.000997000

CBS-QB3 (0 K)= -872.369925

^{1}29

C	1.897282000	0.221197000	0.000001000
C	0.629916000	1.096927000	0.000000000
C	-0.042355000	-0.261273000	-0.000001000
C	1.226919000	-0.957503000	0.000000000

H	0.445521000	1.698810000	-0.891762000
H	0.445517000	1.698811000	0.891760000
H	2.948916000	0.472358000	0.000000000
H	1.509397000	-2.000161000	0.000000000
O	-1.237359000	-0.643239000	0.000000000
O	-2.215131000	0.335001000	0.000000000

CBS-QB3 (0 K)= -304.606914

^{1}30

C	-1.611833000	0.973126000	0.000001000
C	-1.951079000	-0.474152000	0.000001000
C	-0.808771000	-1.194161000	-0.000001000
C	0.277631000	-0.215840000	0.000001000
C	-0.267080000	1.129027000	0.000000000
H	-2.344844000	1.767984000	-0.000006000
H	-2.958319000	-0.865351000	-0.000004000
H	-0.673722000	-2.263993000	0.000003000
H	0.323460000	2.028884000	0.000002000
O	1.504701000	-0.584074000	-0.000001000
O	2.472826000	0.337133000	0.000000000

CBS-QB3 (0 K)= -342.671753

^{1}31

C	0.530804000	-0.443200000	-0.003636000
C	-1.414886000	1.322572000	-0.325537000
C	-2.053241000	0.068575000	0.305868000
H	-1.913967000	2.224054000	0.035255000
H	-3.072327000	-0.080239000	-0.056151000
P	0.398043000	1.347471000	0.194102000
P	-1.005264000	-1.419320000	-0.178321000
H	1.057241000	1.743356000	-0.991586000
H	-0.948481000	-2.106381000	1.061019000
H	-2.093146000	0.163992000	1.393103000
H	-1.510470000	1.300748000	-1.413782000
O	1.690869000	-0.957025000	-0.028996000
O	2.710806000	-0.024910000	0.013403000

CBS-QB3 (0 K)= -949.647368

^{1}32

C	-0.035596000	0.700278000	0.000000000
C	2.234515000	-0.140720000	0.000000000
C	0.911345000	-0.369722000	0.000000000
H	0.248926000	1.747529000	-0.000001000
H	0.489200000	-1.366549000	0.000002000
H	2.642064000	0.865376000	0.000000000

H	2.946554000	-0.956510000	-0.000001000
O	-1.302769000	0.536139000	0.000000000
O	-1.820772000	-0.714747000	0.000000000

CBS-QB3 (0 K)= -266.603032

^{1}33

C	-2.533513000	0.502030000	0.000007000
C	-1.484693000	1.419608000	0.000002000
C	-0.162966000	0.989340000	-0.000001000
C	0.117646000	-0.395084000	0.000000000
C	-0.956190000	-1.315087000	0.000005000
C	-2.266494000	-0.869943000	0.000009000
H	-3.559806000	0.851604000	0.000010000
H	-1.697096000	2.482391000	0.000001000
H	0.667295000	1.677649000	-0.000006000
H	-3.081814000	-1.583677000	0.000013000
C	1.435562000	-0.960360000	-0.000003000
H	1.554196000	-2.039883000	-0.000001000
H	-0.746799000	-2.379609000	0.000007000
O	2.572293000	-0.380454000	-0.000008000
O	2.673695000	0.976516000	-0.000010000

CBS-QB3 (0 K)= -419.976897

^{1}34

C	1.360596000	-0.475136000	0.000000000
C	0.484799000	0.704453000	0.000000000
H	1.113529000	-1.099924000	-0.867298000
H	2.413303000	-0.197702000	-0.000004000
H	1.113536000	-1.099923000	0.867300000
H	0.815717000	1.737888000	0.000001000
O	-0.775541000	0.586062000	0.000000000
O	-1.290517000	-0.675593000	0.000000000

CBS-QB3 (0 K)= -228.586247

^{1}35

C	0.000000000	0.346537000	0.000000000
C	1.403368000	0.321385000	0.000000000
C	0.780027000	1.511665000	0.000000000
H	0.872571000	2.587219000	0.000000000
H	2.328236000	-0.230678000	0.000000000
O	-1.091467000	-0.235184000	0.000000000
O	-0.946180000	-1.694074000	0.000000000

CBS-QB3 (0 K)= -265.337296

[1]36

P	1.239515000	-0.248408000	-0.110961000
H	2.214412000	0.609467000	0.464610000
H	0.938686000	-1.021260000	1.031713000
C	-0.106736000	0.934976000	0.035916000
H	-0.050196000	2.019634000	0.017075000
O	-1.285469000	0.464617000	0.005762000
O	-1.346433000	-0.901063000	-0.013823000

CBS-QB3 (0 K)= -530.860592

[1]37

C	1.044134000	-0.477154000	0.000000000
N	1.939899000	-1.204357000	0.000000000
C	0.000000000	0.488034000	0.000000000
O	0.346863000	1.765931000	0.000000000
H	-0.452942000	2.315170000	0.000000000
O	-1.222336000	0.167371000	0.000000000
O	-1.548421000	-1.177046000	0.000000000

CBS-QB3 (0 K)= -356.607904

[1]38

C	-0.047481000	0.507145000	0.000002000
Si	1.663780000	-0.386420000	0.000000000
C	1.317872000	-2.242975000	0.000004000
H	0.765594000	-2.568170000	-0.886013000
H	2.270969000	-2.782464000	-0.000004000
H	0.765610000	-2.568168000	0.886030000
C	2.588769000	0.038854000	-1.578655000
H	2.768093000	1.111582000	-1.641740000
H	3.549977000	-0.485851000	-1.596479000
H	2.025519000	-0.274850000	-2.462430000
C	2.588781000	0.038857000	1.578647000
H	3.549981000	-0.485863000	1.596473000
H	2.768122000	1.111583000	1.641720000
H	2.025530000	-0.274828000	2.462427000
Si	-1.856209000	-0.126193000	0.000001000
C	-2.122853000	-1.166015000	1.545303000
H	-3.162932000	-1.505596000	1.588012000
H	-1.485374000	-2.053256000	1.560934000
H	-1.925215000	-0.589419000	2.453190000
C	-2.122856000	-1.165994000	-1.545315000
H	-3.162933000	-1.505581000	-1.588023000
H	-1.925228000	-0.589383000	-2.453194000
H	-1.485372000	-2.053231000	-1.560964000
C	-2.994052000	1.364154000	0.000011000
H	-2.834065000	1.989256000	-0.882028000

H	-4.039729000	1.040452000	0.000017000
H	-2.834054000	1.989253000	0.882051000
O	0.003745000	1.786912000	0.000002000
O	1.222558000	2.391458000	0.000002000

CBS-QB3 (0 K)= -1005.312740

^{1}39

C	-0.807716000	-1.185344000	0.000009000
Si	0.649080000	0.051938000	0.000000000
C	2.186916000	-1.033801000	0.000007000
H	2.231480000	-1.675497000	-0.885276000
H	3.089479000	-0.414812000	0.000001000
H	2.231483000	-1.675485000	0.885299000
C	0.556757000	1.073718000	-1.569150000
H	-0.397051000	1.600112000	-1.616990000
H	1.368255000	1.808447000	-1.587611000
H	0.654276000	0.446197000	-2.459383000
C	0.556758000	1.073742000	1.569135000
H	0.654278000	0.446237000	2.459378000
H	1.368255000	1.808472000	1.587581000
H	-0.397050000	1.600137000	1.616966000
H	-0.759773000	-2.275379000	0.000016000
O	-2.014167000	-0.791576000	0.000005000
O	-2.246714000	0.545895000	-0.000003000

CBS-QB3 (0 K)= -597.329913

^{1}40

C	0.000000000	0.460101000	0.000000000
S	-1.583358000	-0.242468000	0.000000000
H	-1.145823000	-1.516188000	0.000000000
H	0.105806000	1.541827000	0.000000000
O	1.038825000	-0.253640000	0.000000000
O	2.257894000	0.390295000	0.000000000

CBS-QB3 (0 K)= -587.100278

^{1}41

C	0.000000000	-0.821812000	0.000000000
H	-0.286552000	-1.864253000	0.000000000
F	1.267722000	-0.534108000	0.000000000
O	-0.876408000	0.061055000	0.000000000
O	-0.513960000	1.389206000	0.000000000

CBS-QB3 (0 K)= -288.510223

^{1}42

C	-0.167447000	-0.102030000	0.000000000
H	-2.695457000	-1.197089000	-0.000001000
H	-2.410055000	0.904767000	1.205194000
H	-2.410056000	0.904770000	-1.205192000
Si	-2.046406000	0.128169000	0.000000000
Si	1.270764000	1.150374000	0.000000000
H	2.064149000	1.007897000	-1.235501000
H	0.604972000	2.477673000	-0.000001000
H	2.064149000	1.007898000	1.235501000
O	0.244116000	-1.313586000	0.000000000
O	1.586630000	-1.485582000	0.000000000

CBS-QB3 (0 K)= -769.854056

^{1}43

C	0.000000000	0.154349000	0.000000000
Cl	-0.334370000	-1.503839000	0.000000000
Cl	-1.270385000	1.292260000	0.000000000
O	1.178726000	0.600634000	0.000000000
O	2.231379000	-0.266791000	0.000000000

CBS-QB3 (0 K)= -1107.660255

^{1}44

C	-1.255192000	-0.359753000	0.000000000
O	-2.305285000	0.240898000	0.000000000
C	0.032329000	0.340591000	0.000000000
H	-1.183614000	-1.463177000	0.000000000
H	0.144437000	1.420700000	0.000000000
O	1.075151000	-0.391032000	0.000000000
O	2.277179000	0.169815000	0.000000000

CBS-QB3 (0 K)= -302.523697

^{1}45

C	0.000000000	0.202180000	0.000000000
Cl	-0.653142000	-1.358513000	0.000000000
C	-0.834285000	1.341431000	0.000000000
N	-1.542900000	2.254726000	0.000000000
O	1.265004000	0.396831000	0.000000000
O	2.098673000	-0.640584000	0.000000000

CBS-QB3 (0 K)= -740.613674

^{1}46

C	0.000000000	0.160155000	0.000000000
C	1.410033000	0.190928000	0.000000000
N	2.564757000	0.236478000	0.000000000

F	-0.661812000	1.279716000	0.000000000
O	-0.603913000	-0.948668000	0.000000000
O	-1.953235000	-0.961243000	0.000000000

CBS-QB3 (0 K)= -380.614111

^{1}47

C	0.000000000	0.388463000	0.000000000
F	1.282330000	0.340244000	0.000000000
F	-0.487848000	1.589243000	0.000000000
O	-0.748030000	-0.583665000	0.000000000
O	-0.145762000	-1.878354000	0.000000000

CBS-QB3 (0 K)= -387.672179

^{1}48

C	0.000000000	0.168186000	0.000000000
C	-0.685289000	-1.069572000	0.000000000
C	-0.681127000	1.407571000	0.000000000
N	-1.297374000	-2.049751000	0.000000000
N	-1.265449000	2.404654000	0.000000000
O	1.294426000	0.217667000	0.000000000
O	1.972855000	-0.907846000	0.000000000

CBS-QB3 (0 K)= -373.562454

^{1}49

C	-0.678022000	1.546196000	0.000000000
C	0.000000000	0.271233000	0.000000000
C	-1.429742000	0.160679000	0.000000000
H	-0.699730000	2.132968000	0.914590000
H	-0.699730000	2.132968000	-0.914590000
H	-1.927020000	-0.151422000	-0.914644000
H	-1.927020000	-0.151422000	0.914644000
O	1.105890000	-0.300434000	0.000000000
O	1.131620000	-1.678534000	0.000000000

CBS-QB3 (0 K)= -266.558336

^{1}50

C	0.813207000	-0.011845000	0.000000000
C	-0.594711000	-0.536401000	0.000000000
F	1.468814000	-0.468363000	1.085329000
F	0.859028000	1.319384000	-0.000002000
F	1.468815000	-0.468366000	-1.085327000
H	-0.813757000	-1.598759000	0.000000000
O	-1.533666000	0.303004000	0.000000000
O	-2.799726000	-0.122461000	0.000000000

CBS-QB3 (0 K)= -526.085049

^{1}51

C	-1.148597000	-0.594129000	0.000000000
C	0.001532000	0.401537000	0.000001000
F	1.723771000	-0.767932000	-1.086428000
F	2.262412000	1.035499000	0.000002000
F	1.723771000	-0.767935000	1.086426000
F	-1.907712000	-0.444411000	-1.088283000
F	-1.907715000	-0.444413000	1.088280000
F	-0.652153000	-1.841313000	0.000001000
C	1.457288000	-0.025800000	0.000001000
O	-0.199500000	1.652482000	0.000000000
O	-1.430837000	2.145630000	0.000001000

CBS-QB3 (0 K)= -862.823051

2. Optimized Geometries of Triplet Criegee Intermediates

Table S2. Optimized XYZ coordinates of triplet Criegee intermediates in Å at the ROB3LYP/CBSB7 level of theory and their ROCBS-QB3 energies in E_h

$^3CH_2OO$

C	-1.117478000	-0.144766000	0.000000000
H	-1.469032000	-0.505416000	0.957607000
H	-1.469029000	-0.505417000	-0.957607000
O	0.078544000	0.545342000	0.000000000
O	1.126822000	-0.310414000	0.000000000

CBS-QB3 (0 K)= -189.294790

^{1}1

C	-1.290394000	-0.599397000	-0.237611000
C	0.970994000	-0.364244000	-0.078034000
N	0.465716000	0.836002000	0.206612000
N	-0.027469000	-1.249367000	-0.296653000
H	1.110336000	1.566528000	0.483697000
H	0.144373000	-2.164097000	-0.684813000
O	2.221773000	-0.662350000	-0.123050000
O	3.053884000	0.427745000	0.195093000
C	-2.453516000	-1.354166000	0.317928000
H	-2.362407000	-1.500167000	1.409526000
H	-3.383016000	-0.809648000	0.138005000
H	-2.555138000	-2.339867000	-0.145868000
C	-1.699286000	2.012368000	-0.237446000
H	-1.648860000	2.125679000	-1.335576000
H	-2.754601000	1.934137000	0.032911000
H	-1.307972000	2.928437000	0.213723000

CBS-QB3 (0 K)= -454.355275

^{3}2

C	-1.572292000	1.046569000	0.058036000
C	-1.999954000	-0.398914000	-0.049890000
C	0.269321000	-0.267307000	-0.011794000
N	-0.159765000	0.992200000	0.011469000
N	-0.775108000	-1.118471000	-0.010813000
H	0.517561000	1.738637000	0.092781000
H	-0.663372000	-2.109244000	-0.160277000
O	1.507686000	-0.654607000	-0.022823000
O	2.412816000	0.396574000	0.028287000
H	-2.811625000	-0.809661000	0.546521000
H	-2.044933000	1.846336000	-0.505441000

CBS-QB3 (0 K)= -375.880704

^{3}3

C	0.093208000	1.941328000	-0.072360000
C	1.483563000	1.396112000	-0.011725000
H	-0.236451000	2.808148000	0.497405000
H	2.290684000	1.765643000	-0.644077000
C	-0.016194000	-0.306955000	0.017142000
N	-0.759177000	0.813267000	0.002880000
N	1.303555000	-0.003428000	-0.013726000
C	-2.214949000	0.944061000	0.043007000
H	-2.458562000	1.742026000	0.748503000
H	-2.589720000	1.216354000	-0.946420000
H	-2.652416000	0.002230000	0.351746000
C	2.384005000	-0.971550000	0.063409000
H	3.107297000	-0.764428000	-0.729537000
H	2.889397000	-0.896891000	1.030259000
H	1.987063000	-1.975735000	-0.065897000
O	-0.366647000	-1.563204000	0.056599000
O	-1.699069000	-1.884820000	-0.106960000

CBS-QB3 (0 K)= -454.321630

^{3}4

C	0.924121000	1.096222000	-0.097492000
C	1.503128000	-0.278417000	0.111767000
C	-0.763184000	-0.404124000	-0.011433000
N	-0.483171000	0.912030000	-0.076572000
N	0.382496000	-1.134220000	0.041946000
C	-1.421351000	2.006556000	-0.348154000
H	-1.418496000	2.707116000	0.489130000
H	-1.097407000	2.524141000	-1.254498000
H	-2.412700000	1.583305000	-0.467969000
C	0.413639000	-2.564218000	0.317995000
H	1.049302000	-3.068789000	-0.411282000
H	0.809938000	-2.742998000	1.322349000
H	-0.594265000	-2.965056000	0.246301000
C	2.789547000	-0.693419000	-0.526715000
H	3.112279000	-1.687013000	-0.205447000
H	2.719401000	-0.696211000	-1.630802000
H	3.583208000	0.006731000	-0.257374000
C	1.514958000	2.303262000	0.553689000
H	1.041538000	3.230750000	0.223776000
H	1.437090000	2.252351000	1.656075000
H	2.577354000	2.374691000	0.310934000
O	-1.895096000	-1.033969000	0.010474000
O	-3.088363000	-0.310889000	0.017432000

CBS-QB3 (0 K)= -532.793798

^{3}5

C	-0.475615000	-0.649376000	0.133396000
C	-0.622020000	0.753700000	0.082581000
C	-1.867740000	1.340858000	-0.084653000
C	-2.972558000	0.491803000	-0.210993000
C	-2.827465000	-0.895940000	-0.166752000
C	-1.573622000	-1.490085000	0.009560000
C	1.584809000	0.289519000	0.496281000
H	-1.982268000	2.417722000	-0.120194000
H	-1.463995000	-2.567133000	0.049584000
H	1.313304000	-1.795515000	0.438493000
H	0.842627000	2.264473000	0.415354000
N	0.870307000	-0.896562000	0.349189000
N	0.649417000	1.292252000	0.242381000
H	-3.957700000	0.922253000	-0.344850000
H	-3.701988000	-1.527680000	-0.266625000
O	2.764777000	0.411531000	-0.441885000
O	3.589876000	-0.602385000	-0.291775000

CBS-QB3 (0 K)= -529.299048

^{3}6

C	-1.779452000	-0.668296000	0.277179000
C	-1.740024000	0.841685000	0.014339000
C	0.368755000	-0.051715000	-0.404550000
H	-1.738019000	-0.873442000	1.355242000
H	-2.662923000	-1.148405000	-0.145321000
H	-2.256780000	1.416384000	0.785190000
H	-2.186336000	1.072550000	-0.961774000
N	-0.293125000	1.096519000	0.038852000
N	-0.548522000	-1.097445000	-0.411781000
H	0.029971000	1.970111000	-0.352588000
H	-0.171602000	-2.007028000	-0.185554000
O	1.576451000	-0.399316000	0.382446000
O	2.646242000	0.255100000	-0.033258000

CBS-QB3 (0 K)= -377.113884

^{3}7

N	-0.856599000	1.255480000	0.066711000
H	-0.143847000	1.957048000	0.185593000
H	-1.653007000	1.300777000	0.682356000
C	-0.482471000	0.013310000	-0.393624000
N	-1.141407000	-1.082667000	0.161105000
H	-1.042672000	-1.918480000	-0.400409000
H	-0.847775000	-1.276177000	1.120412000
O	0.929204000	-0.085365000	-0.628419000

O	1.641816000	-0.083725000	0.525804000

CBS-QB3 (0 K)= -299.867193

^{3}8

C	0.328907000	-1.696766000	0.501593000
C	-1.171071000	-1.445289000	0.340001000
C	-0.010907000	0.347730000	-0.542573000
H	0.652144000	-1.491404000	1.533492000
H	0.625764000	-2.712098000	0.230187000
H	-1.747451000	-1.703992000	1.231353000
H	-1.572088000	-2.011622000	-0.515614000
N	-1.206070000	-0.005161000	0.089603000
N	0.886375000	-0.709114000	-0.427986000
C	-2.451777000	0.582744000	-0.372677000
H	-2.313696000	1.656285000	-0.502869000
H	-2.790831000	0.152291000	-1.327443000
H	-3.228506000	0.426991000	0.379642000
C	2.317554000	-0.480751000	-0.449952000
H	2.692424000	-0.072117000	0.498861000
H	2.828597000	-1.424023000	-0.656082000
H	2.559321000	0.223018000	-1.246962000
O	0.465135000	1.665217000	-0.283227000
O	0.841859000	1.848606000	1.018947000

CBS-QB3 (0 K)= -455.563446

^{3}9

C	1.094715000	0.466697000	0.464940000
C	-0.201030000	0.475770000	-0.297579000
H	0.910930000	0.084582000	1.480143000
H	1.428419000	1.503292000	0.574395000
N	-1.112131000	1.488720000	-0.098382000
H	-2.060101000	1.291161000	-0.384085000
H	-1.050821000	2.022784000	0.760307000
N	2.179122000	-0.320528000	-0.118770000
H	1.901012000	-1.295668000	-0.173561000
H	2.343131000	-0.017528000	-1.074643000
O	-0.752088000	-0.784072000	-0.594195000
O	-1.285865000	-1.393524000	0.510863000

CBS-QB3 (0 K)= -339.084086

^{3}10

C	-0.367858000	1.189990000	-0.428854000
C	0.375969000	-0.110837000	-0.608639000
C	-1.745490000	-0.728380000	0.142917000
C	-1.596058000	0.778463000	0.419771000

H	0.259481000	1.933818000	0.066304000
H	-0.669944000	1.601324000	-1.397917000
H	-0.150700000	-2.090025000	-0.316800000
H	-2.344305000	-0.907023000	-0.761380000
H	-2.205454000	-1.271366000	0.971262000
H	-2.499086000	1.337809000	0.172675000
H	-1.375409000	0.929690000	1.478528000
N	-0.351685000	-1.140785000	-0.032353000
O	1.763231000	-0.168446000	-0.456955000
O	2.167748000	0.127928000	0.814784000

CBS-QB3 (0 K)= -361.076338

^{3}11

C	-2.355149000	-0.454996000	0.197402000
H	-3.108486000	-1.001008000	-0.365813000
H	-2.379688000	-0.758961000	1.246931000
H	-2.537382000	0.618168000	0.117101000
C	0.000002000	-0.370924000	0.228739000
C	2.355152000	-0.454990000	0.197398000
H	3.108491000	-1.000999000	-0.365817000
H	2.537383000	0.618175000	0.117099000
H	2.379693000	-0.758956000	1.246927000
O	-1.098711000	-0.805761000	-0.401235000
O	1.098715000	-0.805758000	-0.401237000
O	0.000001000	1.020272000	0.584938000
O	-0.000010000	1.837378000	-0.499674000

CBS-QB3 (0 K)= -418.032036

^{3}12

C	1.357779000	-0.189671000	-0.028291000
N	2.460848000	-0.553215000	-0.145698000
C	0.061973000	0.263496000	0.125686000
N	-0.350104000	1.567217000	0.048354000
H	0.297736000	2.215751000	-0.375578000
H	-1.312516000	1.690768000	-0.242589000
O	-0.913156000	-0.658445000	0.514329000
O	-1.871712000	-0.772490000	-0.424929000

CBS-QB3 (0 K)= -336.707679

^{3}13

C	0.572150000	-0.000011000	-0.174145000
C	-1.916526000	-0.669987000	0.085201000
C	-1.916511000	0.670021000	0.085204000
H	-2.799061000	-1.290273000	0.161275000
H	-2.799032000	1.290325000	0.161280000

S	-0.371122000	-1.476883000	-0.088224000
S	-0.371089000	1.476883000	-0.088220000
O	1.776157000	-0.000029000	0.555362000
O	2.853693000	0.000005000	-0.239987000

CBS-QB3 (0 K)= -1060.884176

^{3}14

C	2.107029000	0.969215000	0.000000000
C	2.349457000	-0.459977000	-0.000001000
C	1.423023000	-1.468781000	-0.000001000
C	0.918426000	1.629875000	0.000001000
C	0.008998000	-1.399863000	0.000000000
C	-0.419110000	1.105038000	0.000001000
C	-0.766704000	-0.227491000	0.000001000
H	2.999689000	1.586944000	0.000001000
H	3.392432000	-0.756843000	-0.000002000
H	1.824004000	-2.478637000	-0.000002000
H	0.973239000	2.714302000	0.000002000
H	-1.240993000	1.806952000	0.000002000
H	-0.549117000	-2.327653000	0.000001000
O	-2.133312000	-0.580742000	0.000006000
O	-3.007432000	0.401597000	-0.000006000

CBS-QB3 (0 K)= -419.918330

^{3}15

C	0.619486000	-0.015597000	-0.128614000
C	-1.872146000	-0.683432000	0.397728000
C	-1.919935000	0.712267000	-0.215565000
H	-2.712826000	-1.295451000	0.067063000
H	-2.642659000	1.352738000	0.293808000
S	-0.322817000	-1.486177000	-0.194607000
S	-0.265843000	1.492939000	-0.015333000
H	-2.158641000	0.671208000	-1.278916000
H	-1.854181000	-0.642590000	1.487740000
O	1.835253000	-0.043649000	0.566380000
O	2.892552000	0.009458000	-0.257876000

CBS-QB3 (0 K)= -1062.082679

^{3}16

C	0.359784000	-0.066495000	-0.317102000
C	-1.672910000	0.795689000	0.225332000
C	-1.791987000	-0.694871000	-0.076918000
H	-1.720158000	1.012611000	1.296032000
H	-2.178102000	-0.884824000	-1.082193000
O	-0.339063000	1.097719000	-0.253626000

O	-0.420396000	-1.133865000	-0.004487000
H	-2.364501000	-1.258090000	0.657521000
H	-2.382083000	1.419688000	-0.315295000
O	1.524298000	-0.065840000	0.510444000
O	2.644600000	0.040071000	-0.195324000

CBS-QB3 (0 K)= -416.847306

^{3}17

C	-0.160444000	-0.036253000	-0.161051000
C	-2.592231000	0.346751000	0.152411000
C	-1.513039000	-0.440468000	-0.109073000
H	-1.675220000	-1.495931000	-0.306618000
H	-2.507314000	1.407045000	0.356964000
H	-3.588197000	-0.075769000	0.166266000
C	0.390634000	1.251265000	0.047518000
H	-0.324633000	2.034653000	0.277484000
C	1.707364000	1.565990000	-0.019447000
H	2.460793000	0.822140000	-0.243165000
H	2.041733000	2.580261000	0.155432000
O	0.742222000	-1.062271000	-0.526500000
O	1.332670000	-1.612242000	0.542936000

CBS-QB3 (0 K)= -343.825795

^{3}18

C	-0.298311000	-0.000007000	-0.333310000
C	1.769062000	-0.665056000	0.073598000
C	1.769052000	0.665072000	0.073601000
H	2.539987000	-1.404420000	0.192002000
H	2.539966000	1.404447000	0.192013000
O	0.477997000	-1.117703000	-0.120349000
O	0.477980000	1.117701000	-0.120343000
O	-1.440548000	-0.000021000	0.509427000
O	-2.580276000	0.000013000	-0.177153000

CBS-QB3 (0 K)= -415.641817

^{3}19

C	-0.384028000	-0.065734000	-0.475844000
C	0.356934000	1.227634000	-0.315036000
C	0.396525000	-1.251871000	-0.006966000
C	1.660319000	0.790920000	0.397966000
C	1.835744000	-0.698338000	0.026148000
H	0.056525000	-1.539130000	1.000240000
H	-0.230122000	1.951457000	0.259005000
H	1.526106000	0.883739000	1.479793000
H	0.566596000	1.689484000	-1.289584000

H	2.521901000	1.400540000	0.119563000
H	2.479625000	-1.235295000	0.725088000
H	2.283832000	-0.785159000	-0.968605000
H	0.274069000	-2.130467000	-0.647810000
O	-1.768433000	-0.098710000	-0.518439000
O	-2.315505000	0.067355000	0.714026000

CBS-QB3 (0 K)= -345.028772

^{3}20

C	-0.905605000	0.233074000	0.000008000
C	-0.089507000	1.369171000	0.000000000
C	-0.406090000	-1.072042000	0.000012000
H	-0.551610000	2.349077000	-0.000002000
H	-1.096264000	-1.903507000	0.000018000
C	1.276593000	1.203291000	-0.000006000
C	0.959769000	-1.247127000	0.000006000
H	1.952595000	2.049399000	-0.000012000
H	1.401524000	-2.236065000	0.000009000
C	1.869109000	-0.119829000	-0.000003000
O	3.114158000	-0.277845000	-0.000007000
O	-2.290084000	0.522313000	0.000022000
O	-3.065558000	-0.551734000	-0.000029000

CBS-QB3 (0 K)= -455.861366

^{3}21

C	-0.980725000	1.319028000	0.122857000
C	-0.437628000	0.000000000	-0.294949000
H	-0.647691000	2.109381000	-0.555057000
H	-2.072248000	1.302922000	0.139006000
H	-0.629902000	1.583639000	1.132137000
C	-0.980727000	-1.319028000	0.122857000
H	-0.629904000	-1.583640000	1.132137000
H	-2.072250000	-1.302920000	0.139006000
H	-0.647693000	-2.109381000	-0.555057000
O	0.927073000	0.000000000	-0.622631000
O	1.709698000	-0.000001000	0.480535000

CBS-QB3 (0 K)= -267.767292

^{3}22

C	2.303672000	-0.612030000	-0.493419000
C	1.296702000	-0.771831000	0.669891000
H	3.270369000	-1.041293000	-0.216672000
H	1.950338000	-1.121146000	-1.393467000
H	2.448986000	0.441371000	-0.738039000
C	-0.049653000	-0.188445000	0.398077000

H	1.170500000	-1.835877000	0.896598000
H	1.706181000	-0.298173000	1.568118000
C	-1.091701000	-0.777993000	-0.491614000
H	-0.977760000	-0.342076000	-1.496334000
H	-0.893863000	-1.849189000	-0.592197000
C	-2.533116000	-0.544435000	-0.007489000
H	-2.739598000	0.522431000	0.096810000
H	-3.247990000	-0.959944000	-0.721671000
H	-2.703173000	-1.017840000	0.962527000
O	-0.155638000	1.193446000	0.616663000
O	0.213211000	1.915321000	-0.468958000

CBS-QB3 (0 K)= -346.217913

^{3}23

C	-1.593245000	-2.029393000	0.108712000
C	-0.688676000	-0.985274000	0.008495000
C	-1.165871000	0.355027000	-0.127521000
C	-2.536271000	0.632074000	-0.161675000
C	-3.429041000	-0.431967000	-0.059148000
C	-2.965406000	-1.745247000	0.073852000
C	0.780310000	-0.941742000	0.012431000
C	1.177802000	0.425260000	-0.118533000
C	-0.017683000	1.198230000	-0.206191000
H	-1.254205000	-3.054122000	0.213357000
H	-2.891618000	1.650760000	-0.261138000
H	-4.495658000	-0.241579000	-0.081850000
H	-3.679289000	-2.557144000	0.152051000
C	2.530059000	0.782497000	-0.144201000
H	2.825122000	1.820435000	-0.242726000
C	3.483444000	-0.227039000	-0.038019000
H	4.537061000	0.026162000	-0.054058000
C	1.744578000	-1.930594000	0.116090000
H	1.466036000	-2.973826000	0.216454000
C	3.097720000	-1.565887000	0.090022000
H	3.857922000	-2.334289000	0.170889000
O	-0.046850000	2.568445000	-0.410137000
O	-0.312110000	3.237547000	0.730279000

CBS-QB3 (0 K)= -649.396919

^{3}24

C	-3.924295000	-1.013898000	-0.019820000
C	-3.718020000	0.336046000	0.271349000
C	-2.444959000	0.881433000	0.224427000
C	-1.323644000	0.081123000	-0.105808000
C	-1.555814000	-1.280057000	-0.421023000
C	-2.835341000	-1.812587000	-0.372540000

H	-4.922071000	-1.435236000	0.016956000
H	-4.557991000	0.967108000	0.538868000
H	-2.299502000	1.927751000	0.456887000
H	-2.988121000	-2.855297000	-0.627516000
C	-0.010344000	0.662466000	-0.164904000
C	1.285944000	0.053577000	-0.070755000
C	2.429554000	0.730328000	-0.563227000
C	3.688082000	0.157944000	-0.472237000
C	3.857177000	-1.095671000	0.118704000
C	2.745901000	-1.767027000	0.632192000
C	1.480674000	-1.207083000	0.544889000
H	2.311897000	1.701338000	-1.025145000
H	4.545911000	0.691548000	-0.865607000
H	4.843847000	-1.538250000	0.189782000
H	2.870948000	-2.727197000	1.120033000
H	0.639992000	-1.719454000	0.992738000
H	-0.732445000	-1.902990000	-0.743634000
O	-0.012136000	2.055298000	-0.405201000
O	0.291892000	2.761091000	0.697597000

CBS-QB3 (0 K)= -650.567690

^{3}25

C	2.214038000	0.830200000	0.071792000
C	0.831071000	0.974239000	0.031364000
C	-0.007305000	-0.181220000	-0.055856000
C	0.543751000	-1.453150000	-0.099343000
C	1.941603000	-1.578878000	-0.059611000
C	2.764134000	-0.457310000	0.024856000
C	-0.017428000	2.141041000	0.052912000
C	-1.361669000	1.720908000	-0.015777000
C	-1.362893000	0.337015000	-0.080748000
H	2.858811000	1.699926000	0.138469000
H	-0.087558000	-2.329604000	-0.157230000
H	2.385012000	-2.567225000	-0.094096000
H	3.840272000	-0.581750000	0.056055000
H	0.320977000	3.166281000	0.108220000
H	-2.239788000	2.348329000	-0.022208000
O	-2.550186000	-0.374926000	-0.228067000
O	-2.493507000	-1.591703000	0.322224000

CBS-QB3 (0 K)= -496.020726

^{3}26

C	-0.795635000	1.110771000	-0.031591000
C	0.091395000	-0.000001000	-0.519269000
C	-0.795636000	-1.110771000	-0.031589000
C	-1.852340000	0.000001000	0.282650000

H	-0.394550000	1.606245000	0.860409000
H	-1.080887000	1.877590000	-0.757280000
H	-0.394551000	-1.606245000	0.860411000
H	-1.080889000	-1.877590000	-0.757278000
H	-2.227181000	0.000001000	1.305344000
H	-2.693832000	0.000000000	-0.409514000
O	1.471448000	-0.000001000	-0.575972000
O	2.026700000	0.000001000	0.663060000

CBS-QB3 (0 K)= -305.768210

^{3}27

C	1.162140000	-0.725161000	0.024711000
O	2.283891000	-0.273520000	-0.196591000
H	0.973875000	-1.807041000	0.137827000
C	0.012638000	0.116345000	0.162461000
C	-0.018079000	1.583736000	0.025136000
H	-0.752248000	1.871546000	-0.735048000
H	-0.323544000	2.053838000	0.967500000
H	0.971573000	1.940480000	-0.256061000
O	-1.173070000	-0.540028000	0.501936000
O	-2.087052000	-0.424995000	-0.478854000

CBS-QB3 (0 K)= -341.725957

^{3}28

P	1.670825000	-0.725761000	-0.046590000
C	0.000463000	-0.054555000	-0.250786000
P	-1.610822000	-0.756546000	0.183423000
H	-2.301477000	-0.443589000	-1.018021000
H	-1.323804000	-2.097320000	-0.168361000
H	1.948392000	-0.260508000	1.271701000
H	1.272023000	-2.016329000	0.374913000
O	-0.036758000	1.303793000	-0.599849000
O	-0.025488000	2.118667000	0.473848000

CBS-QB3 (0 K)= -872.315911

^{3}29

C	-1.905384000	-0.086981000	-0.224030000
C	-0.936964000	1.073800000	0.053487000
C	0.036451000	-0.079357000	0.263044000
C	-0.919711000	-1.052939000	-0.029065000
H	-1.156102000	1.683970000	0.934058000
H	-0.716427000	1.718821000	-0.801252000
H	-2.961757000	-0.120613000	-0.442283000
H	-0.898989000	-2.133015000	-0.075360000
O	1.376012000	-0.122319000	0.553355000

O	2.134853000	0.087781000	-0.552828000

CBS-QB3 (0 K)= -304.562968

^{3}30

C	-1.691276000	0.928142000	0.000000000
C	-1.989535000	-0.420644000	0.000001000
C	-0.731980000	-1.191551000	0.000000000
C	0.276832000	-0.272367000	-0.000001000
C	-0.281056000	1.063641000	-0.000001000
H	-2.399196000	1.742618000	0.000000000
H	-2.975703000	-0.863490000	0.000003000
H	-0.633488000	-2.266038000	0.000002000
H	0.303676000	1.969892000	-0.000003000
O	1.602401000	-0.602832000	-0.000003000
O	2.423449000	0.449544000	0.000003000

CBS-QB3 (0 K)= -342.642064

^{3}31

C	-0.604060000	-0.054719000	-0.280929000
C	1.802733000	0.790368000	0.472263000
C	1.976732000	-0.631355000	-0.096833000
H	2.666997000	1.412559000	0.230877000
H	2.768902000	-1.166329000	0.431250000
P	0.250257000	1.535349000	-0.284576000
P	0.344699000	-1.536442000	0.119814000
H	-0.326773000	2.124189000	0.876348000
H	0.284303000	-2.227004000	-1.123989000
H	2.243218000	-0.593568000	-1.155062000
H	1.701749000	0.759471000	1.559075000
O	-1.973303000	-0.125776000	-0.500284000
O	-2.691093000	0.010939000	0.636026000

CBS-QB3 (0 K)= -949.594912

^{3}32

C	0.030131000	0.301265000	-0.208791000
C	-2.389462000	0.190895000	0.091559000
C	-1.127130000	-0.382334000	0.061470000
H	0.140217000	1.359516000	-0.402525000
H	-1.024489000	-1.447591000	0.250161000
H	-2.535049000	1.247458000	-0.099446000
H	-3.265795000	-0.406374000	0.302128000
O	1.229990000	-0.428258000	-0.275394000
O	2.220495000	0.251763000	0.310926000

CBS-QB3 (0 K)= -266.564874

^{3}33

C	2.666332000	0.368205000	-0.116388000
C	1.698463000	1.375149000	-0.019068000
C	0.357451000	1.059190000	0.094029000
C	-0.061795000	-0.302660000	0.107631000
C	0.937689000	-1.314235000	0.008018000
C	2.272347000	-0.976062000	-0.101143000
H	3.714943000	0.626998000	-0.202075000
H	2.002111000	2.415910000	-0.030471000
H	-0.387488000	1.840341000	0.172527000
H	3.019349000	-1.758172000	-0.176574000
C	-1.404470000	-0.673131000	0.222866000
H	-1.786348000	-1.684194000	0.219969000
H	0.637350000	-2.356251000	0.018441000
O	-2.379440000	0.321477000	0.369857000
O	-3.370063000	0.140602000	-0.517044000

CBS-QB3 (0 K)= -419.935263

^{3}34

C	1.524309000	-0.375969000	0.060264000
C	0.474252000	0.634243000	-0.196642000
H	1.266371000	-1.333905000	-0.414317000
H	2.483137000	-0.043481000	-0.341211000
H	1.633625000	-0.564241000	1.133094000
H	0.455885000	1.302579000	-1.049992000
O	-0.769642000	0.440571000	0.395772000
O	-1.459155000	-0.554395000	-0.209435000

CBS-QB3 (0 K)= -228.530864

^{3}35

C	-0.322044000	-0.139244000	-0.038149000
C	-1.139728000	0.886497000	0.009860000
C	-1.675853000	-0.528680000	-0.098740000
H	-2.276282000	-1.105316000	0.604336000
H	-1.339434000	1.940555000	0.025673000
O	0.943040000	-0.619877000	-0.022412000
O	1.862143000	0.351543000	0.038933000

CBS-QB3 (0 K)= -265.278899

^{3}36

P	1.393558000	-0.303203000	-0.045090000
H	2.358239000	0.691772000	-0.337569000
H	1.572881000	-0.267263000	1.363413000
C	-0.038330000	0.783464000	-0.153101000

H	-0.176848000	1.502608000	-0.954996000
O	-1.220623000	0.359527000	0.445810000
O	-1.832834000	-0.619510000	-0.255297000

CBS-QB3 (0 K)= -530.804235

^{3}37

C	1.308311000	-0.160261000	-0.001329000
N	2.378528000	-0.605319000	-0.110068000
C	0.035342000	0.355932000	0.185501000
O	-0.271651000	1.601923000	-0.189656000
H	-1.171111000	1.811633000	0.098018000
O	-0.987952000	-0.467180000	0.599238000
O	-1.682959000	-0.978296000	-0.463653000

CBS-QB3 (0 K)= -356.570258

^{3}38

C	0.008959000	0.382375000	-0.257099000
Si	-1.733641000	-0.322334000	-0.016140000
C	-1.849857000	-2.010373000	-0.844167000
H	-1.176383000	-2.740237000	-0.388173000
H	-2.869270000	-2.398542000	-0.747929000
H	-1.616114000	-1.951742000	-1.910824000
C	-2.072892000	-0.498459000	1.828706000
H	-1.988040000	0.468673000	2.330490000
H	-3.084756000	-0.882709000	1.995642000
H	-1.371620000	-1.188881000	2.305778000
C	-2.955586000	0.871412000	-0.795679000
H	-3.980342000	0.517296000	-0.645992000
H	-2.873331000	1.866758000	-0.352607000
H	-2.786985000	0.969231000	-1.871728000
Si	1.762552000	-0.278715000	-0.001809000
C	2.687951000	-0.154368000	-1.637130000
H	3.726522000	-0.479346000	-1.516531000
H	2.227621000	-0.778955000	-2.407731000
H	2.699048000	0.876202000	-2.002117000
C	1.692184000	-2.070046000	0.568856000
H	2.707097000	-2.429571000	0.767134000
H	1.118348000	-2.185740000	1.492550000
H	1.255246000	-2.724643000	-0.189604000
C	2.606284000	0.793438000	1.293155000
H	2.118809000	0.699316000	2.267030000
H	3.655201000	0.500852000	1.407393000
H	2.578125000	1.848442000	1.009190000
O	0.036656000	1.744886000	-0.652694000
O	-0.217429000	2.573164000	0.373878000

CBS-QB3 (0 K)= -1005.263358

^{3}39

C	-0.861650000	-0.405820000	0.879061000
Si	0.735213000	0.023538000	-0.007685000
C	2.022887000	0.329249000	1.326180000
H	2.169091000	-0.555413000	1.952745000
H	2.988335000	0.577771000	0.874873000
H	1.737137000	1.160953000	1.976485000
C	1.228856000	-1.420246000	-1.107824000
H	0.442647000	-1.647971000	-1.833025000
H	2.139960000	-1.182131000	-1.666171000
H	1.418208000	-2.324428000	-0.523011000
C	0.446758000	1.555945000	-1.057012000
H	0.180244000	2.417135000	-0.439135000
H	1.348994000	1.807287000	-1.624036000
H	-0.365442000	1.395385000	-1.771033000
H	-1.058049000	-0.442639000	1.949065000
O	-2.010316000	-0.667261000	0.120384000
O	-2.779085000	0.430980000	0.000666000

CBS-QB3 (0 K)= -597.278089

^{3}40

C	-0.002408000	0.768525000	-0.117348000
S	1.435894000	-0.198930000	-0.062031000
H	1.227299000	-0.691632000	1.173842000
H	-0.135109000	1.423810000	-0.970011000
O	-1.166202000	0.305357000	0.481908000
O	-1.840304000	-0.575412000	-0.295314000

CBS-QB3 (0 K)= -587.055249

^{3}41

C	0.561965000	0.461251000	-0.318917000
H	0.981252000	1.455630000	-0.433720000
F	1.413091000	-0.472833000	0.096720000
O	-0.638048000	0.448585000	0.361372000
O	-1.495810000	-0.444540000	-0.176779000

CBS-QB3 (0 K)= -288.461391

^{3}42

C	0.109695000	0.024102000	-0.151202000
H	2.445426000	0.629139000	1.177538000
H	2.160933000	-1.657258000	0.399437000
H	2.673549000	0.119077000	-1.167072000
Si	1.949652000	-0.230252000	0.077856000

Si	-1.318683000	-1.184025000	-0.006182000
H	-2.386628000	-0.806250000	-0.955886000
H	-0.772566000	-2.516941000	-0.347768000
H	-1.857341000	-1.236980000	1.371363000
O	-0.219817000	1.379320000	-0.422696000
O	-1.249571000	1.761238000	0.350967000

CBS-QB3 (0 K)= -769.804006

^{3}43

C	0.032743000	-0.000003000	-0.126459000
Cl	-0.834722000	1.478634000	-0.025582000
Cl	-0.834904000	-1.478535000	-0.025583000
O	1.251106000	-0.000079000	0.538814000
O	2.272292000	-0.000130000	-0.335245000

CBS-QB3 (0 K)= -1107.615266

^{3}44

C	-1.250074000	0.349882000	0.000000000
O	-2.315714000	-0.259593000	-0.000001000
C	0.004015000	-0.318410000	0.000002000
H	-1.195683000	1.455255000	0.000001000
H	0.137184000	-1.391153000	0.000002000
O	1.111360000	0.472970000	0.000000000
O	2.271211000	-0.244994000	-0.000001000

CBS-QB3 (0 K)= -302.464332

^{3}45

C	-0.096157000	-0.000993000	0.187084000
Cl	0.823970000	-1.408306000	-0.059242000
C	-1.466849000	0.039134000	-0.000605000
N	-2.622466000	0.070144000	-0.141773000
O	0.570166000	1.139797000	0.581778000
O	1.145810000	1.762872000	-0.471697000

CBS-QB3 (0 K)= -740.576803

^{3}46

C	-0.027482000	0.330735000	0.186242000
C	-1.290184000	-0.196968000	-0.001962000
N	-2.359061000	-0.645703000	-0.116127000
F	0.256729000	1.572030000	-0.154965000
O	1.023145000	-0.416382000	0.603267000
O	1.740463000	-0.887486000	-0.465531000

CBS-QB3 (0 K)= -380.578165

^{3}47

C	0.385453000	0.005315000	-0.275264000
F	0.730225000	1.228381000	0.087520000
F	1.355051000	-0.858412000	-0.060321000
O	-0.769729000	-0.443482000	0.390339000
O	-1.865297000	0.023281000	-0.214490000

CBS-QB3 (0 K)= -387.633309

^{3}48

C	0.000003000	-0.090861000	0.180839000
C	1.231176000	-0.718009000	0.003509000
C	-1.231154000	-0.718040000	0.003510000
N	2.262298000	-1.236455000	-0.134765000
N	-2.262264000	-1.236511000	-0.134762000
O	-0.000013000	1.251940000	0.584749000
O	-0.000036000	2.057088000	-0.489806000

CBS-QB3 (0 K)= -373.531784

^{3}49

C	-1.494387000	-0.640514000	-0.035637000
C	-0.203995000	-0.063552000	-0.408982000
C	-1.188919000	0.876658000	0.138920000
H	-2.198083000	-0.908579000	-0.816240000
H	-1.536727000	-1.262076000	0.853771000
H	-1.030129000	1.257751000	1.142846000
H	-1.698231000	1.554042000	-0.537741000
O	0.952492000	-0.446863000	0.287256000
O	2.020880000	0.237276000	-0.138311000

CBS-QB3 (0 K)= -266.516144

^{3}50

C	0.743292000	0.001770000	-0.016162000
C	-0.490256000	-0.651735000	-0.545227000
F	1.022848000	-0.405087000	1.234016000
F	0.633935000	1.346643000	0.017881000
F	1.783891000	-0.308731000	-0.810712000
H	-0.598539000	-0.913775000	-1.588960000
O	-1.619356000	-0.595058000	0.235276000
O	-2.366363000	0.484826000	-0.111947000

CBS-QB3 (0 K)= -526.042368

^{3}51

C	1.337848000	-0.334538000	-0.004237000

C	0.003980000	0.307389000	-0.267210000
F	-1.424037000	-0.778132000	1.259159000
F	-2.324633000	0.483273000	-0.267480000
F	-1.466986000	-1.442651000	-0.805886000
F	1.985919000	0.291940000	0.992414000
F	2.116146000	-0.266097000	-1.097535000
F	1.183916000	-1.622388000	0.329777000
C	-1.322750000	-0.363753000	-0.015799000
O	0.025317000	1.614364000	-0.664635000
O	-0.118742000	2.429626000	0.418316000

CBS-QB3 (0 K)= -862.784877

3. Optimized Geometries of Hydrogenated Compounds

Table S3. Optimized XYZ coordinates of hydrogenated compounds in Å at the B3LYP/CBSB7 level of theory and their CBS-QB3 energies in E_h

CH_4

C	0.000000000	0.000000000	0.000000000
H	0.629738000	0.629738000	0.629738000
H	-0.629738000	-0.629738000	0.629738000
H	-0.629738000	0.629738000	-0.629738000
H	0.629738000	-0.629738000	-0.629738000

CBS-QB3 (0 K)= -40.410008

1-H_2

C	-0.375837000	-0.660585000	0.017256000
C	-0.309475000	0.678501000	-0.026979000
C	1.841122000	-0.079558000	0.177604000
N	0.954969000	-1.230131000	-0.040649000
N	1.042283000	1.101812000	-0.217832000
C	-1.390361000	1.705174000	0.010354000
H	-1.276422000	2.384430000	0.864335000
H	-1.360680000	2.320388000	-0.895786000
H	-2.376690000	1.245601000	0.080836000
C	-1.544859000	-1.582944000	0.053161000
H	-1.581589000	-2.215147000	-0.844261000
H	-1.482377000	-2.258630000	0.912562000
H	-2.488534000	-1.037527000	0.109324000
H	1.280797000	1.928336000	0.318837000
H	1.116731000	-1.630699000	-0.964183000
H	2.105683000	-0.033874000	1.246447000
H	2.758767000	-0.168167000	-0.407129000

CBS-QB3 (0 K)= -305.453757

2-H_2

C	-1.109016000	-0.512114000	0.084151000
C	-0.899332000	0.804293000	0.010863000
H	0.223174000	-1.655595000	-0.939445000
H	-2.042870000	-1.044951000	0.169125000
H	-1.622558000	1.604334000	0.063424000
H	0.820946000	1.895105000	0.263418000
C	1.152473000	-0.173969000	0.149631000
N	0.139726000	-1.228849000	-0.018591000
N	0.469857000	1.086168000	-0.233621000
H	1.457796000	-0.142562000	1.208217000
H	2.031683000	-0.366823000	-0.467131000

CBS-QB3 (0 K)= -226.985759

3-H_2

C	-0.710492000	1.221265000	0.287904000
C	0.549774000	1.219397000	-0.158053000
H	-1.371133000	2.059830000	0.444814000
H	1.182999000	2.062036000	-0.393412000
C	0.047657000	-0.923631000	0.393534000
N	-1.180327000	-0.119952000	0.481161000
N	1.016031000	-0.100087000	-0.355461000
H	0.436839000	-1.110717000	1.413081000
H	-0.136947000	-1.884524000	-0.093716000
C	2.411108000	-0.395746000	-0.094561000
H	2.649188000	-1.401499000	-0.450430000
H	3.047924000	0.306118000	-0.637007000
H	2.664084000	-0.341405000	0.979860000
C	-2.247356000	-0.508774000	-0.447743000
H	-2.580341000	-1.523976000	-0.219482000
H	-3.100636000	0.158176000	-0.304022000
H	-1.946044000	-0.458826000	-1.506077000

CBS-QB3 (0 K)= -305.426329

4-H_2

H	1.742412000	-0.897048000	2.305865000
H	2.770642000	-0.136274000	1.094175000
H	-1.906478000	-0.890350000	0.000000000
H	-2.350719000	0.850220000	0.000000000
C	0.680036000	0.038643000	0.673085000
C	0.680036000	0.038643000	-0.673085000
C	-1.504370000	0.155706000	0.000000000
N	-0.627451000	0.360288000	1.150139000
N	-0.627451000	0.360288000	-1.150139000
C	-1.107956000	-0.258260000	2.372733000
H	-1.243106000	-1.351165000	2.275592000
H	-0.416098000	-0.062698000	3.192907000
H	-2.072009000	0.179521000	2.644792000
C	-1.107956000	-0.258260000	-2.372733000
H	-0.416098000	-0.062698000	-3.192907000
H	-1.243106000	-1.351165000	-2.275592000
H	-2.072009000	0.179521000	-2.644792000
C	1.824091000	-0.040956000	-1.627059000
H	1.742412000	-0.897048000	-2.305865000
H	1.874994000	0.862038000	-2.247718000
H	2.770642000	-0.136274000	-1.094175000
C	1.824091000	-0.040956000	1.627059000
H	1.874994000	0.862038000	2.247718000

CBS-QB3 (0 K)= -383.896732

5-H_2

C	0.182671000	0.700933000	-0.048824000
C	0.177172000	-0.702696000	-0.016316000
C	-1.007210000	-1.413213000	0.027324000
C	-2.214195000	-0.697077000	0.041121000
C	-2.209585000	0.693895000	0.021836000
C	-1.007312000	1.414104000	-0.027025000
C	2.364200000	-0.005400000	0.182530000
H	-0.998569000	-2.496677000	0.062254000
H	-1.011840000	2.497814000	-0.062661000
H	1.731319000	2.007940000	0.312530000
H	1.740958000	-1.665210000	-0.897061000
N	1.509153000	1.150155000	-0.174210000
N	1.518694000	-1.190461000	-0.029271000
H	-3.154577000	-1.234282000	0.078423000
H	-3.148924000	1.234727000	0.045542000
H	3.262198000	-0.048379000	-0.437317000
H	2.670055000	0.042932000	1.238775000

CBS-QB3 (0 K)= -380.366396

6-H_2

C	0.941465000	-0.814809000	0.119484000
C	1.026223000	0.739399000	0.007787000
C	-1.198297000	0.028119000	0.227961000
H	1.599389000	-1.330126000	-0.581728000
H	1.215354000	-1.138163000	1.127675000
H	1.685388000	1.064670000	-0.802195000
H	1.412654000	1.165524000	0.944593000
N	-0.367330000	1.134963000	-0.279179000
N	-0.467200000	-1.175510000	-0.139505000
H	-0.599927000	2.022555000	0.153766000
H	-0.578998000	-1.299683000	-1.141833000
H	-1.316573000	0.043669000	1.324999000
H	-2.191918000	0.039124000	-0.225880000

CBS-QB3 (0 K)= -228.188261

7-H_2

N	0.000000000	1.175432000	-0.316819000
H	-0.051838000	2.027425000	0.231620000
H	0.860847000	1.198057000	-0.855198000
C	0.000000000	0.000000000	0.546201000
H	-0.881810000	0.084696000	1.202707000
H	0.881810000	-0.084696000	1.202707000
N	0.000000000	-1.175432000	-0.316819000

H	0.051838000	-2.027425000	0.231620000
H	-0.860847000	-1.198057000	-0.855198000

CBS-QB3 (0 K)= -150.941213

8-H_2

H	-0.061063000	1.356772000	-2.004218000
H	1.422184000	0.575559000	-1.393927000
N	0.000000000	1.166656000	0.100443000
N	0.000000000	-1.166656000	0.100443000
C	0.778149000	2.294295000	0.570275000
H	0.408438000	2.625988000	1.544421000
H	1.856431000	2.067169000	0.671762000
H	0.669781000	3.131284000	-0.124455000
C	-0.778149000	-2.294295000	0.570275000
H	-1.856431000	-2.067169000	0.671762000
H	-0.669781000	-3.131284000	-0.124455000
H	-0.408438000	-2.625988000	1.544421000
H	0.890844000	-0.027684000	1.641702000
H	-0.890844000	0.027684000	1.641702000
C	-0.333678000	-0.683466000	-1.237976000
C	0.333678000	0.683466000	-1.237976000
C	0.000000000	0.000000000	0.989271000
H	-1.422184000	-0.575559000	-1.393927000
H	0.061063000	-1.356772000	-2.004218000

CBS-QB3 (0 K)= -306.629724

9-H_2

H	-0.896639000	-1.939269000	0.839575000
N	0.427101000	1.825316000	-0.054129000
H	-0.136459000	2.657980000	-0.189784000
H	0.896639000	1.939269000	0.839575000
C	-0.427101000	0.632814000	-0.028687000
C	0.427101000	-0.632814000	-0.028687000
H	-1.119598000	0.597037000	0.831082000
H	-1.045620000	0.625703000	-0.929843000
H	1.045620000	-0.625703000	-0.929843000
H	1.119598000	-0.597037000	0.831082000
N	-0.427101000	-1.825316000	-0.054129000
H	0.136459000	-2.657980000	-0.189784000

CBS-QB3 (0 K)= -190.162489

10-H_2

C	0.101199000	1.024819000	0.778216000
C	0.101199000	-0.468708000	1.161896000
C	0.101199000	-0.468708000	-1.161896000

C	0.101199000	1.024819000	-0.778216000
H	-0.796866000	1.514793000	1.158784000
H	0.963462000	1.546822000	1.197742000
H	-0.407526000	-2.109435000	0.000000000
H	1.139187000	-0.810973000	-1.324043000
H	-0.465100000	-0.674668000	-2.073638000
H	0.963462000	1.546822000	-1.197742000
H	-0.796866000	1.514793000	-1.158784000
N	-0.528944000	-1.102264000	0.000000000
H	-0.465100000	-0.674668000	2.073638000
H	1.139187000	-0.810973000	1.324043000

CBS-QB3 (0 K)= -212.151842

11-H_2

C	0.000000000	2.331370000	0.194874000
H	0.000000000	3.134771000	-0.540851000
H	-0.892781000	2.430437000	0.829536000
H	0.892781000	2.430437000	0.829536000
C	0.000000000	0.000000000	0.314558000
H	0.899103000	0.000000000	0.964358000
H	-0.899103000	0.000000000	0.964358000
C	0.000000000	-2.331370000	0.194874000
H	-0.892781000	-2.430437000	0.829536000
H	0.000000000	-3.134771000	-0.540851000
H	0.892781000	-2.430437000	0.829536000
O	0.000000000	1.115159000	-0.524437000
O	0.000000000	-1.115159000	-0.524437000

CBS-QB3 (0 K)= -269.108806

12-H_2

C	-0.854026000	0.098407000	-0.008478000
N	-1.936965000	-0.294156000	-0.022406000
C	0.522930000	0.602570000	0.048261000
H	0.619514000	1.184269000	0.978391000
H	0.649954000	1.306211000	-0.779741000
N	1.484987000	-0.488904000	-0.113908000
H	2.423027000	-0.107786000	-0.173506000
H	1.457924000	-1.107136000	0.690355000

CBS-QB3 (0 K)= -187.786413

13-H_2

C	-0.448907000	-1.205999000	0.000000000
C	0.089521000	1.283855000	0.666337000
C	0.089521000	1.283855000	-0.666337000
H	-1.534631000	-1.306259000	0.000000000

H	0.133297000	2.171145000	1.283380000
H	0.133297000	2.171145000	-1.283380000
H	0.022547000	-2.186845000	0.000000000
S	0.089521000	-0.281858000	1.492188000
S	0.089521000	-0.281858000	-1.492188000

CBS-QB3 (0 K)= -911.965718

14-H_2

C	1.428440000	0.680873000	0.186120000
C	1.428465000	-0.680824000	0.186122000
C	0.347598000	-1.527601000	-0.266222000
C	0.347545000	1.527612000	-0.266222000
C	-0.962928000	-1.221533000	-0.202000000
C	-0.962971000	1.221500000	-0.201999000
C	-1.460774000	-0.000025000	0.528390000
H	2.365412000	1.177984000	0.423527000
H	2.365455000	-1.177900000	0.423532000
H	0.635557000	-2.476284000	-0.712718000
H	0.635471000	2.476307000	-0.712716000
H	-1.689378000	1.875105000	-0.675825000
H	-1.689311000	-1.875162000	-0.675828000
H	-1.065503000	-0.000018000	1.552871000
H	-2.549956000	-0.000044000	0.592024000

CBS-QB3 (0 K)= -270.966852

15-H_2

C	-0.020826000	-1.349816000	0.125155000
C	-0.692894000	1.247575000	0.372815000
C	0.685216000	1.290556000	-0.272600000
H	-1.327356000	2.066298000	0.025152000
H	1.317148000	2.056551000	0.183374000
S	-1.495306000	-0.307133000	-0.155819000
S	1.511478000	-0.323113000	0.022112000
H	0.609101000	1.477149000	-1.344116000
H	-0.624306000	1.287248000	1.461395000
H	-0.053411000	-1.815914000	1.109018000
H	-0.008902000	-2.117279000	-0.647734000

CBS-QB3 (0 K)= -913.169205

16-H_2

C	-1.177883000	-0.086126000	0.138457000
C	1.036851000	-0.662526000	-0.067369000
C	0.847675000	0.846261000	0.161269000
H	1.638554000	-1.133180000	0.715568000
H	1.512162000	1.473879000	-0.431539000

O	-0.297574000	-1.184816000	-0.045581000
O	-0.490207000	1.068294000	-0.276195000
H	0.952203000	1.106300000	1.223866000
H	1.484515000	-0.877199000	-1.042285000
H	-1.462333000	-0.009956000	1.201639000
H	-2.062712000	-0.213319000	-0.487185000

CBS-QB3 (0 K)= -267.933256

17-H_2

C	0.000000000	0.333629000	0.664508000
C	-2.210155000	-0.524373000	-0.185874000
C	-1.255783000	0.399941000	-0.168758000
H	-1.361168000	1.282892000	-0.797479000
H	-2.144002000	-1.422407000	0.421124000
H	-3.093135000	-0.418342000	-0.806006000
C	1.255782000	0.399941000	-0.168758000
H	1.361168000	1.282892000	-0.797480000
C	2.210155000	-0.524373000	-0.185874000
H	2.144003000	-1.422407000	0.421125000
H	3.093135000	-0.418342000	-0.806007000
H	0.000000000	1.183974000	1.362386000
H	0.000000000	-0.576851000	1.270881000

CBS-QB3 (0 K)= -194.885935

18-H_2

C	-0.229826000	-1.117547000	0.000000000
C	0.073717000	0.976989000	0.663632000
C	0.073717000	0.976989000	-0.663632000
H	-1.304031000	-1.363142000	0.000000000
H	0.116737000	1.771611000	1.387261000
H	0.116737000	1.771611000	-1.387261000
H	0.385434000	-2.017140000	0.000000000
O	0.073717000	-0.323845000	1.147853000
O	0.073717000	-0.323845000	-1.147853000

CBS-QB3 (0 K)= -266.725495

19-H_2

C	-0.615855000	-1.128289000	-0.157326000
C	-1.280159000	0.264800000	0.019596000
C	0.853804000	-0.926043000	0.253358000
C	-0.111454000	1.288960000	0.119879000
C	1.163189000	0.496681000	-0.235598000
H	-0.659763000	-1.433420000	-1.207898000
H	0.950515000	-0.971083000	1.344595000
H	-1.895851000	0.294209000	0.922025000

H	-0.033677000	1.669627000	1.142809000
H	-1.944039000	0.492122000	-0.817834000
H	-0.257998000	2.155490000	-0.529057000
H	2.065657000	0.922123000	0.210654000
H	1.310988000	0.485970000	-1.321694000
H	1.522167000	-1.683065000	-0.164959000
H	-1.115145000	-1.908631000	0.421906000

CBS-QB3 (0 K)= -196.116520

20-H_2

C	1.819570000	0.000000000	0.000000000
C	1.008639000	1.256902000	0.000000000
C	1.008638000	-1.256903000	0.000000000
H	1.555760000	2.195553000	0.000000000
H	1.555759000	-2.195554000	0.000000000
C	-0.329492000	1.255413000	0.000000000
C	-0.329493000	-1.255413000	0.000000000
H	-0.906245000	2.173722000	0.000000000
H	-0.906246000	-2.173721000	0.000000000
C	-1.113583000	0.000000000	0.000000000
O	-2.335104000	0.000000000	0.000000000
H	2.498066000	-0.000001000	0.866662000
H	2.498066000	0.000000000	-0.866663000

CBS-QB3 (0 K)= -306.911168

21-H_2

C	0.000000000	1.277205000	-0.259576000
C	0.000000000	0.000000000	0.585452000
H	0.000000000	2.173329000	0.367158000
H	0.882777000	1.322925000	-0.905306000
H	-0.882777000	1.322925000	-0.905306000
C	0.000000000	-1.277205000	-0.259576000
H	0.875531000	0.000000000	1.244555000
H	-0.875531000	0.000000000	1.244555000
H	0.000000000	-2.173329000	0.367158000
H	-0.882777000	-1.322925000	-0.905306000
H	0.882777000	-1.322925000	-0.905306000

CBS-QB3 (0 K)= -118.855864

22-H_2

H	-0.876174000	1.283086000	-1.182225000
C	0.000000000	2.560065000	0.323653000
H	0.882781000	2.606648000	0.969081000
H	0.000000000	3.455953000	-0.303318000
H	-0.882781000	2.606648000	0.969081000

C	0.000000000	-2.560065000	0.323653000
C	0.000000000	-1.283627000	-0.522422000
H	0.000000000	-3.455953000	-0.303318000
H	0.882781000	-2.606648000	0.969081000
H	-0.882781000	-2.606648000	0.969081000
C	0.000000000	0.000000000	0.315308000
H	0.876174000	-1.283086000	-1.182225000
H	-0.876174000	-1.283086000	-1.182225000
C	0.000000000	1.283627000	-0.522422000
H	-0.876781000	0.000000000	0.976291000
H	0.876781000	0.000000000	0.976291000
H	0.876174000	1.283086000	-1.182225000

CBS-QB3 (0 K)= -197.307278

23-H_2

C	-1.650594000	-1.501978000	-0.000001000
C	-0.734426000	-0.450151000	0.000000000
C	-1.183422000	0.884581000	0.000001000
C	-2.541775000	1.170573000	0.000001000
C	-3.456948000	0.115367000	0.000000000
C	-3.013078000	-1.208995000	-0.000001000
C	0.734426000	-0.450151000	0.000001000
C	1.183422000	0.884581000	0.000000000
C	0.000000000	1.829131000	0.000000000
H	-1.313951000	-2.532990000	-0.000001000
H	-2.893298000	2.197299000	0.000001000
H	-4.520676000	0.325288000	0.000000000
H	-3.736648000	-2.016605000	-0.000001000
C	2.541775000	1.170573000	-0.000001000
H	2.893298000	2.197299000	-0.000001000
C	3.456948000	0.115367000	0.000000000
H	4.520676000	0.325288000	-0.000001000
C	1.650594000	-1.501978000	0.000001000
H	1.313951000	-2.532990000	0.000001000
C	3.013078000	-1.208995000	0.000001000
H	3.736648000	-2.016605000	0.000001000
H	0.000000000	2.483232000	0.879681000
H	0.000000000	2.483231000	-0.879683000

CBS-QB3 (0 K)= -500.467489

24-H_2

C	3.657633000	-0.181725000	-0.866763000
C	3.452708000	0.855654000	0.037592000
C	2.271082000	0.915877000	0.776461000
C	1.277911000	-0.054653000	0.624525000
C	1.495211000	-1.091443000	-0.291153000

C	2.672925000	-1.156520000	-1.028412000
H	4.574861000	-0.231718000	-1.442665000
H	4.210623000	1.619913000	0.170449000
H	2.120480000	1.726453000	1.482627000
H	2.823667000	-1.968248000	-1.731700000
C	-0.000006000	-0.000510000	1.444602000
H	-0.042569000	-0.874814000	2.102795000
C	-1.277913000	0.054210000	0.624546000
C	-2.271142000	-0.916354000	0.775886000
C	-3.452765000	-0.855607000	0.037054000
C	-3.657628000	0.182340000	-0.866664000
C	-2.672861000	1.157174000	-1.027714000
C	-1.495152000	1.091575000	-0.290496000
H	-2.120587000	-1.727374000	1.481551000
H	-4.210724000	-1.619903000	0.169441000
H	-4.574853000	0.232740000	-1.442536000
H	-2.823555000	1.969342000	-1.730504000
H	-0.730574000	1.848882000	-0.429268000
H	0.730679000	-1.848711000	-0.430390000
H	0.042546000	0.873329000	2.103412000

CBS-QB3 (0 K)= -501.637125

25-H_2

C	0.998116000	1.413512000	0.000001000
C	-0.211873000	0.721100000	0.000000000
C	-0.229044000	-0.688691000	0.000000000
C	0.955968000	-1.408094000	-0.000001000
C	2.169011000	-0.711787000	-0.000001000
C	2.187568000	0.684187000	0.000000000
C	-1.599187000	1.194210000	-0.000001000
C	-2.437621000	0.143551000	-0.000001000
C	-1.666256000	-1.154921000	0.000001000
H	1.018103000	2.498130000	0.000001000
H	0.950236000	-2.493415000	-0.000001000
H	3.103976000	-1.260852000	-0.000001000
H	3.137975000	1.206431000	0.000000000
H	-1.887907000	2.237892000	-0.000001000
H	-3.518603000	0.191572000	-0.000001000
H	-1.901936000	-1.769080000	0.878335000
H	-1.901936000	-1.769083000	-0.878330000

CBS-QB3 (0 K)= -347.089898

26-H_2

C	0.000000000	1.084989000	0.122461000
C	1.084989000	0.000000000	-0.122461000
C	0.000000000	-1.084989000	0.122461000

C	-1.084989000	0.000000000	-0.122461000
H	0.000000000	1.960276000	-0.530325000
H	0.000000000	1.427029000	1.160626000
H	1.427029000	0.000000000	-1.160626000
H	1.960276000	0.000000000	0.530325000
H	0.000000000	-1.960276000	-0.530325000
H	0.000000000	-1.427029000	1.160626000
H	-1.427029000	0.000000000	-1.160626000
H	-1.960276000	0.000000000	0.530325000

CBS-QB3 (0 K)= -156.859865

27-H_2

C	-0.999395000	-0.221192000	0.000000000
O	-0.713502000	-1.391346000	0.000000000
H	-2.065754000	0.100110000	0.000000000
C	0.000000000	0.911537000	0.000000000
C	1.457876000	0.462365000	0.000000000
H	-0.231346000	1.542054000	0.869892000
H	-0.231346000	1.542054000	-0.869892000
H	2.129686000	1.323486000	0.000000000
H	1.677946000	-0.146596000	0.878961000
H	1.677946000	-0.146596000	-0.878961000

CBS-QB3 (0 K)= -192.808464

28-H_2

P	1.532052000	-0.259032000	-0.115453000
C	0.004990000	0.810033000	0.042037000
P	-1.622732000	-0.110912000	-0.004139000
H	-0.006052000	1.505179000	-0.802284000
H	0.011542000	1.414691000	0.951169000
H	-1.308029000	-0.996778000	-1.068679000
H	-1.321363000	-1.075231000	0.994025000
H	1.457976000	-0.860734000	1.167390000
H	2.496182000	0.701837000	0.300032000

CBS-QB3 (0 K)= -723.409321

29-H_2

H	0.000000000	1.414432000	1.601208000
H	0.000000000	-1.414432000	1.601208000
C	0.000000000	0.668647000	0.814264000
C	0.000000000	0.786385000	-0.700001000
C	0.000000000	-0.786385000	-0.700001000
C	0.000000000	-0.668647000	0.814264000
H	0.888636000	1.245653000	-1.143394000
H	-0.888636000	1.245653000	-1.143394000

H	0.888636000	-1.245653000	-1.143394000
H	-0.888636000	-1.245653000	-1.143394000

CBS-QB3 (0 K)= -155.646802

30-H_2

C	-0.734362000	0.989283000	0.000000000
C	0.734367000	0.989280000	0.000000000
C	1.179429000	-0.280992000	0.000000000
C	-0.000003000	-1.215579000	0.000000000
C	-1.179430000	-0.280986000	0.000000000
H	-1.347264000	1.881679000	0.000000000
H	1.347274000	1.881673000	0.000000000
H	2.210290000	-0.607670000	0.000000000
H	-2.210293000	-0.607660000	0.000000000
H	-0.000005000	-1.877028000	0.877131000
H	-0.000005000	-1.877028000	-0.877131000

CBS-QB3 (0 K)= -193.712772

31-H_2

C	-0.718461000	1.362866000	0.079565000
C	0.779270000	1.282596000	-0.286853000
H	-1.244232000	2.038564000	-0.599660000
H	1.355478000	2.082929000	0.185953000
P	-1.553461000	-0.335417000	0.008008000
P	1.533858000	-0.368005000	0.148245000
H	-1.544984000	-0.578570000	1.405997000
H	1.243019000	-0.318908000	1.539591000
H	0.914746000	1.400762000	-1.366725000
H	-0.847559000	1.758935000	1.088568000
H	-0.038090000	-2.284630000	0.155917000
H	0.064588000	-1.520769000	-1.420784000
C	0.004369000	-1.316629000	-0.348153000

CBS-QB3 (0 K)= -800.688790

32-H_2

C	1.233545000	-0.162316000	0.000000000
C	-1.280498000	-0.220422000	0.000000000
C	-0.134653000	0.453579000	0.000000000
H	1.807335000	0.153313000	-0.878504000
H	-0.166685000	1.541966000	0.000000000
H	-1.301835000	-1.306403000	0.000000000
H	-2.238894000	0.286426000	0.000001000
H	1.807335000	0.153315000	0.878503000
H	1.182379000	-1.253664000	0.000002000

CBS-QB3 (0 K)= -117.646237

33-H_2

C	-1.901668000	0.000000000	0.008325000
C	-1.199091000	-1.202948000	0.002046000
C	0.193810000	-1.200149000	-0.008696000
C	0.912338000	0.000001000	-0.011403000
C	0.193809000	1.200149000	-0.008696000
C	-1.199092000	1.202947000	0.002046000
H	-2.985822000	-0.000001000	0.013682000
H	-1.735640000	-2.145520000	0.001561000
H	0.731826000	-2.143016000	-0.017351000
H	-1.735642000	2.145520000	0.001560000
C	2.422452000	0.000000000	0.009181000
H	2.828193000	0.884199000	-0.487984000
H	0.731825000	2.143017000	-0.017351000
H	2.801718000	-0.000031000	1.037104000
H	2.828193000	-0.884168000	-0.488037000

CBS-QB3 (0 K)= -271.020470

34-H_2

H	0.000000000	1.018416000	1.163611000
H	-0.881974000	-0.509208000	1.163611000
H	-0.881974000	0.509208000	-1.163611000
H	0.881974000	0.509208000	-1.163611000
H	0.000000000	-1.018416000	-1.163611000
C	0.000000000	0.000000000	0.765213000
C	0.000000000	0.000000000	-0.765213000
H	0.881974000	-0.509208000	1.163611000

CBS-QB3 (0 K)= -79.630568

35-H_2

C	0.000000000	0.000000000	0.863255000
C	0.000000000	0.645007000	-0.501334000
C	0.000000000	-0.645007000	-0.501334000
H	0.912919000	0.000000000	1.460453000
H	-0.912919000	0.000000000	1.460453000
H	0.000000000	-1.575497000	-1.042209000
H	0.000000000	1.575497000	-1.042209000

CBS-QB3 (0 K)= -116.383551

36-H_2

P	0.070338000	-0.675920000	0.000000000
H	-0.886391000	-0.865038000	1.032032000
H	-0.886391000	-0.865038000	-1.032032000

C	0.070338000	1.192449000	0.000000000
H	0.611877000	1.542312000	0.881415000
H	0.611877000	1.542312000	-0.881415000
H	-0.928081000	1.629550000	0.000000000

CBS-QB3 (0 K)= -381.907077

37-H_2

C	-0.656975000	-0.513192000	0.000000000
N	-1.201624000	-1.527566000	0.000000000
C	0.000000000	0.796348000	0.000000000
O	1.403884000	0.604608000	0.000000000
H	1.816250000	1.474108000	0.000000000
H	-0.347053000	1.341528000	0.888326000
H	-0.347053000	1.341528000	-0.888326000

CBS-QB3 (0 K)= -207.655007

38-H_2

H	-2.113662000	-2.739718000	-1.113393000
H	-2.720877000	-1.656500000	0.140996000
H	-2.143605000	-0.996228000	-1.391730000
Si	0.222181000	1.646720000	0.088200000
C	-1.044301000	1.878704000	-1.291451000
H	-0.949457000	2.876705000	-1.731466000
H	-0.912232000	1.151742000	-2.098062000
H	-2.068369000	1.779697000	-0.918572000
C	1.959208000	1.765941000	-0.637620000
H	2.113662000	2.739718000	-1.113393000
H	2.720877000	1.656500000	0.140996000
H	2.143605000	0.996228000	-1.391730000
C	0.000000000	3.044783000	1.337288000
H	0.713127000	2.957099000	2.163029000
H	0.152705000	4.022956000	0.869964000
H	-1.006276000	3.037417000	1.768114000
H	-0.866293000	0.105857000	1.657913000
H	0.866293000	-0.105857000	1.657913000
C	0.000000000	0.000000000	0.989699000
Si	-0.222181000	-1.646720000	0.088200000
C	1.044301000	-1.878704000	-1.291451000
H	2.068369000	-1.779697000	-0.918572000
H	0.949457000	-2.876705000	-1.731466000
H	0.912232000	-1.151742000	-2.098062000
C	0.000000000	-3.044783000	1.337288000
H	-0.713127000	-2.957099000	2.163029000
H	-0.152705000	-4.022956000	0.869964000
H	1.006276000	-3.037417000	1.768114000
C	-1.959208000	-1.765941000	-0.637620000

CBS-QB3 (0 K)= -856.360352

39-H_2

C	-1.088671000	-1.088671000	1.088671000
Si	0.000000000	0.000000000	0.000000000
C	1.088671000	1.088671000	1.088671000
H	1.734558000	0.485622000	1.734556000
H	1.734556000	1.734558000	0.485622000
H	0.485622000	1.734556000	1.734558000
C	1.088671000	-1.088671000	-1.088671000
H	0.485622000	-1.734556000	-1.734558000
H	1.734558000	-0.485622000	-1.734556000
H	1.734556000	-1.734558000	-0.485622000
C	-1.088671000	1.088671000	-1.088671000
H	-0.485622000	1.734556000	-1.734558000
H	-1.734558000	0.485622000	-1.734556000
H	-1.734556000	1.734558000	-0.485622000
H	-1.734558000	-0.485622000	1.734556000
H	-1.734556000	-1.734558000	0.485622000
H	-0.485622000	-1.734556000	1.734558000

CBS-QB3 (0 K)= -448.381563

40-H_2

C	1.163125000	0.020115000	0.000000000
S	-0.665828000	-0.086820000	0.000000000
H	-0.909196000	1.234621000	-0.000001000
H	1.524265000	-1.008363000	0.000001000
H	1.529713000	0.521089000	0.895039000
H	1.529713000	0.521085000	-0.895041000

CBS-QB3 (0 K)= -438.152845

41-H_2

H	0.000000000	1.032490000	-0.993288000
H	0.894163000	-0.516245000	-0.993288000
H	-0.894163000	-0.516245000	-0.993288000
F	0.000000000	0.000000000	0.754277000
C	0.000000000	0.000000000	-0.634772000

CBS-QB3 (0 K)= -139.563780

42-H_2

C	0.000000000	0.000000000	0.813939000
H	0.000000000	2.776172000	0.719810000
H	1.202698000	1.669666000	-1.045219000
H	-1.202698000	1.669666000	-1.045219000

Si	0.000000000	1.598458000	-0.181510000
Si	0.000000000	-1.598458000	-0.181510000
H	0.000000000	-2.776172000	0.719810000
H	-1.202698000	-1.669666000	-1.045219000
H	1.202698000	-1.669666000	-1.045219000
H	0.878278000	0.000000000	1.469948000
H	-0.878278000	0.000000000	1.469948000

CBS-QB3 (0 K)= -620.908391

43-H_2

C	0.000000000	0.000000000	0.770285000
Cl	0.000000000	1.491144000	-0.216811000
Cl	0.000000000	-1.491144000	-0.216811000
H	0.900045000	0.000000000	1.374939000
H	-0.900045000	0.000000000	1.374939000

CBS-QB3 (0 K)= -958.716544

44-H_2

C	0.235639000	0.397225000	0.000000000
O	1.233110000	-0.276593000	0.000000000
C	-1.168815000	-0.147742000	0.000000000
H	-1.155362000	-1.237477000	0.000003000
H	-1.707776000	0.222273000	-0.879037000
H	-1.707778000	0.222277000	0.879034000
H	0.305089000	1.508771000	0.000000000

CBS-QB3 (0 K)= -153.582459

45-H_2

C	0.000000000	0.817934000	0.000000000
Cl	1.389182000	-0.339803000	0.000000000
C	-1.278866000	0.127793000	0.000000000
N	-2.304558000	-0.396342000	0.000000000
H	0.094505000	1.438338000	0.889910000
H	0.094505000	1.438338000	-0.889910000

CBS-QB3 (0 K)= -591.673076

46-H_2

C	0.632309000	-0.510528000	0.000000000
C	0.000000000	0.811312000	0.000000000
N	-0.480963000	1.857424000	0.000000000
H	1.253949000	-0.616183000	0.892761000
H	1.253949000	-0.616183000	-0.892761000
F	-0.326113000	-1.508257000	0.000000000

CBS-QB3 (0 K)= -231.675809

47-H_2

C	0.000000000	0.000000000	0.503272000
H	-0.912701000	0.000000000	1.103952000
H	0.912701000	0.000000000	1.103952000
F	0.000000000	1.108161000	-0.290419000
F	0.000000000	-1.108161000	-0.290419000

CBS-QB3 (0 K)= -238.737918

48-H_2

C	0.000000000	0.000000000	0.832049000
H	0.880850000	0.000000000	1.482213000
H	-0.880850000	0.000000000	1.482213000
C	0.000000000	1.221928000	0.024289000
N	0.000000000	2.195441000	-0.589156000
C	0.000000000	-1.221928000	0.024289000
N	0.000000000	-2.195441000	-0.589156000

CBS-QB3 (0 K)= -224.631424

49-H_2

C	0.000000000	0.870499000	0.000000000
C	0.753874000	-0.435249000	0.000000000
C	-0.753874000	-0.435249000	0.000000000
H	0.000000000	1.459195000	0.909572000
H	0.000000000	1.459195000	-0.909572000
H	1.263700000	-0.729597000	0.909572000
H	1.263700000	-0.729597000	-0.909572000
H	-1.263700000	-0.729597000	-0.909572000
H	-1.263700000	-0.729597000	0.909572000

CBS-QB3 (0 K)= -117.632379

50-H_2

C	0.000000000	0.000000000	-0.025506000
C	0.000000000	0.000000000	1.476927000
F	0.000000000	1.255653000	-0.526911000
F	-1.087428000	-0.627827000	-0.526911000
F	1.087428000	-0.627827000	-0.526911000
H	0.890103000	0.513901000	1.839356000
H	-0.890103000	0.513901000	1.839356000
H	0.000000000	-1.027802000	1.839356000

CBS-QB3 (0 K)= -377.163189

51-H_2

C	-1.285791000	0.000000000	-0.071741000
F	-1.397068000	1.085887000	0.712996000
F	-1.397067000	-1.085888000	0.712994000
F	-2.339056000	0.000001000	-0.916971000
C	0.000000000	0.000001000	-0.878691000
H	0.000000000	0.885755000	-1.514651000
H	0.000000000	-0.885752000	-1.514652000
C	1.285791000	0.000000000	-0.071741000
F	1.397067000	-1.085888000	0.712994000
F	2.339056000	0.000001000	-0.916971000
F	1.397068000	1.085887000	0.712995000

CBS-QB3 (0 K)= -713.909228

4. Optimized Geometries in Water Addition Reactions

Table S4. Optimized XYZ coordinates of structures involved in water addition reactions in Å at the B3LYP/CBSB7 level of theory and their CBS-QB3 energies in E_h

H_2O

O	0.000000000	0.000000000	0.118697000
H	0.000000000	0.757073000	-0.474787000
H	0.000000000	-0.757073000	-0.474787000

CBS-QB3 (0 K)= -76.337479

CH_2OO-A

C	-0.866547000	1.046019000	-0.002986000
H	-1.651771000	1.792470000	0.027448000
O	-0.405213000	-1.179015000	-0.011445000
O	-1.285019000	-0.139510000	0.026066000
O	2.038410000	0.210428000	-0.086471000
H	1.355535000	-0.487437000	-0.126177000
H	2.503376000	0.046583000	0.739716000
H	0.206718000	1.237049000	-0.048269000

CBS-QB3 (0 K)= -265.689212

CH_2OO-B

C	0.044501000	0.996534000	0.248517000
H	0.374719000	1.925087000	-0.209657000
O	-0.936013000	-0.957914000	0.184042000
O	-0.902559000	0.395571000	-0.350812000
O	1.416360000	-0.342825000	-0.214249000
H	0.551872000	-0.943151000	-0.080071000
H	1.987878000	-0.532567000	0.539581000
H	0.196222000	0.812775000	1.307199000

CBS-QB3 (0 K)= -265.673864

CH_2OO-C

C	0.658772000	0.540048000	0.257087000
H	1.163463000	1.445522000	-0.083948000
O	-1.399727000	-0.463090000	0.217467000
O	-0.621384000	0.644861000	-0.331679000
O	1.395352000	-0.556751000	-0.189711000
H	-1.677885000	-0.888265000	-0.604702000
H	1.021386000	-1.339075000	0.229242000
H	0.546477000	0.541374000	1.348280000

CBS-QB3 (0 K)= -265.748138

7-A

C	0.950741000	-0.114157000	0.033040000
O	-0.832212000	1.327725000	0.266012000
O	0.562570000	1.101057000	-0.069982000
O	-2.530552000	-0.600728000	-0.359031000
H	-2.001901000	0.240722000	-0.375307000
H	-3.241119000	-0.412445000	0.262096000
N	2.252827000	-0.347889000	-0.298097000
H	2.715518000	-1.129406000	0.139079000
H	2.815549000	0.483276000	-0.404221000
N	0.150981000	-1.103096000	0.416646000
H	0.444101000	-2.050368000	0.239011000
H	-0.861695000	-0.914375000	0.415259000

CBS-QB3 (0 K)= -376.301883

7-B

C	-0.487313000	-0.184473000	-0.045328000
O	1.718654000	-0.456187000	-0.195191000
O	0.442007000	-0.614203000	-0.892849000
O	0.499422000	1.512011000	0.233346000
H	1.367163000	0.716786000	0.091041000
H	0.426236000	1.691041000	1.176737000
N	-1.677680000	0.094642000	-0.632374000
H	-2.350374000	0.558513000	-0.040890000
H	-1.588002000	0.503437000	-1.551559000
N	-0.510749000	-0.614120000	1.272040000
H	-1.285541000	-1.238352000	1.459643000
H	0.392729000	-1.021210000	1.496891000

CBS-QB3 (0 K)= -376.272445

7-C

C	0.398858000	0.007949000	0.006000000
O	-1.915600000	-0.064002000	-0.193978000
O	-0.693503000	-0.761117000	-0.514932000
O	0.136997000	0.099676000	1.405241000
H	-1.948952000	-0.192013000	0.768119000
H	0.546239000	0.918202000	1.706263000
N	1.539426000	-0.770196000	-0.359281000
H	2.382968000	-0.304257000	-0.045500000
H	1.483162000	-1.684364000	0.075062000
N	0.530669000	1.335163000	-0.518097000
H	0.808157000	1.276847000	-1.492424000
H	-0.378542000	1.786659000	-0.476520000

CBS-QB3 (0 K)= -376.319704

47-A

C	-0.579734000	-0.234830000	0.009714000
O	1.537705000	-1.001718000	0.092357000
O	0.244989000	-0.920531000	-0.591387000
O	0.872196000	1.598537000	-0.317889000
H	1.526961000	0.874248000	-0.200945000
H	1.023457000	2.192096000	0.424433000
F	-1.683328000	0.088859000	-0.573990000
F	-0.573464000	0.014735000	1.268832000

CBS-QB3 (0 K)= -464.023301

47-B

C	-0.505072000	-0.275364000	0.004873000
O	1.690334000	-0.719877000	0.080143000
O	0.384549000	-0.896417000	-0.584669000
O	0.545896000	1.625027000	-0.316701000
H	1.334809000	1.032530000	-0.201983000
H	0.557565000	2.213868000	0.445689000
F	-1.643762000	-0.104280000	-0.579553000
F	-0.559370000	-0.080618000	1.279206000

CBS-QB3 (0 K)= -464.021664

47-C

C	-0.406519000	0.015954000	-0.023228000
O	1.873487000	-0.019612000	0.115167000
O	0.705859000	-0.816284000	-0.220995000
O	-0.329703000	1.222674000	-0.621408000
H	2.391326000	-0.152424000	-0.691651000
H	0.468139000	1.653408000	-0.285854000
F	-1.424988000	-0.669606000	-0.542454000
F	-0.621401000	0.148391000	1.312983000

CBS-QB3 (0 K)= -464.110538

17-A

C	0.835039000	-0.181071000	-0.123538000
O	-1.258821000	-1.009130000	-0.614718000
O	0.052467000	-1.195861000	-0.295103000
O	-3.451753000	-0.048972000	0.802289000
H	-2.656453000	-0.555501000	0.564030000
H	-4.068690000	-0.273728000	0.098809000
C	2.190965000	-0.619765000	0.180746000
H	2.318014000	-1.696975000	0.150398000
C	3.226550000	0.167171000	0.493398000
H	3.153609000	1.245805000	0.556835000
H	4.196305000	-0.264624000	0.706671000

C	0.457438000	1.204015000	-0.240023000
H	1.300549000	1.885377000	-0.226094000
C	-0.779871000	1.723533000	-0.350786000
H	-1.676891000	1.126145000	-0.326574000
H	-0.882315000	2.801919000	-0.422605000

CBS-QB3 (0 K)= -420.201200

17-B

C	0.225623000	-0.097035000	-0.182466000
O	-1.908215000	-0.760590000	-0.502781000
O	-0.546559000	-0.745482000	-1.016714000
O	-0.496683000	-1.148708000	1.386987000
H	-1.389056000	-1.071102000	0.667234000
H	-0.671992000	-0.533241000	2.107757000
C	1.626660000	-0.539352000	-0.292420000
H	1.732386000	-1.580171000	-0.574681000
C	2.695084000	0.233995000	-0.101091000
H	2.621389000	1.283596000	0.156673000
H	3.694513000	-0.169056000	-0.213202000
C	-0.087542000	1.246900000	0.344175000
H	0.628021000	1.628188000	1.064496000
C	-1.112902000	1.998984000	-0.055725000
H	-1.852472000	1.610154000	-0.742841000
H	-1.232669000	3.008928000	0.319790000

CBS-QB3 (0 K)= -420.178591

17-C

C	0.187783000	-0.027214000	0.091488000
O	-1.738254000	-1.341820000	-0.166231000
O	-0.570537000	-0.807005000	-0.853699000
O	0.506113000	-0.786605000	1.226962000
H	-1.491188000	-2.276592000	-0.143263000
H	-0.299466000	-0.841222000	1.753757000
C	1.448193000	0.297303000	-0.675867000
H	1.273145000	0.712947000	-1.662292000
C	2.672396000	0.128495000	-0.192938000
H	2.832323000	-0.284111000	0.795377000
H	3.544976000	0.398217000	-0.776504000
C	-0.533413000	1.248603000	0.485287000
H	-0.041495000	1.793747000	1.286534000
C	-1.638355000	1.713277000	-0.085496000
H	-2.127714000	1.174626000	-0.887676000
H	-2.088783000	2.643049000	0.242968000

CBS-QB3 (0 K)= -420.241773

21-A

C	-0.909392000	0.051516000	0.074521000
O	0.866374000	-1.311223000	0.509615000
O	-0.348596000	-1.064960000	-0.131368000
O	2.360367000	0.670791000	-0.726786000
H	1.978199000	-0.150787000	-0.349525000
H	3.183406000	0.788635000	-0.243410000
C	-0.288228000	1.050079000	0.962146000
H	-0.954968000	1.889448000	1.153514000
H	0.023344000	0.549773000	1.884464000
H	0.645185000	1.384612000	0.484284000
C	-2.193348000	0.262395000	-0.647633000
H	-2.996434000	0.465266000	0.068281000
H	-2.110635000	1.141827000	-1.294815000
H	-2.447457000	-0.609577000	-1.248689000

CBS-QB3 (0 K)= -344.172976

21-B

C	-0.453881000	-0.095151000	-0.184245000
O	1.757479000	-0.062297000	-0.559573000
O	0.430940000	0.304193000	-1.043776000
O	0.505758000	0.805087000	1.308230000
H	1.336904000	0.493453000	0.643821000
H	0.562767000	0.248559000	2.092710000
C	-0.422007000	-1.496602000	0.356759000
H	-0.946428000	-2.131940000	-0.367475000
H	0.604053000	-1.840570000	0.445666000
H	-0.950533000	-1.568903000	1.307571000
C	-1.768594000	0.608705000	-0.301691000
H	-2.429717000	0.041189000	-0.964450000
H	-2.239568000	0.670121000	0.679702000
H	-1.623995000	1.610519000	-0.701528000

CBS-QB3 (0 K)= -344.151873

21-C

C	0.392211000	0.020216000	0.044438000
O	-1.940158000	-0.063818000	-0.169639000
O	-0.691404000	-0.649350000	-0.636435000
O	0.260814000	-0.125224000	1.437205000
H	-2.300478000	-0.819649000	0.313293000
H	-0.473866000	0.436670000	1.708183000
C	0.436790000	1.491731000	-0.362785000
H	0.574474000	1.585984000	-1.441408000
H	-0.500380000	1.983922000	-0.095244000
H	1.259459000	1.994385000	0.149476000
C	1.615451000	-0.774004000	-0.386567000

H	1.700285000	-0.786190000	-1.473767000
H	2.510555000	-0.318560000	0.039468000
H	1.529226000	-1.797093000	-0.019562000

CBS-QB3 (0 K)= -344.218220

5. Optimized Geometries in OH Addition Reactions

Table S5. Optimized XYZ coordinates of structures involved in OH addition reactions in Å at the ROB3LYP/CBSB7 level of theory and their ROCBS-QB3 energies in E_h

$^{\bullet}$OH

O	0.000000000	0.000000000	0.108356000
H	0.000000000	0.000000000	-0.866851000

CBS-QB3 (0 K)= -75.650067

CH_2OO-A$^{\bullet}$

C	-1.085081000	-0.809726000	0.000000000
H	-2.050578000	-1.301374000	0.000000000
O	0.000000000	1.187073000	0.000000000
O	-1.142056000	0.445332000	0.000000000
O	2.041255000	-0.712808000	0.000000000
H	1.483240000	0.108886000	0.000000000
H	-0.115764000	-1.305930000	0.000000000

CBS-QB3 (0 K)= -265.001890

CH_2OO-B$^{\bullet}$

O	1.817417000	-0.092117000	-0.108240000
H	1.151143000	-0.807716000	0.040617000
O	-0.698309000	-1.124077000	0.163846000
O	-0.977059000	0.127391000	-0.310005000
C	-0.340995000	1.088663000	0.197172000
H	-0.503771000	2.050166000	-0.273866000
H	0.262212000	0.935995000	1.085399000

CBS-QB3 (0 K)= -264.999549

CH_2OO-C$^{\bullet}$

C	0.616215000	0.569687000	0.238618000
H	1.038645000	1.477026000	-0.188313000
O	-1.367562000	-0.554473000	0.127937000
O	-0.758937000	0.535896000	-0.295297000
O	1.350664000	-0.510482000	-0.181581000
H	0.967719000	-1.299071000	0.222567000
H	0.503029000	0.636398000	1.325563000

CBS-QB3 (0 K)= -265.110112

7-A$^{\bullet}$

C	0.813147000	0.042730000	0.059991000
O	-1.137549000	1.215515000	0.224382000
O	0.081610000	0.923178000	-0.527755000

O	-2.042113000	-1.216107000	-0.476377000
H	-1.920529000	-0.234157000	-0.326939000
N	1.871913000	-0.431131000	-0.627268000
H	2.662551000	-0.802418000	-0.127023000
H	2.046777000	-0.014759000	-1.528810000
N	0.515250000	-0.340818000	1.295288000
H	0.801668000	-1.243771000	1.634958000
H	-0.395073000	0.061670000	1.549719000

CBS-QB3 (0 K)= -375.618612

7-B•

H	1.181335000	1.085897000	1.498787000
O	0.763504000	1.322939000	0.660081000
O	1.633731000	-0.387674000	-0.371355000
O	0.366806000	-0.333612000	-1.045461000
C	-0.539080000	-0.190821000	-0.097285000
N	-1.655970000	0.447982000	-0.482139000
H	-2.428073000	0.512237000	0.161127000
H	-1.509207000	1.234057000	-1.096825000
N	-0.559350000	-1.066353000	0.939982000
H	-0.991040000	-0.736096000	1.790380000
H	0.376379000	-1.435797000	1.079218000

CBS-QB3 (0 K)= -375.600413

7-C•

C	0.473289000	-0.012526000	0.099895000
O	-1.978100000	0.013300000	-0.108288000
O	-0.898409000	0.192397000	-0.810816000
O	0.003771000	-0.066321000	1.373453000
H	-0.980569000	-0.123346000	1.289582000
N	1.089010000	-1.199072000	-0.318180000
H	1.249311000	-1.226717000	-1.317200000
H	0.602907000	-2.021245000	0.013154000
N	1.225990000	1.111006000	-0.294095000
H	2.202082000	0.987390000	-0.053701000
H	0.863444000	1.960522000	0.119928000

CBS-QB3 (0 K)= -375.683313

47-A•

C	-0.659214000	-0.132492000	0.027659000
O	1.354570000	-1.154349000	0.180733000
O	0.090610000	-0.945933000	-0.506494000
O	1.392443000	1.496387000	-0.387306000
H	1.764869000	0.593617000	-0.189607000
F	-1.746688000	0.216591000	-0.568716000

F	-0.532264000	0.342575000	1.205180000

CBS-QB3 (0 K)= -463.335976

47-B•

O	0.635203000	1.671657000	-0.306190000
H	1.392085000	1.005037000	-0.267707000
O	1.675327000	-0.679498000	0.098395000
O	0.373061000	-0.889201000	-0.550863000
C	-0.514188000	-0.236753000	0.016295000
F	-1.651726000	-0.091801000	-0.573371000
F	-0.545572000	0.046447000	1.266616000

CBS-QB3 (0 K)= -463.333794

47-C•

C	-0.402709000	0.068527000	-0.000004000
O	1.922793000	-0.066063000	0.000006000
O	0.829268000	-0.783699000	-0.000274000
O	-0.114253000	1.355524000	-0.000067000
H	0.864788000	1.424229000	0.000182000
F	-1.086385000	-0.326727000	-1.078489000
F	-1.085948000	-0.326771000	1.078769000

CBS-QB3 (0 K)= -463.469021

17-A•

C	0.668468000	-0.115229000	0.000015000
O	-1.523464000	0.599864000	0.000074000
O	-0.592474000	-0.397476000	0.000060000
O	-3.881139000	-0.941218000	-0.000073000
H	-3.084107000	-0.356609000	0.000000000
C	1.468689000	-1.332896000	0.000011000
H	0.876701000	-2.242189000	0.000044000
C	2.804414000	-1.404014000	-0.000027000
H	3.447158000	-0.532430000	-0.000060000
H	3.299077000	-2.367095000	-0.000026000
C	1.232013000	1.209865000	-0.000028000
H	2.315581000	1.226407000	-0.000068000
C	0.573263000	2.383933000	-0.000026000
H	-0.503162000	2.426006000	0.000013000
H	1.144276000	3.306600000	-0.000064000

CBS-QB3 (0 K)= -419.518712

17-B•

O	-0.338871000	-1.357990000	1.733002000
H	-1.187656000	-1.421427000	1.253407000

O	-1.874169000	-0.700602000	-0.829522000
O	-0.527872000	-0.851746000	-0.880968000
C	0.252285000	0.028290000	-0.308749000
C	1.646357000	-0.369056000	-0.428912000
H	1.782511000	-1.362983000	-0.840895000
C	2.709524000	0.366539000	-0.085887000
H	2.632654000	1.365224000	0.325393000
H	3.709760000	-0.028534000	-0.210849000
C	-0.175463000	1.281817000	0.261091000
H	0.624452000	1.830524000	0.743291000
C	-1.405285000	1.823285000	0.241233000
H	-2.241634000	1.312634000	-0.206689000
H	-1.557294000	2.802008000	0.683590000

CBS-QB3 (0 K)= -419.512208

17-C•

C	0.179598000	0.028249000	0.116908000
O	-1.426107000	-1.645724000	-0.172797000
O	-0.586680000	-0.882768000	-0.831791000
O	0.494855000	-0.676358000	1.258493000
H	-0.336908000	-1.052990000	1.583022000
C	1.412623000	0.399106000	-0.654890000
H	1.217602000	0.831476000	-1.630813000
C	2.646181000	0.243616000	-0.191131000
H	2.826947000	-0.186594000	0.786009000
H	3.505788000	0.541280000	-0.779847000
C	-0.691885000	1.230493000	0.414317000
H	-0.233707000	1.902473000	1.134968000
C	-1.886875000	1.494701000	-0.101341000
H	-2.363440000	0.841433000	-0.821296000
H	-2.430669000	2.384724000	0.193539000

CBS-QB3 (0 K)= -419.605019

21-A•

C	0.858400000	-0.036504000	0.067210000
O	-1.006269000	1.174405000	0.581297000
O	0.219446000	1.046883000	-0.076464000
O	-2.436581000	-0.702974000	-0.790235000
H	-2.051698000	0.093548000	-0.327582000
C	0.313957000	-1.126606000	0.897257000
H	-0.051767000	-0.702414000	1.837098000
H	-0.576019000	-1.520681000	0.387814000
H	1.047142000	-1.915398000	1.057409000
C	2.154988000	-0.112649000	-0.658321000
H	2.969697000	-0.283804000	0.052875000
H	2.144346000	-0.966356000	-1.343872000

H	2.341467000	0.803152000	-1.217392000

CBS-QB3 (0 K)= -343.486984

21-B•

O	0.609554000	1.877719000	0.478142000
H	1.386699000	1.352018000	0.196909000
O	1.676414000	-0.722405000	-0.436833000
O	0.441722000	-0.323118000	-0.902402000
C	-0.517431000	-0.300904000	-0.056801000
C	-0.332229000	-0.879796000	1.290398000
H	0.115246000	-1.873346000	1.183465000
H	0.392994000	-0.274710000	1.837360000
H	-1.276146000	-0.921088000	1.832145000
C	-1.816342000	0.196390000	-0.579402000
H	-2.565983000	-0.601249000	-0.541135000
H	-2.168746000	1.012500000	0.057157000
H	-1.709581000	0.554168000	-1.602322000

CBS-QB3 (0 K)= -343.482173

21-C•

C	-0.384577000	-0.030296000	0.070572000
O	1.936348000	0.171091000	-0.122436000
O	0.812250000	0.530751000	-0.693054000
O	-0.165252000	0.160602000	1.419703000
H	0.699748000	-0.227057000	1.618049000
C	-0.471716000	-1.499597000	-0.320114000
H	-0.616566000	-1.614337000	-1.395908000
H	0.450224000	-2.011978000	-0.036045000
H	-1.308480000	-1.962953000	0.205872000
C	-1.544056000	0.829302000	-0.379459000
H	-1.645254000	0.797956000	-1.465298000
H	-2.466848000	0.463846000	0.074313000
H	-1.377510000	1.858525000	-0.060680000

CBS-QB3 (0 K)= -343.583298

6. Additional Information

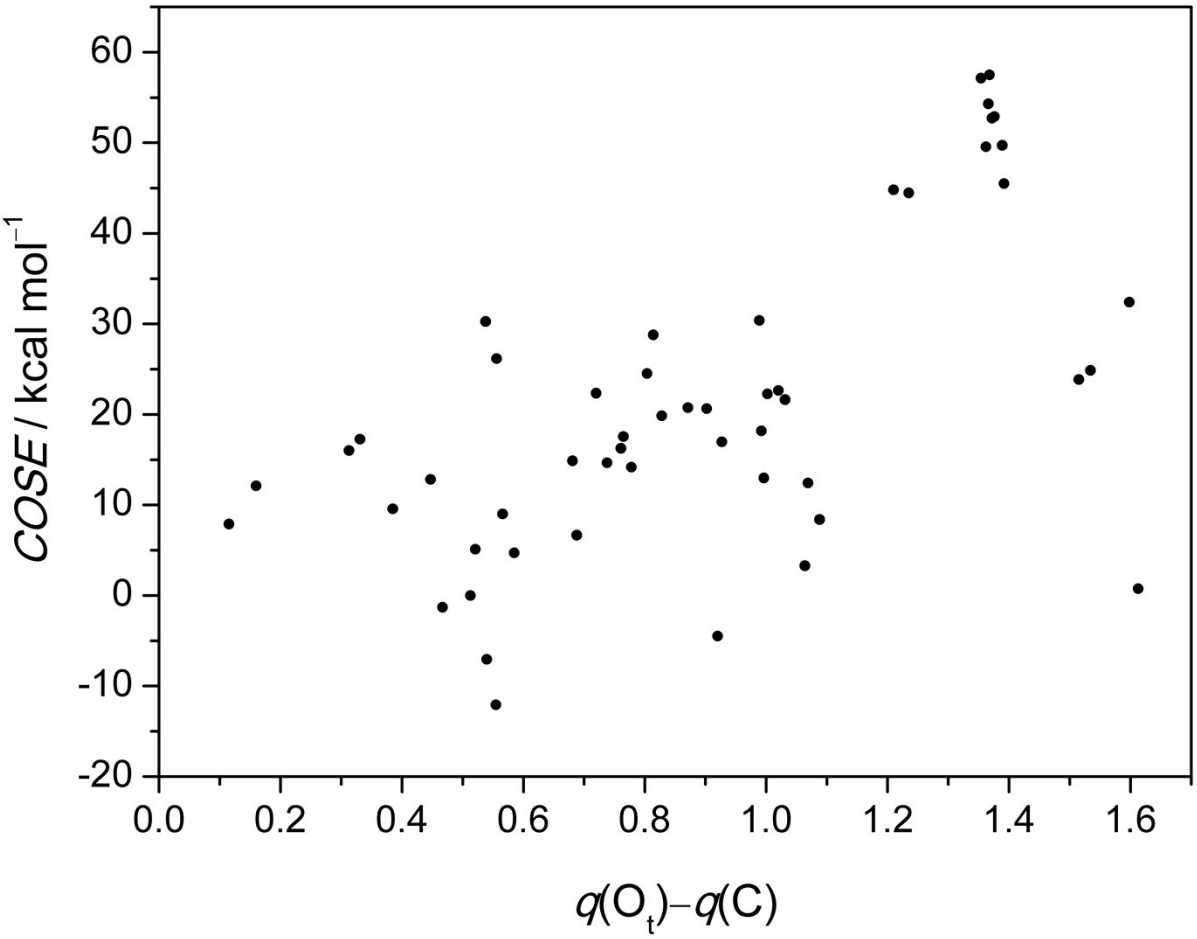
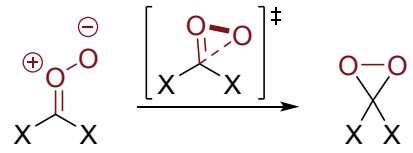


Figure S1. The plot shows the dependence of the carbonyl oxide stabilization energy on the difference in natural charges of the terminal oxygen and the carbonyl carbon atom.

Table S6. Reaction energetics for the cyclization of selected carbonyl oxides to dioxiranes at the CBS-QB3 level of theory in kcal mol^{-1}



X=			
H	0.0	19.0	–25.5
NH_2	0.0	14.5	–9.0
F	0.0	9.5	–44.6
C_2H_3	0.0	20.8	–22.7
CH_3	0.0	22.3	–16.7

Table S7. *COSE* values of selected carbonyl oxides computed with W1 theory and several density functionals in combination with a def2-TZVP basis set. The energies are given in kcal mol^{-1}

Structure	CBS-QB3	W1	B3LYP	M06-2X
7	49.6	50.3	52.0	54.2
47	0.7	1.7	3.3	5.3
17	24.5	23.4	25.9	23.5
21	22.3	22.1	22.9	23.8