Supplementary Information

Mechanistic Investigation on the Initial Thermal Decomposition of Energetic Materials FOX-7 and RDX in Crystal and Gas Phase: An MM/DFT-based ONIOM Calculation

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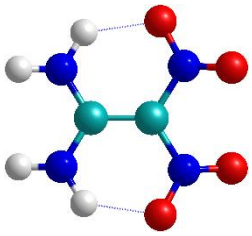
[e]College of Science, Shenyang University of Chemical Technology, Shenyang 110142, P. R. China

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[*] Corresponding author: beam@dicp.ac.cn; pwzhou@sdu.edu.cn;

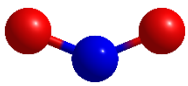
Coordinates of the optimized structures for gas phase FOX-7 initial decomposition, obtained with the M06-2X functional and the SVP basis set.

FOX-7 (gas phase)



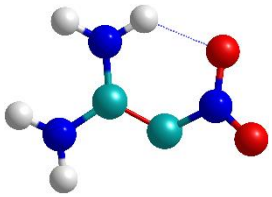
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N	-0.805265000000	-1.213505000000	0.101496000000
O	-1.918321000000	-1.173521000000	0.550931000000
O	-0.254770000000	-2.257948000000	-0.241610000000
N	-0.805204000000	1.213555000000	-0.101538000000
O	-1.918405000000	1.173603000000	-0.550626000000
O	-0.254522000000	2.258014000000	0.241248000000
N	2.065227000000	-1.135377000000	-0.143078000000
H	1.537677000000	-1.994532000000	-0.281608000000
H	3.061105000000	-1.141265000000	0.023745000000
N	2.065299000000	1.135229000000	0.143216000000
H	1.537756000000	1.994428000000	0.281544000000
H	3.061186000000	1.141051000000	-0.023560000000

NO_2



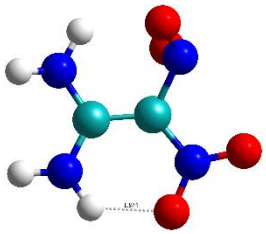
N	0.000000000000	0.312991000000	0.000000000000
O	1.089411000000	-0.136936000000	0.000000000000
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IM_F1



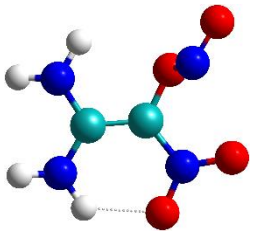
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N	-1.306401000000	-0.128992000000	0.048065000000
O	-2.213228000000	-0.862546000000	-0.276049000000
O	-1.414673000000	1.101049000000	0.104379000000
N	1.246780000000	1.238905000000	-0.092145000000
H	0.382762000000	1.777751000000	-0.043127000000
H	2.126722000000	1.664982000000	-0.344879000000
N	2.211891000000	-0.865657000000	-0.099057000000
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H	3.136943000000	-0.469705000000	-0.183660000000

TS_F1



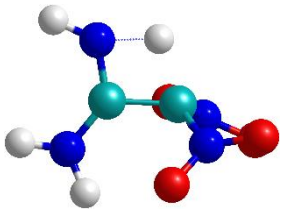
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N	1.517252000000	-0.311975000000	-0.009304000000
O	1.916911000000	-1.448725000000	0.003103000000
O	2.236353000000	0.684142000000	-0.107837000000
N	-0.715948000000	-1.332389000000	-0.203361000000
O	-1.665633000000	-1.405749000000	-0.952025000000
O	-0.914900000000	-1.179484000000	1.077532000000
N	0.149861000000	2.280383000000	-0.182515000000
H	1.162699000000	2.213396000000	-0.253458000000
H	-0.324847000000	3.170612000000	-0.144989000000
N	-1.857074000000	1.199709000000	0.225008000000
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IM_F2



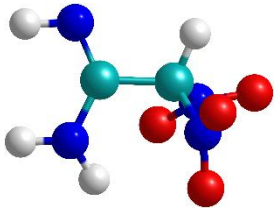
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N	0.289021000000	-1.417368000000	0.077492000000
O	-0.713857000000	-2.091048000000	0.162352000000
O	1.405884000000	-1.881280000000	-0.154254000000
N	-1.969861000000	0.374991000000	-0.551508000000
O	-3.037432000000	0.645826000000	-0.226440000000
O	-1.069559000000	0.434217000000	0.592932000000
N	2.466579000000	0.532749000000	-0.233357000000
H	2.636502000000	-0.462255000000	-0.361019000000
H	3.102266000000	1.221065000000	-0.610376000000
N	0.897976000000	2.211322000000	0.073723000000
H	-0.007075000000	2.448791000000	0.459968000000
H	1.649757000000	2.854504000000	0.285111000000

TS_F2



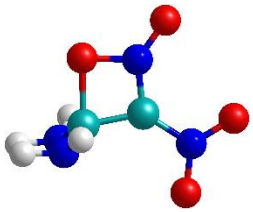
C	0.062725000000	0.037093000000	0.432089000000
C	-1.371091000000	-0.308034000000	0.132589000000
N	0.451457000000	1.339438000000	-0.133788000000
O	1.614945000000	1.560818000000	-0.335831000000
O	-0.461731000000	2.115992000000	-0.316039000000
N	1.048841000000	-1.005243000000	0.122226000000
O	2.118272000000	-0.949550000000	0.656479000000
O	0.687198000000	-1.876894000000	-0.651700000000
N	-1.860859000000	-0.692738000000	-1.039077000000
H	-1.197582000000	-1.013490000000	-1.736003000000
H	-2.834978000000	-0.944414000000	-1.145277000000
N	-1.942825000000	-0.102043000000	1.279849000000
H	-0.712220000000	0.165980000000	1.640887000000
H	-2.950785000000	-0.161264000000	1.424582000000

IM_F3



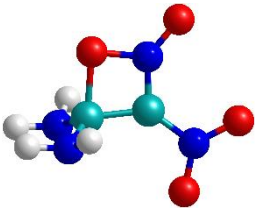
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N	0.817104000000	-1.179185000000	-0.145775000000
O	1.898644000000	-1.275421000000	-0.656429000000
O	0.331046000000	-1.910967000000	0.674614000000
N	0.687075000000	1.216653000000	0.016935000000
O	1.146416000000	1.070091000000	1.121724000000
O	0.657838000000	2.220966000000	-0.633004000000
N	-1.662950000000	0.193329000000	1.164765000000
H	-0.899307000000	0.019591000000	1.810317000000
H	-2.590156000000	0.009484000000	1.527911000000
N	-2.269255000000	-0.282964000000	-1.098705000000
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H	-3.231082000000	-0.347953000000	-0.754686000000

TS_F3



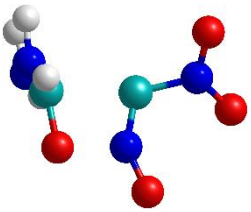
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C	1.190445000000	-0.329549000000	0.004615000000
N	-1.477934000000	-0.728983000000	-0.001445000000
O	-2.504649000000	-0.087122000000	0.032201000000
O	-1.377196000000	-1.936776000000	-0.028310000000
N	-0.088964000000	1.313542000000	-0.009186000000
O	-0.748200000000	2.298687000000	-0.015569000000
O	1.274271000000	1.323668000000	0.001781000000
N	1.706182000000	-0.861674000000	1.170922000000
H	1.394384000000	-0.386787000000	2.010828000000
H	2.713452000000	-0.990185000000	1.167917000000
N	1.729699000000	-0.870088000000	-1.147139000000
H	1.381982000000	-0.442566000000	-1.998262000000
H	2.744065000000	-0.923714000000	-1.150552000000

IM_F4



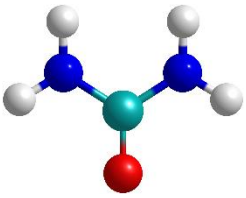
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C	1.191713000000	-0.322240000000	0.004615000000
N	-1.485778000000	-0.722916000000	-0.001445000000
O	-2.507630000000	-0.073258000000	0.033001000000
O	-1.393080000000	-1.930854000000	-0.029110000000
N	-0.086472000000	1.310116000000	-0.009186000000
O	-0.730484000000	2.304924000000	-0.015969000000
O	1.284333000000	1.300878000000	0.001781000000
N	1.703569000000	-0.867673000000	1.172122000000
H	1.404924000000	-0.380687000000	2.010428000000
H	2.711333000000	-0.995093000000	1.163517000000
N	1.727036000000	-0.876620000000	-1.147539000000
H	1.386179000000	-0.441160000000	-1.997862000000
H	2.742361000000	-0.921997000000	-1.148552000000

TS_F4



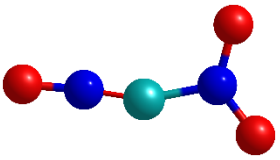
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C	-1.685434000000	-0.184842000000	0.049098000000
N	1.794296000000	-0.605136000000	0.079817000000
O	2.606645000000	0.108351000000	0.618175000000
O	2.026511000000	-1.670560000000	-0.444698000000
N	0.206612000000	1.048027000000	-0.129407000000
O	0.739969000000	2.072999000000	-0.370538000000
O	-1.383870000000	1.115672000000	-0.085798000000
N	-2.102775000000	-0.836198000000	-1.062048000000
H	-1.691744000000	-0.495180000000	-1.923732000000
H	-2.204934000000	-1.843347000000	-1.014436000000
N	-2.179990000000	-0.561612000000	1.243875000000
H	-1.811637000000	-0.061172000000	2.043869000000
H	-2.438368000000	-1.528208000000	1.396513000000

IM_F5



C	0.000000000000	0.143489000000	-0.003118000000
O	0.000005000000	1.354263000000	0.011420000000
N	1.157920000000	-0.597064000000	-0.039495000000
H	2.012526000000	-0.077788000000	0.103309000000
H	1.171936000000	-1.590321000000	0.136821000000
N	-1.157923000000	-0.597054000000	-0.039478000000
H	-2.012535000000	-0.077781000000	0.103294000000
H	-1.171949000000	-1.590329000000	0.136729000000

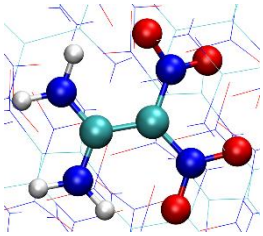
IM_F6



C	-0.316074000000	-0.258521000000	0.000245000000
N	1.084815000000	0.008324000000	-0.000163000000
O	1.397027000000	1.169793000000	0.000116000000
O	1.810883000000	-0.948575000000	-0.000077000000
N	-1.465786000000	-0.075049000000	0.000042000000
O	-2.637505000000	0.031058000000	-0.000118000000

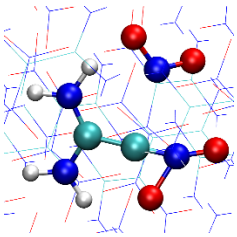
Coordinates of the optimized structures for crystal phase FOX-7 initial decomposition, obtained with the M06-2X functional and the SVP basis set based on the ONIOM model.

FOX-7(crystal phase)



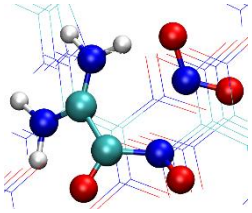
C	1.417628000000	-1.785292000000	2.173420000000
C	0.293346000000	-1.220540000000	1.474427000000
N	1.643054000000	-3.183345000000	2.291607000000
N	2.507874000000	-0.949357000000	2.502439000000
O	2.552720000000	-3.561552000000	2.984236000000
O	0.861573000000	-3.959783000000	1.741891000000
O	2.241580000000	0.174051000000	2.941356000000
O	3.643711000000	-1.311665000000	2.343971000000
N	-0.598121000000	-2.006430000000	0.904732000000
H	-1.433037000000	-1.618507000000	0.467937000000
H	-0.427101000000	-3.002792000000	0.948482000000
N	0.139543000000	0.097905000000	1.365045000000
H	-0.660175000000	0.455222000000	0.837293000000
H	0.753806000000	0.737342000000	1.859734000000

TS_F5



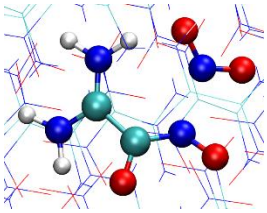
C	0.914192000000	-2.327071000000	2.155739000000
C	0.138470000000	-1.366596000000	1.390503000000
N	1.719964000000	-3.189160000000	2.574549000000
N	2.639190000000	-0.741574000000	2.528826000000
O	2.675611000000	-3.625332000000	3.084705000000
O	0.518228000000	-3.835014000000	2.094032000000
O	2.433515000000	0.476137000000	2.750078000000
O	3.777625000000	-1.136568000000	2.516643000000
N	-0.725189000000	-1.980641000000	0.616772000000
H	-1.466103000000	-1.506316000000	0.101194000000
H	-0.663641000000	-2.983616000000	0.584587000000
N	0.243770000000	-0.066548000000	1.489438000000
H	-0.365632000000	0.499708000000	0.895751000000
H	1.034754000000	0.385580000000	2.053301000000

IM_F7



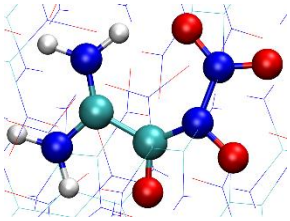
C	0.814650000000	-2.558563000000	2.029883000000
C	0.149528000000	-1.367376000000	1.326466000000
N	2.228140000000	-2.643170000000	2.059285000000
N	2.916924000000	-0.699016000000	2.612649000000
O	2.754027000000	-3.357090000000	2.848696000000
O	0.184584000000	-3.577965000000	2.133153000000
O	2.557805000000	0.479481000000	2.822201000000
O	4.076231000000	-0.986104000000	2.649441000000
N	-0.813228000000	-1.798611000000	0.561266000000
H	-1.449950000000	-1.198902000000	0.034519000000
H	-0.969276000000	-2.791693000000	0.580823000000
N	0.434992000000	-0.103824000000	1.469617000000
H	-0.140408000000	0.570917000000	0.962537000000
H	1.233164000000	0.276117000000	2.063133000000

TS_F6



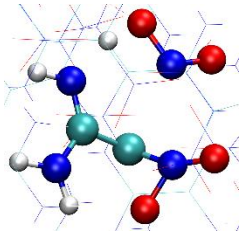
C	-0.795695000000	2.482046000000	2.049797000000
C	-0.112835000000	1.330944000000	1.310291000000
N	-2.171896000000	2.490339000000	2.138076000000
N	-2.931190000000	0.785383000000	2.596774000000
O	-2.791627000000	3.286032000000	2.782141000000
O	-0.202080000000	3.540743000000	2.102852000000
O	-2.488083000000	-0.328504000000	2.891656000000
O	-4.094728000000	1.024476000000	2.593404000000
N	0.835524000000	1.807705000000	0.558726000000
H	1.494002000000	1.247271000000	0.016321000000
H	0.946223000000	2.807438000000	0.623562000000
N	-0.368716000000	0.051455000000	1.402517000000
H	0.210893000000	-0.601975000000	0.874695000000
H	-1.128040000000	-0.315237000000	2.011034000000

IM_F8



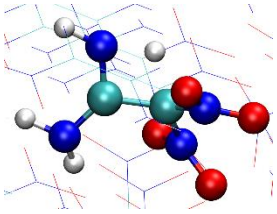
C	1.422655000000	-0.907257000000	2.123042000000
C	0.140658000000	-0.828547000000	1.326087000000
N	1.738560000000	-3.344654000000	2.519464000000
N	2.238946000000	-1.995500000000	2.288563000000
O	2.450779000000	-4.009695000000	3.188675000000
O	0.688583000000	-3.706895000000	2.012579000000
O	1.879376000000	0.180547000000	2.468702000000
O	3.397296000000	-1.790777000000	2.710787000000
N	-0.588503000000	-1.806415000000	0.856241000000
H	-1.452073000000	-1.595294000000	0.353481000000
H	-0.333017000000	-2.761244000000	1.107488000000
N	-0.172225000000	0.426753000000	1.118299000000
H	-1.012018000000	0.682533000000	0.588131000000
H	0.450230000000	1.120034000000	1.538268000000

TS_F7



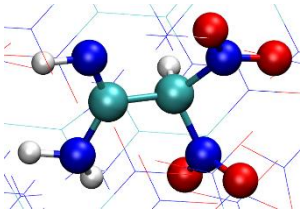
C	1.236947000000	-1.056636000000	2.760872000000
C	0.154386000000	-0.981765000000	1.750485000000
N	1.633805000000	-3.463510000000	2.515800000000
N	2.503773000000	-0.921862000000	2.613309000000
O	2.424641000000	-4.039288000000	3.171984000000
O	0.659243000000	-4.185130000000	2.034574000000
O	2.101635000000	0.314814000000	2.991137000000
O	3.579131000000	-1.315857000000	2.347685000000
N	-0.438613000000	-2.036933000000	1.336436000000
H	-1.190481000000	-1.846059000000	0.668907000000
H	0.056351000000	-3.408549000000	1.649526000000
N	-0.069993000000	0.290452000000	1.385568000000
H	-0.940068000000	0.518638000000	0.898059000000
H	0.455219000000	1.038298000000	1.828370000000

TS_F8



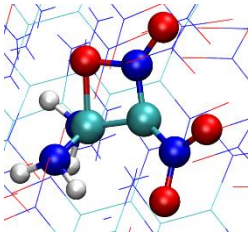
C	-1.185051000000	1.688665000000	2.344751000000
C	-0.101897000000	1.045241000000	1.524026000000
N	-1.651737000000	3.040852000000	2.017195000000
N	-2.204422000000	0.775360000000	2.803244000000
O	-2.569143000000	3.450234000000	2.681283000000
O	-0.982072000000	3.701701000000	1.263237000000
O	-1.773187000000	-0.223328000000	3.351548000000
O	-3.367786000000	0.975840000000	2.570594000000
N	0.942007000000	1.713486000000	1.862874000000
H	1.856667000000	1.558118000000	1.429527000000
H	0.017447000000	2.051882000000	2.796187000000
N	-0.247815000000	-0.038992000000	0.749719000000
H	0.644090000000	-0.499837000000	0.532128000000
H	-0.953548000000	-0.704467000000	1.067552000000

IM_F9



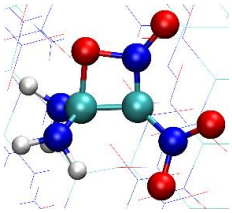
C	1.222889000000	-1.911475000000	2.399115000000
C	0.178850000000	-1.368502000000	1.423683000000
N	1.699966000000	-3.350013000000	2.271383000000
N	2.438450000000	-1.054677000000	2.490130000000
O	2.569926000000	-3.609362000000	3.062818000000
O	1.182346000000	-4.099838000000	1.506528000000
O	2.305745000000	-0.066586000000	3.183219000000
O	3.423940000000	-1.347236000000	1.884387000000
N	-0.644444000000	-2.207420000000	0.987190000000
H	-1.387959000000	-1.775715000000	0.425665000000
H	0.775882000000	-1.871431000000	3.383197000000
N	0.252341000000	-0.009428000000	1.221674000000
H	-0.625324000000	0.401482000000	0.888198000000
H	0.723929000000	0.575259000000	1.907576000000

TS_F9



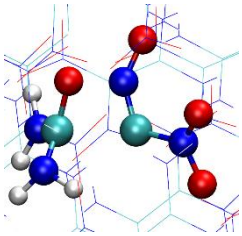
C	1.388716000000	-1.896956000000	1.796390000000
C	0.089238000000	-1.188098000000	1.526475000000
N	1.683670000000	-3.230153000000	2.097006000000
N	1.892667000000	-0.860783000000	2.462267000000
O	2.663742000000	-3.457435000000	2.763408000000
O	0.880042000000	-4.064642000000	1.700265000000
O	0.838656000000	-0.039178000000	2.405133000000
O	2.923103000000	-0.573210000000	2.977977000000
N	-0.972261000000	-1.804228000000	2.090701000000
H	-1.891022000000	-1.500994000000	1.770401000000
H	-0.857627000000	-2.810519000000	2.137441000000
N	-0.099941000000	-0.488215000000	0.320485000000
H	-0.816769000000	-0.999701000000	-0.203195000000
H	-0.482712000000	0.437429000000	0.542739000000

IM_F10



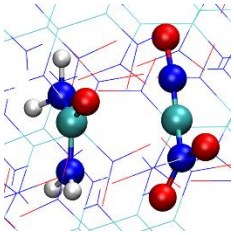
C	1.377480000000	-1.877552000000	1.807809000000
C	0.115626000000	-1.095844000000	1.548922000000
N	1.651512000000	-3.219906000000	2.101941000000
N	1.927333000000	-0.839379000000	2.417164000000
O	2.636906000000	-3.462444000000	2.754055000000
O	0.829564000000	-4.032587000000	1.709267000000
O	0.875009000000	0.015940000000	2.276623000000
O	2.946626000000	-0.544191000000	2.945766000000
N	-0.953600000000	-1.626590000000	2.249120000000
H	-1.852980000000	-1.262568000000	1.927034000000
H	-0.948741000000	-2.637874000000	2.124506000000
N	-0.119587000000	-0.553142000000	0.269461000000
H	-0.810263000000	-1.159878000000	-0.182876000000
H	-0.590299000000	0.350409000000	0.420486000000

TS_F10



C	1.338822000000	-2.355038000000	1.919516000000
C	0.204785000000	-0.526338000000	1.759266000000
N	1.730107000000	-3.712410000000	2.167862000000
N	2.143873000000	-1.463545000000	2.408964000000
O	2.444678000000	-3.950275000000	3.113111000000
O	1.186442000000	-4.559459000000	1.479638000000
O	1.348175000000	-0.248029000000	2.473656000000
O	3.287603000000	-1.329359000000	2.758179000000
N	-0.929196000000	-1.083295000000	2.258966000000
H	-1.788743000000	-0.758174000000	1.819189000000
H	-0.901819000000	-2.088494000000	2.337954000000
N	0.105253000000	0.302974000000	0.749843000000
H	-0.789106000000	0.378823000000	0.254236000000
H	0.778898000000	1.062357000000	0.687718000000

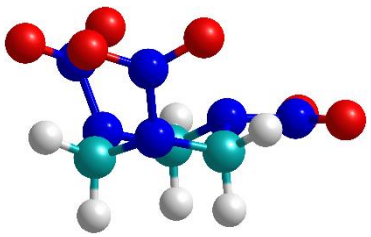
IM_F11



C	2.316501000000	-2.487714000000	2.046500000000
C	-0.070094000000	-0.870714000000	2.010077000000
N	1.787759000000	-3.735174000000	2.458268000000
N	2.830196000000	-1.479839000000	2.313330000000
O	2.385658000000	-4.267643000000	3.351401000000
O	0.825882000000	-4.164932000000	1.873658000000
O	0.424887000000	-1.104887000000	3.111228000000
O	3.289147000000	-0.412609000000	2.499192000000
N	-0.788064000000	-1.791606000000	1.330463000000
H	-1.332292000000	-1.552229000000	0.507130000000
H	-1.100328000000	-2.584181000000	1.870833000000
N	0.203441000000	0.294438000000	1.340936000000
H	-0.570434000000	0.693761000000	0.804559000000
H	0.697369000000	0.964607000000	1.925864000000

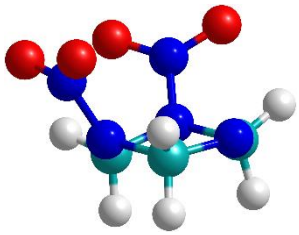
Coordinates of the optimized structures for gas phase RDX initial decomposition, obtained with the M06-2X functional and the SVP basis set.

RDX (gas phase)



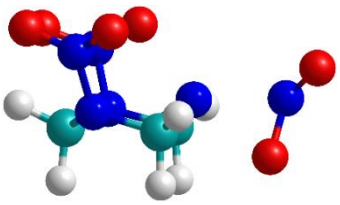
C	-0.756709000000	-1.232574000000	0.792018000000
C	-0.757143000000	1.232384000000	0.792174000000
C	1.272604000000	0.000243000000	1.358847000000
H	-1.119945000000	2.090238000000	0.224475000000
H	-1.087280000000	-1.311236000000	1.843079000000
H	-1.119168000000	-2.090478000000	0.224174000000
H	2.352826000000	0.000425000000	1.201398000000
H	1.048576000000	0.000190000000	2.433933000000
H	-1.087671000000	1.310776000000	1.843267000000
N	0.684427000000	1.203844000000	0.794739000000
N	0.684846000000	-1.203519000000	0.794665000000
N	-1.249914000000	-0.000143000000	0.185691000000
N	1.318760000000	1.741715000000	-0.343758000000
O	0.650031000000	2.445464000000	-1.049982000000
O	2.484436000000	1.489782000000	-0.469437000000
N	1.319521000000	-1.741353000000	-0.343646000000
O	0.651073000000	-2.445267000000	-1.049976000000
O	2.485188000000	-1.489252000000	-0.469066000000
N	-2.559305000000	-0.000364000000	-0.255361000000
O	-3.068597000000	1.076079000000	-0.434131000000
O	-3.068155000000	-1.076992000000	-0.434267000000

IM_R1



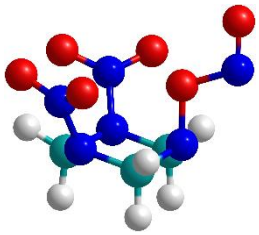
C	-1.219497000000	1.644646000000	0.034547000000
C	1.219724000000	1.644577000000	0.034654000000
C	0.000033000000	-0.039518000000	1.330040000000
H	2.031070000000	1.708532000000	-0.697705000000
H	-1.477144000000	2.332567000000	0.866076000000
H	-2.030764000000	1.708578000000	-0.697906000000
H	-0.000013000000	-1.097927000000	1.597873000000
H	0.000051000000	0.579748000000	2.238186000000
H	1.477297000000	2.332438000000	0.866254000000
N	1.192584000000	0.291113000000	0.578942000000
N	-1.192462000000	0.291207000000	0.578889000000
N	0.000152000000	2.130909000000	-0.534279000000
N	1.776998000000	-0.726357000000	-0.176846000000
O	2.536615000000	-0.389017000000	-1.047666000000
O	1.513517000000	-1.854137000000	0.144020000000
N	-1.777100000000	-0.726191000000	-0.176806000000
O	-2.536655000000	-0.388677000000	-1.047611000000
O	-1.513884000000	-1.854035000000	0.144067000000

TS_R1



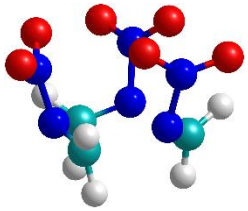
C	-0.801550000000	-1.109502000000	0.844432000000
C	-0.602885000000	1.289886000000	0.747735000000
C	1.351328000000	-0.066707000000	1.314456000000
H	-0.912464000000	2.185200000000	0.204368000000
H	-1.094063000000	-1.010672000000	1.900870000000
H	-1.276899000000	-1.980607000000	0.387556000000
H	2.420229000000	-0.159006000000	1.110438000000
H	1.171944000000	-0.034783000000	2.397390000000
H	-0.949544000000	1.326989000000	1.792295000000
N	0.842866000000	1.173869000000	0.751777000000
N	0.639382000000	-1.223973000000	0.795874000000
N	-1.086081000000	0.099534000000	0.056692000000
N	1.520652000000	1.690216000000	-0.374236000000
O	0.907634000000	2.457914000000	-1.061678000000
O	2.665091000000	1.355518000000	-0.500655000000
N	1.187602000000	-1.864751000000	-0.335078000000
O	0.445177000000	-2.571885000000	-0.956119000000
O	2.355688000000	-1.680142000000	-0.534322000000
N	-2.889312000000	0.480238000000	-0.459884000000
O	-3.491141000000	-0.130250000000	-1.261532000000
O	-2.950741000000	0.131955000000	0.779471000000

IM_R2



C	-0.304922000000	-1.201583000000	1.491853000000
C	-0.308070000000	1.200799000000	1.492018000000
C	1.732170000000	0.002366000000	0.872499000000
H	-0.893392000000	2.086154000000	1.233458000000
H	-0.051982000000	-1.224834000000	2.560999000000
H	-0.887883000000	-2.088428000000	1.233062000000
H	2.542735000000	0.003315000000	0.140997000000
H	2.145484000000	0.002930000000	1.891030000000
H	-0.055051000000	1.224532000000	2.561127000000
N	0.934230000000	1.208150000000	0.734246000000
N	0.937430000000	-1.205493000000	0.734190000000
N	-1.089054000000	-0.001400000000	1.254866000000
N	0.906690000000	1.822881000000	-0.524082000000
O	0.033209000000	2.628214000000	-0.709786000000
O	1.793635000000	1.538678000000	-1.281750000000
N	0.911996000000	-1.820580000000	-0.523942000000
O	0.040760000000	-2.628319000000	-0.709797000000
O	1.798482000000	-1.534161000000	-1.281317000000
N	-2.868344000000	-0.003835000000	-0.198028000000
O	-3.178161000000	-0.004068000000	-1.307248000000
O	-1.443627000000	-0.001746000000	-0.097556000000

TS_R2



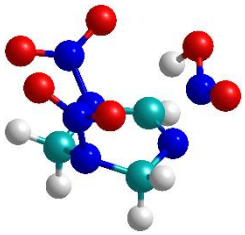
C	-0.691145000000	-1.546699000000	1.367883000000
C	-0.993104000000	1.371874000000	1.367977000000
C	1.685983000000	0.175149000000	1.368172000000
H	-1.071972000000	2.312752000000	0.816701000000
H	-0.834401000000	-1.356429000000	2.433828000000
H	-1.466687000000	-2.085131000000	0.816414000000
H	2.539802000000	-0.228075000000	0.817033000000
H	1.592286000000	-0.043774000000	2.434124000000
H	-0.756065000000	1.400502000000	2.433778000000
N	1.046876000000	1.214000000000	0.925182000000
N	0.528445000000	-1.512784000000	0.925557000000
N	-1.573294000000	0.298765000000	0.925423000000
N	1.345219000000	1.539130000000	-0.433077000000
O	0.399489000000	1.915395000000	-1.072807000000
O	2.483527000000	1.464256000000	-0.792339000000
N	0.661295000000	-1.934193000000	-0.432386000000
O	0.026623000000	-2.882060000000	-0.791887000000
O	1.460947000000	-1.304232000000	-1.071958000000
N	-2.006940000000	0.394995000000	-0.431890000000
O	-2.510634000000	1.418933000000	-0.790126000000
O	-1.863025000000	-0.612439000000	-1.071850000000

IM_R3



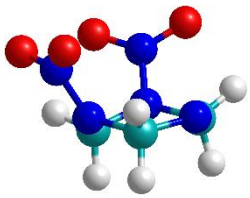
C	-1.740829000000	0.009712000000	0.000049000000
H	-2.714359000000	-0.489085000000	0.000217000000
H	-1.675230000000	1.105337000000	0.000212000000
N	-0.721977000000	-0.737774000000	-0.000145000000
N	0.540614000000	0.021650000000	0.000015000000
O	0.510152000000	1.222020000000	-0.000050000000
O	1.502861000000	-0.679726000000	0.000073000000

TS_R3



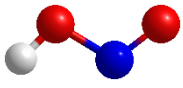
C	-0.196681000000	-1.248148000000	1.073261000000
N	1.015293000000	-0.724876000000	1.298161000000
C	1.214565000000	0.703208000000	1.412911000000
N	0.175589000000	1.500542000000	0.775180000000
C	-1.159602000000	1.032769000000	1.114412000000
N	-1.290415000000	-0.362953000000	0.762519000000
N	1.888601000000	-1.099255000000	-0.325802000000
N	0.367592000000	1.744915000000	-0.595194000000
N	-2.133151000000	-0.712731000000	-0.282757000000
O	1.168162000000	-1.918483000000	-0.903318000000
O	2.986120000000	-0.806605000000	-0.624671000000
O	1.504491000000	1.757386000000	-0.988148000000
O	-0.620019000000	1.950639000000	-1.248075000000
O	-3.004377000000	0.063778000000	-0.567686000000
O	-1.944863000000	-1.800046000000	-0.772125000000
H	0.234888000000	-1.858529000000	-0.136586000000
H	-0.463795000000	-2.145701000000	1.646085000000
H	1.193620000000	0.942135000000	2.486153000000
H	2.194782000000	0.976994000000	1.010724000000
H	-1.264484000000	1.151924000000	2.200972000000
H	-1.925374000000	1.613363000000	0.596585000000

IM_R4



C	-0.599546000000	1.524109000000	-0.404845000000
C	1.544401000000	1.391638000000	0.536759000000
C	-0.062539000000	-0.317425000000	1.141536000000
H	2.508945000000	1.493462000000	0.030856000000
H	-1.384884000000	1.987491000000	-1.008518000000
H	-0.250483000000	-1.390797000000	1.190847000000
H	-0.213988000000	0.136948000000	2.131404000000
H	1.634351000000	1.857296000000	1.529398000000
N	1.288958000000	-0.035813000000	0.733883000000
N	-0.952301000000	0.289042000000	0.157734000000
N	0.523281000000	2.074885000000	-0.220313000000
N	1.779360000000	-0.885668000000	-0.275892000000
O	2.767802000000	-0.523171000000	-0.852350000000
O	1.192162000000	-1.922708000000	-0.440447000000
N	-2.179553000000	-0.287757000000	-0.105252000000
O	-2.857026000000	0.236953000000	-0.948307000000
O	-2.453694000000	-1.260718000000	0.547879000000

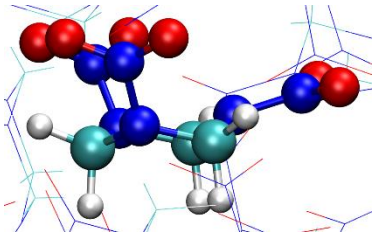
HONO



H	1.706638000000	0.413874000000	-0.000020000000
N	-0.150391000000	0.476362000000	0.000044000000
O	-1.088772000000	-0.212921000000	0.000017000000
O	1.007034000000	-0.255630000000	-0.000053000000

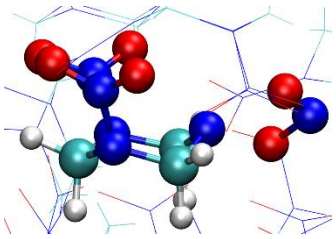
Coordinates of the optimized structures for crystal phase RDX initial decomposition, obtained with the M06-2X functional and the SVP basis set based on the ONIOM model.

RDX (crystal phase)



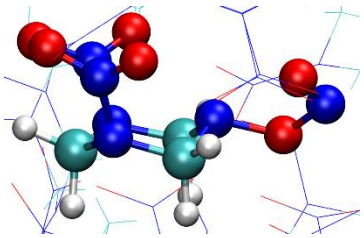
C	2.438058000000	-1.604883000000	-4.339070000000
C	0.661931000000	-2.970944000000	-3.357575000000
C	1.832784000000	-1.305868000000	-1.986030000000
H	3.232766000000	-2.328619000000	-4.078152000000
H	2.709999000000	-1.045692000000	-5.233552000000
H	-0.336286000000	-3.361123000000	-3.564999000000
H	1.319124000000	-3.798381000000	-3.062050000000
H	2.605824000000	-2.018216000000	-1.638871000000
H	1.667242000000	-0.543823000000	-1.223467000000
N	2.222273000000	-0.688482000000	-3.236688000000
N	1.222654000000	-2.361139000000	-4.553849000000
N	0.617592000000	-2.049921000000	-2.237684000000
N	2.912497000000	0.493461000000	-3.224849000000
N	0.308760000000	-1.809202000000	-5.439615000000
N	-0.580922000000	-1.374476000000	-2.015524000000
O	2.981478000000	1.070967000000	-2.161462000000
O	3.363828000000	0.858921000000	-4.273391000000
O	-0.815429000000	-2.221704000000	-5.401854000000
O	0.734015000000	-0.993276000000	-6.228749000000
O	-1.559189000000	-1.814827000000	-2.561927000000
O	-0.549874000000	-0.462879000000	-1.235329000000

TS_R4



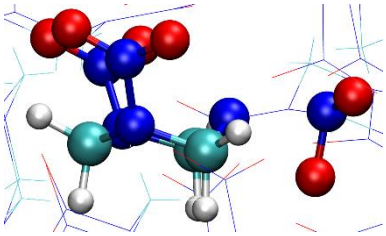
C	-2.115402000000	-1.764728000000	4.381536000000
C	-0.438092000000	-3.161012000000	3.320812000000
C	-1.549684000000	-1.287534000000	2.164641000000
H	-2.907944000000	-2.416331000000	3.964778000000
H	-2.425998000000	-1.358445000000	5.344118000000
H	0.542800000000	-3.616542000000	3.465185000000
H	-1.163871000000	-3.918996000000	2.998352000000
H	-2.408111000000	-1.914827000000	1.849365000000
H	-1.350722000000	-0.521659000000	1.415002000000
N	-1.653593000000	-0.745978000000	3.485749000000
N	-0.939628000000	-2.623737000000	4.579497000000
N	-0.378159000000	-2.178944000000	2.247715000000
N	-3.438447000000	0.789866000000	3.742152000000
N	0.024590000000	-2.040112000000	5.393912000000
N	0.842903000000	-1.567446000000	2.009904000000
O	-3.062865000000	1.015444000000	2.657168000000
O	-2.988666000000	0.838337000000	4.809196000000
O	1.154724000000	-2.418204000000	5.268395000000
O	-0.360334000000	-1.231563000000	6.210659000000
O	1.819167000000	-2.064818000000	2.516032000000
O	0.845732000000	-0.636520000000	1.249080000000

IM_R5



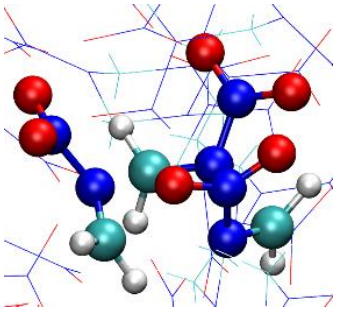
C	-2.328170000000	-1.620056000000	4.419765000000
C	-0.569560000000	-3.040226000000	3.482922000000
C	-1.882264000000	-1.572914000000	2.062218000000
H	-3.137749000000	-2.353172000000	4.238785000000
H	-2.572094000000	-1.002332000000	5.285564000000
H	0.446163000000	-3.386247000000	3.681943000000
H	-1.221048000000	-3.895522000000	3.269596000000
H	-2.649472000000	-2.358291000000	1.926234000000
H	-1.826575000000	-0.952738000000	1.165758000000
N	-2.151127000000	-0.759099000000	3.250856000000
N	-1.103577000000	-2.349533000000	4.647172000000
N	-0.612558000000	-2.212009000000	2.297918000000
N	-3.360589000000	1.013605000000	2.364482000000
N	-0.182716000000	-1.771364000000	5.500123000000
N	0.515428000000	-1.431358000000	2.026132000000
O	-2.396340000000	1.147973000000	1.720607000000
O	-3.379050000000	-0.096548000000	3.148585000000
O	0.942108000000	-2.183439000000	5.463903000000
O	-0.597429000000	-0.932347000000	6.272103000000
O	1.531502000000	-1.742450000000	2.593335000000
O	0.392758000000	-0.576226000000	1.195663000000

TS_R5



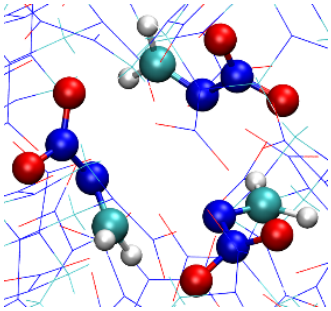
C	-2.433906000000	-1.406807000000	4.262986000000
C	-0.681974000000	-2.936469000000	3.468626000000
C	-1.760002000000	-1.362492000000	1.946691000000
H	-3.258660000000	-2.081187000000	3.970479000000
H	-2.724621000000	-0.781357000000	5.110010000000
H	0.295293000000	-3.334209000000	3.751425000000
H	-1.348797000000	-3.763019000000	3.195289000000
H	-2.568907000000	-2.082525000000	1.729583000000
H	-1.591419000000	-0.703024000000	1.087765000000
N	-1.983222000000	-0.574888000000	3.152572000000
N	-1.276068000000	-2.222746000000	4.592301000000
N	-0.564782000000	-2.098884000000	2.291382000000
N	-2.989128000000	0.920744000000	2.686102000000
N	-0.391964000000	-1.707725000000	5.531203000000
N	0.657448000000	-1.447599000000	2.081218000000
O	-2.731013000000	1.448461000000	1.654672000000
O	-3.839051000000	-0.034270000000	2.671727000000
O	0.716543000000	-2.161138000000	5.552560000000
O	-0.832475000000	-0.880734000000	6.296724000000
O	1.595254000000	-1.853634000000	2.714712000000
O	0.669488000000	-0.597432000000	1.237472000000

TS_R6



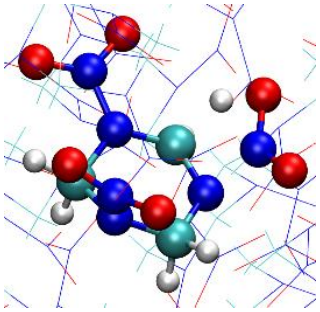
C	-3.182636000000	1.506999000000	-3.842379000000
C	-0.338912000000	3.159310000000	-4.026819000000
C	-1.795431000000	1.383626000000	-1.438051000000
H	-3.167651000000	2.571825000000	-3.628983000000
H	-3.536068000000	1.119837000000	-4.802196000000
H	0.720325000000	2.893227000000	-3.954835000000
H	-0.757849000000	3.889462000000	-3.333097000000
H	-2.590660000000	2.096986000000	-1.194703000000
H	-1.784823000000	0.444676000000	-0.875049000000
N	-2.787778000000	0.731185000000	-2.910577000000
N	-1.141258000000	2.655584000000	-4.881946000000
N	-0.675492000000	1.914424000000	-1.886635000000
N	-2.893395000000	-0.675916000000	-3.174370000000
N	-0.553652000000	1.655592000000	-5.698413000000
N	0.431516000000	1.095378000000	-1.781160000000
O	-2.788197000000	-1.344061000000	-2.184504000000
O	-3.088696000000	-1.014703000000	-4.296692000000
O	0.637002000000	1.620183000000	-5.853700000000
O	-1.350971000000	0.909173000000	-6.209059000000
O	1.412698000000	1.476116000000	-2.383700000000
O	0.407984000000	0.124775000000	-1.067188000000

IM_R6



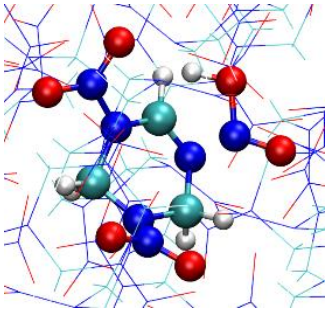
C	-3.302724000000	-1.516937000000	4.277875000000
C	0.479330000000	-3.160530000000	4.244629000000
C	-1.296833000000	-1.042455000000	1.328128000000
H	-3.036195000000	-2.568720000000	4.272319000000
H	-4.075868000000	-1.122855000000	4.947766000000
H	1.424299000000	-2.894353000000	4.728208000000
H	0.467559000000	-3.809518000000	3.365644000000
H	-2.279947000000	-1.486636000000	1.151157000000
H	-1.179129000000	0.044492000000	1.257802000000
N	-2.655858000000	-0.772206000000	3.480095000000
N	-0.651104000000	-2.746502000000	4.648556000000
N	-0.343177000000	-1.837234000000	1.588524000000
N	-3.057062000000	0.588349000000	3.546992000000
N	-0.570249000000	-1.850781000000	5.757058000000
N	0.911139000000	-1.209254000000	1.716421000000
O	-2.994973000000	1.172867000000	2.493085000000
O	-3.371378000000	1.025886000000	4.612555000000
O	0.489073000000	-1.416892000000	6.129943000000
O	-1.631395000000	-1.576120000000	6.250322000000
O	1.644648000000	-1.685343000000	2.549516000000
O	1.204928000000	-0.338037000000	0.946377000000

TS_R7



C	2.508900000000	-1.628058000000	-4.453253000000
C	0.769944000000	-3.003267000000	-3.425249000000
C	1.890637000000	-1.299164000000	-2.088312000000
H	3.290092000000	-2.379869000000	-4.252045000000
H	2.752826000000	-1.043265000000	-5.339461000000
H	-0.294967000000	-3.232633000000	-3.535387000000
H	1.302576000000	-3.951700000000	-3.302261000000
H	2.583198000000	-1.308076000000	-1.232444000000
H	0.884874000000	-0.424062000000	-1.560265000000
N	2.369234000000	-0.747456000000	-3.317118000000
N	1.256841000000	-2.339859000000	-4.627252000000
N	1.004546000000	-2.277713000000	-2.206849000000
N	2.944988000000	0.481598000000	-3.322480000000
N	0.307777000000	-1.714519000000	-5.410001000000
N	-0.610791000000	-1.324699000000	-2.042300000000
O	2.930551000000	1.076191000000	-2.261855000000
O	3.407090000000	0.865326000000	-4.362079000000
O	-0.837984000000	-2.052310000000	-5.282009000000
O	0.710433000000	-0.904585000000	-6.218396000000
O	-1.706655000000	-1.716238000000	-2.225946000000
O	-0.302390000000	-0.301442000000	-1.428952000000

IM_R7



C	2.315013000000	-1.541734000000	-4.744831000000
C	0.980199000000	-3.029532000000	-3.278306000000
C	2.558812000000	-1.565630000000	-2.326035000000
H	3.141897000000	-2.240204000000	-4.937715000000
H	2.203151000000	-0.836583000000	-5.569621000000
H	-0.060525000000	-2.952600000000	-2.942032000000
H	1.180129000000	-4.082911000000	-3.448210000000
H	3.198305000000	-1.198242000000	-1.512492000000
H	1.315186000000	0.412557000000	-1.724426000000
N	2.576815000000	-0.818955000000	-3.517240000000
N	1.103036000000	-2.287846000000	-4.540590000000
N	1.860111000000	-2.605183000000	-2.230378000000
N	3.024786000000	0.463108000000	-3.534315000000
N	-0.046554000000	-1.806263000000	-5.102196000000
N	-0.171255000000	-0.705407000000	-1.957003000000
O	3.021022000000	1.028289000000	-2.447939000000
O	3.345853000000	0.922047000000	-4.586860000000
O	-1.078578000000	-2.314051000000	-4.764300000000
O	0.071694000000	-0.943909000000	-5.955861000000
O	-1.035683000000	-1.217888000000	-1.357428000000
O	0.613982000000	0.039567000000	-1.158115000000