Electronic Supporting Information

Understanding the Reactivity of Bis(propargyl) Aromatic Esters towards GAP: A Theoretical Exploration

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Table of content

Electronic Supporting Information

Cartesian coordinates of all the optimized stationary points at M052X/6-311G(d,p) in the gas phase, including corresponding charge, multiplicity, thermodynamic data generated from frequency calculation and imaginary frequencies of all the transition state geometries.

GAP-2

Zero-point correction=	0.215759 (Hartree/Particle)
Thermal correction to Energy=	0.231702
Thermal correction to Enthalpy=	0.232647
Thermal correction to Gibbs Free Energy=	0.169468
Sum of electronic and zero-point Energies=	-789.765955
Sum of electronic and thermal Energies=	-789.750012
Sum of electronic and thermal Enthalpies=	-789.749068
Sum of electronic and thermal Free Energies=	-789.812247

Charge = 0; Multiplicity = 1

C	-0.76699600	0.77006300	-0.29937600
C	-1.21147100	1.83118100	0.68629700
H	-0.32939100	2.39127200	1.00382800
H	-1.66389300	1.33471100	1.54776900
O	-2.14211400	2.66044300	0.00579400
H	-2.43509800	3.34689100	0.60413300
O	0.18624900	-0.01227900	0.39533000
C	0.76228200	-1.05349700	-0.36859100
H	0.04538400	-1.85469100	-0.55529100
H	1.13874900	-0.67474500	-1.32528400
C	1.93239400	-1.60835400	0.41786300
H	1.55458600	-2.12782200	1.30593700
C	2.86339200	-0.50113800	0.90150100
H	2.35555700	0.07720600	1.67357900
H	3.76204100	-0.94598300	1.32810600
O	2.57060300	-2.50960700	-0.46736900
H	3.32257700	-2.90256400	-0.02287500
N	3.31021400	0.36839900	-0.20119600
N	2.69500600	1.41830500	-0.31424600
N	2.20176800	2.41049500	-0.49846600
C	-1.94173000	-0.04315500	-0.81780800
H	-2.67934600	0.65726000	-1.21163500
H	-1.62379200	-0.71329300	-1.61959100
N	-2.49700000	-0.82843500	0.30129200
N	-3.62052400	-1.27011500	0.10395600
N	-4.64630800	-1.71711800	0.01437200
H	-0.29458600	1.26198100	-1.15800300

1

Zero-point correction=	0.208732 (Hartree/Particle)
Thermal correction to Energy=	0.225565
Thermal correction to Enthalpy=	0.226510
Thermal correction to Gibbs Free Energy=	0.161352
Sum of electronic and zero-point Energies=	-840.195150
Sum of electronic and thermal Energies=	-840.178316
Sum of electronic and thermal Enthalpies=	-840.177372
Sum of electronic and thermal Free Energies=	-840.242530

Charge = 0; Multiplicity = 1

C	-0.24245400	1.37131700	-0.00013600
C	1.06237400	0.90707300	0.00000600

C	1.29978500	-0.46571500	0.00004400
C	0.24245500	-1.37131800	-0.00005900
C	-1.06237300	-0.90707400	-0.00019900
C	-1.29978400	0.46571400	-0.00023900
H	-0.46343700	2.42880400	-0.00017100
H	1.89467300	1.59426900	0.00008600
H	0.46343800	-2.42880500	-0.00002600
H	-1.89467300	-1.59427000	-0.00028000
C	-2.67993200	1.02478000	-0.00039700
O	-2.93908700	2.19838500	-0.00032800
O	-3.61991000	0.06729600	-0.00034400
C	-4.97033500	0.56305300	-0.00035600
H	-5.12444700	1.18285400	0.88167500
H	-5.12443600	1.18283300	-0.88240400
C	-5.87418400	-0.57954900	-0.00035100
C	-6.64379600	-1.49566800	-0.00032500
H	-7.32271100	-2.31242400	0.00035300
C	2.67993200	-1.02478000	0.00019500
O	2.93908700	-2.19838600	0.00023700
O	3.61991100	-0.06729600	0.00030800
C	4.97033500	-0.56305300	0.00047400
H	5.12455400	-1.18283700	-0.88155100
H	5.12433100	-1.18285100	0.88252800
C	5.87418500	0.57954900	0.00059600
C	6.64379500	1.49566900	0.00070700
H	7.32267900	2.31245000	0.00104800

1TS

Zero-point correction=	0.425714 (Hartree/Particle)
Thermal correction to Energy=	0.458930
Thermal correction to Enthalpy=	0.459874
Thermal correction to Gibbs Free Energy=	0.352670
Sum of electronic and zero-point Energies=	-1629.937705
Sum of electronic and thermal Energies=	-1629.904489
Sum of electronic and thermal Enthalpies=	-1629.903545
Sum of electronic and thermal Free Energies=	-1630.010749

1 Imaginary frequency = -468.0 cm^{-1}

Charge = 0; Multiplicity = 1

C	-4.28514300	-1.04532800	1.13066700
C	-5.54675200	-0.86647000	0.58816400
C	-5.77222900	0.19724500	-0.28287200
C	-4.74492900	1.07742700	-0.61161300
C	-3.48339400	0.89754600	-0.06943500
C	-3.25786400	-0.16547600	0.80211100
H	-4.07433400	-1.85814400	1.81035000
H	-6.35512600	-1.53885300	0.83187300
H	-4.95548600	1.89149800	-1.28990400
H	-2.67406400	1.56925300	-0.31182600
C	-1.92223800	-0.40541500	1.41960000
O	-1.68263200	-1.30240300	2.18390500
O	-1.01162300	0.49383300	1.02856500
C	0.29792400	0.31932400	1.60931200
H	0.21848700	0.38722200	2.69292900
H	0.66800400	-0.67503300	1.36548300
C	1.18624100	1.35255100	1.08256600

C	1.57970400	2.32298600	0.44266700
H	1.62798900	3.13229400	-0.24670900
C	-7.10628800	0.44066700	-0.89570700
O	-7.35740800	1.34340400	-1.64864500
O	-8.01781300	-0.46820000	-0.51464800
C	-9.32351200	-0.27218000	-1.08462100
H	-9.24727000	-0.29215700	-2.17069200
H	-9.70086000	0.70541200	-0.78849800
C	-10.19373600	-1.33655000	-0.60241400
C	-10.93179800	-2.19882800	-0.22371000
H	-11.58245200	-2.96677100	0.11510700
C	4.85628700	-1.02222200	-0.18761500
C	5.77808600	-1.48207000	0.92602900
H	5.52391500	-0.94099000	1.83953800
H	6.80396800	-1.23512000	0.63778500
O	5.59553500	-2.88156800	1.07291100
H	6.18706300	-3.20152400	1.75406900
O	5.22456400	0.32348500	-0.43445600
C	4.34313700	1.02520900	-1.28979700
H	4.46185300	0.71675400	-2.33000800
H	3.30331000	0.87061700	-0.98512800
C	4.67069700	2.50143800	-1.17236000
H	5.63258000	2.69674000	-1.65646300
C	4.78462000	2.95047900	0.28099400
H	5.68562100	2.52912600	0.72045300
H	4.84956700	4.03760100	0.31561200
O	3.61995800	3.17928700	-1.85156200
H	3.91889300	4.06010800	-2.08018900
N	3.61878300	2.55682100	1.07438800
N	3.65080900	1.51415900	1.74553100
N	2.96051800	0.69523800	2.16438300
C	4.97716700	-1.90885300	-1.42364400
H	4.66624900	-2.91768200	-1.15424700
H	4.32714000	-1.54270800	-2.21397500
N	6.34529500	-1.89809200	-1.97126400
N	7.08462400	-2.77686000	-1.54805000
N	7.83990000	-3.54214300	-1.22631900
H	3.81492900	-1.06310400	0.15526300

1P

Zero-point correction=	0.432342 (Hartree/Particle)
Thermal correction to Energy=	0.463424
Thermal correction to Enthalpy=	0.464368
Thermal correction to Gibbs Free Energy=	0.363259
Sum of electronic and zero-point Energies=	-1630.084372
Sum of electronic and thermal Energies=	-1630.053291
Sum of electronic and thermal Enthalpies=	-1630.052347
Sum of electronic and thermal Free Energies=	-1630.153456

Charge = 0; Multiplicity = 1

C	-4.68111000	-1.67576300	-0.55632600
C	-5.90425000	-1.03815200	-0.42945100
C	-5.96407500	0.21082800	0.18425200
C	-4.81125600	0.82075000	0.67119600
C	-3.58871300	0.18297400	0.54320100
C	-3.52754100	-1.06459700	-0.07341000

H	-4.59684700	-2.64541500	-1.02523600
H	-6.80898300	-1.49625900	-0.79894900
H	-4.89630000	1.78819000	1.14457600
H	-2.68482100	0.63706800	0.91959000
C	-2.23974700	-1.79692300	-0.24062100
O	-2.14181100	-2.89037800	-0.72859100
O	-1.19165900	-1.09630100	0.21445400
C	0.08555800	-1.75054300	0.08014200
H	0.11368300	-2.64325800	0.70072200
H	0.21210800	-2.04598700	-0.96011300
C	1.12766900	-0.79132300	0.53148200
C	1.25783900	0.55443600	0.28871000
H	0.68141400	1.26255100	-0.27476000
C	-7.24906500	0.94486700	0.34670200
O	-7.35557800	2.02822000	0.85679100
O	-8.29377800	0.26126400	-0.14440700
C	-9.55800600	0.93508100	-0.01333300
H	-9.51013700	1.89031600	-0.53388200
H	-9.75203300	1.13156900	1.03991900
C	-10.58982600	0.07907900	-0.58339300
C	-11.46039100	-0.60149600	-1.04212300
H	-12.22965600	-1.20940700	-1.45023400
C	5.84862500	-0.29828400	-0.10189100
C	6.61405500	-0.53147200	1.18492300
H	5.90700900	-0.50884300	2.01582100
H	7.33876700	0.27984400	1.29995400
O	7.25602300	-1.79316300	1.06539000
H	7.76754100	-1.95484100	1.85793400
O	5.42138100	1.05168300	-0.03748300
C	4.44617400	1.41212900	-0.98914100
H	4.89773400	1.74916800	-1.92446500
H	3.77606500	0.57232900	-1.20494600
C	3.63119400	2.54460700	-0.39311800
H	4.27520400	3.41891900	-0.26639900
C	3.07776800	2.16922500	0.97899400
H	3.88989900	2.05038300	1.68988000
H	2.38610100	2.93463500	1.33050800
O	2.58444700	2.80839500	-1.31881000
H	2.30407100	3.71910600	-1.22346300
N	2.39133000	0.89058100	0.93976800
N	2.93205000	-0.17136900	1.53450600
N	2.17227700	-1.18843200	1.29770800
C	6.69986900	-0.57950100	-1.33518700
H	6.95298500	-1.63929900	-1.34926100
H	6.13761400	-0.33884800	-2.23489200
N	7.91110400	0.26028000	-1.36845300
N	8.90789600	-0.23633500	-0.86132400
N	9.87719700	-0.59845700	-0.42679800
H	4.97476500	-0.95907700	-0.12854600

2

Zero-point correction=	0.211428	(Hartree/Particle)
Thermal correction to Energy=	0.230895	
Thermal correction to Enthalpy=	0.231839	
Thermal correction to Gibbs Free Energy=	0.158913	

Sum of electronic and zero-point Energies= -1044.705856
Sum of electronic and thermal Energies= -1044.686389
Sum of electronic and thermal Enthalpies= -1044.685445
Sum of electronic and thermal Free Energies= -1044.758371

Charge = 0; Multiplicity = 1

C	-0.51315800	-2.18578800	0.03081200
C	0.85977100	-2.19551900	0.22685800
C	1.58827700	-1.01725800	0.10845200
C	0.95552100	0.17549500	-0.22402900
C	-0.41040100	0.15724300	-0.42358100
C	-1.16670100	-1.00078200	-0.28123300
H	-1.09618500	-3.09064200	0.12396000
H	1.38489500	-3.10670400	0.47447000
H	1.50776100	1.09533300	-0.33764300
C	3.06073100	-1.08576800	0.33149000
O	3.65147300	-2.09239000	0.61371800
C	-2.65898200	-1.03673800	-0.40625600
O	-3.25240300	-1.85519200	-1.04674400
O	-3.22550800	-0.09852200	0.35428400
N	-1.04242500	1.40148500	-0.89337900
O	-1.98704600	1.28720600	-1.63989000
O	-0.54813500	2.44145000	-0.53484500
O	3.65000700	0.10488700	0.18131700
C	-4.65021200	0.03488000	0.17182200
H	-4.83144100	0.37821700	-0.84627800
H	-5.12055500	-0.93721100	0.30473100
C	-5.14619000	0.99707900	1.14467900
C	-5.58399400	1.78438800	1.93203800
H	-5.96479800	2.48722600	2.63152000
C	5.07763200	0.09426400	0.38555700
H	5.53239400	-0.59115000	-0.32780200
H	5.28920800	-0.26737800	1.39039200
C	5.57125300	1.45098100	0.19971500
C	6.00161300	2.55753600	0.05295300
H	6.37762400	3.54232700	-0.07805400

2TS

Zero-point correction= 0.428513 (Hartree/Particle)
Thermal correction to Energy= 0.464331
Thermal correction to Enthalpy= 0.465275
Thermal correction to Gibbs Free Energy= 0.351923
Sum of electronic and zero-point Energies= -1834.447057
Sum of electronic and thermal Energies= -1834.411239
Sum of electronic and thermal Enthalpies= -1834.410295
Sum of electronic and thermal Free Energies= -1834.523647

1 Imaginary frequency = -465.5 cm^{-1}

Charge = 0; Multiplicity = 1

C	3.79423900	1.31592100	1.58708000
C	5.08503000	1.16520000	1.10063100
C	5.39305800	0.11578800	0.24292400
C	4.37502900	-0.75743000	-0.12510500
C	3.08806800	-0.63606500	0.35638200
C	2.80250700	0.41411700	1.22272300
H	3.53797700	2.12476100	2.25597900
H	5.86711100	1.85190800	1.38865300

H	2.32591400	-1.33698100	0.05292900
C	1.43185500	0.61945000	1.77756000
O	1.14492200	1.50873200	2.53292700
O	0.56993400	-0.29635400	1.33569600
C	-0.77941600	-0.16087900	1.84204800
H	-0.75662800	-0.23463500	2.92775200
H	-1.15689600	0.82603700	1.58097100
C	-1.60399800	-1.21389600	1.25874000
C	-1.92751100	-2.19407700	0.59540600
H	-1.90652600	-3.00283200	-0.09622100
C	6.82155900	-0.13002700	-0.13226700
O	7.36239700	-1.19458800	-0.05725800
O	7.43097800	1.00663100	-0.48122000
C	8.82815000	0.84598600	-0.80469000
H	8.91476000	0.17717000	-1.65948600
H	9.33988000	0.39022700	0.04122500
C	9.37849500	2.15966600	-1.10632500
C	9.86277200	3.22356100	-1.36081900
H	10.28744800	4.16985300	-1.58883600
C	-5.29654200	1.04365100	-0.22807500
C	-6.32661300	1.45912500	0.80533900
H	-6.13084500	0.92113300	1.73509700
H	-7.31316800	1.17476000	0.42862300
O	-6.21220500	2.86343500	0.97396900
H	-6.90148000	3.16170300	1.56750100
O	-5.59242900	-0.31255100	-0.51189900
C	-4.62593900	-0.97151100	-1.30719700
H	-4.68679200	-0.66264200	-2.35223400
H	-3.61648900	-0.77424600	-0.93251800
C	-4.89521400	-2.46145600	-1.21611100
H	-5.81237300	-2.69694600	-1.76457500
C	-5.08628800	-2.92320700	0.22514400
H	-6.03032500	-2.54180500	0.60728100
H	-5.10784900	-4.01205000	0.25235400
O	-3.77086000	-3.08752900	-1.82277100
H	-4.01692400	-3.97264200	-2.09405400
N	-3.99120400	-2.48784800	1.09395800
N	-4.10109000	-1.44843100	1.76091200
N	-3.47031400	-0.60757000	2.22645700
C	-5.34439600	1.93671200	-1.46394900
H	-5.08736700	2.95177200	-1.16290400
H	-4.62138800	1.59660400	-2.20092400
N	-6.66293500	1.89012100	-2.12061300
N	-7.45471300	2.75202300	-1.76274400
N	-8.25096500	3.50041700	-1.50685600
H	-4.29003200	1.11985300	0.20170700
N	4.61819700	-1.79947500	-1.13691200
O	5.36760000	-1.51751700	-2.04045300
O	4.01267200	-2.83643900	-1.01453700

2P

Zero-point correction=	0.434972 (Hartree/Particle)
Thermal correction to Energy=	0.469554
Thermal correction to Enthalpy=	0.470498
Thermal correction to Gibbs Free Energy=	0.359602

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Sum of electronic and zero-point Energies=          -1834.594408
Sum of electronic and thermal Energies=             -1834.559825
Sum of electronic and thermal Enthalpies=           -1834.558881
Sum of electronic and thermal Free Energies=          -1834.669777
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Charge = 0; Multiplicity = 1

C	4.08261500	2.12803300	-0.87914900
C	5.18069000	1.29808500	-0.70168600
C	5.04455800	0.08484000	-0.03681100
C	3.78166000	-0.28052900	0.41745700
C	2.67855000	0.53189300	0.26079900
C	2.83854100	1.75084600	-0.38978400
H	4.17306300	3.07677000	-1.38840300
H	6.15561900	1.58827900	-1.06422700
H	1.71592500	0.20901500	0.62481100
C	1.69174000	2.68502300	-0.58918400
O	1.77309000	3.73614600	-1.16172700
O	0.56657800	2.21102900	-0.04876700
C	-0.59601300	3.05125700	-0.17810100
H	-0.37737200	4.02186400	0.26474500
H	-0.83206400	3.19645900	-1.23018700
C	-1.69869800	2.34170800	0.52409500
C	-1.63300300	1.34372700	1.46319400
H	-0.82277000	0.79756900	1.90491300
C	6.26903600	-0.70734000	0.30352400
O	6.49792900	-1.15461500	1.38941700
O	7.10341300	-0.77562900	-0.73675000
C	8.33441200	-1.47616800	-0.45687000
H	8.09863600	-2.50752700	-0.19981300
H	8.82168100	-1.01140400	0.39844300
C	9.17538100	-1.40636500	-1.64295000
C	9.89309700	-1.36386000	-2.59924200
H	10.52516000	-1.32607600	-3.45213300
C	-5.54257300	-0.34963200	-0.66696600
C	-6.86510200	0.29521300	-0.30465100
H	-6.66842300	1.12677100	0.37435800
H	-7.47918300	-0.45396800	0.20365600
O	-7.46515400	0.72847200	-1.51719000
H	-8.32121200	1.10765900	-1.31903700
O	-5.09297400	-0.96369300	0.52869800
C	-3.74436300	-1.37441600	0.51599200
H	-3.63394100	-2.38866200	0.12708200
H	-3.13105700	-0.69800400	-0.08993600
C	-3.24318200	-1.33548200	1.94809500
H	-3.79013600	-2.07576700	2.53762700
C	-3.47830300	0.03463600	2.58130700
H	-4.54294000	0.23390700	2.65913600
H	-3.01694900	0.08130800	3.56718000
O	-1.85753100	-1.64437100	1.88785900
H	-1.58669500	-2.06889000	2.70245000
N	-2.92757900	1.09079600	1.75122600
N	-3.73572300	1.87112200	1.03788800
N	-3.00085300	2.63024400	0.29274000
C	-5.68535400	-1.34601800	-1.81233600
H	-5.98515800	-0.80542300	-2.70966400
H	-4.73128000	-1.83509000	-1.99685300

N	-6.64383600	-2.41837000	-1.48896200
N	-7.79746100	-2.21560500	-1.84236600
N	-8.88044600	-2.13159600	-2.12521400
H	-4.83174500	0.42716000	-0.97051500
N	3.55272100	-1.61042400	1.00715800
O	4.17674200	-2.53017300	0.53880400
O	2.72177700	-1.68739600	1.88073900

3

```
Zero-point correction=                           0.214301 (Hartree/Particle)
Thermal correction to Energy=                    0.236230
Thermal correction to Enthalpy=                  0.237174
Thermal correction to Gibbs Free Energy=         0.159478
Sum of electronic and zero-point Energies=          -1249.217637
Sum of electronic and thermal Energies=             -1249.195708
Sum of electronic and thermal Enthalpies=           -1249.194764
Sum of electronic and thermal Free Energies=        -1249.272460
```

Charge = 0; Multiplicity = 1

C	-0.48223000	1.51909800	-0.13263600
C	0.86314600	1.75120900	0.07450500
C	1.74019000	0.67574900	0.05268300
C	1.26776200	-0.60750800	-0.18032000
C	-0.08594900	-0.78959600	-0.40322100
C	-1.00277900	0.25526300	-0.38774900
H	1.22703600	2.75181800	0.25585600
H	1.93262700	-1.45723900	-0.19236200
N	-0.53986200	-2.16652100	-0.68897500
O	-1.61469200	-2.29369900	-1.22248800
O	0.20538000	-3.06240100	-0.38067400
C	3.18675600	0.95548300	0.29255800
O	3.62446100	2.04935100	0.51636300
O	3.92535400	-0.15307100	0.22753800
C	-2.47060800	0.06064200	-0.70714800
N	-1.39153000	2.67822200	-0.03264400
O	-2.54030300	2.44809800	0.25639300
O	-0.91133100	3.76685000	-0.22230700
O	-2.94593000	0.37255900	-1.75479900
O	-3.10152100	-0.47970700	0.32448900
C	5.33805600	0.05228100	0.45040100
H	5.71182800	0.75986100	-0.28761400
H	5.47966100	0.48067400	1.44113600
C	6.00415700	-1.23579800	0.33190600
C	6.57855900	-2.28103900	0.24044100
H	7.08414500	-3.21175200	0.15854500
C	-4.50223800	-0.73497400	0.07728000
H	-4.98484800	0.20353700	-0.18972500
H	-4.58324200	-1.42607800	-0.76050300
C	-5.08164300	-1.30076500	1.28609500
C	-5.59286400	-1.76745100	2.26171100
H	-6.04069300	-2.18213400	3.13084400

3TS

```
Zero-point correction=                           0.431132 (Hartree/Particle)
Thermal correction to Energy=                    0.469416
Thermal correction to Enthalpy=                  0.470360
```

```
Thermal correction to Gibbs Free Energy=          0.351057
Sum of electronic and zero-point Energies=          -2038.961586
Sum of electronic and thermal Energies=             -2038.923303
Sum of electronic and thermal Enthalpies=           -2038.922359
Sum of electronic and thermal Free Energies=        -2039.041662
```

1 Imaginary frequency = -466.3 cm^{-1}

Charge = 0; Multiplicity = 1

C	3.36380000	-1.38021100	-1.36653700
C	4.64662500	-1.08982100	-0.94023100
C	4.97170200	0.08712900	-0.27424700
C	3.92274800	0.97192700	-0.05437000
C	2.62984800	0.73334700	-0.48213000
C	2.35424600	-0.45636900	-1.14134600
H	3.14952000	-2.31029900	-1.87159800
H	1.85716500	1.46385900	-0.29856100
C	0.98148100	-0.79086600	-1.63063700
O	0.71774800	-1.80858800	-2.20948200
O	0.10808500	0.17040300	-1.34653200
C	-1.24716400	-0.07492600	-1.80393800
H	-1.23107700	-0.20843400	-2.88382600
H	-1.60562900	-0.99952400	-1.35535100
C	-2.08067800	1.05774800	-1.42000900
C	-2.41872600	2.13710400	-0.94404400
H	-2.40344400	3.05800300	-0.41039800
C	6.39085300	0.43736100	0.12018600
O	7.04618400	1.23274500	-0.47912500
O	6.75896100	-0.25003000	1.19170100
C	8.12542100	-0.00695200	1.59187100
H	8.24957100	1.05794400	1.78048100
H	8.78045300	-0.30025500	0.77268800
C	8.39501900	-0.78820900	2.78959100
C	8.65073000	-1.41493100	3.77605000
H	8.87108100	-1.97287000	4.65249200
C	-5.75439500	-0.96449800	0.45702200
C	-6.76551500	-1.55190000	-0.50994200
H	-6.55143600	-1.17981500	-1.51393800
H	-7.75892100	-1.20967600	-0.20629800
O	-6.64867700	-2.96381200	-0.43423700
H	-7.32689400	-3.36166800	-0.98021000
O	-6.04820100	0.42096800	0.49546200
C	-5.08245700	1.21019300	1.16223100
H	-5.13389300	1.08129200	2.24476700
H	-4.07376800	0.95982100	0.81847100
C	-5.36652600	2.66165200	0.82480100
H	-6.28245300	2.97724900	1.33367800
C	-5.57325800	2.87263500	-0.67171500
H	-6.51700100	2.42546300	-0.97489600
H	-5.60394000	3.94077700	-0.88285900
O	-4.24526600	3.39190000	1.30834900
H	-4.50135000	4.30638400	1.43358200
N	-4.48231800	2.30445400	-1.46640800
N	-4.58198800	1.16091200	-1.93475200
N	-3.94382300	0.25841400	-2.24942400
C	-5.83486200	-1.62839000	1.82856200
H	-5.57800500	-2.68107000	1.71481100

H	-5.12709000	-1.16791400	2.51304400
N	-7.16819600	-1.46468400	2.43443900
N	-7.95644600	-2.37443900	2.21239900
N	-8.75067900	-3.15406900	2.06953600
H	-4.74018400	-1.11595700	0.06696300
N	4.16178500	2.21416300	0.70647700
O	5.10243700	2.22070500	1.46249600
O	3.38402500	3.11919400	0.53480400
N	5.69883100	-2.08262900	-1.23990800
O	6.84339900	-1.69954200	-1.21067600
O	5.33553000	-3.20023100	-1.50608000

3P

```
Zero-point correction=                           0.437404 (Hartree/Particle)
Thermal correction to Energy=                    0.474563
Thermal correction to Enthalpy=                  0.475507
Thermal correction to Gibbs Free Energy=         0.358355
Sum of electronic and zero-point Energies=          -2039.108313
Sum of electronic and thermal Energies=             -2039.071154
Sum of electronic and thermal Enthalpies=           -2039.070210
Sum of electronic and thermal Free Energies=        -2039.187362
```

Charge = 0; Multiplicity = 1

C	3.66448300	2.04022700	-0.76281300
C	4.72562500	1.19546800	-0.49394400
C	4.58330300	0.00366200	0.20864800
C	3.29600400	-0.30275500	0.63200900
C	2.20933500	0.51951800	0.40124200
C	2.40130100	1.70131500	-0.30054500
H	3.81644400	2.95409600	-1.31792400
H	1.23365400	0.23029800	0.75861900
C	1.27699200	2.64700100	-0.57591100
O	1.40331500	3.67125000	-1.18467900
O	0.13219600	2.20925000	-0.05431900
C	-1.01642300	3.06254100	-0.24165500
H	-0.78761500	4.04621600	0.16546500
H	-1.22833700	3.16611200	-1.30363400
C	-2.14266900	2.39739400	0.46610300
C	-2.10995800	1.44981600	1.45767300
H	-1.31718000	0.92391400	1.95265100
C	5.76117400	-0.87577500	0.57230500
O	6.21013600	-0.92238900	1.67575700
O	6.17904400	-1.55216800	-0.48674300
C	7.34890300	-2.36224100	-0.23317200
H	7.11786000	-3.06886700	0.56200800
H	8.15398900	-1.70754200	0.09735000
C	7.70017400	-3.04994700	-1.46620500
C	8.01707700	-3.62741000	-2.46472600
H	8.29320600	-4.13639000	-3.35507000
C	-5.98895600	-0.38293800	-0.69357200
C	-7.33100400	0.25981300	-0.40647900
H	-7.16519300	1.13815800	0.22014500
H	-7.94407800	-0.46475700	0.13739200
O	-7.90886000	0.60065800	-1.65821500
H	-8.78066700	0.96520700	-1.50625800
O	-5.55722600	-0.90265800	0.55240500

C	-4.20765100	-1.30694500	0.59095700
H	-4.08407700	-2.33898400	0.25630500
H	-3.58326800	-0.65805700	-0.03387400
C	-3.74177200	-1.19448900	2.03063600
H	-4.30323100	-1.90407800	2.64341800
C	-3.99271900	0.20624800	2.58637300
H	-5.05863000	0.41046400	2.62059700
H	-3.56098600	0.30338900	3.58182900
O	-2.35396700	-1.50241100	2.02327300
H	-2.11181400	-1.91614400	2.85219700
N	-3.41357200	1.21690300	1.71921500
N	-4.19607900	1.96176200	0.94246700
N	-3.43590000	2.67816100	0.18087500
C	-6.08502700	-1.45858000	-1.76981500
H	-6.38082900	-0.98775100	-2.70681300
H	-5.11569000	-1.93340000	-1.90493800
N	-7.02130900	-2.53208100	-1.39107500
N	-8.17562200	-2.37841900	-1.76706900
N	-9.25696600	-2.33653300	-2.06465400
H	-5.28424100	0.38346900	-1.03523200
N	3.03721500	-1.57647900	1.33101700
O	3.80309600	-2.48387900	1.12014400
O	2.06392300	-1.62050900	2.04283000
N	6.06148000	1.61929700	-0.96176500
O	7.01823400	1.12245400	-0.41832400
O	6.09595800	2.44225500	-1.84087500

4

```
Zero-point correction=                           0.209357 (Hartree/Particle)
Thermal correction to Energy=                    0.226064
Thermal correction to Enthalpy=                  0.227008
Thermal correction to Gibbs Free Energy=         0.162434
Sum of electronic and zero-point Energies=           -840.194989
Sum of electronic and thermal Energies=              -840.178282
Sum of electronic and thermal Enthalpies=            -840.177338
Sum of electronic and thermal Free Energies=         -840.241912
```

Charge = 0; Multiplicity = 1

C	1.19790300	1.44141100	-0.00002500
C	-0.00000100	0.73543400	0.00000000
C	-1.19790400	1.44141000	0.00000300
C	-1.19983100	2.83427900	-0.00001900
C	-0.00000200	3.53037900	-0.00004400
C	1.19982800	2.83428000	-0.00004700
H	0.00000000	-0.34359200	0.00001800
H	-2.15053000	3.34816700	-0.00001600
H	2.15052600	3.34816900	-0.00006700
C	2.51633700	0.75382800	-0.00002900
C	-2.51633900	0.75382600	0.00003200
O	-3.57781000	1.31831800	0.00001000
O	-2.39779100	-0.58245500	0.00002400
O	3.57780800	1.31832100	-0.00004400
O	2.39779100	-0.58245300	-0.00000200
C	-3.65214300	-1.28653900	0.00002000
H	-4.22339500	-1.00103100	-0.88190400
H	-4.22339600	-1.00103800	0.88194600

C	-3.37275000	-2.71622500	0.00001500
C	-3.17860100	-3.89683700	0.00001000
H	-2.99928600	-4.94361500	-0.00004000
C	3.65214400	-1.28653600	0.00000300
H	4.22340400	-1.00101000	0.88191600
H	4.22338800	-1.00104900	-0.88193400
C	3.37275400	-2.71622200	0.00003700
C	3.17860800	-3.89683400	0.00006500
H	2.99929400	-4.94361200	0.00013100
H	-0.00000200	4.61083500	-0.00006200

4TS

```
Zero-point correction=                           0.425738 (Hartree/Particle)
Thermal correction to Energy=                    0.458962
Thermal correction to Enthalpy=                  0.459906
Thermal correction to Gibbs Free Energy=         0.352551
Sum of electronic and zero-point Energies=          -1629.937928
Sum of electronic and thermal Energies=             -1629.904703
Sum of electronic and thermal Enthalpies=           -1629.903759
Sum of electronic and thermal Free Energies=        -1630.011114
```

1 Imaginary frequency = -469.2cm^{-1}

Charge = 0; Multiplicity = 1

C	4.65626600	-0.24062100	-0.04632600
C	5.76548200	-0.74181000	-0.71566600
C	5.68707200	-1.95021500	-1.40493100
C	4.49578000	-2.65935300	-1.42776100
C	3.38200300	-2.16520500	-0.76125000
C	3.46570900	-0.95778700	-0.07191300
H	4.70301300	0.69410500	0.49221300
H	4.43378400	-3.59619400	-1.96260300
H	2.44683200	-2.70500600	-0.76804400
C	2.30131200	-0.38863200	0.66121900
O	2.32466500	0.64714500	1.27106800
O	1.21299200	-1.16439000	0.56697500
C	0.05385100	-0.66448200	1.26522200
H	0.28768400	-0.57129800	2.32423600
H	-0.18876700	0.32864200	0.89089500
C	-1.05690600	-1.58931500	1.05090300
C	-1.69393300	-2.55851800	0.65010400
H	-1.97399600	-3.44402000	0.13100700
C	-4.42089600	1.21684600	-0.17181800
C	-5.09896300	1.99927300	0.93704200
H	-4.82843300	1.55631000	1.89763400
H	-6.18023300	1.91391600	0.79505300
O	-4.65881900	3.34417100	0.83290200
H	-5.12615700	3.87519200	1.47778000
O	-5.04170100	-0.05667900	-0.15214800
C	-4.40822500	-1.03176800	-0.95769900
H	-4.60735900	-0.86834900	-2.01832800
H	-3.32666200	-1.02907300	-0.78967400
C	-4.96050800	-2.38568600	-0.55454800
H	-5.99931400	-2.46571400	-0.88979500
C	-4.94572600	-2.58409200	0.95811300
H	-5.69332800	-1.93960500	1.41472300
H	-5.18821500	-3.62180800	1.18547300

O	-4.14337600	-3.34236800	-1.21926800
H	-4.60724500	-4.18016900	-1.24397500
N	-3.63154800	-2.30540600	1.54095000
N	-3.39230400	-1.18443800	2.01641800
N	-2.52286300	-0.45544100	2.20258600
C	-4.54832500	1.92203000	-1.51883700
H	-4.02747300	2.87695000	-1.45581200
H	-4.08904000	1.32420300	-2.30181700
N	-5.95806300	2.10620000	-1.90796000
N	-6.45871200	3.16982900	-1.56776300
N	-7.01005200	4.11151800	-1.30543500
H	-3.35240100	1.10985300	0.05174100
C	7.06834600	-0.02539200	-0.72913100
O	8.05865600	-0.42374200	-1.28296600
O	7.02431600	1.13028200	-0.05002800
C	8.26499000	1.85783800	-0.03865700
H	8.56651500	2.06780700	-1.06372900
H	9.03662500	1.24374700	0.42320300
C	8.06178600	3.09199600	0.70820800
C	7.92327000	4.11363200	1.31522400
H	7.79151100	5.01884700	1.85460900
H	6.56926900	-2.31196500	-1.91362300

4P

Zero-point correction=	0.432031 (Hartree/Particle)
Thermal correction to Energy=	0.464162
Thermal correction to Enthalpy=	0.465106
Thermal correction to Gibbs Free Energy=	0.357996
Sum of electronic and zero-point Energies=	-1630.085132
Sum of electronic and thermal Energies=	-1630.053000
Sum of electronic and thermal Enthalpies=	-1630.052056
Sum of electronic and thermal Free Energies=	-1630.159166

Charge = 0; Multiplicity = 1

C	-4.45027500	0.15586500	-0.01601300
C	-5.13315000	1.13625100	0.69236100
C	-4.46591600	1.92444300	1.62752900
C	-3.11170400	1.73294600	1.85572400
C	-2.42185500	0.75356600	1.15313800
C	-3.09341600	-0.03345900	0.22024000
H	-4.95507700	-0.46092500	-0.74453800
H	-2.59268600	2.34522500	2.57901100
H	-1.36672200	0.59424400	1.31989100
C	-2.40210200	-1.09954500	-0.55543900
O	-2.93343400	-1.79283500	-1.37977100
O	-1.10543900	-1.20614000	-0.22815600
C	-0.37707600	-2.22980100	-0.93477900
H	-0.89788100	-3.17666200	-0.80256900
H	-0.34165600	-1.99715300	-1.99655300
C	1.00165500	-2.25367400	-0.38002600
C	1.43040400	-2.21958200	0.92466500
H	0.92442300	-2.12582000	1.86631300
C	4.81083700	0.55095300	-0.69921900
C	5.96805100	-0.08981800	-1.43903800
H	5.77732400	-1.16160000	-1.51460300
H	6.87859800	0.07838200	-0.85638900

O	6.04140400	0.52975200	-2.71509000
H	6.78269000	0.16118500	-3.19523200
O	4.91978100	0.07985000	0.63365000
C	3.79399300	0.32785400	1.44471300
H	3.85800800	1.30019500	1.93765400
H	2.86873400	0.29075500	0.85868200
C	3.74911200	-0.76157500	2.49935500
H	4.62751200	-0.67032400	3.14366300
C	3.77540300	-2.15141100	1.86802200
H	4.73245400	-2.32562100	1.38555700
H	3.59797200	-2.91424600	2.62599700
O	2.54998600	-0.55042600	3.23559700
H	2.65785000	-0.90691400	4.11793000
N	2.77491900	-2.27411200	0.82338700
N	3.15460900	-2.33442100	-0.45201100
N	2.09059000	-2.32006200	-1.18397100
C	4.84929200	2.07292500	-0.78103100
H	4.72273100	2.36926900	-1.82177800
H	4.03725100	2.49559800	-0.19338000
N	6.09556100	2.62092900	-0.21565300
N	7.00915500	2.77952100	-1.01422800
N	7.90723000	2.96724100	-1.66071900
H	3.86641800	0.20543600	-1.13456700
C	-6.58500100	1.38708400	0.49039700
O	-7.22077500	2.21808600	1.08302800
O	-7.11962300	0.57710400	-0.43454400
C	-8.52516600	0.78317300	-0.66190900
H	-8.68901000	1.81107400	-0.98173200
H	-9.06478700	0.62740800	0.27090200
C	-8.96304500	-0.15785600	-1.68394700
C	-9.34897500	-0.91827100	-2.52319800
H	-9.68341400	-1.59551600	-3.26979400
H	-5.02676300	2.67877700	2.16093000

5

```
Zero-point correction=                           0.211563 (Hartree/Particle)
Thermal correction to Energy=                    0.231047
Thermal correction to Enthalpy=                  0.231991
Thermal correction to Gibbs Free Energy=         0.159798
Sum of electronic and zero-point Energies=          -1044.717134
Sum of electronic and thermal Energies=             -1044.697651
Sum of electronic and thermal Enthalpies=           -1044.696706
Sum of electronic and thermal Free Energies=        -1044.768900
```

Charge = -1; Multiplicity = 1

C	-1.20305300	-0.54458600	0.00000200
C	0.00000000	-1.24018500	0.00001000
C	1.20305400	-0.54458900	0.00000300
C	1.21516600	0.84589900	-0.00001500
C	0.00000300	1.50715700	-0.00002500
C	-1.21516300	0.84590200	-0.00001600
H	-0.00000200	-2.32116500	0.00002600
H	2.13986700	1.40127700	-0.00002200
H	-2.13986300	1.40128200	-0.00002500
N	0.00000400	2.98277100	-0.00004500
O	-1.07375000	3.53566900	-0.00012700

O	1.07375900	3.53566700	-0.00010200
C	-2.46632500	-1.33570600	0.00001700
C	2.46632400	-1.33571200	0.00001600
O	2.51036900	-2.53501600	0.00003200
O	3.54976700	-0.55106300	0.00003000
O	-2.51037100	-2.53501000	0.00001700
O	-3.54976700	-0.55105400	-0.00000100
C	4.80331600	-1.26350500	0.00005800
H	4.85002700	-1.89914400	-0.88267300
H	4.84999200	-1.89913500	0.88279800
C	5.87956200	-0.28319200	0.00007500
C	6.78300800	0.50087300	0.00009700
H	7.58130200	1.20151700	0.00028700
C	-4.80331600	-1.26349800	0.00000100
H	-4.85001000	-1.89912500	0.88274100
H	-4.85000600	-1.89913900	-0.88273000
C	-5.87956700	-0.28319000	-0.00001000
C	-6.78302100	0.50086400	-0.00002100
H	-7.58132300	1.20149900	-0.00002800

5TS

Zero-point correction=	0.428209 (Hartree/Particle)
Thermal correction to Energy=	0.463339
Thermal correction to Enthalpy=	0.464283
Thermal correction to Gibbs Free Energy=	0.353292
Sum of electronic and zero-point Energies=	-1834.460758
Sum of electronic and thermal Energies=	-1834.425628
Sum of electronic and thermal Enthalpies=	-1834.424684
Sum of electronic and thermal Free Energies=	-1834.535675

1 Imaginary frequency = -465.8 cm^{-1}

Charge = 0; Multiplicity = 1

C	-4.27229200	0.45942800	-0.21550100
C	-5.41496900	-0.07515800	0.36800400
C	-5.41723000	-1.37793700	0.85389500
C	-4.25800200	-2.12100000	0.73699700
C	-3.10253100	-1.62012800	0.16244800
C	-3.12128600	-0.31493400	-0.31414500
H	-4.26286700	1.47091600	-0.59417500
H	-2.21652100	-2.23143600	0.09209300
C	-1.91618800	0.30515400	-0.93974200
O	-1.88819000	1.42840200	-1.36465900
O	-0.87912400	-0.53273700	-0.96614300
C	0.32834200	0.00794800	-1.55358500
H	0.11981900	0.30143200	-2.58079900
H	0.61954000	0.90029900	-1.00269300
C	1.37053500	-1.01208700	-1.49827500
C	1.92423200	-2.08774800	-1.29392100
H	2.12473000	-3.07865100	-0.96087300
C	4.88451400	1.17692200	0.40464600
C	5.66663300	2.13065900	-0.47878600
H	5.40842300	1.93684200	-1.52194000
H	6.73140200	1.92880900	-0.33134800
O	5.32073200	3.44929000	-0.08553400
H	5.86337400	4.07092400	-0.57078400
O	5.41129400	-0.10543600	0.11295400

C	4.68196200	-1.18147600	0.67085100
H	4.86053000	-1.27470100	1.74357000
H	3.60925900	-1.05436700	0.49426900
C	5.14180400	-2.45200500	-0.01857600
H	6.15708000	-2.69417500	0.31043700
C	5.17079400	-2.30364600	-1.53655300
H	5.98016900	-1.63547400	-1.82089700
H	5.34299600	-3.28000300	-1.98835000
O	4.22605900	-3.46003100	0.39301000
H	4.62617300	-4.31873600	0.25042000
N	3.90330200	-1.79594200	-2.06537200
N	3.76434200	-0.58457500	-2.29075600
N	2.95973400	0.23522000	-2.33633300
C	5.00009500	1.54837200	1.87990400
H	4.56172600	2.53602700	2.01956100
H	4.45491500	0.83423400	2.49139500
N	6.39807400	1.51260700	2.34544700
N	7.00364900	2.57250200	2.25826400
N	7.64431900	3.49319500	2.22181100
H	3.82218300	1.21009400	0.13229300
C	-6.67631300	0.70688500	0.50429800
O	-7.67746200	0.28556700	1.01587600
O	-6.56546800	1.93654900	-0.00989400
C	-7.75854900	2.73786600	0.10115800
H	-8.01387200	2.85062100	1.15355300
H	-8.57942300	2.22449900	-0.39672800
C	-7.49528900	4.02954100	-0.51692900
C	-7.30439200	5.09827100	-1.01960900
H	-7.12800800	6.04474900	-1.46821300
H	-6.30366600	-1.79325200	1.30871900
N	-4.24904500	-3.50512700	1.24799900
O	-3.22408700	-4.13299000	1.12569100
O	-5.26623200	-3.91528500	1.75289800

5P

Zero-point correction=	0.435301 (Hartree/Particle)
Thermal correction to Energy=	0.469752
Thermal correction to Enthalpy=	0.470696
Thermal correction to Gibbs Free Energy=	0.359521
Sum of electronic and zero-point Energies=	-1834.610069
Sum of electronic and thermal Energies=	-1834.575618
Sum of electronic and thermal Enthalpies=	-1834.574674
Sum of electronic and thermal Free Energies=	-1834.685849

Charge = 0; Multiplicity = 1

C	-3.71903200	-0.41354300	-0.05446100
C	-4.15958300	0.84679400	0.33715300
C	-3.26809000	1.78440000	0.84754600
C	-1.93715000	1.42651000	0.95383700
C	-1.46660500	0.18382200	0.57175100
C	-2.37289600	-0.73868000	0.06512900
H	-4.40846400	-1.14316200	-0.45408500
H	-0.42023300	-0.05592500	0.66470200
C	-1.91660700	-2.09170500	-0.37523500
O	-2.63566000	-2.93297400	-0.83864900
O	-0.60528900	-2.23221400	-0.18710900

C	0.00378200	-3.46845400	-0.63852800
H	-0.35845500	-4.28128100	-0.01337900
H	-0.28052300	-3.64343200	-1.67250000
C	1.46467700	-3.24751900	-0.52270600
C	2.28530800	-3.32071200	0.57656700
H	2.13841600	-3.61731100	1.59807700
C	3.63797500	0.87722100	-0.77701600
C	4.56437000	0.96726400	-1.97322200
H	4.72467900	-0.03929200	-2.36336400
H	5.51781000	1.38176300	-1.63302800
O	3.93456900	1.81326300	-2.92465800
H	4.51438500	1.91445100	-3.67926900
O	4.39416600	0.21251800	0.22348900
C	3.64057900	-0.25477300	1.31598500
H	3.51304300	0.52626200	2.07377900
H	2.64658100	-0.58807100	0.99596300
C	4.38856500	-1.43419600	1.91799300
H	5.35572400	-1.09672600	2.30075200
C	4.66129400	-2.52095700	0.88908700
H	5.38827300	-2.17436200	0.16178000
H	5.02330400	-3.41405200	1.39484500
O	3.61385100	-2.02772500	2.95339100
H	3.41335400	-1.36007800	3.61227500
N	3.46355200	-2.84090600	0.13130800
N	3.38129400	-2.49383300	-1.15464300
N	2.18125600	-2.73652500	-1.55573500
C	3.14894700	2.24850300	-0.32320900
H	2.54310100	2.68010700	-1.11962700
H	2.53433800	2.15858400	0.56935600
N	4.27594400	3.13359300	0.02694200
N	4.67098300	3.86052200	-0.87386300
N	5.10662600	4.56911900	-1.62768600
H	2.76469400	0.26843900	-1.03983400
C	-5.58925100	1.25593400	0.22831400
O	-6.00598100	2.33373300	0.55381600
O	-6.35449300	0.28288000	-0.27546900
C	-7.74811600	0.62858400	-0.40964900
H	-7.83710600	1.49394500	-1.06439900
H	-8.14309600	0.89716700	0.56867000
C	-8.44752700	-0.52262800	-0.96175300
C	-9.04643000	-1.45408500	-1.41403800
H	-9.57170300	-2.28479600	-1.81655900
H	-3.61222000	2.76206000	1.14965400
N	-0.97156900	2.40203100	1.49242000
O	0.18190100	2.04319200	1.58914100
O	-1.39153600	3.48820400	1.80276000

6

```
Zero-point correction=                           0.500675 (Hartree/Particle)
Thermal correction to Energy=                    0.529350
Thermal correction to Enthalpy=                  0.530294
Thermal correction to Gibbs Free Energy=         0.433356
Sum of electronic and zero-point Energies=          -1111.462901
Sum of electronic and thermal Energies=             -1111.434226
Sum of electronic and thermal Enthalpies=           -1111.433282
```

Sum of electronic and thermal Free Energies= -1111.530220

Charge = 0; Multiplicity = 1

N	2.66600200	-0.00384500	0.07354300
C	1.89397100	0.27798500	-1.05719000
C	2.23464900	0.04951400	1.40978600
N	0.97264200	1.27528300	-0.92921300
H	0.46812300	1.41607800	-1.78956400
N	0.90543200	-0.18716100	1.63673200
H	0.70602300	-0.10801300	2.62168500
C	1.00423900	2.39694900	0.00333500
H	0.21976100	2.28429800	0.75476400
H	1.95903900	2.38827300	0.52820500
C	0.83867900	3.71750700	-0.73813100
H	1.64683900	3.82489400	-1.46583500
H	-0.10086800	3.70370900	-1.30033800
C	0.83478400	4.90920800	0.21498800
H	1.76954200	4.91925300	0.78036900
H	0.02951300	4.78625800	0.94327100
C	0.66432500	6.23297700	-0.52453400
H	1.47360400	6.38232200	-1.24051400
H	-0.27694900	6.24972000	-1.07583700
C	3.99521200	-0.58792900	-0.15280700
H	4.65868800	-0.16883400	0.60055000
H	4.32303500	-0.26956600	-1.13905400
C	3.97011000	-2.10819400	-0.07349200
H	3.60197700	-2.40748100	0.91286100
H	3.26837600	-2.48069100	-0.82273800
C	5.35281600	-2.70961600	-0.30465800
H	6.05084700	-2.30411200	0.43229200
H	5.71755200	-2.40144400	-1.28771500
C	5.33825500	-4.23308000	-0.21633900
H	5.00073000	-4.55841200	0.76877000
H	4.65907400	-4.65458600	-0.95877800
O	2.05669300	-0.32208500	-2.10314700
O	3.01058000	0.28971900	2.31029900
C	0.05900300	-1.12402000	0.90021800
H	0.01222200	-2.07248000	1.44404500
H	0.51665400	-1.33799500	-0.06250300
C	-1.34796600	-0.57796400	0.69796600
H	-1.27718900	0.37697800	0.17524400
H	-1.80960000	-0.38611600	1.67086500
C	-2.21519600	-1.54666600	-0.09974700
H	-2.26174200	-2.51056600	0.41612100
H	-1.74686300	-1.73226200	-1.07100200
C	-3.63316300	-1.02310000	-0.31209500
H	-3.58968400	-0.06366500	-0.83767100
H	-4.08612700	-0.82926300	0.66363600
C	-4.49561500	-1.99736200	-1.10812500
H	-4.59310000	-2.93932600	-0.56444800
H	-4.00661800	-2.22048500	-2.06000500
C	-5.88838500	-1.45900700	-1.41752200
H	-6.43448100	-2.16422500	-2.03880400
H	-5.81584300	-0.51634300	-1.96374200
N	-6.67280000	-1.24977000	-0.21588100
C	-6.68387300	-0.54328200	0.74670300

O	-6.78063500	0.09305000	1.72067300
H	6.32913000	-4.65264500	-0.38823800
H	0.66524400	7.07618200	0.16509800

6TS

```
Zero-point correction=                           0.714495 (Hartree/Particle)
Thermal correction to Energy=                    0.759429
Thermal correction to Enthalpy=                  0.760374
Thermal correction to Gibbs Free Energy=         0.621821
Sum of electronic and zero-point Energies=          -1901.197639
Sum of electronic and thermal Energies=             -1901.152705
Sum of electronic and thermal Enthalpies=           -1901.151761
Sum of electronic and thermal Free Energies=        -1901.290313
```

1 Imaginary frequency = -1564.5 cm^{-1}

Charge = 0; Multiplicity = 1

C	-5.61986600	-0.39478900	-0.62938600
H	-5.70675000	-0.02204200	-1.65138200
O	-5.23332000	-1.76872900	-0.71163800
H	-4.45930200	-2.22804000	0.06512400
C	-1.90798000	-3.10308000	-0.56589000
H	-1.70341500	-3.59903400	0.38137100
N	-3.25630600	-2.55199200	-0.47853300
C	-3.82735600	-2.02224500	-1.51167300
O	-3.72891800	-1.66943600	-2.63533600
H	-1.87156100	-3.86172200	-1.35274700
C	-4.57061000	0.42060600	0.10828600
H	-3.62743600	0.40620200	-0.44149800
C	-6.97612600	-0.35613600	0.04728700
H	-7.66739000	-0.98882400	-0.51272000
H	-6.87999300	-0.73086000	1.07139100
O	-7.39686500	0.99281900	0.04208000
C	-8.40569200	1.30442400	0.98517600
H	-8.03461000	1.11510000	2.00046300
C	-8.66559500	2.78750400	0.79559600
H	-7.77196500	3.34577800	1.08241100
H	-8.86086700	2.95942500	-0.26610300
O	-9.78196900	3.12964400	1.60140700
H	-10.05620200	4.02208200	1.38970400
C	-9.67932800	0.48386100	0.80064200
H	-9.46695100	-0.57504400	0.92314600
H	-10.39348800	0.78911100	1.56488400
N	-10.24022400	0.64208400	-0.55244700
N	-11.06709000	1.53663500	-0.66987300
N	-11.83426000	2.32893500	-0.87766100
H	-4.92956300	1.44545100	0.18532500
N	-4.40728100	-0.14195600	1.46353100
N	-3.25286800	-0.32669600	1.82374700
N	-2.23211300	-0.53291900	2.23958400
C	-0.85553000	-2.03109800	-0.83435100
H	-1.11048400	-1.50808600	-1.75932800
H	-0.88206000	-1.30149600	-0.02219700
C	0.54499600	-2.62491800	-0.94907300
H	0.78659900	-3.17314800	-0.03365600
H	0.56782500	-3.35101400	-1.76710300
C	1.60859200	-1.55832100	-1.19389500

H	1.59439800	-0.83983400	-0.36893400
H	1.35535800	-1.00058900	-2.10041900
C	3.00951900	-2.14626600	-1.33136000
H	3.27770700	-2.69453000	-0.42492100
H	3.02518700	-2.86902400	-2.15198100
C	4.05183900	-1.06881600	-1.59526200
H	4.07726100	-0.35348600	-0.77631700
H	3.78154300	-0.50863100	-2.49516400
N	5.39111700	-1.64140800	-1.76107200
H	5.53774900	-2.08805000	-2.65326200
C	6.54464100	-0.98562900	-1.39820800
O	7.51145100	-0.96685500	-2.14233800
N	6.52725100	-0.38688100	-0.14078100
C	7.35230300	0.71394100	0.21425300
O	7.20063900	1.23623600	1.30510900
C	5.79470100	-0.98902200	0.98795000
H	5.27552800	-0.19528100	1.52118200
H	5.06800300	-1.68536800	0.58402300
N	8.24502900	1.14064900	-0.69697900
H	8.40765300	0.56566800	-1.50797500
C	9.08200100	2.28901600	-0.38814400
H	9.41458600	2.20929000	0.64726200
H	9.95865700	2.23613000	-1.03382400
C	6.72362100	-1.74118700	1.93401300
H	7.46908500	-1.04966000	2.32621900
H	7.24782600	-2.52029900	1.37346200
C	8.35667800	3.61552000	-0.58808200
H	8.01535600	3.68480000	-1.62435100
H	7.47203900	3.62009400	0.05152000
C	9.24520300	4.80841400	-0.25016900
H	10.14060500	4.78636800	-0.87780500
H	9.58535500	4.71989600	0.78459900
C	8.51824500	6.13689600	-0.43945200
H	9.15832900	6.98292300	-0.19010200
H	8.19131700	6.25378400	-1.47375900
H	7.63346200	6.18292100	0.19704500
C	5.94680100	-2.36791900	3.08874000
H	5.18789100	-3.04903000	2.69306200
H	5.41411100	-1.58202000	3.63002300
C	6.86197600	-3.12192400	4.04929600
H	7.60918400	-2.44959200	4.47273000
H	6.30044800	-3.56444300	4.87161000
H	7.38985200	-3.92345400	3.53032500

6P

```
Zero-point correction=                           0.721335 (Hartree/Particle)
Thermal correction to Energy=                    0.765030
Thermal correction to Enthalpy=                  0.765974
Thermal correction to Gibbs Free Energy=         0.633461
Sum of electronic and zero-point Energies=          -1901.282226
Sum of electronic and thermal Energies=             -1901.238531
Sum of electronic and thermal Enthalpies=           -1901.237587
Sum of electronic and thermal Free Energies=        -1901.370100
```

Charge = 0; Multiplicity = 1

C	5.81336200	-0.06990900	0.38895500

H	6.06585900	-0.55886000	1.32858000
O	4.90513300	-0.89277000	-0.35824400
H	3.17812700	-1.96334300	-1.45974600
C	1.79383300	-2.63998900	0.03010600
H	1.46593000	-3.43127700	-0.64396100
N	3.05361800	-2.11705000	-0.47452600
C	3.89179800	-1.46045500	0.35174200
O	3.78311800	-1.37260000	1.55194600
H	1.99617900	-3.08830800	1.00161100
C	5.16821500	1.27701800	0.68537700
H	4.33653400	1.13811700	1.37647600
C	7.04157300	0.04888900	-0.48937500
H	7.42712200	-0.95161500	-0.69656900
H	6.77174600	0.54154100	-1.42896200
O	7.98212100	0.82038100	0.22897300
C	9.02678900	1.36220600	-0.55558100
H	8.60870300	2.02037300	-1.32788000
C	9.86012700	2.17266200	0.42002700
H	9.26690600	3.01717900	0.77686100
H	10.10183600	1.52910400	1.27021300
O	11.02542600	2.59980700	-0.26784100
H	11.61271900	3.02884300	0.35453900
C	9.86433100	0.29929300	-1.26210500
H	9.24605300	-0.27360600	-1.94830800
H	10.64576100	0.80307000	-1.83039600
N	10.43382400	-0.67022600	-0.30994000
N	11.53932800	-0.38103700	0.12824600
N	12.54989100	-0.20742500	0.58442100
H	5.91187000	1.92673700	1.13516500
N	4.72136300	1.94302400	-0.55335500
N	3.67355100	1.51043100	-1.01476900
N	2.71515500	1.19455700	-1.50769200
C	0.71865600	-1.56648600	0.16655200
H	1.09031300	-0.79337300	0.84278900
H	0.55118600	-1.09479400	-0.80513200
C	-0.58945400	-2.13935100	0.70227600
H	-0.94692400	-2.92794100	0.03283500
H	-0.40965200	-2.60928000	1.67370400
C	-1.67381600	-1.07583400	0.84996500
H	-1.85425800	-0.60685500	-0.12193600
H	-1.31399900	-0.28641800	1.51617700
C	-2.98193800	-1.64467200	1.39083200
H	-3.34870300	-2.43417800	0.73035800
H	-2.80583800	-2.10836400	2.36545800
C	-4.05074200	-0.56984800	1.53452800
H	-4.26591000	-0.11206700	0.57142400
H	-3.68306800	0.22752000	2.18677200
N	-5.29562400	-1.11290200	2.08574400
H	-5.26756900	-1.27766300	3.08011500
C	-6.54575000	-0.65045500	1.74722100
O	-7.38990900	-0.45433500	2.60635300
N	-6.76958300	-0.45827400	0.38588900
C	-7.75828000	0.42276900	-0.13038800
O	-7.84155800	0.57290400	-1.33690600
C	-6.16935900	-1.35297400	-0.62049500

H	-5.85752100	-0.74848000	-1.46915300
H	-5.29999700	-1.82516800	-0.17795300
N	-8.53525500	1.07179400	0.75518300
H	-8.50991600	0.77213200	1.71671700
C	-9.54368700	1.99977600	0.26775600
H	-10.01853800	1.56705800	-0.61332700
H	-10.29793700	2.09997100	1.04835400
C	-7.14424700	-2.43506000	-1.06972200
H	-8.03006100	-1.96236200	-1.49386100
H	-7.45676500	-3.01599900	-0.19726300
C	-8.96554200	3.36539700	-0.08709700
H	-8.48490200	3.79258200	0.79687500
H	-8.19421300	3.22299900	-0.84635900
C	-10.03676900	4.31716200	-0.61015100
H	-10.82062200	4.43392600	0.14359500
H	-10.51042700	3.87376900	-1.48948700
C	-9.46395100	5.68500400	-0.97048500
H	-10.23590900	6.35584000	-1.34681800
H	-9.00592800	6.15321800	-0.09796800
H	-8.69583800	5.58847300	-1.73907300
C	-6.50915300	-3.35867100	-2.10568200
H	-5.60311100	-3.80783000	-1.68873500
H	-6.19929300	-2.76689500	-2.97060100
C	-7.46767200	-4.45870300	-2.55288900
H	-8.36834500	-4.02714100	-2.99088100
H	-7.00933300	-5.11021500	-3.29641300
H	-7.77073800	-5.07437400	-1.70470100

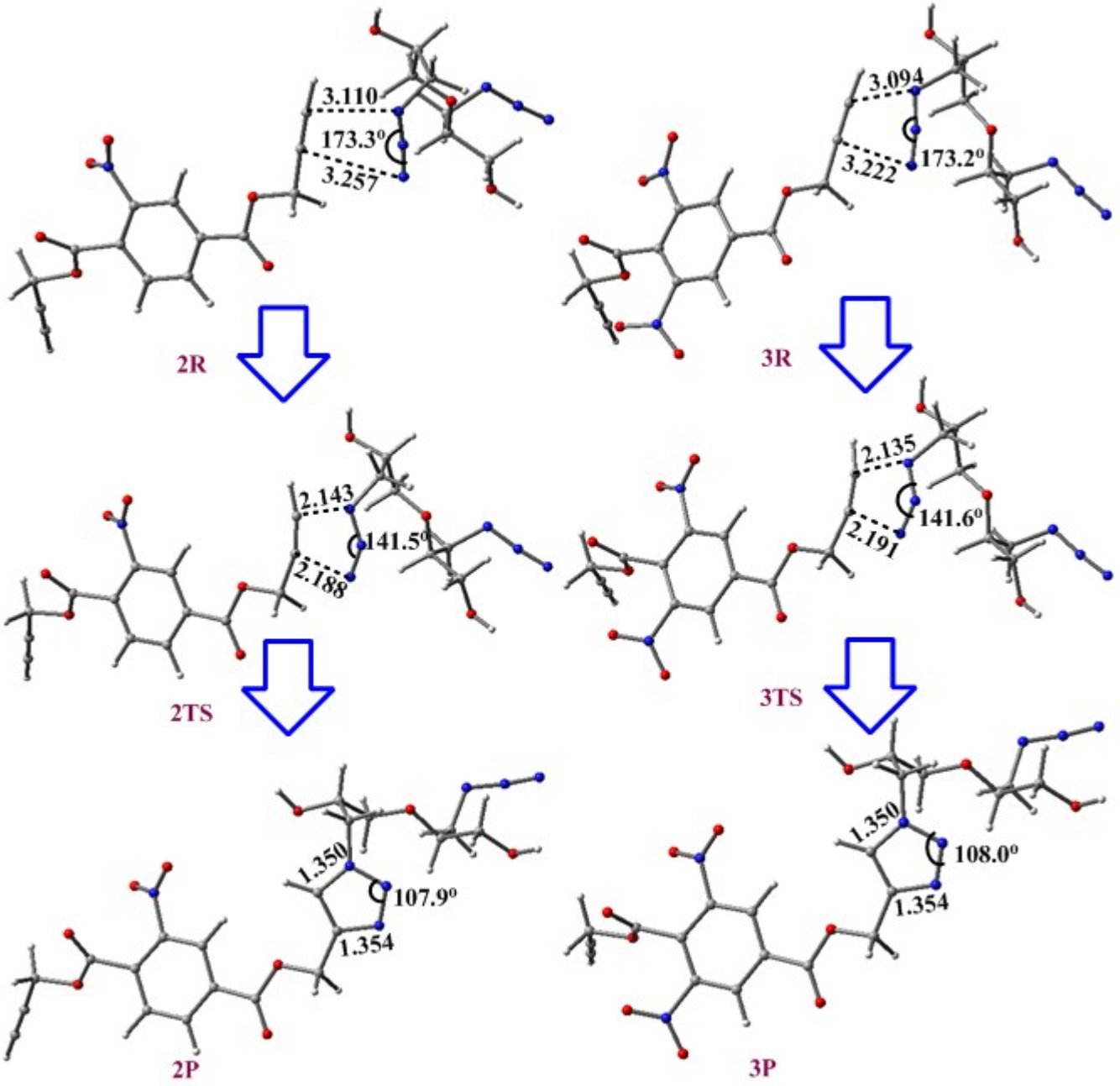

Fig. S1 M052X/6-311G(d,p) optimized geometries and selected bond distances (Å) for bis(propargyl) aromatic esters (**2** & **3**) involved in the curing reaction with **GAP-2**. (Red = oxygen; gray = carbon; blue = nitrogen; white = hydrogen)

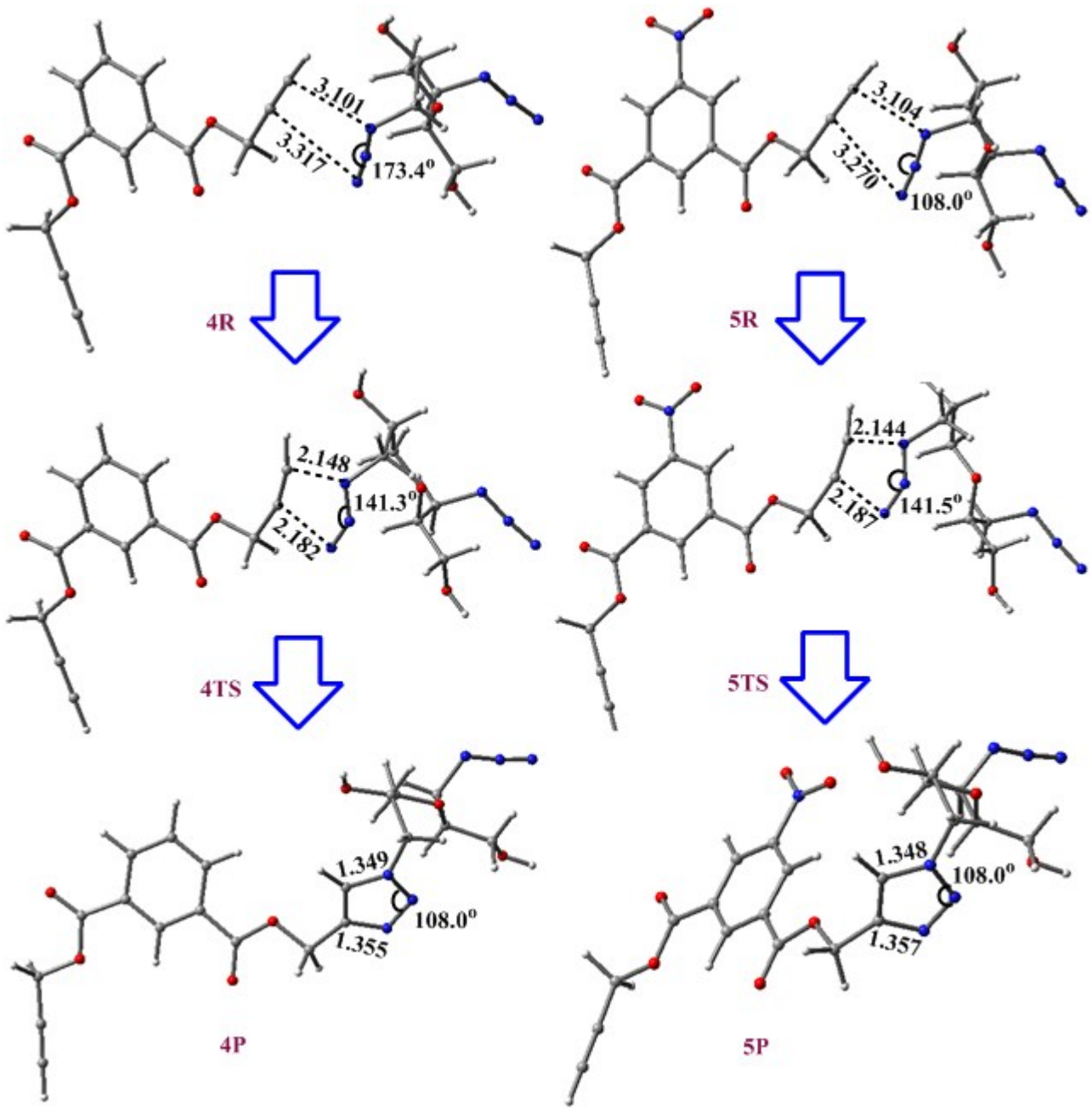

Fig. S2 M052X/6-311G(d,p) optimized geometries and selected bond distances (Å) for bis(propargyl) aromatic esters (**4** & **5**) involved in the curing reaction with **GAP-2**. (Red = oxygen; gray = carbon; blue = nitrogen; white = hydrogen)