

Supporting Information for

DFT Study of Intermolecular [4+2] versus [3+2] Cycloadditions in the Dimerization of 2,4,6-trinitrotoluene (TNT): Regioselectivity and Stereoselectivity

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Supplementary material includes three parts

Part I: Optimized geometries for all important species during the dimerization of TNT, as calculated at the B3LYP/6-31+G(d,p) level. S2–S20

Part II: Harmonic frequencies for all important species during the dimerization of TNT, as calculated at the B3LYP/6-31+G(d,p) level. S21–S25

Part III: Electronic energies (E), zero-point energies (ZPE), sum of electronic and zero-point energies (Es), sum of electronic and thermal Energies(tEs), sum of electronic and thermal enthalpies(tH), and sum of electronic and thermal free energies(tG) at 298.15K for all important species, as calculated at the B3LYP/6-31+G(d,p) level. (Energies in Hartree) S26–S27

Part I: Optimized geometries for all important species during the dimerization of TNT, as calculated at the B3LYP/6-31+G(d,p) level.

#	TNT			
C	-1.55762300	-0.00005700	-0.03970900	
C	-0.88014500	-1.21112100	-0.01077300	
C	0.51017200	-1.18249900	0.02258000	
C	1.27820000	-0.00001600	0.05225400	
C	0.51012600	1.18239000	0.02261600	
C	-0.88017900	1.21102600	-0.01080500	
H	-1.41770800	-2.15077900	-0.01281400	
H	-1.41775600	2.15067800	-0.01280200	
C	2.77936400	0.00024900	0.18950300	
H	3.12303400	0.88878900	0.71845200	
H	3.12341100	-0.88782900	0.71894700	
H	3.25259600	0.00008400	-0.79660100	
N	1.16856100	-2.50903500	0.01601800	
N	-3.03346300	-0.00007600	-0.09332600	
N	1.16867500	2.50882500	0.01633400	
O	0.62723700	3.40366600	0.66153400	
O	2.19150700	2.63157400	-0.65403700	
O	0.62774700	-3.40356200	0.66217500	
O	2.19071200	-2.63221200	-0.65531300	
O	-3.59562200	1.09248200	-0.11390100	
O	-3.59559700	-1.09264600	-0.11388700	

#	TS ₃ ³			
C	-0.01067300	-0.00328100	-0.03234200	
C	-0.02428000	-0.00100200	1.45180500	
C	1.36125800	0.02407500	1.95023700	
C	2.21710400	0.88222600	1.36607400	
C	1.62427800	1.63459000	0.27429800	
C	0.79962600	0.86707300	-0.69210800	
H	-0.64444200	-0.76594400	1.90862100	
N	1.73542000	-0.72090900	3.15374100	
N	-1.00837800	-0.85244400	-0.68684200	
N	2.50412500	2.70499600	-0.29147200	
O	1.99754600	3.45987700	-1.11935400	
O	3.65769500	2.77044400	0.11870500	
O	0.82676400	-1.28562600	3.76149000	
O	2.92460100	-0.73122200	3.46255400	
O	-0.74499800	-1.35238000	-1.77688400	
O	-2.06273100	-1.01971300	-0.06786800	

O	1.21958300	2.77050900	3.40297200
N	0.99131400	3.33922300	2.33845600
C	0.09773100	2.63038700	1.35038400
O	1.45123000	4.42409700	1.99605000
C	-0.51606100	3.51537400	0.39942900
C	-0.70399900	1.51143100	1.92359100
C	-1.77279800	3.24778300	-0.03144600
H	0.04162600	4.35776200	0.01136300
C	-2.14939400	1.53001200	1.56138600
H	-0.58786500	1.46456900	3.00549800
C	-2.69992700	2.30132100	0.57489000
N	-2.23925400	4.06146100	-1.17792700
N	-2.97379500	0.64509600	2.40131800
C	-4.15383100	2.33092200	0.17312000
O	-2.24272100	5.28034500	-1.05580300
O	-2.55960900	3.42975600	-2.18309900
O	-2.40687600	0.10228600	3.35483900
O	-4.16164000	0.49459700	2.12500900
H	-4.78851400	2.49278600	1.04627100
H	-4.35150300	3.10852900	-0.56183000
H	-4.45120100	1.36789500	-0.25013200
C	0.87579500	1.09880300	-2.17658900
H	0.41977400	2.05616500	-2.44163000
H	1.91914600	1.14314900	-2.50363800
H	0.37648600	0.29726100	-2.71334800
H	3.21799200	1.08830200	1.72158100

$\mathbf{P}_3^3$

C	0.00136200	0.02402300	-0.07718400
C	-0.04535400	-0.01191800	1.43644300
C	1.37743700	-0.05942800	1.91228300
C	2.17134400	0.90094700	1.44361700
C	1.44279800	1.80168600	0.46732400
C	0.79290200	0.94784600	-0.65111600
H	-0.65006500	-0.82239300	1.83109100
N	1.83767500	-1.06486500	2.86961200
N	-0.88407600	-0.86978200	-0.81661100
N	2.44878100	2.78816900	-0.12666300
O	3.48758400	2.29152500	-0.53737800
O	2.15459500	3.97762900	-0.17002000
O	1.02918600	-1.93257700	3.19667100
O	2.99905700	-0.97850800	3.26430800
O	-0.55384400	-1.22485700	-1.94716400

O	-1.92352900	-1.20397800	-0.24208400
O	1.79388000	3.23121700	2.82460700
N	0.74916700	3.51944600	2.25607300
C	0.20265700	2.51707300	1.18692600
O	0.05171600	4.49692300	2.47565500
C	-0.62544400	3.31154200	0.22457500
C	-0.59527200	1.40477200	1.94734700
C	-1.94084000	3.11373700	0.08750300
H	-0.12445000	4.07067200	-0.36151000
C	-2.09803900	1.49230000	1.81890400
H	-0.34436100	1.45177800	3.00801400
C	-2.77826900	2.19779300	0.87925100
N	-2.61319700	4.02262500	-0.87525000
N	-2.79976800	0.68654700	2.82948000
C	-4.25193600	2.10372500	0.57995700
O	-2.19201600	4.03180500	-2.02916100
O	-3.52292400	4.71546500	-0.43179200
O	-2.09594500	-0.02558900	3.55490800
O	-4.02056100	0.78833200	2.93643400
H	-4.82597600	2.77714100	1.22385400
H	-4.44882600	2.38606600	-0.45525500
H	-4.61731700	1.09393700	0.75472700
C	1.01794600	1.26901000	-2.09413900
H	2.01877500	0.93673200	-2.39450700
H	0.29168300	0.76335500	-2.72720500
H	0.96446500	2.34816900	-2.27019800
H	3.21138600	1.05010300	1.69644600

endo-TS₂⁵

C	-2.11424600	1.27509100	-0.21843700
C	-0.79771900	1.02724900	-0.78045100
C	-0.66618200	-0.28149700	-1.42635400
C	-1.60926700	-1.35021600	-1.27205100
C	-2.74496500	-1.01626600	-0.54001000
C	-3.04522600	0.29491700	-0.08483400
H	-0.41900600	1.86253500	-1.36550400
H	-4.01756900	0.51148400	0.34096400
C	-1.41092000	-2.69557600	-1.91955800
H	-0.57883400	-3.23026900	-1.45007700
H	-2.30038900	-3.31360500	-1.83482500
H	-1.14172100	-2.56988600	-2.96964600
N	0.53710200	-0.45204900	-2.07139400
N	-2.44742900	2.64770200	0.15979000

N	-3.78805400	-2.01882900	-0.25063500
O	-4.95626100	-1.65298200	-0.37345600
O	-3.42556500	-3.13395800	0.11996300
O	1.34196700	0.60376200	-1.99463800
O	0.95891000	-1.48268500	-2.61338100
O	-3.58336100	2.88140000	0.56217300
O	-1.54777500	3.48564800	0.03489200
C	2.42206300	-0.99570700	0.85023200
C	1.26971800	-0.89301900	1.69131600
C	2.79834700	-0.06037600	-0.08085200
C	0.44980700	0.17598700	1.55389200
C	1.80893800	0.99387900	-0.33626600
C	0.57244100	1.14794300	0.47075500
C	4.04895300	-0.12370500	-0.91936700
H	4.91889900	0.17861500	-0.33157100
H	4.22557200	-1.14395500	-1.26631000
H	3.96552000	0.52478900	-1.79001500
N	2.39406700	2.35821400	-0.67410300
O	3.49118300	2.60570600	-0.18846700
O	1.69734400	3.12036000	-1.32666800
H	0.36171000	2.17647500	0.76317200
H	1.10233500	-1.62548800	2.47080300
N	3.24651500	-2.20036600	1.08870200
O	4.46759100	-2.09462000	1.02146700
O	2.62986500	-3.23267500	1.34897000
N	-0.59542700	0.38942900	2.55724100
O	-1.22847100	1.44725800	2.47810100
O	-0.77472400	-0.47616700	3.41075800

endo- $\mathbf{P}_2^5$

C	-2.09229000	1.29265600	-0.06768300
C	-0.76121800	0.96652700	-0.66269900
C	-0.77074600	-0.40121800	-1.31319500
C	-1.83598100	-1.37759500	-1.17246000
C	-2.93134600	-0.93730200	-0.46511600
C	-3.10351500	0.41194300	0.01097500
H	-0.55451200	1.72615400	-1.42539200
H	-4.06341500	0.71444800	0.41135300
C	-1.73200600	-2.72908100	-1.82715000
H	-0.95043000	-3.32862800	-1.34827200
H	-2.66617000	-3.27878300	-1.75945400
H	-1.43946600	-2.61680100	-2.87320800
N	0.35891300	-0.69324000	-1.95114000

N	-2.31801100	2.68452800	0.31687600
N	-4.09102600	-1.81411800	-0.22585300
O	-5.20278200	-1.29672300	-0.33694300
O	-3.88132300	-2.98427100	0.09042600
O	1.30343800	0.42901400	-1.96456500
O	0.75617000	-1.68776700	-2.54782300
O	-3.39815700	2.99187300	0.81113600
O	-1.38754000	3.47025700	0.09598700
C	2.62823000	-0.92737900	0.79682700
C	1.46931900	-0.83725600	1.66143300
C	2.86098400	-0.10771700	-0.25431400
C	0.52393700	0.09147400	1.45366200
C	1.72618500	0.82629400	-0.65261700
C	0.50582600	1.05013000	0.29887000
N	2.34590300	2.24192500	-0.89199000
O	3.08878000	2.61606400	0.00698000
O	2.02515200	2.85852200	-1.88976300
N	3.57994400	-1.99930000	1.15942100
O	4.76372400	-1.85509300	0.86444000
O	3.10447100	-2.97571000	1.73845000
N	-0.47968800	0.27705500	2.50974000
O	-1.05616000	1.36842400	2.52915100
O	-0.66846200	-0.63470100	3.31075300
H	0.53086200	2.07106200	0.68940900
C	4.05709200	-0.11050300	-1.16332500
H	4.91708200	0.32979800	-0.64975500
H	4.34155800	-1.12752500	-1.44135400
H	3.85337700	0.45347700	-2.07462900
H	1.41356400	-1.48611400	2.52683900

$exo-TS_3^4$

C	0.00385700	-0.00815000	0.01032100
C	0.01396100	-0.00013500	1.45608800
C	1.34281200	0.00538000	2.04431200
C	2.52139000	0.14896700	1.33592500
C	2.36997500	0.27794400	-0.09909500
C	1.17696000	0.15360600	-0.75421600
H	-0.69619800	-0.65247700	1.95065000
H	1.12125300	0.21717500	-1.83422700
C	3.89390000	0.03609000	1.94743500
H	4.22174500	1.01235000	2.31733700
H	3.89086300	-0.64638700	2.79622700
H	4.62177200	-0.30154800	1.21121600

N	1.35138600	-0.25562400	3.49244300
N	-1.21510200	-0.02638700	-0.60005300
N	3.53532100	0.59044100	-0.94838500
O	3.57048000	0.08240000	-2.06801500
O	4.37139600	1.36694100	-0.49047500
O	0.39574700	-0.89616700	3.94655000
O	2.27245600	0.19244900	4.17049300
O	-1.43973600	-0.03604800	-1.80363400
O	-2.25614500	0.05250900	0.27626900
C	-2.29189400	1.44409700	1.05668100
C	-1.07492700	1.61712000	1.91242800
C	-3.57510000	1.36026300	1.77910600
C	-1.25310100	1.61579800	3.34925600
C	-3.71205300	1.27071300	3.13306200
C	-2.46369200	1.33912800	3.88815000
N	-2.49168000	1.14441000	5.35357100
O	-3.22224800	0.24875500	5.77410000
O	-1.76675300	1.85788600	6.04145300
N	-0.13466400	2.66062400	1.41698600
O	-0.20485200	2.96443600	0.22357100
O	0.70282300	3.08843700	2.20871200
N	-4.74520900	1.45557200	0.88924900
O	-5.73781700	0.78440000	1.16340300
O	-4.64349500	2.20300600	-0.08490000
H	-2.33369200	2.15742100	0.23517400
H	-0.40532100	1.80696800	3.99457500
C	-5.03316600	1.27282800	3.85787200
H	-5.81427100	1.73523900	3.25750700
H	-5.34393000	0.24643200	4.07392900
H	-4.95059200	1.79696700	4.81105700

$exo-P_3^4$

C	-0.00873200	-0.08327800	0.05519800
C	0.05222400	-0.02748700	1.55817100
C	1.49184100	0.08073100	2.02085500
C	2.59846300	0.19198500	1.23191000
C	2.35681900	0.22482700	-0.21596100
C	1.12697100	0.07701200	-0.77404900
H	-0.36583400	-0.95806700	1.96003900
H	0.99819400	0.10024700	-1.84961300
C	4.01020300	0.23585300	1.76331900
H	4.53602400	1.10024700	1.34680800
H	4.03570700	0.31539500	2.84484400

H	4.56065700	-0.64825400	1.43651900
N	1.64128400	-0.15027500	3.46966300
N	-1.20812900	-0.25121900	-0.50144900
N	3.46283100	0.37490300	-1.17915900
O	3.22538900	1.00530900	-2.20880000
O	4.53660700	-0.16776800	-0.91693100
O	1.00992400	-1.11082900	3.92809500
O	2.33636000	0.60832900	4.13863400
O	-1.52537300	-0.42688900	-1.67102600
O	-2.27021100	-0.14679700	0.44849600
C	-2.15057400	1.14110800	1.14441100
C	-0.95378700	1.09056800	2.12534700
C	-3.48809100	1.40099200	1.75580600
C	-1.35025400	0.84423300	3.54846500
C	-3.77305600	1.28548000	3.07351500
C	-2.63673600	0.87809000	3.91924400
N	-2.92875300	0.45188600	5.31098100
O	-3.89628100	-0.29395700	5.45131800
O	-2.17909500	0.83552500	6.20134100
N	-0.21965200	2.46301300	2.05212000
O	0.09182700	2.85783700	0.93534100
O	0.01944600	3.02482800	3.11070800
N	-4.49386400	1.85670200	0.77977900
O	-5.66863800	1.55611300	0.97762200
O	-4.08164000	2.50753300	-0.18185200
H	-1.95771100	1.89990900	0.38308000
H	-0.60055400	0.60175600	4.28920100
C	-5.08058600	1.65221600	3.72427200
H	-5.61524700	2.40113500	3.14260700
H	-5.72337300	0.77071600	3.80264100
H	-4.91234300	2.03125500	4.73442800

$anti-TS_1^2$

C	0.00018300	0.03071400	-0.02709700
C	-0.01288800	0.00461600	1.42469400
C	1.31750800	-0.03021600	2.06891300
C	2.53956700	0.27449500	1.31354700
C	2.37011800	0.44423700	-0.03713600
C	1.12925000	0.25743000	-0.73358600
H	-0.75316200	-0.65349300	1.86811800
H	1.11241500	0.28808800	-1.81565000
C	3.82548700	0.49213700	2.06556100
H	3.73557200	0.18018500	3.10294400

H	4.65530600	-0.05248800	1.60865400
H	4.08339000	1.55437200	2.02945500
N	1.42029400	-1.11112200	3.10331600
N	-1.27482700	-0.18243200	-0.71801200
N	3.51896900	0.76919000	-0.91344900
O	3.48124600	0.31874900	-2.05707100
O	4.42304700	1.46255800	-0.45418800
O	0.46495200	-1.23759600	3.86709500
O	2.42497700	-1.81480000	3.09701700
O	-1.28440900	-0.10777900	-1.94418300
O	-2.25474700	-0.42649300	-0.00991900
O	-0.59301900	1.54097700	1.87893100
N	-0.10606400	1.71311000	3.09404400
C	-0.93321200	1.34068100	4.21624400
O	1.17869400	1.46509400	3.09889600
C	-0.48492200	1.63398200	5.52656800
C	-2.19804700	0.81635500	3.94767300
C	-1.37639300	1.26586600	6.55062400
C	-3.02670200	0.50877000	5.01800700
H	-2.53874400	0.65382800	2.93347700
C	-2.63922400	0.72386200	6.33193600
N	-1.00499400	1.45108000	7.97173300
N	-4.36319300	-0.06139400	4.74817000
O	0.16054200	1.22228100	8.28999400
O	-1.89750200	1.79600700	8.74327800
O	-4.68283200	-0.21797200	3.57197200
O	-5.06238600	-0.34108100	5.71984600
C	0.81381400	2.35317400	5.79369000
H	0.75284400	2.94391100	6.70742800
H	1.63629600	1.64374300	5.92220200
H	1.06621700	3.01244600	4.96246700
H	-3.29807100	0.48872700	7.15741800

$anti-P_1^2$

C	-2.48873100	1.53620700	-0.11804100
C	-1.20320700	0.79685500	-0.03114000
C	-1.36758900	-0.71825500	0.26905700
C	-2.74842900	-1.35032400	0.17009100
C	-3.78870800	-0.51648000	-0.07244800
C	-3.68172700	0.92828900	-0.17102100
H	-0.52508600	1.26093500	0.68976200
H	-4.58826300	1.51371500	-0.26692500
C	-2.78046700	-2.84421500	0.31357800

H	-3.41190900	-3.30729700	-0.44718100
H	-1.77374700	-3.25838300	0.24219400
H	-3.21362200	-3.11491800	1.28247900
N	-0.86297000	-0.94596100	1.74483100
N	-2.39942600	2.99727700	-0.15917800
N	-5.16012300	-1.03821800	-0.25902100
O	-5.93757200	-0.32205400	-0.88875300
O	-5.43646200	-2.13733300	0.21655500
O	-1.70813000	-0.76179100	2.61313800
O	0.30627600	-1.24302300	1.90826300
O	-3.43729200	3.64101500	-0.28372500
O	-1.26622200	3.47646300	-0.05967300
O	-0.59285700	0.76219500	-1.34889400
N	0.24024900	-0.35889200	-1.39628100
C	1.54400200	-0.13217900	-0.79963800
O	-0.51542400	-1.36262400	-0.62883200
C	2.43440200	-1.23303300	-0.76519900
C	1.93655000	1.15777500	-0.44943100
C	3.71667700	-0.95349500	-0.26349800
C	3.23674100	1.35631800	0.00622900
H	1.27004400	2.00512200	-0.54779400
C	4.14611600	0.31705600	0.11122300
N	4.71809800	-2.03289600	-0.11263500
N	3.65944700	2.71985800	0.38597900
O	4.31403800	-3.14269000	0.23079400
O	5.89434800	-1.73927800	-0.31712000
O	2.83247500	3.62166200	0.26520400
O	4.80861100	2.86025300	0.79981000
H	5.15570200	0.48628100	0.46135100
C	2.02432600	-2.58049800	-1.29997000
H	1.59576800	-3.19769400	-0.50527500
H	1.27237100	-2.45891500	-2.08176800
H	2.87775400	-3.12350300	-1.70559400

$syn-TS_l^2$

C	-0.00555300	-0.01382400	0.00568300
C	-0.00286000	-0.00548400	1.46161700
C	1.34841200	-0.01352000	2.07964700
C	2.56669400	0.13629400	1.29029300
C	2.37914800	0.27386800	-0.06791700
C	1.11789900	0.16304500	-0.73056400
O	-0.68604300	1.43413600	2.00373500
N	0.32097000	2.19807700	2.39665100

C	0.75712000	3.25640000	1.51824700
O	1.20392200	1.50067600	3.05029700
C	1.80571700	4.11369700	1.93422700
C	0.03567700	3.46517600	0.34124200
C	2.14792600	5.11725200	1.00846700
C	0.41627700	4.50331600	-0.49624100
H	-0.80701100	2.83958100	0.08362900
C	1.47516200	5.34499700	-0.18729300
N	3.29003700	6.02041700	1.27700400
N	-0.33253100	4.71862300	-1.75287000
O	4.29891200	5.52301000	1.77450400
O	3.16007500	7.19900100	0.95654100
O	-1.25816300	3.94760800	-1.99547800
O	0.02425600	5.65315200	-2.46591600
H	-0.72063900	-0.66723100	1.93386800
N	3.51456300	0.57021300	-0.96187700
O	3.27582200	1.31406200	-1.91509100
O	4.60596900	0.06488400	-0.71195900
N	-1.29026200	-0.25062500	-0.66243100
O	-1.31005100	-0.24188300	-1.89114400
O	-2.26490800	-0.44645700	0.06688000
N	1.41141900	-0.95925100	3.26127600
O	2.41404700	-1.65751700	3.37474600
O	0.43481700	-0.97739400	3.99674600
H	1.06941400	0.20125700	-1.81189000
C	3.90075300	0.26037300	1.98318800
H	4.47388900	-0.66460200	1.88689500
H	4.49605600	1.05657200	1.53016400
H	3.76842000	0.47133100	3.04367000
H	1.75942200	6.15497400	-0.84646200
C	2.44191200	4.01996600	3.29971700
H	1.72130300	3.65508600	4.03275100
H	3.29167800	3.33230800	3.29779900
H	2.81323500	4.99227100	3.62253400

$_{syn}P_1^2$

C	-0.00122000	0.02045000	0.03027600
C	0.00378700	0.00372300	1.51854200
C	1.44850400	0.05036400	2.14419400
C	2.65140000	0.25541700	1.23793200
C	2.40909700	0.33374100	-0.09216800
C	1.10209300	0.19445200	-0.70969500
O	-0.56242700	1.22471300	2.00977200

N	-0.07067600	1.25500600	3.33715100
C	-0.22093300	2.57956700	3.88442400
O	1.41134100	1.07812500	3.06253000
C	-0.55525800	3.65685400	3.06660600
C	-0.04418400	2.69692100	5.28251100
C	-0.75189100	4.89785800	3.65932300
C	-0.23743000	3.99203700	5.80024800
C	-0.60900300	5.08733300	5.02648200
N	-1.11798100	6.04896200	2.80932300
N	-0.05649100	4.26471900	7.24340000
O	-1.24060600	5.84331900	1.60318100
O	-1.27213900	7.13463800	3.36444100
O	0.83247800	3.65254400	7.83268000
O	-0.79517300	5.10602100	7.75071800
H	-0.55553500	-0.84617800	1.91919500
N	3.50620000	0.59238900	-1.04981900
O	3.19748300	1.17065600	-2.09095000
O	4.63887100	0.21814000	-0.75379700
N	-1.29337600	-0.20543400	-0.62618500
O	-1.34785800	-0.11353900	-1.85005000
O	-2.24022000	-0.48093900	0.11396300
N	1.66284200	-1.33511700	2.87233800
O	1.76220800	-1.34689300	4.08461200
O	1.70516900	-2.30016300	2.11481800
H	-0.77888000	6.05618400	5.47795900
H	-0.67892300	3.53627600	1.99921800
C	0.29959900	1.49556300	6.12246500
H	-0.19742800	1.53218600	7.09302500
H	0.02283900	0.57925300	5.60241400
H	1.37580400	1.46437600	6.31860800
C	3.97300400	0.37455900	1.94008900
H	4.50146800	-0.58567300	1.89615500
H	4.62385300	1.10713200	1.46158700
H	3.82597200	0.64459800	2.98704300
H	1.03324400	0.20760700	-1.79091400

$syn-TS_l^5$

C	0.00095500	-0.00680300	-0.00774700
C	-0.02934300	-0.00263100	1.47660200
C	1.27087000	-0.03146200	2.12210000
C	2.43600400	0.02101100	1.43034200
C	2.40081700	0.00383000	0.00532900
C	1.25258000	-0.04692400	-0.75798200

H	-0.78106300	-0.64864400	1.91615600
N	1.29381300	-0.15074100	3.58230800
N	-1.14242200	-0.79888800	-0.61341700
N	3.73077100	0.06840900	-0.63134600
O	3.97050600	-0.69524600	-1.56250400
O	4.51871900	0.88666200	-0.15488000
O	0.20529500	-0.27854000	4.14684800
O	2.38641400	-0.11376100	4.14638800
O	-1.53292200	-0.47835300	-1.72493800
O	-1.57818100	-1.72564100	0.06431900
O	-0.75166400	1.64001700	-0.30146100
N	-0.54684400	2.26025600	0.81911300
C	0.54849000	3.19663400	0.91040100
O	-0.77501300	1.45686400	1.85111700
C	0.74218200	3.92929800	2.10730800
C	1.30708900	3.41280400	-0.23978900
C	1.83461100	4.81755600	2.07975000
C	2.35078000	4.32444100	-0.18701700
H	1.09033900	2.88554800	-1.15756500
C	2.63576600	5.04358800	0.96479600
N	2.19661900	5.59608700	3.28680300
N	3.17574900	4.53260800	-1.39436400
O	2.11415200	5.02825500	4.37337400
O	2.58099600	6.75028600	3.11186000
O	2.91509000	3.84340200	-2.38007100
O	4.06385600	5.37766100	-1.33184600
C	1.23397600	-0.07582500	-2.26446900
H	2.18187800	0.25918800	-2.68095100
H	1.06663200	-1.09776400	-2.62487300
H	0.42197100	0.54133200	-2.64781200
H	3.38651100	0.04030300	1.94945500
H	3.44436400	5.76238100	0.99330900
C	-0.20250000	3.82931000	3.27942200
H	-0.23386800	4.76692000	3.83416100
H	-1.20914900	3.58385200	2.93931700
H	0.11007600	3.04879000	3.97864000

$syn-P_1^5$

C	1.61764068	-0.80729442	-0.82162035
C	1.56819357	-1.20999267	0.70225247
C	2.62864674	-0.55992774	1.52087003
C	3.47828249	0.35760674	1.03992880
C	3.44447517	0.75604682	-0.35643281

C	2.61064274	0.24252922	-1.29142081
H	1.58306623	-2.29833040	0.80612365
N	2.74705562	-1.00061998	2.91590029
N	1.94510099	-2.12480086	-1.62738318
N	4.40603865	1.82498320	-0.70434451
O	4.85326544	1.85707971	-1.84842314
O	4.69251357	2.61490128	0.19464317
O	2.03734115	-1.95085510	3.25037756
O	3.53702989	-0.40772798	3.64715594
O	1.13026059	-2.53462540	-2.43046163
O	3.03846861	-2.61617732	-1.35957694
O	0.34254142	-0.36620066	-1.11908583
N	-0.49457535	-1.01599505	-0.06844695
C	-1.77382939	-0.34182122	-0.01249479
O	0.28602006	-0.70429818	1.09462665
C	-2.82876353	-1.24742073	-0.11428692
C	-1.97304481	1.05471232	0.11331259
C	-4.13416717	-0.77373246	-0.06626016
C	-3.32366058	1.45582127	0.13045660
C	-4.40335023	0.57932436	0.06761478
N	-5.25587336	-1.72774972	-0.16273260
N	-3.68404677	2.88950373	0.21787817
O	-4.97428016	-2.91975232	-0.26735268
O	-6.39403780	-1.26459530	-0.13201198
O	-3.00283219	3.68790005	-0.42317688
O	-4.65889716	3.17972858	0.90722559
C	2.52401980	0.60468842	-2.74570262
H	2.73999928	1.65921263	-2.91816944
H	3.27291421	0.03689421	-3.31202980
H	1.53598435	0.36038240	-3.13962004
H	4.22371170	0.80064463	1.68957153
H	-5.42107378	0.94521639	0.11604513
C	-0.83818588	2.03865194	0.24509678
H	0.05047391	1.55012140	0.63216267
H	-0.60981778	2.48287342	-0.72830132
H	-1.10640662	2.85967948	0.91191420
H	-2.62571111	-2.30516827	-0.22522765

$anti-T_I^2$

C	-1.69798000	0.10710700	0.27036600
C	-2.51326200	-1.04194500	0.15673400
C	-3.89568500	-0.78250100	0.09394000
C	-4.45234000	0.49054400	0.17925100

C	-3.58754700	1.57047900	0.29831900
C	-2.21114900	1.40342300	0.34283700
N	-4.86423700	-1.89054100	-0.06255200
N	-0.26256800	-0.02121000	0.35950800
N	-4.15006700	2.93486800	0.37254000
O	-3.35672100	3.86629500	0.48943400
O	-5.37289500	3.04470700	0.31180900
O	-4.52527000	-2.85071900	-0.75258600
O	-5.95475000	-1.76489300	0.49052900
O	0.42125400	0.89012200	0.89983500
O	0.20662600	-0.62061100	-0.82788400
C	2.10913600	-0.84227800	-0.94274100
C	2.55720200	-1.27274500	0.36837600
C	2.50094000	0.41477300	-1.49650600
C	3.29899300	-0.32175000	1.07227800
C	3.21628700	1.28485900	-0.70995900
C	3.62158200	0.94714300	0.58109900
H	4.17719000	1.64896700	1.18984600
H	2.21633300	0.66047700	-2.51147300
C	2.12835400	-2.59327500	0.94216800
H	1.27101800	-2.98945300	0.40211100
H	2.93885000	-3.32426700	0.87179000
H	1.88193500	-2.48832700	2.00080800
N	3.79884600	-0.60873900	2.43914200
O	4.10591000	-1.76922300	2.70262000
O	3.89175300	0.34484300	3.20686500
N	3.59001700	2.60895300	-1.25534700
O	3.19573800	2.88095400	-2.38560600
O	4.26876000	3.33746600	-0.53652900
N	1.90996900	-1.89909400	-2.01990000
O	2.36582600	-3.01514700	-1.79938700
O	1.35951100	-1.53595000	-3.04778500
H	-5.52491500	0.63208900	0.15573700
C	-1.92417800	-2.42722500	0.18474400
H	-1.75423300	-2.79837500	-0.82994300
H	-0.96973600	-2.41172400	0.71095000
H	-2.59179500	-3.13337800	0.67911000
H	-1.54640300	2.25192400	0.44137800

$anti-PP_1^2$

C	0.09315500	0.40371800	0.03013900
C	0.16951600	0.35008000	1.43209900
C	1.32383500	0.10868600	2.11311600

C	2.60295800	-0.07922400	1.36902000
C	2.52418700	-0.02829200	-0.14537500
C	1.27864000	0.18752700	-0.69852900
O	3.62373000	-0.01981900	3.94393700
N	3.85388100	0.96183000	3.22276200
C	5.07237100	1.73007100	3.37271600
O	3.63337900	0.80783500	1.73193400
C	5.05371900	3.11243600	3.09919500
C	6.19520800	1.04038800	3.82545300
C	6.29597800	3.75809500	3.26950100
C	7.37639100	1.75269100	3.97921900
C	7.45360900	3.10757800	3.68668500
N	6.44301700	5.20942400	3.01190000
N	8.58695700	1.04871600	4.45233000
O	5.47438000	5.93329300	3.23447700
O	7.53684200	5.59461500	2.60614800
O	9.61574700	1.71149100	4.56317100
O	8.47877900	-0.14946200	4.70124600
H	8.38679400	3.64675800	3.78649500
N	3.13311900	-1.59163600	1.71351200
O	4.33691500	-1.77408500	1.71544900
O	2.25697600	-2.42568900	1.87589600
C	3.80304500	-0.21641500	-0.91052600
H	4.66179800	0.02773600	-0.28675100
H	3.90161200	-1.25943100	-1.23543200
H	3.82310200	0.39338600	-1.81530800
N	1.11938000	0.23860200	-2.17371000
O	0.29894700	1.04129300	-2.61302100
O	1.79968400	-0.52734700	-2.85140400
H	-0.84221700	0.60475500	-0.47307100
N	-1.07887700	0.56555500	2.20907500
O	-2.11550100	0.71837000	1.56808400
O	-0.98879700	0.58018000	3.43327800
H	1.32946400	0.05180300	3.19261800
C	3.78951300	3.81209500	2.67241900
H	3.96642000	4.46327900	1.81306700
H	3.01584900	3.09293300	2.41294900
H	3.42625500	4.45364500	3.47974900
H	6.14806800	-0.01995000	4.04156100

$anti-TT_I^2$

C	0.12188600	-0.03689300	-0.07329000
C	-0.06956600	-0.13349400	1.34357000

C	1. 15184800	-0. 01214600	2. 18872400
C	2. 49918100	-0. 18632800	1. 49903100
C	2. 52715600	0. 03846900	0. 09683600
C	1. 34491700	0. 04156200	-0. 69646900
O	1. 12865700	-0. 91960600	3. 28502200
N	2. 21238500	-1. 85017900	3. 13347100
C	3. 20062400	-1. 73637400	4. 17444900
O	2. 61539900	-1. 80043700	1. 87529400
C	4. 54383800	-1. 66560700	3. 79849800
C	2. 77838700	-1. 82479900	5. 52340200
C	5. 50310200	-1. 62601800	4. 80226600
C	3. 81203300	-1. 74452700	6. 47163600
C	5. 16366900	-1. 66246100	6. 14622300
N	6. 93135600	-1. 55014600	4. 42457900
N	3. 50557300	-1. 76210300	7. 92018000
O	7. 19807400	-1. 57764900	3. 22629000
O	7. 74922800	-1. 46740500	5. 33808700
O	4. 30742400	-2. 33520200	8. 65395400
O	2. 48657200	-1. 18382400	8. 29245000
H	5. 92315000	-1. 63851100	6. 91681100
C	1. 33460700	-2. 06201500	5. 88366200
H	0. 81327600	-1. 11334400	6. 04037200
H	0. 82787300	-2. 60418900	5. 08371800
H	1. 24748500	-2. 63410300	6. 80730400
H	4. 84343500	-1. 64362300	2. 75804600
H	3. 34624500	0. 22986300	2. 04145700
H	1. 41866500	0. 12921600	-1. 77209500
N	3. 81049600	0. 23406900	-0. 52283600
O	3. 82796200	0. 48606100	-1. 73326700
O	4. 81749300	0. 13591000	0. 19683800
N	-1. 04918100	0. 01473800	-0. 96868500
O	-0. 92679400	-0. 47280600	-2. 09169500
O	-2. 06660900	0. 55888000	-0. 53835200
N	1. 20937000	1. 44148500	2. 89666700
O	0. 53321500	2. 31301000	2. 37757000
O	1. 93946700	1. 54820700	3. 86815200
C	-1. 38850600	-0. 32092800	2. 02852200
H	-1. 24302200	-0. 68591600	3. 04672300
H	-1. 94263100	0. 62467300	2. 06747600
H	-2. 02378000	-1. 03206300	1. 49371300

$syn-T_I^2$

C	0. 00428700	0. 07782400	0. 03809200
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C	0.02130100	-0.01713400	1.44870300
C	1.30679900	-0.04884600	2.02236700
C	2.48870400	0.04869200	1.29254100
C	2.39086500	0.14920200	-0.09014500
C	1.16332500	0.16358000	-0.73767100
N	1.47248500	-0.18312400	3.49104200
N	-1.25018000	0.14034700	-0.67136200
N	3.63279000	0.23735500	-0.89434900
O	3.50996500	0.33827200	-2.10721800
O	4.69598500	0.20140800	-0.28977300
O	0.67652600	-0.89754400	4.08731700
O	2.41003900	0.41162000	4.00434700
O	-1.33229600	0.70588900	-1.78845200
O	-1.97669200	-1.03409100	-0.44154400
C	-3.75200100	-0.99171700	-1.28508500
C	-4.33954900	-2.04799000	-0.48501700
C	-3.35587800	-1.20205100	-2.64172300
C	-4.26381600	-3.31486000	-1.06305200
C	-3.30082500	-2.49703300	-3.10613000
C	-3.72442700	-3.57575200	-2.32930600
H	3.45243000	0.05027000	1.78802500
N	-4.18985300	0.42546000	-0.98696900
O	-4.02396000	0.86950600	0.13442800
O	-4.72667300	1.00436900	-1.91744800
N	-2.80930500	-2.75451000	-4.48326700
O	-2.46891800	-1.78656700	-5.14433600
O	-2.78082500	-3.92055100	-4.85170000
N	-4.78957700	-4.51165400	-0.35433700
O	-5.89810300	-4.42676200	0.15420000
O	-4.07848400	-5.50504400	-0.36146100
C	-4.88183700	-1.76788600	0.88598200
H	-4.14486500	-1.20299700	1.46209500
H	-5.78377500	-1.14483400	0.82180900
H	-5.14869600	-2.68148100	1.41307400
H	-3.66361600	-4.58959700	-2.70956700
H	-3.06300800	-0.36152400	-3.25779700
C	-1.25145700	0.00327500	2.25361700
H	-1.55506400	-1.01540800	2.51831100
H	-1.11533500	0.54877500	3.19035100
H	-2.05299500	0.46932000	1.67847200
H	1.09789800	0.25057500	-1.81626100

$syn-PP_I^2$

C	-0.02779300	0.09970800	0.07790900
C	-0.01573100	-0.12404700	1.57702000
C	1.21462900	-0.09651000	2.20539000
C	2.44223400	0.17237600	1.57439600
C	2.42730300	0.38773900	0.18518600
C	1.29409300	0.35008400	-0.56707200
H	1.33057400	0.51487900	-1.63402200
N	1.30744400	-0.32897700	3.66925000
N	3.71829000	0.67552500	-0.49139300
O	3.68571000	0.92773300	-1.69209800
O	4.73083300	0.64188700	0.20365400
O	0.54983400	-1.15742900	4.16823700
O	2.15539000	0.31836900	4.27881600
C	-2.22095400	2.44224500	-1.70213200
C	-3.44639200	2.59211800	-1.02062100
C	-1.67871500	3.41324600	-2.54228000
C	-4.08318900	3.83187100	-1.22577500
C	-2.37892100	4.60070000	-2.70449600
C	-3.58758600	4.82892300	-2.06074800
H	-4.13219900	5.75290300	-2.20640900
H	-0.74244600	3.24500100	-3.05980200
C	-4.03319900	1.46756100	-0.20969200
H	-3.57526700	0.51808800	-0.48662500
H	-3.87301600	1.64138700	0.85803300
H	-5.11285400	1.40125200	-0.35712200
N	-5.36428200	4.14242800	-0.55147700
O	-5.54125100	3.68110000	0.57465300
O	-6.15562400	4.86139400	-1.15670300
N	-1.82288300	5.64895700	-3.58536100
O	-0.75591200	5.40528800	-4.14447400
O	-2.46507900	6.69050500	-3.69561800
N	-1.49728700	1.19809300	-1.59167000
O	-0.77072700	0.78323200	-2.50582700
O	-0.99178600	1.09979400	-0.17256100
C	-1.33101700	-0.36698600	2.25994700
H	-1.36750000	0.11520700	3.23901300
H	-2.15194100	-0.00225900	1.64680600
H	-1.47881600	-1.43901100	2.43548200
H	3.36264600	0.21786800	2.13953600
N	-0.60069100	-1.31004000	-0.55466500
O	0.25180100	-2.11676200	-0.88194700
O	-1.81016700	-1.45792100	-0.58573900

#	$syn-TT_1^2$		
C	0.36349200	-0.30023200	-0.25428700
C	-0.15483500	0.21384500	1.09746600
C	0.84938400	0.52082400	2.07642700
C	2.14564500	-0.02168400	2.00215200
C	2.50179100	-0.76552300	0.88798200
C	1.69276600	-0.94780200	-0.27051100
N	0.47118200	1.36380700	3.17373300
N	0.28556600	0.94134700	-1.27071100
N	3.84342900	-1.37170600	0.93546600
O	3.98839200	-2.45910500	0.37158600
O	4.72397400	-0.77231100	1.55050800
O	-0.70408600	1.76839900	3.21356900
O	1.33645000	1.63639900	4.01465100
O	1.34735300	1.47485700	-1.54277400
O	-0.82832900	1.27407600	-1.64575800
O	-0.63340400	-1.20834200	-0.73956300
N	-1.60230200	-1.34704400	0.30867200
C	-2.38862000	-2.52810100	0.22467100
O	-0.98319700	-1.11116900	1.46665200
C	-2.32457500	-3.44741300	1.27515400
C	-3.23864000	-2.67897200	-0.89873100
C	-3.14036900	-4.56758500	1.20916700
C	-3.99989800	-3.86091000	-0.89977500
C	-3.98899900	-4.79390500	0.13403600
N	-3.09291700	-5.55422700	2.31002600
N	-4.89807800	-4.17599200	-2.03463900
O	-2.33104700	-5.31582500	3.24378600
O	-3.81793300	-6.54044200	2.21107800
O	-4.52004000	-3.85937200	-3.16041300
O	-5.94817400	-4.75544700	-1.77033200
H	2.85803200	0.16114700	2.79532600
H	-4.62515200	-5.66921000	0.09955600
C	2.11093200	-1.64911900	-1.53293800
H	2.09856400	-2.73744600	-1.41405200
H	3.12897500	-1.37494700	-1.82326800
H	1.44129000	-1.38890600	-2.35678200
H	-0.94241400	0.96136500	1.01987400
H	-1.66189300	-3.29803100	2.11758000
C	-3.33752100	-1.61200600	-1.95639800
H	-3.03996000	-0.64278700	-1.55585800
H	-2.68358600	-1.84625200	-2.80187500
H	-4.35199600	-1.54185900	-2.35055200

Part II: Harmonic frequencies for all important species during the dimerization of TNT, as calculated at the B3LYP/6-31+G(d,p).

TNT

45	49	53	92	118	149	175	182	185	288	315	321	353	359	375
466	473	532	543	646	666	704	732	738	778	778	801	831	916	943
950	956	1049	1049	1101	1185	1222	1223	1356	1383	1391	1400	1422	1427	1479
1480	1501	1600	1616	1620	1657	1661	3079	3148	3175	3255	3255			

TS_3^3

-369	19	29	46	49	52	59	65	77	78	84	86	103	112	131
138	151	159	179	184	196	198	230	280	302	306	309	323	331	338
347	357	368	400	402	417	426	466	516	532	533	545	566	582	618
625	664	690	703	709	724	736	750	760	767	772	782	793	804	820
826	835	892	904	912	922	942	948	994	1020	1040	1047	1060	1077	1114
1132	1150	1157	1173	1183	1224	1262	1295	1320	1329	1353	1360	1370	1373	1379
1386	1410	1411	1415	1425	1432	1466	1473	1499	1502	1554	1598	1607	1613	1619
1625	1632	1640	1671	1681	3070	3080	3129	3141	3149	3184	3207	3208	3254	3266

P_3^3

28	43	46	47	50	57	62	65	77	87	91	107	118	122	139
147	162	175	187	204	218	242	254	278	296	308	312	324	337	346
355	384	387	411	428	438	462	482	486	500	553	593	597	615	651
678	696	709	716	735	739	744	749	767	774	782	802	819	831	841
869	882	892	902	916	931	943	970	1000	1019	1043	1047	1054	1067	1112
1115	1138	1145	1156	1197	1209	1238	1264	1271	1322	1350	1354	1371	1373	1374
1383	1398	1405	1412	1418	1419	1469	1472	1482	1500	1593	1603	1616	1628	1640
1652	1657	1681	1720	1723	3051	3074	3110	3119	3142	3183	3185	3206	3251	3279

$endo-TS_2^5$

-605	22	36	44	45	52	61	64	81	87	90	101	122	132	144
154	168	170	180	195	204	216	232	263	292	307	312	325	334	343
349	352	360	374	388	414	458	467	469	511	532	540	565	592	620
649	672	680	690	700	704	737	742	753	755	773	776	780	791	809
815	824	891	902	922	934	956	966	1009	1024	1045	1048	1051	1076	1098
1113	1152	1161	1181	1203	1212	1232	1254	1312	1344	1358	1362	1371	1382	1385
1392	1401	1419	1422	1428	1443	1472	1474	1479	1498	1533	1551	1573	1601	1602
1622	1627	1655	1663	1675	3071	3078	3135	3143	3144	3155	3178	3201	3248	3251

$endo-P_2^5$

15	35	43	46	51	57	60	82	89	94	98	118	132	146	155
160	169	179	186	198	217	258	274	290	309	318	323	335	342	348
362	373	390	410	432	452	470	485	509	522	550	560	592	615	636
661	667	685	689	696	728	737	741	765	768	776	790	794	812	823
827	861	896	918	954	956	960	966	968	1030	1043	1049	1059	1066	1099
1121	1132	1153	1197	1205	1212	1255	1273	1317	1325	1347	1363	1367	1377	1383
1394	1399	1403	1414	1418	1426	1471	1478	1481	1499	1571	1604	1605	1613	1621
1658	1663	1676	1704	1716	3059	3067	3068	3108	3129	3135	3161	3205	3246	3248

$exo-TS_3^4$

-461	21	32	46	51	54	58	60	76	92	92	94	99	115	144
151	166	172	184	188	200	217	250	263	275	314	321	332	333	344
353	363	374	397	406	429	472	477	499	519	536	546	573	580	629
647	654	665	676	701	717	730	739	752	756	771	776	780	798	807
821	830	880	915	919	928	946	949	1006	1039	1040	1045	1051	1063	1105
1131	1152	1168	1183	1215	1219	1250	1303	1312	1348	1352	1366	1373	1379	1381
1391	1408	1415	1420	1429	1464	1470	1479	1498	1500	1535	1570	1587	1601	1610
1613	1618	1626	1654	1683	3077	3078	3144	3150	3158	3181	3182	3209	3247	3251

$exo-P_3^4$

12	28	41	48	51	55	58	63	76	89	92	98	121	141	150
171	179	188	194	204	226	250	256	258	298	316	322	333	341	353
356	364	399	402	417	461	470	478	488	547	567	578	601	609	618
640	671	681	703	712	730	735	753	759	763	771	800	803	809	832
850	859	882	907	916	926	945	970	991	1016	1033	1039	1052	1056	1107
1120	1127	1162	1212	1224	1259	1267	1318	1338	1352	1367	1373	1374	1377	1385
1395	1398	1407	1420	1421	1469	1471	1472	1497	1500	1567	1601	1610	1611	1627
1644	1652	1660	1673	1720	3056	3074	3079	3117	3139	3140	3177	3219	3243	3262

$anti-TS_l^2$

-533	19	29	33	42	46	50	56	63	69	86	98	112	132	137
144	157	173	185	190	207	213	232	266	300	306	322	324	332	338
351	356	369	371	397	408	435	470	498	519	531	537	542	561	617
635	664	674	699	702	716	732	747	754	759	770	778	781	798	805
824	835	897	917	938	942	948	954	965	1022	1041	1047	1053	1074	1097
1111	1140	1165	1170	1203	1208	1217	1244	1257	1326	1356	1359	1369	1373	1383
1389	1396	1417	1424	1430	1442	1473	1483	1487	1495	1503	1571	1601	1608	1614
1622	1637	1647	1658	1687	3074	3075	3133	3143	3168	3194	3207	3254	3256	3260

$anti-P_1^2$

14	23	32	36	41	48	51	57	66	80	94	118	130	134	142
157	163	176	199	209	218	231	281	301	312	318	332	337	338	349
356	365	381	392	434	476	479	491	516	524	544	581	600	606	646
677	694	698	712	721	741	745	756	765	780	781	792	800	814	819
830	891	896	911	941	946	956	957	971	984	1018	1040	1048	1054	1069
1082	1112	1129	1161	1199	1202	1225	1238	1268	1319	1338	1359	1368	1381	1383
1394	1398	1410	1418	1421	1433	1471	1479	1488	1493	1503	1602	1608	1613	1613
1647	1655	1658	1669	1724	3063	3072	3104	3130	3140	3162	3165	3247	3247	3261

$syn-TS_I^2$

-507	14	22	33	44	46	50	52	59	69	88	101	117	128	143
151	172	178	189	202	210	235	239	275	302	302	312	324	335	340
348	350	366	374	396	413	460	472	475	507	518	529	541	579	621
640	663	681	700	702	714	738	745	753	765	777	779	781	798	809
825	835	905	912	931	939	942	948	949	1018	1041	1049	1051	1068	1092
1113	1137	1168	1193	1205	1210	1222	1261	1277	1326	1357	1360	1370	1379	1384
1391	1398	1420	1425	1429	1432	1478	1482	1484	1497	1503	1558	1602	1607	1616
1619	1646	1650	1659	1674	3075	3078	3140	3145	3169	3171	3214	3248	3257	3270

$syn-P_1^2$

10	22	32	41	45	50	50	58	64	70	98	104	123	132	135
141	160	171	180	193	214	232	262	286	293	313	327	334	339	346
354	357	379	393	419	465	478	488	517	534	541	582	594	618	643
660	693	700	703	717	730	733	746	752	775	779	784	802	806	822
834	884	907	912	944	950	956	971	977	1006	1041	1050	1055	1060	1068
1083	1111	1145	1185	1199	1207	1225	1242	1269	1318	1341	1358	1368	1382	1384
1395	1401	1412	1420	1420	1436	1470	1477	1485	1493	1498	1601	1609	1614	1614
1649	1659	1660	1665	1725	3054	3073	3106	3128	3138	3167	3177	3245	3257	3265

$syn-TS_I^5$

-504	18	23	26	36	46	50	57	57	68	81	102	116	127	133
142	156	166	177	181	195	202	230	285	303	304	313	326	338	341
351	358	369	373	381	403	463	468	492	507	532	542	556	571	606
641	665	680	704	707	716	739	744	747	762	773	779	787	798	814
825	835	904	913	931	941	944	947	950	1010	1041	1051	1053	1066	1099
1117	1125	1168	1190	1207	1219	1224	1261	1270	1326	1357	1365	1370	1383	1385
1393	1399	1423	1426	1429	1439	1478	1481	1484	1484	1500	1562	1601	1604	1617
1619	1647	1650	1658	1673	3060	3077	3143	3145	3169	3189	3216	3247	3259	3273

$syn-P_1^5$

17	25	31	43	48	51	52	56	62	69	106	113	124	133	139
145	158	164	183	194	217	229	262	282	295	315	333	337	344	349
353	361	375	394	412	459	471	477	521	538	550	579	598	628	638
674	693	704	710	717	730	741	748	755	772	779	784	795	814	823
835	881	893	907	934	952	962	968	972	1006	1041	1049	1054	1059	1067
1085	1111	1144	1183	1199	1209	1224	1239	1271	1312	1341	1349	1369	1383	1384
1396	1400	1412	1419	1420	1432	1471	1474	1485	1495	1507	1599	1610	1615	1616
1648	1659	1661	1667	1725	3052	3077	3107	3127	3140	3170	3211	3245	3252	3255

$anti-T_I^2$

-343	8	19	32	44	45	48	50	52	57	61	91	108	124	129
142	151	164	174	188	192	197	214	233	255	294	306	310	315	325
343	348	350	354	361	367	436	455	460	476	507	511	533	536	576
620	632	652	657	691	695	709	724	733	745	750	768	774	784	793
808	828	865	894	923	931	932	939	944	950	989	1024	1034	1052	1054
1090	1098	1151	1183	1194	1216	1216	1223	1346	1359	1368	1380	1382	1384	1391
1395	1404	1410	1420	1425	1442	1465	1478	1485	1495	1498	1558	1591	1597	1611
1630	1643	1654	1655	1656	3074	3076	3135	3145	3169	3184	3256	3258	3259	3259

$anti-PP_I^2$

11	16	23	37	43	47	49	53	63	72	95	101	121	132	136
137	151	158	172	178	183	202	232	242	290	292	302	307	330	337
338	347	349	371	391	405	419	466	480	501	513	530	539	557	566
619	646	659	676	686	702	710	723	726	739	747	770	776	785	802
812	822	842	850	879	906	928	944	951	957	968	1028	1038	1049	1056
1084	1100	1126	1167	1194	1211	1223	1228	1276	1345	1355	1381	1383	1385	1393
1398	1401	1419	1420	1431	1467	1473	1483	1489	1497	1500	1531	1586	1602	1615
1628	1649	1650	1659	1669	3052	3077	3126	3135	3177	3189	3249	3258	3268	3271

$anti-TT_I^2$

-560	18	21	35	38	46	49	51	54	63	77	84	112	124	132
140	150	159	174	176	200	218	237	271	287	297	311	321	332	338
343	350	355	357	389	440	453	462	488	510	521	542	553	564	573
643	651	680	685	698	714	720	731	740	745	762	771	778	793	807
814	837	850	884	898	927	937	946	953	976	1009	1015	1043	1050	1055
1096	1114	1129	1173	1182	1211	1224	1227	1241	1301	1315	1348	1356	1359	1382
1385	1390	1396	1411	1420	1424	1465	1475	1481	1484	1489	1503	1550	1558	1601
1612	1614	1644	1658	1668	3045	3073	3108	3141	3149	3165	3167	3246	3259	3262

$syn-T_I^2$

-351	10	22	27	43	47	49	53	59	65	74	89	102	111	115
124	141	150	161	170	176	188	201	225	250	287	303	306	312	325
343	345	350	352	359	387	410	453	453	490	507	524	534	548	571
578	639	657	668	689	695	711	725	737	742	749	769	777	786	800
811	840	870	899	905	928	932	937	939	943	991	1025	1037	1052	1052
1095	1095	1165	1188	1190	1212	1216	1222	1341	1363	1375	1380	1381	1383	1393
1397	1407	1410	1415	1423	1442	1469	1479	1483	1489	1498	1560	1594	1597	1610
1628	1641	1644	1651	1654	3060	3074	3135	3140	3175	3203	3250	3252	3258	3275

$syn-PP_l^2$

12	17	23	40	47	49	50	61	67	77	102	110	122	127	132
149	156	161	167	182	201	217	227	246	285	294	297	306	319	336
338	346	351	359	386	415	436	457	467	482	508	528	536	558	581
588	632	662	681	683	698	706	722	726	742	745	769	778	781	803
805	822	844	852	885	905	929	943	948	955	970	1023	1035	1055	1056
1082	1100	1124	1167	1195	1211	1222	1228	1269	1343	1358	1376	1383	1385	1393
1397	1402	1417	1422	1430	1468	1477	1488	1488	1502	1506	1528	1587	1602	1615
1628	1649	1650	1658	1669	3057	3072	3124	3137	3170	3192	3249	3257	3270	3277

$syn-TT_l^2$

-739	12	21	36	43	48	50	52	58	65	73	92	110	123	128
140	155	167	178	181	187	204	231	254	282	286	300	313	328	341
343	349	350	362	382	402	422	441	505	511	521	533	545	553	581
637	652	671	684	698	711	726	734	740	749	754	770	777	784	803
816	848	856	887	901	928	935	946	953	985	1016	1023	1036	1048	1060
1094	1104	1134	1170	1201	1211	1224	1241	1269	1309	1322	1352	1357	1360	1383
1392	1395	1414	1420	1426	1427	1451	1473	1478	1482	1496	1502	1533	1557	1600
1605	1615	1644	1659	1667	3050	3073	3111	3132	3141	3168	3172	3254	3258	3262

Part III: Electronic energies (E), zero-point energies (ZPE), sum of electronic and zero-point energies (Es), Sum of electronic and thermal Energies(tEs), sum of electronic and thermal enthalpies(tH), and sum of electronic and thermal free energies(tG) at 298.15K for all important species, as calculated at the B3LYP/6-31+G(d,p) level. (Energies in Hartree)

S3.1. Single state

Species	ZPE	E	Es = ZPE + E	298.15K		
				tEs	tH	tG
TNT	0.134972	1770.181100	-884.955578	-884.941910	-884.940966	-884.997656
${}^aP_3^3$	0.270465	-1770.073709	-1769.803244	-1769.775444	-1769.774500	-1769.863555
<i>endo</i> - TS_2^5	0.269954	-1770.082367	-1769.812413	-1769.784811	-1769.783867	-1769.871782
<i>exo</i> - TS_3^4	0.270615	-1770.083071	-1769.812456	-1769.784911	-1769.783967	-1769.872158
<i>anti</i> - TS_1^2	0.269788	-1770.104018	-1769.834230	-1769.806380	-1769.805435	-1769.895434
<i>syn</i> - TS_1^2	0.270028	-1770.103330	-1769.833302	-1769.805551	-1769.804607	-1769.894669
<i>syn</i> - TS_1^5	0.269846	-1770.104147	-1769.834301	-1769.806345	-1769.805401	-1769.896170
${}^aP_3^3$	0.272582	-1770.088889	-1769.816307	-1769.788453	-1769.787509	-1769.876135
<i>endo</i> - P_2^5	0.272326	-1770.100502	-1769.828176	-1769.800566	-1769.799622	-1769.887973
<i>anti</i> - P_1^2	0.271629	-1770.130769	-1769.859140	-1769.831269	-1769.830325	-1769.921336
<i>syn</i> - P_1^2	0.271418	-1770.137299	-1769.865881	-1769.837726	-1769.836782	-1769.928923
<i>syn</i> - P_1^5	0.271554	-1770.131541	-1769.859987	-1769.831913	-1769.830969	-1769.922209

^a The barrier energy (E_{retro}^a) for intermolecular [4+2] cycloreversion ($2\text{TNT} \rightarrow P_3^3$) is 8.20 kcal/mol, as calculated at B3LYP/6-31+G(d,p) level.

S3.2. Triplet state

Species	ZPE	E	Es = ZPE + E	298.15K		
				tE	tH	tG
<i>anti</i> - T_1^2	0.266865	-1770.074669	-1769.807804	-1769.778956	-1769.778012	-1769.873060
<i>anti</i> - PP_1^2	0.267226	-1770.099495	-1769.832269	-1769.802930	-1769.801985	-1769.898226
<i>anti</i> - TT_1^2	0.266622	-1770.054561	-1769.787939	-1769.759675	-1769.758731	-1769.851441
<i>syn</i> - T_1^2	0.266568	-1770.086477	-1769.819909	-1769.790843	-1769.789899	-1769.885208
<i>syn</i> - PP_1^2	0.267219	-1770.098185	-1769.830966	-1769.801713	-1769.800769	-1769.896169
<i>syn</i> - TT_1^2	0.266491	-1770.051041	-1769.784550	-1769.756131	-1769.755186	-1769.848382