Electronic Supplementary Information

How and Why [Bu_4P][Im]/CO_2 System Efficiently Catalyzes the Hydration of Propargylic Alcohols to α-Hydroxy Ketones: Electrostatically Controlled Reactivity

Xueli Mu, Chengbu Liu,* and Dongju Zhang*

Institute of Theoretical Chemistry, School of Chemistry and Chemical Engineering,

Shandong University, Jinan 250100, China

Corresponding authors:

Email: cbliu@sdu.edu.cn

Email: zhangdj@sdu.edu.cn

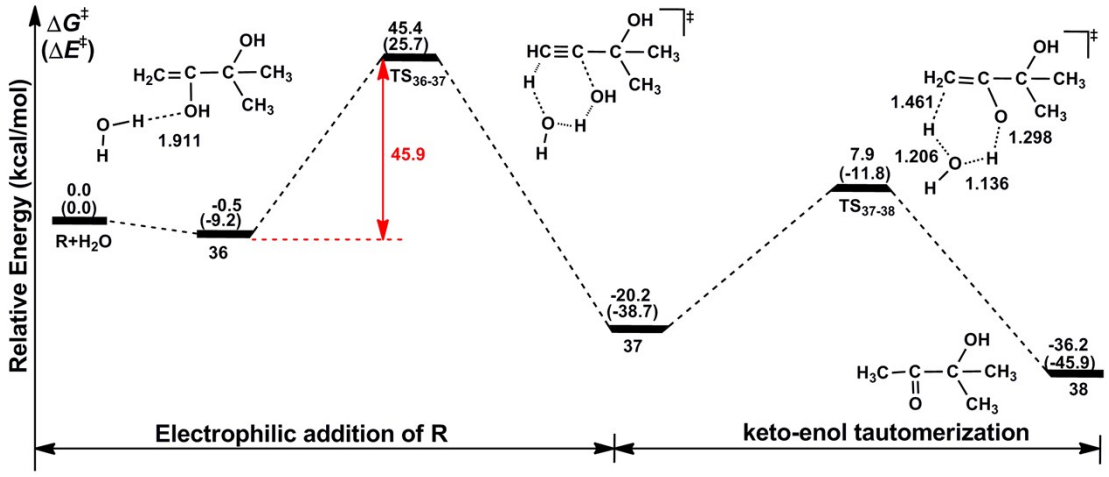

Fig. S1 Calculated relative energy profiles with schematic structures (distances in Å) for the hydration of (2-methylbut-3-yn-2-ol) to the α-hydroxy ketone (3-hydroxy-3-methyl-2-butanone, **P**) catalyzed by H_2O. $\Delta E^{‡}$: electronic energy and $\Delta G^{‡}$: Gibbs free energy.

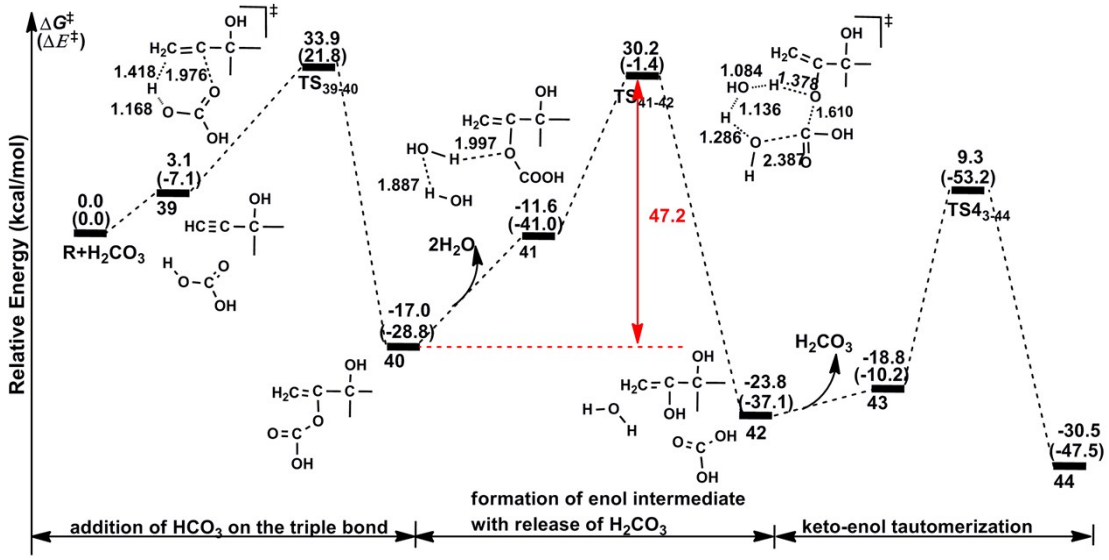

Fig. S2 Calculated relative energy profiles with schematic structures (distances in Å) for the hydration of (2-methylbut-3-yn-2-ol, **R**) to the α-hydroxy ketone (3-hydroxy-3-methyl-2-butanone, **P**) catalyzed by H_2CO_3. $\Delta E^{‡}$: electronic energy and $\Delta G^{‡}$: Gibbs free energy.

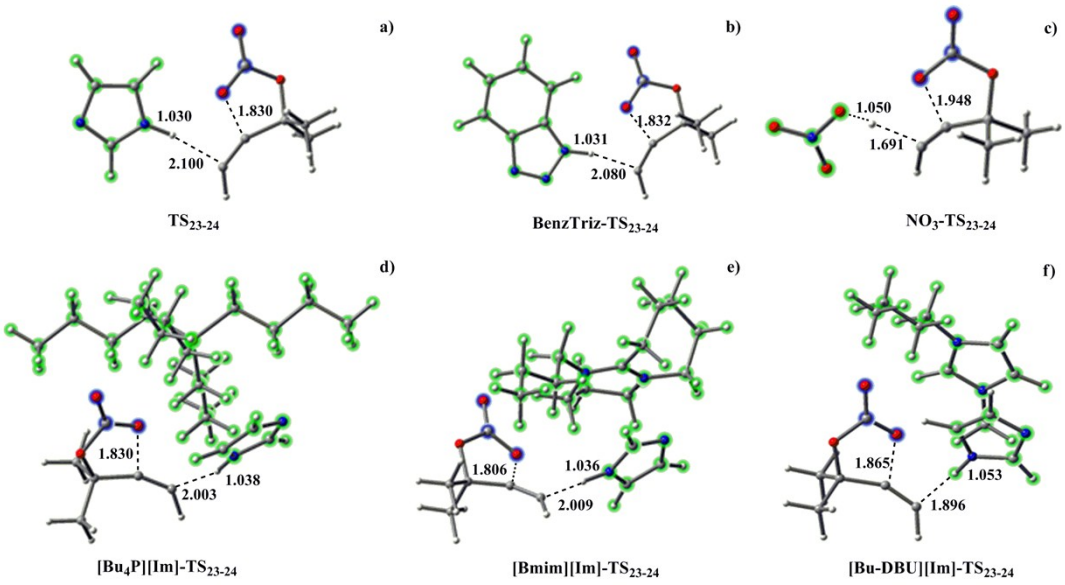

Fig. S3 The optimized geometries of $\mathbf{TS_{23\text{-}24}}$ with $[Im]^-$ (a), $[BenzTriz]^-$ (b), $[NO_3]^-$ (c), $[Bu_4P][Im]$ (d), [Bmim][Im] (e) and [Bu-DBU][Im] (f) as the catalyst.

The complete citation information of official Gaussian 09:

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, Revision B.01, Gaussian, Inc., Wallingford CT, 2010.

Following are the charge, multiplicity, and cartesian coordinates of the optimized intermediates, transition states and products, along with the calculated absolute energies (in hartree).

1

0 1

C	-0.70066300	2.11696100	-0.03098000
H	-1.25499700	3.02575500	-0.03528700
C	-0.05366800	1.10364100	-0.03250500
C	0.77092000	-0.12814400	-0.00874000
C	0.46740200	-0.92459800	1.26201500
H	-0.57933300	-1.23337800	1.27974400
H	1.10835000	-1.80827900	1.27836400
H	0.67285200	-0.32146800	2.15009500
C	0.50845200	-0.96201900	-1.25814300
H	0.73657800	-0.37651300	-2.14921700
H	1.16117900	-1.83664200	-1.23310900
H	-0.53321100	-1.28386000	-1.28082600
O	2.14821400	0.23185700	-0.05933800
H	2.34383700	0.79987300	0.69201700
O	-2.62385400	-0.70028600	0.05482100
H	-2.27802200	0.19806400	0.00932200
H	-3.52676500	-0.65116500	-0.26484400

Sum of electronic and zero-point Energies: -346.750052;
Sum of electronic and thermal Free Energies: -346.784045.

TS_{1-2}

0 1

C	1.67326600	1.36121300	0.18218100
H	1.53453200	2.42744100	0.28387600
C	0.76394500	0.45982900	0.08995900
C	-0.64451000	-0.02521000	-0.03157200
C	-1.00995400	-0.98108200	1.10657000
H	-0.85711600	-0.51050500	2.08017200
H	-2.05850600	-1.26682900	1.00646800
H	-0.41116900	-1.89364400	1.05399000
C	-1.55512200	1.19857900	-0.02976000
H	-1.28093900	1.86629200	-0.84639100
H	-2.58363700	0.86497200	-0.17659300
H	-1.48227900	1.73358200	0.91823600
O	-0.83244500	-0.67016400	-1.28301900

H	-0.08080900	-1.25463300	-1.42945900
O	1.78216900	-0.91369600	-0.14499800
H	2.40125000	0.05156200	-0.04203700
H	1.85513700	-1.42732800	0.67160500

Sum of electronic and zero-point Energies: -346.661939;
Sum of electronic and thermal Free Energies: -346.693968.

2

0 1

C	-1.62666300	1.25392200	0.13382300
H	-2.70984700	1.23907100	0.18174500
C	-0.92457500	0.13162300	0.01351900
C	0.58760400	-0.00438400	-0.03090100
C	1.29019400	1.33045400	-0.20787100
H	1.12748100	1.97933100	0.65412300
H	2.36049500	1.14489900	-0.30783300
H	0.93783000	1.82871500	-1.11178000
C	1.06213400	-0.70732000	1.24559200
H	0.58096200	-1.68203300	1.34712200
H	2.14264600	-0.85207500	1.19061400
H	0.82333200	-0.10936800	2.12799400
O	0.93882000	-0.78345700	-1.17074200
H	0.39166600	-1.57602900	-1.16553900
O	-1.48934000	-1.11293500	-0.07232900
H	-1.13477600	2.21300200	0.18278400
H	-2.44779300	-1.04014900	-0.07963300

Sum of electronic and zero-point Energies: -346.787421;
Sum of electronic and thermal Free Energies: -346.818906.

$TS_{2\text{-}3}$

0 1

C	-1.82388000	1.01859300	0.04618300
H	-2.42912200	0.95367200	0.95029500
C	-0.87181900	-0.02598900	-0.03311800
C	0.63447700	-0.01020600	-0.02279200
C	1.17209800	1.19086400	-0.79141700
H	0.87860400	2.12638100	-0.31405200
H	2.26113100	1.12625000	-0.80703500
H	0.81095100	1.17843800	-1.82082500
C	1.06712700	0.03219000	1.45266500
H	0.67393700	-0.83453500	1.98871900
H	2.15722000	-0.00282400	1.48608300
H	0.71727000	0.94243400	1.94227400
O	1.14562200	-1.17016900	-0.64750500

H	0.53998500	-1.89975200	-0.47361700
O	-1.47981800	-1.14976000	-0.13496600
H	-1.60422700	2.02843300	-0.27718200
H	-2.40019000	-0.29176900	-0.32402400

Sum of electronic and zero-point Energies: -346.703356;
Sum of electronic and thermal Free Energies: -346.735371.

3

0 1

C	-1.83481200	-0.94681300	0.05164600
H	-1.91215800	-1.37257800	-0.95303000
C	-0.90690300	0.24014300	-0.00440900
C	0.60752200	-0.00247400	-0.01476000
C	1.03995300	-0.49802200	1.37219600
H	0.62939200	-1.48174500	1.60727900
H	2.12921400	-0.56363500	1.38203500
H	0.73322400	0.21292200	2.14239200
C	0.98301000	-1.00899000	-1.10187000
H	0.64037700	-0.66027300	-2.07830400
H	2.07059600	-1.09398200	-1.13266700
H	0.56157300	-1.99659600	-0.90309700
O	1.26273400	1.21322200	-0.29046700
H	0.59780300	1.91357500	-0.23782100
O	-1.32544700	1.37246700	-0.05045000
H	-1.45954400	-1.72866600	0.71237900
H	-2.82139500	-0.61759400	0.37135200

Sum of electronic and zero-point Energies: -346.8086;
Sum of electronic and thermal Free Energies: -346.840869
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4

0 1

C	0.09941300	0.30283000	2.20901400
H	-0.35097100	0.52468000	3.14782300
C	0.61760200	0.02702600	1.15949700
C	1.25100000	-0.30468200	-0.14261400
C	2.51161400	0.54467800	-0.32405000
H	3.22262100	0.35992300	0.48306100
H	2.97290600	0.28535700	-1.27879800
H	2.25742100	1.60703100	-0.33252300
C	1.57318900	-1.79562000	-0.18627300
H	0.65767000	-2.37711800	-0.08040800
H	2.03029000	-2.02278200	-1.15096400
H	2.26412900	-2.06052100	0.61518300

O	0.33413900	-0.05789000	-1.19923700
H	0.16000100	0.89729500	-1.21438500
C	-2.15117800	-0.66692900	-0.18379300
O	-2.46333800	0.44456600	-0.28095000
O	-1.89435300	-1.78481800	-0.06985300
O	-0.35975400	2.56749700	-0.37405200
H	-0.24797000	2.26533700	0.53526600
H	-1.30948400	2.52214700	-0.52220600

Sum of electronic and zero-point Energies: -535.322389;
Sum of electronic and thermal Free Energies: -535.362609

TS_{4-5}

0 1

C	-0.03517300	1.96234000	0.23283600
H	-0.28133000	3.00103100	0.37630600
C	-0.66691900	0.89701100	0.09754700
C	-1.64327900	-0.20503000	-0.01834300
C	-1.54649100	-1.16966200	1.16472400
H	-1.66232300	-0.64046500	2.11262200
H	-2.34818000	-1.90312100	1.06322000
H	-0.58441800	-1.67894800	1.14934200
C	-3.00436900	0.51639600	-0.03215700
H	-3.06311600	1.20181000	-0.87742200
H	-3.76370000	-0.25750100	-0.15503500
H	-3.18314200	1.05171800	0.90086000
O	-1.52367200	-0.86104400	-1.25000900
H	-0.61222000	-1.18603200	-1.30227500
C	2.15696500	-0.41488800	-0.06524500
O	3.13502100	-1.03200600	0.24694200
O	0.97153700	-0.66875700	-0.32971200
O	2.36134800	1.05941100	-0.15849600
H	1.19563900	1.62731500	0.09453500
H	3.18452600	1.28635400	0.29186900

Sum of electronic and zero-point Energies: -535.240432;
Sum of electronic and thermal Free Energies: -535.276936.

5

0 1

C	0.51673900	-2.19592300	-0.21411600
H	1.48945500	-2.64321500	-0.36033400
C	0.44088600	-0.88449400	-0.02057100
C	1.60648800	0.09432600	0.04054200
C	1.66890700	0.74875400	1.41766200
H	1.85102100	-0.00789200	2.18253700

H	2.48094200	1.47780500	1.43361200
H	0.73080400	1.25788600	1.64086500
C	2.93887700	-0.54813900	-0.31758800
H	2.90523800	-1.00654400	-1.30934600
H	3.70826000	0.22503600	-0.31521200
H	3.21436600	-1.31421800	0.40874200
O	1.33676300	1.17226800	-0.87795900
H	1.33881500	0.81676800	-1.77328100
C	-1.98524900	-0.61398100	0.07180100
O	-2.29856900	-1.76157100	0.01770300
O	-0.70662200	-0.14151900	0.16225000
O	-2.81413200	0.40960400	0.06580200
H	-0.35706200	-2.82723000	-0.22065000
H	-2.30691000	1.25197000	0.02238500
O	-1.11382100	2.52532600	-0.18938900
H	-0.26203400	2.12661000	-0.43823000
H	-1.14173500	3.40689300	-0.56471800

Sum of electronic and zero-point Energies: -611.756971;
Sum of electronic and thermal Free Energies: -611.79623.

$TS_{5\text{-}6}$

0 1

C	0.66682700	-1.99534300	-0.77274800
H	1.62268000	-2.49055000	-0.68073100
C	0.52573400	-0.72819500	-0.40551800
C	1.60185300	0.19269900	0.14418200
C	1.24597200	0.62251200	1.56479000
H	1.18763200	-0.24962900	2.21816800
H	2.01098800	1.30505300	1.93874000
H	0.28783600	1.14365400	1.58439400
C	2.99020200	-0.42961500	0.09989500
H	3.25472400	-0.73476600	-0.91620500
H	3.71636500	0.30820200	0.44442400
H	3.04928000	-1.30507600	0.74875400
O	1.57955800	1.39789200	-0.63833700
H	1.93612500	1.19151700	-1.50840000
C	-2.04290900	-0.65087500	0.19214500
O	-1.97303000	-1.78874000	0.49421600
O	-0.68328100	-0.07762100	-0.50123600
O	-2.83107100	0.29687200	0.21217700
H	-0.17867000	-2.56397500	-1.13219200
H	-2.22350500	1.55085100	-0.08668300
O	-1.38160500	2.15660200	-0.31008000
H	-0.77304700	1.21627800	-0.49326600

H	-1.50104800	2.68130200	-1.10739400

Sum of electronic and zero-point Energies: -611.722031;
Sum of electronic and thermal Free Energies: -611.760496.

6

0 1

C	0.55642400	-1.75457900	-1.09108900
H	0.24941300	-2.71753800	-0.71467600
C	-0.07446600	-0.63379700	-0.73683700
C	-1.28304100	-0.56915400	0.19128300
C	-2.52081700	-0.13237500	-0.59028600
H	-2.77628300	-0.89319000	-1.32910600
H	-3.35634700	-0.00938400	0.10197800
H	-2.35626200	0.81531300	-1.10507300
C	-1.54560100	-1.88403300	0.91474900
H	-0.66745000	-2.19913400	1.48350000
H	-2.37637900	-1.73733800	1.60636200
H	-1.81171000	-2.67630900	0.21375900
O	-1.05576400	0.46034200	1.17346400
H	-0.21629800	0.28122500	1.61430700
C	2.60630100	0.14599600	0.47622200
O	3.31946400	-0.05280000	-0.40454700
O	0.37488000	0.55515000	-1.21486700
O	1.92564300	0.34928800	1.39349700
H	1.38376900	-1.70594000	-1.78724600
H	-0.76982400	3.63006200	-0.04121200
O	-1.10504900	2.76338100	-0.27768500
H	-0.16766400	1.31165200	-0.92876100
H	-1.24114100	2.26534200	0.54300500

Sum of electronic and zero-point Energies: -611.772374;
Sum of electronic and thermal Free Energies: -611.813956.

7

0 1

C	-0.83963400	1.44258200	-0.32516200
H	-0.28751400	2.31221400	-0.00259800
C	-0.26386900	0.23682100	-0.30108600
C	1.18009100	-0.01851600	0.10025900
C	1.21665600	-0.76158000	1.43195200
H	0.65948100	-1.69597800	1.35772400
H	2.25288500	-0.97765000	1.69870600
H	0.77578100	-0.13759100	2.21131900
C	1.88185100	-0.82210400	-0.99740900
H	1.85492400	-0.27644600	-1.94541600

H	2.92320700	-0.97902800	-0.71027500
H	1.39582900	-1.78583300	-1.14752800
O	1.86413700	1.20472500	0.32068300
H	1.91559600	1.67458900	-0.51766100
O	-0.88710400	-0.92047900	-0.63480100
H	-1.85325000	1.57164500	-0.68562500
O	-3.44088900	-0.16849100	0.23059900
H	-4.07827800	-0.72162600	0.68806700
H	-1.84691300	-0.77988000	-0.62789500
H	-3.05147100	0.40633600	0.89800700

Sum of electronic and zero-point Energies: -423.196254;
Sum of electronic and thermal Free Energies: -423.232277.

TS_{7-8}

0 1

C	-1.06370100	1.35669200	-0.25725200
H	-0.55437900	2.21944400	0.14674300
C	-0.35584800	0.14335800	-0.35420500
C	1.10137100	0.00258100	0.08734300
C	1.14806100	-0.80430900	1.38160500
H	0.68578400	-1.78000700	1.23110900
H	2.18803100	-0.93517200	1.68528400
H	0.62086500	-0.26818300	2.17366600
C	1.87933400	-0.69458800	-1.03025300
H	1.85420000	-0.09846400	-1.94765000
H	2.91844600	-0.81258400	-0.71792500
H	1.44449800	-1.67002700	-1.24658700
O	1.68007300	1.25988600	0.39208900
H	1.73060000	1.77983800	-0.41600100
O	-0.93484500	-0.94122800	-0.68943400
H	-1.77259800	1.55655600	-1.05915700
O	-2.97892400	-0.22786900	0.29164700
H	-3.15195100	-0.66488300	1.13118800
H	-2.15176500	-0.76223500	-0.27516000
H	-2.19746700	0.68700000	0.37663500

Sum of electronic and zero-point Energies: -423.15347;
Sum of electronic and thermal Free Energies: -423.187433.

8

0 1

C	-0.87954900	1.45104700	-0.10825100
H	-0.33705700	2.12285400	0.55861300
C	-0.29151700	0.06775700	-0.04969500
C	1.24029900	-0.05870400	-0.00706900

C	1.63754900	-0.12962900	1.46667600
H	1.17302700	-0.99385500	1.94320700
H	2.72352800	-0.21322900	1.53588500
H	1.32905400	0.77770700	1.98992100
C	1.69523800	-1.29755500	-0.76754900
H	1.41949000	-1.22852400	-1.82439600
H	2.78004600	-1.39101600	-0.69062100
H	1.22181800	-2.18984300	-0.35990900
O	1.85342000	1.11647000	-0.52186100
H	1.87652500	1.06512400	-1.48151400
O	-0.97448800	-0.93260300	-0.00059500
H	-0.74380900	1.84825600	-1.11841800
O	-3.71250800	-0.17664700	0.00446500
H	-4.37715800	-0.82253200	0.24760300
H	-2.86687900	-0.64785200	0.01190000
H	-1.94210600	1.41765200	0.12697700

Sum of electronic and zero-point Energies: -423.212926;
Sum of electronic and thermal Free Energies: -423.250798.

9

-1 1

C	0.00014300	-1.41968500	-0.08264900
H	1.01356600	-1.76345400	-0.10938000
C	-1.11113900	-0.96339800	-0.05664800
C	-2.41633200	-0.26929200	-0.00132900
C	-3.54575100	-1.21244700	-0.40961600
H	-3.59662200	-2.06819200	0.26665600
H	-4.49201800	-0.66634400	-0.38011200
H	-3.37392800	-1.56883200	-1.42613500
C	-2.62971700	0.26048600	1.42354200
H	-1.83221400	0.96678300	1.66175800
H	-3.59340300	0.77512000	1.46986100
H	-2.61398200	-0.55575600	2.14984400
O	-2.44150000	0.80647200	-0.92102500
H	-1.64376900	1.34848800	-0.74256500
C	2.61140200	0.12766100	-1.04922900
C	2.59590200	0.25484800	1.07873200
C	3.39510300	-0.80407900	0.68544000
H	2.38005800	0.34158700	-2.08554200
H	2.34278800	0.60058100	2.07124500
H	3.95772800	-1.49553800	1.29828300
N	2.09326900	0.85406400	-0.04065100
N	3.40207200	-0.88418100	-0.68082400
O	-0.20109300	2.16289600	-0.10243000

H	0.68814400	1.65002900	-0.08083300
H	0.03934100	3.04684100	-0.38457400

Sum of electronic and zero-point Energies: -572.353523;
Sum of electronic and thermal Free Energies: -572.395606.

$TS_{9\text{-}10}$

-1 1

C	-0.93860700	1.79537300	-0.93005900
H	-1.13343300	2.83620800	-0.75514900
C	-1.33700300	0.69118800	-0.50502000
C	-2.30503300	-0.10425000	0.32809700
C	-2.76799900	0.75386900	1.50307700
H	-3.26012500	1.66026300	1.14611000
H	-3.46576200	0.17640100	2.11597800
H	-1.90585000	1.03281700	2.11041700
C	-3.50063400	-0.51386700	-0.54354900
H	-3.14156100	-1.12931400	-1.37015100
H	-4.20471300	-1.09555800	0.05898500
H	-4.00468600	0.36718600	-0.94873500
O	-1.71764000	-1.26834100	0.88585800
H	-1.17039800	-1.61151700	0.16130300
C	2.87771400	-1.13344000	0.07824800
C	2.43670100	0.99221900	-0.07621300
C	3.70704200	0.79625000	0.41100200
H	2.72744800	-2.20084800	0.01614200
H	1.85453500	1.87253800	-0.29381600
H	4.43368800	1.54082400	0.69936700
N	1.91884000	-0.25392000	-0.28371300
N	3.97926200	-0.54587700	0.50700900
O	-0.47653500	-0.80667400	-1.29080400
H	0.95274300	-0.47658800	-0.68170400
H	-0.44828700	-0.43776600	-2.17574800

Sum of electronic and zero-point Energies: -572.298062;
Sum of electronic and thermal Free Energies: -572.340427.

10

-1 1

C	-0.84667800	-1.34628800	-0.95504500
H	-1.58230600	-2.12631700	-1.09848700
C	-1.17771300	-0.15855300	-0.38677000
C	-2.62114300	0.10582900	0.12276800
C	-3.69471400	-0.32386300	-0.87171800
H	-3.69227300	-1.40509100	-1.02172500
H	-4.67619800	-0.02309300	-0.49215200

H	-3.52459600	0.16297200	-1.83344400
C	-2.81574000	-0.60138400	1.46892600
H	-2.03065200	-0.28467700	2.15957400
H	-3.78723600	-0.32536300	1.89123300
H	-2.76112300	-1.68641700	1.35217400
O	-2.75862900	1.50342700	0.32529000
H	-1.83187300	1.81216800	0.28108900
C	3.20630900	1.05727500	-0.30927400
C	2.65133300	-0.91758000	0.40405500
C	4.01971700	-0.78829200	0.36319100
H	3.09109500	2.06605200	-0.67651000
H	2.00596300	-1.73182300	0.69075900
H	4.76869800	-1.51905200	0.62893900
N	2.14323800	0.27358200	-0.03021000
N	4.36377300	0.46011400	-0.08770200
O	-0.38034700	0.84242200	-0.15857600
H	0.16708100	-1.53064000	-1.29005500
H	1.08792500	0.52576000	-0.11652500

Sum of electronic and zero-point Energies: -572.400946;
Sum of electronic and thermal Free Energies: -572.443543.

$TS_{10\text{-}11}$

-1 1

C	0.58631100	0.72795700	1.47823400
H	0.63824700	-0.19066500	2.06140500
C	1.55340100	0.84691300	0.43012000
C	2.07743600	-0.44974300	-0.25240300
C	2.86181500	-1.30638500	0.74321800
H	2.21364200	-1.71758900	1.51909200
H	3.33173200	-2.13199100	0.20167400
H	3.64732800	-0.71143900	1.21548000
C	0.91094500	-1.23372300	-0.85262900
H	0.35625200	-0.60735700	-1.55429500
H	1.30452400	-2.10104700	-1.39045600
H	0.21128300	-1.56873800	-0.08417000
O	2.96244600	-0.06741700	-1.28918100
H	2.92543900	0.90589500	-1.27220300
C	-2.52103300	0.82186700	-0.69746700
C	-2.66309200	-0.65774400	0.85696400
C	-3.78116600	-0.71366600	0.05028400
H	-2.11939700	1.62576400	-1.29920100
H	-2.38552900	-1.23955100	1.72436100
H	-4.63521400	-1.37200900	0.12516700
N	-1.86055100	0.33427000	0.37104600

N	-3.68677300	0.22913500	-0.93651400
O	1.95697400	1.90967800	-0.05547900
H	0.48845300	1.62693300	2.08338200
H	-0.64855500	0.58701100	0.84740800

Sum of electronic and zero-point Energies: -572.385996;
Sum of electronic and thermal Free Energies: -572.427714.

11

-1 1

C	0.96087700	1.84580900	0.24106700
H	0.70727600	1.80683000	1.30519600
C	2.01676700	0.82011800	-0.03889400
C	1.64856900	-0.66659600	0.05502600
C	0.92708600	-0.97626300	1.36307500
H	-0.06144700	-0.51091400	1.38512200
H	0.79604900	-2.05829300	1.43032200
H	1.52138300	-0.64682800	2.22004300
C	0.75794600	-1.01607700	-1.14218700
H	1.27309300	-0.77836600	-2.07704700
H	0.56279100	-2.09009100	-1.11707700
H	-0.19831700	-0.48875100	-1.10281500
O	2.84563100	-1.42668900	0.00588000
H	3.53238700	-0.81703200	-0.29651600
C	-2.74686400	0.00552400	-1.14125200
C	-2.35314400	0.77017100	0.79530600
C	-3.06377400	-0.41630900	0.90722200
H	-2.76393700	-0.08760900	-2.22174300
H	-1.99733400	1.43215300	1.57641600
H	-3.40253100	-0.92675700	1.79988900
N	-2.14387300	1.04055800	-0.52856000
N	-3.31479700	-0.90763000	-0.34059300
O	3.15255800	1.12228200	-0.35004200
H	1.34666300	2.83364400	-0.00635500
H	0.02431700	1.63851400	-0.29425300

Sum of electronic and zero-point Energies: -572.397267;
Sum of electronic and thermal Free Energies: -572.437624.

12

-1 1

C	3.26504200	-1.19647400	2.08997200
H	3.24505800	-1.68820400	3.03180100
C	3.25284000	-0.64712600	1.02202300
C	3.25645600	0.05349200	-0.28057400
C	2.66286400	-0.83943800	-1.36215200

H	1.61169500	-1.02997100	-1.13807400
H	2.73852800	-0.31502900	-2.31763000
H	3.22370600	-1.77384200	-1.42273800
C	2.48002100	1.36344500	-0.16283400
H	2.92123800	1.99971200	0.61076700
H	2.53358900	1.88310200	-1.12253200
H	1.43122600	1.18019300	0.08316700
O	4.61786900	0.30706100	-0.66414000
H	5.00840900	0.85863400	0.01963500
C	-3.16641500	-1.10237900	-0.39060500
C	-4.79519100	0.13442700	0.20789600
C	-3.66054000	0.88159100	0.38567900
H	-2.54123100	-1.90808400	-0.74091300
H	-5.81851600	0.41872300	0.40273000
H	-3.47399200	1.88085400	0.73966300
N	-4.47797100	-1.11380400	-0.28103200
N	-2.62183400	0.07748600	-0.00163600
C	-1.15654200	0.43645700	0.00364100
O	-0.93542700	1.57524600	0.40826400
O	-0.43397700	-0.47678700	-0.39981000

Sum of electronic and zero-point Energies: -684.515375;
Sum of electronic and thermal Free Energies: -684.562537.

$TS_{12\text{-}13}$

-1 1

C	-1.95792700	-0.82047500	1.95313700
H	-1.19074400	-1.11312700	2.66121900
C	-1.69828600	-0.22792800	0.84758100
C	-2.57617900	0.27035200	-0.27541200
C	-2.49274200	1.79224600	-0.42018800
H	-1.48436700	2.10338400	-0.69841200
H	-3.19831800	2.12008200	-1.18925400
H	-2.76359600	2.25969000	0.52838000
C	-2.24724400	-0.41531400	-1.60333100
H	-2.26370900	-1.49771700	-1.47088300
H	-2.99993600	-0.12886600	-2.34351900
H	-1.26014700	-0.12360400	-1.96813700
O	-3.91295300	-0.06804600	0.07926400
H	-3.81754000	-0.51297100	0.94153800
C	2.46182100	1.11457900	0.38683000
C	4.19013200	0.04209900	-0.25927900
C	3.14176400	-0.81801800	-0.41789100
H	1.76853600	1.85048900	0.76127300
H	5.23229100	-0.13364400	-0.47624000

H	3.05296200	-1.83034900	-0.77165100
N	3.75576700	1.25074600	0.24586800
N	2.03138900	-0.12176000	-0.00073700
C	0.67033300	-0.63905200	0.00498100
O	0.49969700	-1.78100000	-0.34182700
O	-0.15368700	0.26314500	0.38896300

Sum of electronic and zero-point Energies: -684.47217;
Sum of electronic and thermal Free Energies: -684.51331.

13

-1 1

C	2.00562600	-1.01558700	-1.81211200
H	1.21136200	-1.36305900	-2.47800100
C	1.62095400	-0.29559900	-0.79277400
C	2.50730800	0.31917000	0.27696200
C	2.42588000	1.84974600	0.25394200
H	1.41478300	2.19509300	0.48338700
H	3.12086000	2.26387400	0.99072700
H	2.70983300	2.20778200	-0.73754300
C	2.15877000	-0.21009000	1.67214600
H	2.19405700	-1.30039800	1.66671200
H	2.88809100	0.17135500	2.39300300
H	1.15977500	0.10686300	1.98514100
O	3.83537600	-0.06474300	-0.02967400
H	3.72446100	-0.60227400	-0.84686700
C	-2.38960900	1.08133200	-0.47903900
C	-4.12485700	0.10571800	0.29366500
C	-3.09783500	-0.77087400	0.48535900
H	-1.68927000	1.77027300	-0.92327700
H	-5.16408600	-0.02275600	0.55206700
H	-3.02558800	-1.75730800	0.90925700
N	-3.67282600	1.26217000	-0.31047900
N	-1.98091600	-0.13874500	-0.01365300
C	-0.65172800	-0.70026000	-0.01609700
O	-0.48152600	-1.80642500	0.41554300
O	0.18425800	0.15682300	-0.51311800

Sum of electronic and zero-point Energies: -684.471837;
Sum of electronic and thermal Free Energies: -684.513275.

14

-1 1

C	1.90784200	-1.21374800	-0.87040500
H	1.22737100	-1.97112900	-1.27369100
C	1.29444900	-0.15040100	-0.40821900

C	1.90259800	1.10562400	0.19132000
C	1.56046100	2.33752300	-0.65681400
H	0.48256200	2.51262400	-0.68688300
H	2.05355400	3.21631500	-0.23176900
H	1.92671500	2.18729800	-1.67427200
C	1.44486700	1.31595000	1.63802800
H	1.66435900	0.42243100	2.22392900
H	1.98364100	2.16768900	2.06264000
H	0.37193100	1.51854700	1.69527500
O	3.31096600	0.95260400	0.20365100
H	3.48593800	0.12641400	-0.27893400
C	-2.84455100	0.38376200	-1.02811100
C	-4.51357100	-0.31849700	0.10427100
C	-3.41096500	-0.76307100	0.77088400
H	-2.19437100	0.83935700	-1.75753500
H	-5.54999400	-0.46969000	0.36121700
H	-3.26148000	-1.34079600	1.66623800
N	-4.14995300	0.39752600	-1.01954000
N	-2.33536300	-0.30874400	0.03888500
C	-0.95797500	-0.53626200	0.37892700
O	-0.68031000	-1.18534400	1.34694700
O	-0.19229600	0.06044400	-0.48890300
O	4.63066500	-2.18259000	-0.51794000
H	3.70635500	-1.88196700	-0.74643400
H	4.64949500	-2.07476000	0.43548500

Sum of electronic and zero-point Energies: -760.892095;
Sum of electronic and thermal Free Energies: -760.938699.

$TS_{14\text{-}15}$

-1 1

C	1.82694500	-1.50766300	-0.74794700
H	1.11723800	-2.22336900	-1.16928500
C	1.29576900	-0.39468900	-0.29077000
C	1.96789700	0.84831900	0.28424200
C	2.03456300	1.92127000	-0.81624600
H	1.04111800	2.14161000	-1.21812000
H	2.46773000	2.83772400	-0.40541000
H	2.67225800	1.55834600	-1.62512400
C	1.19923800	1.38769300	1.49497400
H	1.08251100	0.59908000	2.24026600
H	1.78316500	2.20131600	1.93140400
H	0.21465700	1.77338000	1.21754200
O	3.26249300	0.57099800	0.75443300
H	3.75314100	-0.04940600	0.15185900

C	-2.73944300	0.49471200	-1.06211000
C	-4.50230400	-0.04184000	0.01817800
C	-3.46910600	-0.58884700	0.71834500
H	-2.02667400	0.88589000	-1.77024900
H	-5.55586000	-0.09088900	0.24315600
H	-3.40454200	-1.17603700	1.61773100
N	-4.03662700	0.63377400	-1.09324600
N	-2.33246600	-0.24194800	0.01978500
C	-0.99827500	-0.60326000	0.40220900
O	-0.80970100	-1.25722900	1.38652700
O	-0.15245200	-0.11146200	-0.46161900
O	4.40916500	-1.30204400	-0.77016100
H	3.22503500	-1.55687800	-0.77710500
H	4.84613000	-1.93982100	-0.20113600

Sum of electronic and zero-point Energies: -760.892751;
Sum of electronic and thermal Free Energies: -760.936077.

15

-1 1

C	1.72013100	-1.38091700	-1.20235300
H	1.10814400	-1.86893700	-1.95080600
C	1.22101900	-0.47334700	-0.38570100
C	1.96972900	0.31794800	0.69133400
C	1.87688200	1.81755700	0.29818000
H	0.84709100	2.17645200	0.18763200
H	2.37388500	2.39437700	1.08291400
H	2.42093900	1.96790700	-0.63752100
C	1.22354300	0.10708500	2.03264500
H	1.23940300	-0.95441900	2.28850600
H	1.77336500	0.65894100	2.79879400
H	0.18541500	0.46330600	2.02321100
O	3.24961500	-0.10054900	0.77935400
H	4.09528100	0.12126600	-0.43668900
C	-2.59159800	1.09940400	-0.64530900
C	-4.47320800	0.30065200	-0.02227300
C	-3.56007800	-0.66627800	0.26969900
H	-1.79180000	1.71475400	-1.02554100
H	-5.53834800	0.27831400	0.14390800
H	-3.62450200	-1.64476200	0.71269700
N	-3.85874600	1.39933000	-0.59292900
N	-2.34514700	-0.15145700	-0.13438300
C	-1.09829500	-0.83102100	-0.01687100
O	-1.02510200	-1.90912800	0.49209200
O	-0.15288700	-0.08649100	-0.54694000

O	4.71502300	0.25727300	-1.25519900
H	2.77315800	-1.61020100	-1.10642100
H	5.54326900	0.53253500	-0.86007100

Sum of electronic and zero-point Energies: -760.915795;
Sum of electronic and thermal Free Energies: -760.960804.

16

-1 1

C	2.10552800	-1.31998300	1.55980200
H	2.00615800	-1.38714400	2.63476900
C	1.45850300	-0.37534600	0.86883300
C	1.50608900	-0.17463100	-0.64583800
C	2.92953000	0.11405300	-1.11824100
H	3.57062000	-0.75791500	-0.96662300
H	2.91376200	0.36566700	-2.18200400
H	3.33759200	0.95835200	-0.56110700
C	0.91478500	-1.36328000	-1.41019700
H	-0.11376900	-1.55812900	-1.10358000
H	0.92560300	-1.13939800	-2.48046100
H	1.50998900	-2.26210200	-1.22814100
O	0.74301000	0.99696900	-0.83754400
H	2.74250600	-2.02732400	1.04589000
C	-1.69261200	-0.75176900	0.88448800
C	-3.11722300	-0.58156800	-0.69081700
C	-2.21640300	0.44059200	-0.86535200
H	-1.13611800	-1.07006000	1.75161300
H	-3.98321700	-0.81764000	-1.29135600
H	-2.12901900	1.23025200	-1.59294700
N	-2.78353700	-1.32721000	0.41184000
N	-1.30948300	0.31759800	0.14691200
C	-0.09648600	1.27253300	0.31114900
O	-0.38675900	2.44284000	0.51677500
O	0.67584400	0.55633100	1.40823200

Sum of electronic and zero-point Energies: -684.528796;
Sum of electronic and thermal Free Energies: -684.56746.

$TS_{16\text{-}17}$

-1 1

C	1.72359500	-1.36318500	1.75153600
H	1.63040900	-1.21694900	2.81853700
C	1.37132700	-0.40604600	0.90018600
C	1.43449100	-0.43348100	-0.61800600
C	2.88353800	-0.49727000	-1.09903000
H	3.32775000	-1.45621700	-0.82350200

H	2.91139700	-0.38759700	-2.18581500
H	3.46593200	0.30644800	-0.64542200
C	0.59541300	-1.54262800	-1.24342000
H	-0.43475700	-1.50899100	-0.89130900
H	0.60752200	-1.42690200	-2.33013100
H	1.03241900	-2.51222500	-0.98907100
O	0.93028200	0.85644600	-0.96339000
H	2.07898500	-2.31326000	1.37661000
C	-1.88776200	-0.46280500	1.00507200
C	-3.19609300	-0.50503300	-0.66330400
C	-2.22452100	0.45196100	-0.89942700
H	-1.42290200	-0.68734400	1.95680100
H	-4.02962900	-0.79391200	-1.28970800
H	-2.06896000	1.10508000	-1.74675400
N	-2.97855900	-1.08908700	0.55488100
N	-1.38890400	0.47280100	0.17616800
C	0.45419300	1.50502400	0.14939400
O	0.20202100	2.66876400	0.17606900
O	0.93632000	0.81562000	1.27912200

Sum of electronic and zero-point Energies: -684.559413;
Sum of electronic and thermal Free Energies: -684.519803.

17

-1 1

C	1.26254800	-1.51274700	1.80185500
H	1.28156000	-1.27424700	2.85575600
C	1.26527600	-0.55360500	0.89074200
C	1.26443100	-0.65916300	-0.61934100
C	2.64649700	-1.07801400	-1.12298500
H	2.84555400	-2.11235600	-0.83533500
H	2.67721500	-0.99414700	-2.21157500
H	3.42170900	-0.43888100	-0.69462100
C	0.16461900	-1.52910800	-1.19899000
H	-0.82009600	-1.20481300	-0.86612300
H	0.21388600	-1.48607200	-2.28975500
H	0.32827600	-2.56340200	-0.88458700
O	1.07364400	0.71748400	-1.00035000
H	1.17836100	-2.54472900	1.49155900
C	-2.14724300	-0.38329900	1.03242600
C	-3.19570000	-0.06798400	-0.77943300
C	-2.21230800	0.90280300	-0.65286300
H	-1.83673800	-0.81826900	1.97601900
H	-3.91994300	-0.20692600	-1.57222800
H	-1.95081300	1.71153100	-1.32320100

N	-3.15206900	-0.89689800	0.30723200
N	-1.53319300	0.69550600	0.51294700
C	1.12922700	1.51594500	0.07466000
O	1.10386100	2.70036400	0.05920100
O	1.36171800	0.77378800	1.19820200

Sum of electronic and zero-point Energies: -458.939389;
Sum of electronic and thermal Free Energies: -458.973028.

18

-1 1

C	-4.70231400	-1.13882800	-0.32621500
H	-5.76072100	-1.18851600	-0.40785500
C	-3.50480500	-1.07557900	-0.24255700
C	-2.03010400	-1.01287600	-0.12691000
C	-1.62036800	-1.28183000	1.32724200
H	-1.98136800	-2.26042100	1.65381100
H	-0.52925400	-1.26864300	1.38531900
H	-2.04006500	-0.50821400	1.97195400
C	-1.40179500	-2.05405900	-1.06239300
H	-1.75133600	-3.05850400	-0.81131500
H	-1.67144200	-1.82570400	-2.09495500
H	-0.31637100	-2.01542300	-0.94250300
O	-1.65180600	0.29252100	-0.51869600
H	-0.66749400	0.35172900	-0.45715900
C	-3.50098400	2.00798100	0.29522900
O	-3.33473400	1.73656100	1.40762200
O	-3.73475800	2.35192300	-0.78279300
C	3.69383600	1.28510900	-0.39647400
C	5.41996700	0.17088000	0.17374600
C	4.35174200	-0.66186000	0.36758800
H	3.00347400	2.04013200	-0.73706300
H	6.46489500	-0.03411300	0.35065900
H	4.24868700	-1.67305900	0.72109800
N	4.99942100	1.39271600	-0.30680300
N	3.24720300	0.06344000	-0.00106300
C	1.83861700	-0.40503300	0.02553700
O	1.69082800	-1.55755300	0.41887500
O	1.03195500	0.45707600	-0.36071800

Sum of electronic and zero-point Energies: -873.104829;
Sum of electronic and thermal Free Energies: -873.156078.

$TS_{18\text{-}19}$

-1 1

C	4.67996700	-0.80629400	-1.25166100

H	5.63329800	-0.79380600	-1.72020900
C	3.61308800	-0.76367800	-0.70161900
C	2.28048100	-0.82569400	-0.05967800
C	1.46672400	-1.91585300	-0.77372500
H	2.01209400	-2.86112200	-0.74563800
H	0.50885900	-2.03966700	-0.26503900
H	1.29774900	-1.63221800	-1.81378300
C	2.41173100	-1.16865600	1.42850700
H	2.88134500	-2.14905500	1.54427700
H	3.01338900	-0.41499200	1.93244100
H	1.40650700	-1.19339400	1.85591700
O	1.58520500	0.39812100	-0.24452200
H	0.29301800	0.37952200	-0.43181400
C	2.16334000	1.81009600	0.33881800
O	3.25817900	1.65897500	0.81803400
O	1.32255100	2.64142300	0.12605900
C	-3.51988800	0.61380400	-0.98255600
C	-5.06871500	-0.27637200	0.18742300
C	-3.90073500	-0.66092200	0.77669900
H	-2.94400400	1.16246000	-1.71037400
H	-6.07553500	-0.52237000	0.48627300
H	-3.65943700	-1.26403700	1.63461000
N	-4.82100300	0.52112800	-0.91297400
N	-2.90430100	-0.08642600	0.01887500
C	-1.49155600	-0.22604300	0.25770700
O	-1.12559600	-0.86953900	1.21433800
O	-0.80243500	0.37144900	-0.64234100

Sum of electronic and zero-point Energies: -873.083734;
Sum of electronic and thermal Free Energies: -873.130175.

19

-1 1

C	4.68794700	-0.79354900	-1.26225300
H	5.63865300	-0.77946600	-1.73606300
C	3.62500700	-0.74997700	-0.70474000
C	2.29571400	-0.81763500	-0.05728500
C	1.48025300	-1.90473400	-0.77316900
H	2.02493800	-2.85045700	-0.74981900
H	0.52345800	-2.02973000	-0.26257200
H	1.30910400	-1.61745000	-1.81189900
C	2.43167700	-1.16649600	1.42881400
H	2.90187300	-2.14729500	1.53847500
H	3.03402400	-0.41422400	1.93371400
H	1.42766200	-1.19382500	1.85909400

O	1.58983500	0.40208800	-0.23614200
H	0.25600200	0.39412900	-0.43648600
C	2.15245500	1.78090000	0.33734900
O	3.25616900	1.64980400	0.81311400
O	1.31109100	2.62280000	0.14237600
C	-3.53009100	0.61361100	-0.98136200
C	-5.07272600	-0.29067200	0.18641100
C	-3.90278100	-0.66964000	0.77465500
H	-2.95810600	1.16867300	-1.70740900
H	-6.07795100	-0.54393400	0.48436000
H	-3.65793500	-1.27381700	1.63080800
N	-4.83001000	0.51197200	-0.91159200
N	-2.90976500	-0.08612900	0.01849400
C	-1.49918200	-0.21866500	0.25761300
O	-1.12444500	-0.85945000	1.21073200
O	-0.81426600	0.38571200	-0.64591900

Sum of electronic and zero-point Energies: -873.082852;
Sum of electronic and thermal Free Energies: -873.130086.

20

-1 1

C	-3.63110400	-0.71011100	2.41828600
H	-3.72968000	-0.81381600	3.47126900
C	-3.46126000	-0.57103600	1.23832100
C	-3.35957700	-0.46273800	-0.23099200
C	-2.40202700	-1.51339800	-0.80151800
H	-2.78533200	-2.51024800	-0.57182200
H	-2.36407500	-1.39046000	-1.88677900
H	-1.39661700	-1.41017100	-0.39685900
C	-4.76089300	-0.64741200	-0.82104900
H	-5.43017300	0.12249500	-0.43606900
H	-4.69982900	-0.55728800	-1.90721200
H	-5.15156600	-1.63083100	-0.55525900
O	-2.99789900	0.86225400	-0.64604900
H	-0.05882600	0.87508900	0.54536900
C	-1.76064700	1.38755600	-0.35884200
O	-1.11806400	0.71522000	0.54409300
O	-1.42518700	2.38806000	-0.93564100
C	4.09663500	0.76567900	0.54793100
C	5.34084600	-0.76628900	-0.26136000
C	4.05559000	-1.16105800	-0.50604500
H	3.70333400	1.65197900	1.01921800
H	6.25456900	-1.27832300	-0.52086000
H	3.61623600	-2.01843200	-0.98544600

N	5.35905000	0.44386300	0.40051400
N	3.26139400	-0.17076300	0.01784400
C	1.79387400	-0.14630100	0.00214900
O	1.24580400	-1.09173000	-0.53658800
O	1.32412600	0.87606300	0.56601700

Sum of electronic and zero-point Energies: -873.095345;
Sum of electronic and thermal Free Energies: -873.144069.

$TS_{20\text{-}21}$

-1 1

C	1.06756900	-1.57212100	-0.31274200
H	0.71518500	-2.56062300	-0.52122500
C	2.03012400	-0.82262800	-0.10301600
C	3.47113300	-0.50883300	0.13770900
C	3.76797000	-0.56900300	1.63953800
H	3.57896400	-1.57273300	2.02670500
H	4.81397600	-0.30205700	1.80918200
H	3.12595400	0.13888100	2.16558300
C	4.33974400	-1.49292500	-0.63957900
H	4.13505400	-1.39899200	-1.70644300
H	5.39326600	-1.26939800	-0.45668200
H	4.12593900	-2.51571000	-0.32326200
O	3.76123800	0.78826000	-0.34342600
H	-0.27682600	-0.55151200	-0.16143000
C	2.65726000	1.65727800	-0.22844400
O	1.60406600	1.04762600	0.12941800
O	2.85704000	2.82504600	-0.48273500
C	-3.60440900	1.20182900	0.14374800
C	-5.54733600	0.31261000	0.12453700
C	-4.67580100	-0.72457500	-0.01923100
H	-2.76229600	1.87498400	0.18197400
H	-6.62449600	0.27354600	0.16156600
H	-4.79286700	-1.78868800	-0.12751400
N	-4.86915200	1.51220000	0.22553300
N	-3.42258200	-0.14940000	-0.00665800
C	-2.18781700	-0.86395300	-0.12915100
O	-2.20003700	-2.06101900	-0.25850400
O	-1.18484800	-0.04658500	-0.07735300

Sum of electronic and zero-point Energies: -873.045673;
Sum of electronic and thermal Free Energies: -873.093796.

21

-1 1

C	1.03634500	-0.70746200	-0.02278100

H	0.98605400	-1.79082900	-0.02373500
C	2.22931400	-0.14794200	-0.00643900
C	3.59410700	-0.80837300	0.01333700
C	3.84050800	-1.59972000	1.28890400
H	3.15098300	-2.44473300	1.33249400
H	4.86755400	-1.97121500	1.30771000
H	3.66854400	-0.97018700	2.16298100
C	3.86589900	-1.62888300	-1.23795900
H	3.71690500	-1.01862400	-2.12965900
H	4.89147300	-2.00467700	-1.22473200
H	3.17443400	-2.47239600	-1.27854000
O	4.47894300	0.33374400	0.00913000
H	0.08285700	-0.18430000	-0.03490100
C	3.77424500	1.48116300	0.00408400
O	2.45244800	1.22393300	-0.00272500
O	4.25491300	2.56730400	0.00534400
C	-4.59366100	1.18468900	0.00623300
C	-6.09358300	-0.32861800	0.04891600
C	-4.89033600	-0.98291200	0.01997300
H	-4.04962700	2.11559500	-0.01023400
H	-7.08471600	-0.75593300	0.07630400
H	-4.60653500	-2.02127900	0.01548600
N	-5.90055200	1.03524700	0.04024200
N	-3.93507000	-0.00152200	-0.00743900
C	-2.44438800	-0.20257100	-0.04604500
O	-2.11013100	-1.38744700	-0.05095400
O	-1.80858300	0.85325000	-0.06481200

Sum of electronic and zero-point Energies: -873.117244;
Sum of electronic and thermal Free Energies: -873.168224.

22

-1 1

C	1.58754800	-0.02769600	2.31376400
H	1.70986600	-0.54664100	3.23310800
C	1.41636800	0.55296000	1.27448900
C	1.20300000	1.24426800	-0.02789100
C	0.19638900	2.38623900	0.18268700
H	0.58785900	3.11661100	0.89602400
H	0.02637400	2.87320300	-0.78111200
H	-0.75359100	1.99232400	0.54519500
C	2.54515500	1.80280900	-0.51180100
H	3.24621400	0.98385400	-0.67532600
H	2.37687400	2.31864400	-1.46005900
H	2.96454400	2.50226400	0.21566000

O	0.75516800	0.33369600	-0.99339300
H	-0.25045100	0.10641900	-0.81990900
C	-2.84567000	0.42320300	-0.97707200
C	-2.18589800	-0.82609800	0.62508800
C	-3.54884600	-0.61494100	0.72953100
H	-2.81700600	1.03961600	-1.86774600
H	-1.51434700	-1.40052800	1.24766600
H	-4.23795300	-0.99176300	1.47362600
N	-1.73661400	-0.15723600	-0.47836200
N	-3.96866400	0.18444000	-0.29756100
C	1.90605600	-1.98647700	-0.47123900
O	0.89946500	-2.48621600	-0.20917600
O	2.96461100	-1.58623400	-0.72255700

Sum of electronic and zero-point Energies: -684.509479;
Sum of electronic and thermal Free Energies: -684.555773.

$TS_{22\text{-}23}$

-1 1

C	-2.67747400	-0.70900700	2.17547900
H	-3.12534300	-0.57730200	3.13003400
C	-2.15944300	-0.83073800	1.09527000
C	-1.50168600	-0.98121600	-0.24108100
C	-0.71271500	-2.30784600	-0.21451600
H	-1.36390400	-3.16256400	-0.01026000
H	-0.23569200	-2.43884900	-1.19031100
H	0.06246600	-2.26070000	0.55335300
C	-2.61146700	-1.07515800	-1.30699200
H	-3.17581000	-0.14249700	-1.32318600
H	-2.13111100	-1.21463900	-2.27913900
H	-3.29311200	-1.90890000	-1.11180700
O	-0.66212800	0.07582100	-0.50946300
H	0.73065200	-0.04115400	-0.27170700
C	2.68319800	-1.11393200	-0.29011400
C	2.62171400	0.95874100	0.33733100
C	3.91043100	0.47908100	0.39442000
H	2.33424100	-2.07446200	-0.64114600
H	2.19515700	1.92359400	0.55656600
H	4.80660300	1.00137900	0.69558900
N	1.84376400	-0.07365700	-0.10244100
N	3.94394900	-0.83266000	-0.00325100
C	-1.30153100	2.15797800	-0.23925200
O	-0.23184800	2.60673400	-0.13215500
O	-2.45906200	2.03905700	-0.31230800

Sum of electronic and zero-point Energies: -684.506582;

Sum of electronic and thermal Free Energies: -684.553952.

23

-1 1

C	3.72329100	-0.43443300	-1.66490100
H	4.44523300	-0.32731400	-2.43710600
C	2.89999800	-0.48569500	-0.79173900
C	1.89707200	-0.68733900	0.27856400
C	1.38202200	-2.12792500	0.17526300
H	2.20376000	-2.83731600	0.29059300
H	0.64279900	-2.29532100	0.96198800
H	0.91024400	-2.28206000	-0.79635800
C	2.53363800	-0.46175700	1.65556300
H	2.93480700	0.54651200	1.72243000
H	1.76046000	-0.59945900	2.41592000
H	3.33104200	-1.19122500	1.81905700
O	0.74350500	0.11370700	0.08904600
H	-1.50572900	1.07038800	-0.09801300
C	-2.33824200	-0.91163100	-0.14665500
C	-3.66679700	0.81177500	-0.06801300
C	-4.39233400	-0.35496800	-0.09112000
H	-1.40858200	-1.45718800	-0.18024800
H	-3.96266200	1.84692600	-0.02984800
H	-5.46527300	-0.47392900	-0.07500200
N	-2.35320500	0.43725600	-0.10397600
N	-3.55011800	-1.43622200	-0.14072700
C	0.87261800	1.54571000	0.06785500
O	-0.24341700	2.07883100	-0.07242600
O	1.99610800	2.01125300	0.18720700

Sum of electronic and zero-point Energies: -684.521946;
Sum of electronic and thermal Free Energies: -684.565572.

$TS_{23\text{-}24}$

-1 1

C	0.40718300	-2.01039600	-0.15353200
H	0.55366900	-3.04993500	-0.38188800
C	1.15916700	-1.01899200	-0.03047400
C	2.51543900	-0.38294100	0.01443300
C	3.06850500	-0.41673300	1.44161800
H	3.19816300	-1.44979100	1.77149100
H	4.03010800	0.10213700	1.47368300
H	2.36935700	0.08028300	2.11616400
C	3.45611600	-1.07480800	-0.96354600
H	3.05978000	-0.98964400	-1.97574200

H	4.44196000	-0.60516100	-0.92229500
H	3.54853700	-2.13173100	-0.70638700
O	2.39394100	0.97531300	-0.39378000
H	-1.37044300	-0.90424300	0.02147300
C	-3.47066400	-1.25006100	-0.04037400
C	-2.68607700	0.78968500	0.06724300
C	-4.05861700	0.79429300	0.03002500
H	-3.46291700	-2.32847000	-0.08636400
H	-1.93759700	1.56349600	0.12073500
H	-4.72015700	1.64672400	0.04684900
N	-2.32917300	-0.52784700	0.02197700
N	-4.54601500	-0.48959500	-0.03651000
C	1.13047900	1.48247900	-0.10833500
O	0.93010500	2.66172700	-0.29406800
O	0.33678900	0.57711800	0.32305700

Sum of electronic and zero-point Energies: -684.483081;
Sum of electronic and thermal Free Energies: -684.526107.

24

-1 1

C	0.47174300	1.97678300	0.54282300
H	-0.55809200	1.78846100	0.83601400
C	1.23619200	0.95186800	0.21625100
C	0.91279800	-0.52576200	0.18724700
C	0.37323600	-1.02920200	1.51105600
H	-0.57611200	-0.52412900	1.70446300
H	0.19713600	-2.10538600	1.45512300
H	1.08009500	-0.81428400	2.31485100
C	0.03349600	-0.90843100	-0.99204500
H	0.45403800	-0.51871400	-1.92201800
H	-0.03130800	-1.99665700	-1.05554700
H	-0.97059300	-0.49963300	-0.85614400
O	2.24360500	-1.09468600	-0.03019300
H	0.86428000	2.98427600	0.49613800
C	-2.85940800	1.06848000	-0.46099500
C	-3.09992500	-0.62246700	0.79478100
C	-3.66180300	-0.88907600	-0.44510800
H	-2.57036100	2.05533600	-0.80663400
H	-3.04819000	-1.25586100	1.67196600
H	-4.16157200	-1.78571200	-0.78825300
N	-2.57691200	0.64008300	0.78391500
N	-3.50543500	0.20031400	-1.25217800
C	3.13308800	-0.13835200	-0.28573900
O	4.27901000	-0.30680300	-0.56263900

O	2.55996200	1.08729800	-0.17988600

Sum of electronic and zero-point Energies: -684.535812;
Sum of electronic and thermal Free Energies: -684.577478.

26

-1 1

C	0.39709600	-1.25450700	-0.95899600
H	1.25517100	-0.81987800	-1.45835000
C	-0.67382000	-0.54044200	-0.67439200
C	-1.91785500	-0.92163700	0.10063800
C	-2.82022600	-1.85948400	-0.69324400
H	-2.32522200	-2.82507700	-0.81544900
H	-3.76482000	-2.00413600	-0.16358100
H	-3.02391000	-1.44529600	-1.68262000
C	-1.61366000	-1.44414700	1.49433700
H	-1.03705500	-0.69699900	2.03930200
H	-2.54810300	-1.65691100	2.02019700
H	-1.03389600	-2.36675100	1.41626000
O	-2.59268400	0.35006500	0.21144600
H	0.45981300	-2.27684300	-0.61090300
C	2.83738900	-0.61993600	0.89165700
C	3.72182900	0.00043500	-0.92885600
C	2.90119600	1.01700600	-0.46710800
H	2.56685500	-1.22332400	1.75076300
H	4.33371300	-0.02585500	-1.82110300
H	2.68346100	1.98124800	-0.90580200
N	3.67731700	-1.05032500	-0.05512200
N	2.33389100	0.61503400	0.70765300
C	-1.90327600	1.30478500	-0.43068800
O	-2.22474200	2.44872600	-0.49617000
O	-0.83067100	0.77782100	-1.05786300
O	-0.08945700	1.29602400	1.67851100
H	-0.15719500	2.25141500	1.62589100
H	0.84111600	1.08192300	1.35019400

Sum of electronic and zero-point Energies: -760.94981;
Sum of electronic and thermal Free Energies: -760.995385.

$TS_{26\text{-}27}$

-1 1

C	0.11177400	-1.63324800	-1.03763900
H	1.03857200	-1.41204300	-1.55150900
C	-0.72938600	-0.66398700	-0.70334200
C	-2.02261800	-0.76376100	0.09084300
C	-3.10982700	-1.48415500	-0.70149800

H	-2.84117900	-2.53455800	-0.83489800
H	-4.05833400	-1.42251400	-0.16191700
H	-3.22871500	-1.02230400	-1.68308500
C	-1.82051700	-1.37852000	1.47042600
H	-1.10011400	-0.77370600	2.02115800
H	-2.77476100	-1.39585100	2.00425300
H	-1.45257900	-2.40297000	1.37004300
O	-2.40943300	0.60531100	0.21104200
H	-0.10018100	-2.65165800	-0.73998200
C	2.77904800	-0.59926400	1.03141800
C	3.71806100	-0.06804900	-0.79821200
C	2.64502700	0.77858600	-0.63011100
H	2.52338000	-1.09180700	1.95865000
H	4.42779600	-0.09825500	-1.61194700
H	2.24184600	1.56268600	-1.25048900
N	3.79854900	-0.93960200	0.25758800
N	2.05616300	0.43262000	0.55097300
C	-1.39024700	1.41831800	-0.22175900
O	-1.51643200	2.59880000	-0.38391500
O	-0.55740200	0.63880400	-1.04069300
O	-0.21100600	1.18753700	1.35965100
H	-0.24709500	2.08461900	1.69860000
H	1.05467200	0.82810300	0.95176400

Sum of electronic and zero-point Energies: -760.933764;
Sum of electronic and thermal Free Energies: -760.976511.

27

-1 1

C	-0.46497500	-2.09710700	-0.82160900
H	0.43756900	-2.21671600	-1.40500100
C	-0.96991900	-0.88442000	-0.56678600
C	-2.20644400	-0.58985900	0.28140900
C	-3.44747300	-1.29146300	-0.26103000
H	-3.34308000	-2.37629200	-0.18241400
H	-4.32339600	-0.97548800	0.31206700
H	-3.59346000	-1.02280300	-1.30794000
C	-1.97312500	-0.94414400	1.75252700
H	-1.10294200	-0.40627800	2.12803200
H	-2.85001500	-0.65146200	2.33698900
H	-1.80861300	-2.01892000	1.86417300
O	-2.38820300	0.79880100	0.11391800
H	-0.95352200	-2.97904300	-0.42909200
C	3.18673500	0.10850600	1.17261700
C	3.94220100	-0.56130200	-0.70162400

C	2.65479700	-0.14614100	-0.93279400
H	3.07484500	0.36620700	2.21466800
H	4.64794500	-0.96703100	-1.41003400
H	2.02979600	-0.10988600	-1.80902100
N	4.26929200	-0.39927100	0.62292400
N	2.18666700	0.27916400	0.27760300
C	-1.17788900	1.44263700	-0.30517100
O	-1.28124800	2.47561400	-0.96446500
O	-0.46899100	0.26390100	-1.00999400
O	-0.32562300	1.56095000	0.89425200
H	-0.21195000	2.51385800	0.95626900
H	1.25417700	0.67023100	0.45269300

Sum of electronic and zero-point Energies: -760.942213;
Sum of electronic and thermal Free Energies: -760.985894.

28

-1 1

C	-0.15206300	1.75943700	-1.21689100
H	-1.06557800	1.56850400	-1.76777300
C	0.47983100	0.73431200	-0.61298100
C	1.76854200	0.91640800	0.20096900
C	2.36916800	2.31131400	0.07841200
H	1.68734300	3.06400400	0.47744500
H	3.30215000	2.33725000	0.64388700
H	2.58765800	2.53737300	-0.96593900
C	1.49563700	0.60830100	1.67736500
H	1.04150000	-0.37248900	1.80976400
H	2.43554200	0.64385400	2.23461200
H	0.81373900	1.36178600	2.07833400
O	2.82901900	0.07158800	-0.31119900
H	0.23075100	2.76796900	-1.19477700
C	-3.63487000	-1.33818800	-0.20128700
C	-4.59908700	0.43878900	0.46493800
C	-3.27532300	0.75764300	0.29222800
H	-3.42391300	-2.34988700	-0.51237600
H	-5.40166600	1.08116700	0.79282700
H	-2.71756500	1.67007200	0.42078300
N	-4.81747500	-0.87952800	0.15280000
N	-2.67020100	-0.39217000	-0.13586600
C	2.92090500	-1.28736500	-0.07091600
O	4.02855500	-1.76528800	-0.03977100
O	0.01419000	-0.50445900	-0.62068700
O	1.80641000	-1.92698200	0.07178800
H	0.92051400	-1.30496200	-0.24928700

H	-1.65856900	-0.50554000	-0.35810900

Sum of electronic and zero-point Energies: -760.978258;
Sum of electronic and thermal Free Energies: -761.023663.

$TS_{28\text{-}29}$

-1 1

C	-0.14952400	1.75583200	-1.22845600
H	-1.05575200	1.56078000	-1.78986700
C	0.48552900	0.73294400	-0.62627900
C	1.76346500	0.91469100	0.20342000
C	2.35697400	2.31391600	0.09373000
H	1.66767900	3.06151600	0.48970100
H	3.28412700	2.34136300	0.66858400
H	2.58508600	2.54596400	-0.94730200
C	1.47223200	0.60049900	1.67559300
H	1.02159500	-0.38310900	1.79863800
H	2.40544100	0.63711600	2.24386800
H	0.78286900	1.34991500	2.07155600
O	2.83207100	0.07800300	-0.29878900
H	0.22403900	2.76746500	-1.19407100
C	-3.63622700	-1.34040800	-0.19593900
C	-4.58688300	0.44329900	0.47232800
C	-3.26329800	0.75591100	0.28858500
H	-3.43208400	-2.35396800	-0.50544900
H	-5.38399100	1.09010700	0.80467600
H	-2.70019100	1.66598600	0.41004100
N	-4.81355200	-0.87504800	0.16583600
N	-2.66692900	-0.39822600	-0.14068700
C	2.92029100	-1.28686800	-0.06387400
O	4.03089600	-1.75964400	-0.02638800
O	0.02467700	-0.51029900	-0.65177500
O	1.80573100	-1.92152400	0.06541100
H	0.90217200	-1.28528700	-0.27773800
H	-1.65997800	-0.51612500	-0.37099700

Sum of electronic and zero-point Energies: -760.979539;
Sum of electronic and thermal Free Energies: -761.024661.

29

-1 1

C	3.29836500	-1.81793500	-0.92289300
H	4.21431500	-1.78882900	-1.49929700
C	2.78710300	-0.67240100	-0.45176100
C	1.51986500	-0.59305900	0.40394100
C	0.78151100	-1.92612100	0.48369600

H	1.39926300	-2.69376100	0.95213100
H	-0.11941500	-1.78454900	1.08499700
H	0.49001500	-2.25636300	-0.51517500
C	1.87661200	-0.13439600	1.82438100
H	2.45088300	0.78951600	1.82111200
H	0.95387800	0.02884100	2.38784900
H	2.46021300	-0.91715500	2.31467900
O	0.54735900	0.27750500	-0.20285100
H	2.82204000	-2.77087800	-0.75567500
C	-3.36145400	0.81173900	-0.06559400
C	-4.28364800	-1.11059500	-0.10807700
C	-2.93449700	-1.32907200	-0.23114400
H	-3.14959600	1.86849300	-0.01961400
H	-5.07626200	-1.84277100	-0.08846400
H	-2.35188900	-2.22852500	-0.33766700
N	-4.54359700	0.23306000	-0.00475400
N	-2.36117900	-0.08724300	-0.20116200
C	0.58686700	1.70781600	-0.10284600
O	-0.52493000	2.20265400	-0.21160700
O	3.41151400	0.49239300	-0.66701800
O	1.71302000	2.22104500	0.05264500
H	-1.36967700	0.15387700	-0.26622600
H	2.80962300	1.25673800	-0.38480200

Sum of electronic and zero-point Energies: -760.981913;
Sum of electronic and thermal Free Energies: -761.027459.

$TS_{29\text{-}30}$

-1 1

C	2.70078500	-0.78426000	1.79767300
H	3.50866000	-0.30812700	2.34548400
C	2.38399200	-0.38905300	0.56315800
C	1.28894100	-0.95837500	-0.34020100
C	1.99608900	-1.59407200	-1.55573100
H	2.69077600	-2.38668800	-1.25732200
H	1.23083600	-2.00986700	-2.21559200
H	2.53787900	-0.81843100	-2.09810100
C	0.49191100	-2.04091800	0.40110800
H	-0.00255100	-1.61727900	1.27866700
H	-0.28430500	-2.41452200	-0.27107500
H	1.12222300	-2.88051300	0.70840400
O	0.44903600	0.04946000	-0.79312300
H	2.13852700	-1.55472000	2.30127200
C	-2.55453300	0.32668500	0.96556500
C	-4.19385900	-0.46129500	-0.13624200

C	-3.07691900	-0.59675100	-0.92776600
H	-1.93574500	0.78060100	1.72620200
H	-5.21121500	-0.74611100	-0.36088800
H	-2.94258800	-0.99762300	-1.91938100
N	-3.85811600	0.12205400	1.05759000
N	-2.03356800	-0.08596100	-0.20957600
C	0.61223200	1.98003400	-0.22752300
O	0.58160700	2.51902800	-1.26793000
O	3.06192800	0.61170700	-0.07516200
O	0.63816200	1.91979000	0.94944800
H	-0.95971500	-0.05777100	-0.48834900
H	3.61131300	1.06655000	0.56850000

Sum of electronic and zero-point Energies: -760.943675;
Sum of electronic and thermal Free Energies: -760.987997.

30

-1 1

C	1.32081000	-0.70848600	2.02956600
H	1.42155600	-0.16449400	2.96292500
C	1.84153800	-0.22950800	0.90240800
C	1.72090500	-0.84963200	-0.48430500
C	3.10438100	-0.91143800	-1.13223300
H	3.77876700	-1.54589200	-0.55017600
H	2.99958900	-1.32315900	-2.13852500
H	3.52506500	0.09156200	-1.20269200
C	1.09797000	-2.24591700	-0.43294300
H	0.08028100	-2.19979600	-0.03917000
H	1.04580400	-2.63192000	-1.45332800
H	1.69711100	-2.92862000	0.17596100
O	0.93517900	0.00823500	-1.28386800
H	0.72876700	-1.61102300	2.03221100
C	-2.03186800	-0.27964500	0.98006900
C	-3.58011400	-1.09279600	-0.21547200
C	-2.57609800	-0.64048400	-1.05158900
H	-1.45369800	0.04361100	1.83698800
H	-4.51922600	-1.56276700	-0.47555800
H	-2.50886200	-0.65852900	-2.13064600
N	-3.22965400	-0.85893800	1.08565100
N	-1.57605900	-0.11498100	-0.27932600
C	-0.38681100	2.40126200	-0.25307500
O	-0.71205500	2.64645400	-1.33262300
O	2.52749800	0.96021000	0.86049300
O	-0.04156600	2.27529700	0.84714400
H	-0.00857100	-0.03093900	-0.93739800

H	2.11667700	1.55768500	1.49140600

Sum of electronic and zero-point Energies: -760.955346;
Sum of electronic and thermal Free Energies: -761.002663.

31

-1 1

C	0.84624700	-1.34597000	-0.95513700
H	-0.16753600	-1.53001700	-1.29023400
C	1.17758200	-0.15830100	-0.38690400
C	2.62103900	0.10570300	0.12275100
C	2.81506900	-0.60094400	1.46928000
H	2.75982300	-1.68600600	1.35310100
H	3.78667000	-0.32529300	1.89159600
H	2.03008500	-0.28340600	2.15966800
C	3.69463800	-0.32486500	-0.87131900
H	3.52481600	0.16143500	-1.83336600
H	4.67613300	-0.02415500	-0.49174500
H	3.69192600	-1.40618400	-1.02066900
O	2.75904900	1.50334500	0.32466500
H	1.58166800	-2.12618800	-1.09858700
C	-3.20618400	1.05724700	-0.30916700
C	-4.01945800	-0.78840300	0.36318600
C	-2.65106500	-0.91759800	0.40406700
H	-3.09104900	2.06606000	-0.67633900
H	-4.76838200	-1.51923900	0.62888300
H	-2.00562700	-1.73179600	0.69073400
N	-4.36360300	0.45998400	-0.08767000
N	-2.14304700	0.27362500	-0.03014300
O	0.38047100	0.84290600	-0.15877600
H	1.83240500	1.81238500	0.28045600
H	-1.08774100	0.52591500	-0.11646200

Sum of electronic and zero-point Energies: -572.400945;
Sum of electronic and thermal Free Energies: -572.443536.

$TS_{31\text{-}32}$

-1 1

C	0.58641200	0.73005000	1.47745600
H	0.48912000	1.62961400	2.08182200
C	1.55355800	0.84739200	0.42928100
C	2.07684300	-0.45023400	-0.25198700
C	2.86050800	-1.30650900	0.74451500
H	2.21193800	-1.71667100	1.52061400
H	3.33003000	-2.13285700	0.20375800
H	3.64628800	-0.71164300	1.21643500

C	0.90996700	-1.23401500	-0.85172500
H	0.35589500	-0.60796100	-1.55415800
H	1.30309400	-2.10212500	-1.38861500
H	0.20987600	-1.56782500	-0.08313000
O	2.96227200	-0.06941500	-1.28896400
H	0.63748400	-0.18815400	2.06135300
C	-2.52098400	0.82118600	-0.69871800
C	-3.78019900	-0.71399500	0.05133700
C	-2.66233300	-0.65598000	0.85813800
H	-2.11976300	1.62433200	-1.30172000
H	-4.63379800	-1.37280600	0.12714300
H	-2.38452500	-1.23617300	1.72653000
N	-3.68625900	0.22724700	-0.93699400
N	-1.86040200	0.33579400	0.37074700
O	1.95788700	1.90945400	-0.05729300
H	2.92593000	0.90394200	-1.27280300
H	-0.64884500	0.58935600	0.84677600

Sum of electronic and zero-point Energies: -572.385993;
Sum of electronic and thermal Free Energies: -572.427682.

32

-1 1

C	-0.89733300	1.86736100	0.13121300
H	-1.33608100	2.81709600	0.43412700
C	-1.98057200	0.84009700	-0.00910600
C	-1.57898700	-0.63560800	-0.10716300
C	-0.48436400	-0.83788600	-1.15095500
H	0.44335000	-0.33077400	-0.87418300
H	-0.27295000	-1.90587000	-1.22963600
H	-0.82639200	-0.48044900	-2.12619900
C	-1.10622000	-1.08605600	1.28090400
H	-1.90114400	-0.93138900	2.01624400
H	-0.88329300	-2.15394800	1.22928000
H	-0.20032400	-0.55597600	1.58232400
O	-2.72169700	-1.38699800	-0.48680200
H	-0.40496000	1.98134100	-0.84036100
C	2.43477200	-0.73609600	0.81507400
C	3.13567000	0.24052200	-0.92510700
C	2.47253000	1.16164500	-0.12672400
H	2.23289700	-1.51545100	1.54243300
H	3.62067500	0.39153700	-1.88111300
H	2.30592700	2.21884000	-0.29536500
N	3.11034700	-0.98047000	-0.31681700
N	2.01572800	0.52999700	0.99605000

O	-3.15952700	1.13576300	-0.03860700
H	-3.47756200	-0.79578100	-0.37109300
H	-0.10585500	1.54014500	0.81335100

Sum of electronic and zero-point Energies: -572.399297;
Sum of electronic and thermal Free Energies: -572.439692.

33

-1 1

C	-0.85955500	-2.31854200	0.02626100
H	-0.06228000	-2.92382900	-0.38875000
C	-1.06340100	-1.06788700	-0.46561200
C	-2.28208200	-0.24707700	0.02214800
C	-3.40736500	-0.41023000	-0.99505000
H	-3.74731100	-1.44726000	-0.99592000
H	-4.24266100	0.25073700	-0.74682000
H	-3.02722600	-0.15590400	-1.98534400
C	-2.76533600	-0.56213900	1.43183500
H	-1.94633100	-0.48348100	2.14663000
H	-3.55661500	0.14158600	1.70468400
H	-3.17550000	-1.57232600	1.47212000
O	-1.98890600	1.18210500	-0.05269100
H	-1.46200700	-2.73745700	0.81907800
C	3.14564300	0.28158400	-1.00804300
C	3.76216200	-0.48637600	0.87772300
C	2.45417900	-0.87356300	0.70116300
H	3.11622900	0.78924800	-1.96030300
H	4.41281200	-0.69329300	1.71411600
H	1.76814900	-1.44684700	1.30367800
N	4.19242900	0.23955000	-0.20324700
N	2.07273000	-0.37406100	-0.51533700
C	-0.79228000	1.66163300	0.25472600
O	-0.38303900	2.71417900	-0.15099700
O	-0.35951300	-0.46901200	-1.36598300
O	-0.13750000	0.90255500	1.15503400
H	0.79062700	1.17196400	1.14405600
H	1.07587700	-0.45459800	-0.95094400

Sum of electronic and zero-point Energies: -760.957372;
Sum of electronic and thermal Free Energies: -761.00145.

$TS_{33\text{-}34}$

-1 1

C	-0.40262200	-2.20867700	-0.71443300
H	-0.24323900	-2.71177300	-1.66634100
C	-1.05012200	-0.93727500	-0.84579300

C	-1.83599800	-0.39491900	0.38672200
C	-3.28040700	-0.86881600	0.24429200
H	-3.31673500	-1.95964900	0.25925800
H	-3.88438500	-0.47524100	1.06623400
H	-3.68575000	-0.50830500	-0.70238400
C	-1.26595400	-0.80114900	1.74472700
H	-0.19396800	-0.61620400	1.80097300
H	-1.77447900	-0.22673100	2.52432200
H	-1.45369300	-1.86091100	1.92549900
O	-1.95585900	1.04560600	0.29833200
H	-0.73444900	-2.86238100	0.08819000
C	2.40624600	-0.12232700	-1.01844900
C	3.31813600	0.28537400	0.85939300
C	2.62829900	-0.90017600	0.97808600
H	2.04188700	-0.02758200	-2.03207800
H	3.90308000	0.80433700	1.60501600
H	2.50296900	-1.56119200	1.82256700
N	3.16943300	0.78240800	-0.41156800
N	2.05447800	-1.16287500	-0.23639900
C	-0.88342000	1.80526500	0.05475200
O	-0.97261100	2.93397600	-0.34027700
O	-1.00833200	-0.21992700	-1.84140000
O	0.25066100	1.19232200	0.39369500
H	1.02665000	1.65880700	0.04395100
H	0.92892200	-1.74950800	-0.41802100

Sum of electronic and zero-point Energies: -760.942968;
Sum of electronic and thermal Free Energies: -760.98497.

34

-1 1

C	4.05750300	0.02223000	-0.14543400
H	4.68332200	0.24918900	-1.00706100
C	2.67758600	-0.35163000	-0.63692900
C	1.56621000	-0.67366600	0.39836200
C	1.16185900	-2.13007600	0.17260700
H	2.00380200	-2.80183000	0.36549100
H	0.34309500	-2.38681400	0.84847900
H	0.83660100	-2.25504700	-0.86066800
C	1.98946100	-0.46177700	1.85233600
H	2.25665000	0.57999800	2.02663900
H	1.14345000	-0.71994900	2.49347900
H	2.83383100	-1.10283800	2.12077200
O	0.40577300	0.08639800	0.11477800
H	4.49333000	-0.81242500	0.41336100

C	-3.96064600	0.79920400	0.10265500
C	-2.63873500	-0.89258600	-0.27029300
C	-3.94646000	-1.30717800	-0.19756800
H	-4.26481300	1.82008000	0.27712400
H	-1.70771200	-1.40670100	-0.43802700
H	-4.33609900	-2.30842900	-0.30149900
N	-2.66535700	0.45828400	-0.07508600
N	-4.77365100	-0.23735400	0.03857500
C	0.57824900	1.49783000	0.01648900
O	-0.50633400	2.08830500	-0.09851600
O	2.45215600	-0.50993400	-1.81129600
O	1.73819200	1.91046000	0.06127500
H	-1.82877900	1.09437500	-0.07792600
H	3.98792300	0.88793700	0.51213000

Sum of electronic and zero-point Energies: -760.992863;
Sum of electronic and thermal Free Energies: -761.038063.

$TS_{34\text{-}35}$

-1 1

C	3.50383000	-1.11601100	0.70463300
H	4.48749000	-1.08059300	0.23884300
C	2.45573600	-0.73575900	-0.32345300
C	0.96177400	-0.78089800	0.08332200
C	0.41493400	-2.06436100	-0.57765400
H	0.95786900	-2.95622100	-0.24457000
H	-0.64085100	-2.17871700	-0.32110700
H	0.51381500	-1.96690700	-1.66013900
C	0.75714500	-0.86434400	1.60509700
H	1.16719200	0.02164500	2.09316900
H	-0.31827100	-0.89744700	1.79587200
H	1.20814500	-1.75828500	2.04593800
O	0.31753200	0.33454900	-0.43557600
H	3.31175300	-2.11840600	1.09716400
C	-2.88070000	0.44002900	0.91127800
C	-3.01197200	-0.52162200	-1.01179900
C	-4.24595300	-0.52112000	-0.39746000
H	-2.45048600	0.95688400	1.75854100
H	-2.69416500	-0.90316400	-1.97015600
H	-5.18068200	-0.91984900	-0.76521800
N	-2.13974700	0.10004000	-0.16357500
N	-4.15747500	0.09076500	0.82397200
C	1.23694900	2.16897500	-0.06601300
O	0.51485400	2.87542600	-0.64678800
O	2.77785500	-0.46200000	-1.45302200

O	2.14329200	1.82732500	0.59998800
H	-0.91749200	0.24964600	-0.31706700
H	3.45750700	-0.41597000	1.54141800

Sum of electronic and zero-point Energies: -760.972879;
Sum of electronic and thermal Free Energies: -761.019331.

35

-1 1

C	3.01282400	-2.13852800	0.44174100
H	3.97209400	-2.28648600	-0.05215500
C	2.29593300	-0.96816900	-0.21423000
C	0.77775900	-0.87279400	-0.02808000
C	0.13083200	-1.99167100	-0.87102800
H	0.43626600	-2.99178700	-0.55277400
H	-0.95293700	-1.90523800	-0.76447700
H	0.39003900	-1.84981400	-1.92286100
C	0.42203300	-1.05400600	1.45860500
H	0.90848600	-0.27588300	2.05160000
H	-0.66019200	-0.94546000	1.55821100
H	0.71126700	-2.03688400	1.84031000
O	0.35987500	0.37273900	-0.48913100
H	2.42731100	-3.05773100	0.42388400
C	-2.99357800	0.59741300	0.92190200
C	-3.18771500	-0.18904900	-1.05101200
C	-4.42505400	-0.17570600	-0.43245400
H	-2.54291400	1.02028400	1.81225100
H	-2.91089600	-0.51002800	-2.04617600
H	-5.38205800	-0.49477800	-0.82323300
N	-2.26470100	0.31053800	-0.17456500
N	-4.29761400	0.32845700	0.83090800
C	2.00008700	2.29334800	0.07694000
O	1.86842100	2.81740400	-0.94261500
O	2.92935300	-0.15419500	-0.83996200
O	2.19350400	1.87904500	1.14286100
H	-0.65975400	0.41619000	-0.39226900
H	3.19153900	-1.88033000	1.48975800

Sum of electronic and zero-point Energies: -760.976377;
Sum of electronic and thermal Free Energies: -761.023833.

[BenzTriz]$^{-}$-23

-1 1

C	-2.97720500	0.37877400	2.26360200
H	-3.14206700	0.94135300	3.15005100
C	-2.76326600	-0.26058800	1.26777500

C	-2.49666500	-1.02774500	0.02008900
C	-1.86371900	-2.37500700	0.38623800
H	-2.54909400	-2.96105200	1.00378300
H	-1.63911700	-2.91743500	-0.53467800
H	-0.92376200	-2.22936500	0.91771500
C	-3.82106300	-1.24081200	-0.71877800
H	-4.24525500	-0.27786700	-1.00483800
H	-3.61725400	-1.82127600	-1.62118500
H	-4.53387300	-1.77964000	-0.09027000
O	-1.65981800	-0.28193700	-0.83104700
H	-0.69276400	-0.44798000	-0.59308500
C	-2.28691400	2.26747700	-0.52653000
O	-1.24918900	2.54442600	-0.10179700
O	-3.35019700	2.09673200	-0.95110200
C	2.00714100	0.01279900	-0.08467800
C	3.13060300	-0.84042700	-0.08297600
C	4.42784100	-0.32271000	0.08165500
C	4.55951300	1.04111400	0.24221900
C	3.42666800	1.89636800	0.24237100
C	2.14828700	1.40294100	0.08240000
H	5.28977900	-0.98118300	0.08216700
H	5.54529900	1.47580400	0.37215400
H	3.57650500	2.96295600	0.37404100
H	1.28070500	2.05227400	0.08556200
N	0.92145600	-0.78217600	-0.25901400
N	1.36969200	-2.03164100	-0.35738400
N	2.67702400	-2.11239300	-0.25648200

Sum of electronic and zero-point Energies: -854.112545;
Sum of electronic and thermal Free Energies: -854.162994.

[BenzTriz]$^{-}$-TS$_{23\text{-}24}$

-1 1

C	1.57398000	-2.07575800	-0.29969800
H	1.85976300	-3.07707200	-0.56326200
C	2.17390300	-0.99706100	-0.09738700
C	3.42216800	-0.17812300	0.03565800
C	3.92258100	-0.19938500	1.48170300
H	4.19001700	-1.21806000	1.77051500
H	4.79695500	0.44996300	1.57593000
H	3.13597200	0.15767200	2.14839200
C	4.48808600	-0.67672400	-0.93060100
H	4.12102000	-0.59974400	-1.95435100
H	5.39394100	-0.07454200	-0.82649200
H	4.72205200	-1.72123100	-0.71602300

O	3.11366400	1.16871100	-0.31881600
C	1.78096300	1.46060900	-0.08027500
O	1.39723200	2.59968900	-0.23458700
O	1.11666100	0.42701400	0.27924800
C	-2.11735600	-0.18056800	-0.01550300
C	-3.41642100	-0.71116200	0.03218500
C	-4.54089400	0.12935400	0.04829300
C	-4.31381500	1.48738000	0.01212300
C	-2.99769800	2.01199900	-0.03827200
C	-1.87943600	1.20563300	-0.05084700
H	-5.53950800	-0.28914500	0.08673700
H	-5.15305900	2.17384800	0.02177600
H	-2.86287300	3.08736700	-0.06529800
H	-0.87632800	1.61180000	-0.08247000
N	-1.32731500	-1.28739900	-0.02201300
N	-2.07428000	-2.39142600	0.01354100
N	-3.32576600	-2.08127500	0.04976300
H	-0.29325600	-1.40062600	-0.07552500

Sum of electronic and zero-point Energies: -854.075868;
Sum of electronic and thermal Free Energies: -854.121749.

NO_3^--23

-1 1

C	-0.92629300	2.33292600	-0.75196200
H	-0.30771500	3.12723300	-1.09415000
C	-1.54451900	1.39073300	-0.34221100
C	-2.31694900	0.23756600	0.15476800
C	-2.33324600	0.20863100	1.68553700
H	-2.83790700	1.10162200	2.06091100
H	-2.88431000	-0.67744200	2.01083000
H	-1.31970000	0.17420100	2.07683200
C	-3.74564400	0.31842600	-0.38803900
H	-3.72525800	0.31168500	-1.47781400
H	-4.30933900	-0.54844200	-0.03702000
H	-4.22697900	1.23426900	-0.04112800
O	-1.82253300	-0.99558300	-0.38809400
C	-0.49207200	-1.34455200	-0.30721300
O	-0.12873200	-2.30676200	-0.92938800
O	0.19269500	-0.56923000	0.47242500
H	1.25814100	-0.67521900	0.40554900
N	3.25669300	0.28263400	0.07336500
O	2.60125500	1.23478100	-0.34760300
O	2.64061100	-0.77049300	0.46863200
O	4.48027400	0.29619600	0.13367200

Sum of electronic and zero-point Energies: -739.260121;
Sum of electronic and thermal Free Energies: -739.303426.

NO_3^--TS_{23-24}

-1 1

C	-0.49167800	-1.30659300	-0.39769200
H	-1.03956600	-2.18590400	-0.66314100
C	0.59687300	-0.76975200	-0.16176900
C	2.07183000	-0.73901800	0.07061200
C	2.36271600	-0.94417900	1.56110600
H	1.99234900	-1.91618700	1.89459300
H	3.44157800	-0.88704200	1.72543500
H	1.86857600	-0.16082500	2.13747200
C	2.73783200	-1.81823100	-0.77788700
H	2.53902000	-1.62963500	-1.83329000
H	3.81666900	-1.79588500	-0.60798100
H	2.34925200	-2.80273800	-0.51039400
O	2.59475100	0.50694500	-0.33941900
C	1.67688000	1.56289500	-0.14376100
O	2.09796600	2.68352500	-0.33173400
O	0.53243900	1.14314000	0.20156600
H	-1.62619700	-0.08510000	-0.11398100
N	-3.56026000	-0.00392800	0.02387600
O	-3.58249000	-1.19828300	-0.19317300
O	-2.38659700	0.61838600	0.05811100
O	-4.52439000	0.69379700	0.21721100

Sum of electronic and zero-point Energies: -739.210559;
Sum of electronic and thermal Free Energies: -739.253601.

[Bu_4P][Im]

0 1

P	-0.48153300	0.01028300	-0.50279100
C	-1.06891000	-1.26709200	0.64000200
C	-2.15206000	-2.17349400	0.05173900
H	-1.43100000	-0.74300600	1.53079900
H	-0.17116000	-1.81555300	0.95577200
C	-2.55290100	-3.26865200	1.04108200
H	-3.04165400	-1.59043200	-0.21571600
H	-1.79457400	-2.64618900	-0.87060600
C	-3.62920400	-4.18920600	0.47360000
H	-1.66435000	-3.84725800	1.30980000
H	-2.90931200	-2.80221500	1.96514100
H	-3.90438700	-4.96497900	1.18978900
H	-4.53361000	-3.62825900	0.22330700

H	-3.27979700	-4.68373300	-0.43645800
C	0.39725700	-0.75718900	-1.89691000
C	1.77824600	-1.30415700	-1.52384800
H	0.47403700	0.00064200	-2.68418300
H	-0.25273500	-1.55033200	-2.28234800
C	2.42532300	-2.04646800	-2.69067900
H	2.42277900	-0.47565400	-1.21226500
H	1.70470400	-1.95695700	-0.64747600
C	3.82365800	-2.54207400	-2.33144600
H	1.79340600	-2.89432500	-2.97784500
H	2.47714700	-1.38601900	-3.56398500
H	4.28173500	-3.08183100	-3.16216500
H	4.47573600	-1.70447900	-2.07182100
H	3.78695200	-3.21125000	-1.46864400
C	-1.93158900	0.85438100	-1.21535700
C	-2.80676600	1.53548600	-0.16065700
H	-2.50333500	0.10922300	-1.77821600
H	-1.55619000	1.58442600	-1.93926700
C	-3.99941700	2.25714200	-0.78663600
H	-3.17016500	0.79097400	0.55686700
H	-2.20746700	2.25312300	0.41111500
C	-4.87734300	2.93631900	0.26029900
H	-3.63215800	2.99995300	-1.50271900
H	-4.59295400	1.53773600	-1.36088400
H	-5.72292100	3.44659700	-0.20357500
H	-5.27457600	2.20702000	0.97064800
H	-4.30777600	3.67731300	0.82644900
C	0.57396600	1.22716000	0.31047600
C	0.91961200	2.42754500	-0.57373900
H	1.48422600	0.69852200	0.61833000
H	0.08377300	1.53242500	1.23971700
C	1.91883300	3.34149800	0.13691900
H	1.35972800	2.08775000	-1.52058900
H	0.01954800	3.00070300	-0.82825000
C	2.30772800	4.54276100	-0.71879500
H	1.48466700	3.67392800	1.08489800
H	2.80229700	2.75378100	0.40260200
H	3.01610000	5.18679100	-0.19522300
H	2.77582400	4.22272500	-1.65377600
H	1.43202500	5.14651400	-0.97332800
C	1.31380400	-0.56864000	2.78792100
C	3.17867500	0.33165700	2.36018800
C	3.03782300	-0.80443500	1.57424600
H	0.35233300	-0.76280000	3.25272700

H	4.01263400	1.01795700	2.42090900
H	3.73372400	-1.23482200	0.86501900
N	2.06690500	0.48090900	3.13579900
N	1.82728600	-1.38055400	1.84089900

Sum of electronic and zero-point Energies: -1197.595013;
Sum of electronic and thermal Free Energies: -1197.657583.

[Bu_4P][Im]-23

0 1

C	-3.38742300	-2.79504900	-2.01712800
H	-3.00866700	-3.73904500	-2.32966500
C	-3.78470500	-1.72071000	-1.65481500
C	-4.38596200	-0.43832900	-1.22979700
C	-4.20320800	0.63468200	-2.30707600
H	-4.71983500	0.33107900	-3.21984500
H	-4.64339000	1.56616200	-1.94320200
H	-3.14813700	0.78853500	-2.51864700
C	-5.87644100	-0.67306500	-0.96852900
H	-6.00153300	-1.42091100	-0.18556700
H	-6.32782200	0.26446100	-0.63892700
H	-6.37014500	-1.01752000	-1.87835300
O	-3.87735300	-0.01653500	0.03526200
H	-1.03224500	-1.64312800	-1.24479200
C	0.87464200	-2.61748100	-1.36237300
C	-0.63273200	-3.22856800	0.09931500
C	0.53740500	-3.92088200	0.29105400
H	1.31208300	-2.11535100	-2.21228900
H	-1.58028500	-3.23401700	0.61295700
H	0.74929700	-4.67785000	1.02967300
N	-0.40282200	-2.40487400	-0.96683700
N	1.47829000	-3.52911300	-0.62856900
C	-2.51597800	0.19338900	0.22085600
O	-2.21307100	0.50955800	1.37292500
O	-1.75905400	0.03482000	-0.77239300
P	1.71804400	0.85491000	0.56482600
C	0.75061000	-0.45867500	1.33928000
C	0.54719600	-0.29233300	2.84655300
H	1.23914500	-1.40932000	1.09594000
H	-0.22173500	-0.43704700	0.84070000
C	-0.28883700	-1.44614800	3.39708800
H	1.50727100	-0.23839800	3.37736400
H	0.00367200	0.63970900	3.03401700
C	-0.55220500	-1.29661900	4.89213400
H	-1.23557200	-1.45710300	2.84913800

H	0.21963700	-2.39438900	3.19250800
H	-1.15476800	-2.12371700	5.27181400
H	0.38270600	-1.27521100	5.45964400
H	-1.09353000	-0.36947700	5.09614000
C	1.24522300	1.02408600	-1.17353200
C	1.97465000	2.15377600	-1.90212000
H	0.15388400	1.13946300	-1.17655000
H	1.44598000	0.05823900	-1.64440800
C	1.54586200	2.24368600	-3.36669900
H	1.76810000	3.11180000	-1.41125700
H	3.06050500	2.00219200	-1.85322800
C	2.25871500	3.36967100	-4.10969700
H	1.74802800	1.28627400	-3.85829600
H	0.46233700	2.39098300	-3.40955700
H	1.93831200	3.42166000	-5.15147200
H	2.04927100	4.33737900	-3.64672700
H	3.34168700	3.22142800	-4.09926700
C	3.49097500	0.45368000	0.67512600
C	3.89097600	-0.69570400	-0.25768700
H	3.68413700	0.19110300	1.72146800
H	4.06619600	1.35877300	0.45674500
C	5.32081800	-1.17397700	-0.01140100
H	3.21056300	-1.54581600	-0.13637300
H	3.79597500	-0.36633500	-1.29923200
C	5.70189700	-2.30363700	-0.96457800
H	6.01574600	-0.33423700	-0.12180000
H	5.40673700	-1.51862300	1.02432800
H	6.70762000	-2.67436700	-0.75990800
H	5.00208200	-3.13741700	-0.87022700
H	5.67575300	-1.96185000	-2.00256000
C	1.40569100	2.43592600	1.39801700
C	-0.04219600	2.89529800	1.17812000
H	2.13123700	3.16836100	1.03063400
H	1.61198600	2.27936800	2.46188800
C	-0.45184500	4.00035800	2.14881100
H	-0.15536800	3.24993000	0.14703200
H	-0.73380800	2.05143700	1.29313700
C	-1.89791700	4.42919500	1.91441400
H	-0.34183200	3.62693300	3.17298600
H	0.22293600	4.85888900	2.05197100
H	-2.21193900	5.18602400	2.63554700
H	-2.02097200	4.84825200	0.91224400
H	-2.56569600	3.56879500	2.00134300

Sum of electronic and zero-point Energies: -1656.549714;

Sum of electronic and thermal Free Energies: -1656.625413.

[Bu_4P][Im]-$TS_{23\text{-}24}$

0 1

C	-1.79486800	1.61328300	-2.59033700
H	-1.99499900	2.34524100	-3.35380100
C	-2.54630100	0.94614000	-1.84218500
C	-3.88647000	0.57375700	-1.27980100
C	-4.23203600	1.48176800	-0.09896900
H	-4.31322300	2.51784600	-0.43270100
H	-5.17843900	1.16419500	0.34415700
H	-3.44607300	1.41574400	0.65699500
C	-4.95159800	0.62395200	-2.36467000
H	-4.69402500	-0.06270700	-3.17099200
H	-5.91749400	0.33750800	-1.94415100
H	-5.02180400	1.63501200	-2.76880400
O	-3.82189300	-0.77546900	-0.80013100
H	-0.21583000	0.38503500	-2.69621800
C	1.88820600	-0.01934500	-2.77752000
C	0.44047800	-1.64944500	-2.92645900
C	1.72376000	-2.13392300	-2.98392200
H	2.26899200	0.99018200	-2.71961900
H	-0.52156000	-2.13440900	-2.94687700
H	2.04465100	-3.15808100	-3.09139800
N	0.56286000	-0.29499700	-2.79259900
N	2.62709900	-1.10467700	-2.88213600
C	-2.55623000	-1.11766500	-0.41385200
O	-2.35865800	-2.16698600	0.16562900
O	-1.68633800	-0.22534400	-0.72991400
P	1.27323400	0.16358000	1.19074300
C	1.03041000	-1.39251800	0.30539600
C	0.97926400	-2.63446600	1.19920000
H	1.82943200	-1.46683100	-0.44013400
H	0.08765200	-1.28346300	-0.23697000
C	0.72322200	-3.88141100	0.35362900
H	1.91029000	-2.75346500	1.76872300
H	0.15993100	-2.53877800	1.91981800
C	0.63110400	-5.14076800	1.20946800
H	-0.21351700	-3.72736400	-0.19047000
H	1.51951700	-3.98410500	-0.39074400
H	0.43175800	-6.02126600	0.59614300
H	1.56129100	-5.31752100	1.75713700
H	-0.17930300	-5.05317200	1.93763600
C	0.67932300	1.56204800	0.20746900

C	0.74933400	2.91053200	0.92449300
H	-0.34239500	1.31485300	-0.09789600
H	1.27147200	1.57421300	-0.71085400
C	0.21589600	4.02608700	0.02458800
H	0.15350600	2.87926400	1.84438700
H	1.78048300	3.14128000	1.22171000
C	0.23898100	5.38710400	0.71264500
H	0.81213200	4.05843300	-0.89322500
H	-0.80194100	3.76920000	-0.28566800
H	-0.14252200	6.16891000	0.05389700
H	-0.37799400	5.38064100	1.61508100
H	1.25576100	5.66314400	1.00503200
C	3.04401900	0.38880900	1.55009100
C	3.86498900	0.70689700	0.29410400
H	3.39065500	-0.54106300	2.01461500
H	3.14520300	1.18184500	2.29791800
C	5.36701200	0.71798400	0.57377500
H	3.65432300	-0.02121800	-0.49756500
H	3.56588600	1.68678500	-0.09533100
C	6.16789100	1.05817000	-0.68034100
H	5.58620000	1.43960400	1.36850100
H	5.66801700	-0.26500500	0.95055300
H	7.24095500	1.04202400	-0.48315200
H	5.95670000	0.34261300	-1.47860800
H	5.90939500	2.05455400	-1.04778600
C	0.36257300	0.11608900	2.76051900
C	-1.14618400	-0.00760600	2.51948400
H	0.61323700	1.01468400	3.33251900
H	0.74243700	-0.74408600	3.32186500
C	-1.92673400	-0.31321100	3.79520400
H	-1.51801800	0.92066800	2.07039000
H	-1.34391400	-0.80171400	1.79280300
C	-3.42050200	-0.43590800	3.50273400
H	-1.55488700	-1.25202600	4.22032600
H	-1.74665500	0.46617600	4.54419000
H	-3.98102000	-0.71399900	4.39697800
H	-3.82291800	0.51223900	3.13608600
H	-3.59767600	-1.19332800	2.73435700

Sum of electronic and zero-point Energies: -1656.513825;
Sum of electronic and thermal Free Energies: -1656.589551.

[Bu-DBU][Im]-23

0 1

N	-2.94005200	-0.48528300	0.45532600
N	-1.19784300	1.00534600	0.81946200

C	-0.84144900	0.29584000	2.06360100
H	-0.16064600	-0.52562100	1.81977700
H	-0.27003300	0.98052100	2.68391200
C	-2.10813100	-0.18712100	2.74162500
H	-1.85507400	-0.73200800	3.65142100
H	-2.73064400	0.66828400	3.02127700
C	-2.85880900	-1.09425300	1.78974300
H	-3.88454100	-1.25979700	2.13089800
H	-2.36744700	-2.06546600	1.69160800
C	-2.19762800	0.56094600	0.07968400
C	-2.57303800	1.22532200	-1.22042600
C	-4.04649800	-0.95406900	-0.38482200
C	-3.96705500	1.91089900	-1.19011000
H	-2.52687600	0.44849100	-1.98681600
H	-1.81864800	1.95599500	-1.48846200
C	-5.29468800	-0.07459200	-0.23207200
H	-4.24748800	-1.98388100	-0.08603300
H	-3.70646500	-1.00575700	-1.41722000
C	-4.94204800	1.40981500	-0.12032900
H	-4.41923000	1.80100200	-2.17950500
H	-3.81874200	2.98175000	-1.03311900
H	-5.94048700	-0.25043900	-1.09728100
H	-5.86501900	-0.37296300	0.65256000
H	-5.85694500	2.00441800	-0.17387400
H	-4.51472100	1.60345300	0.86973700
C	-0.34038100	2.14856700	0.42935000
C	0.69194100	1.83393900	-0.65164000
H	0.20023000	2.42922800	1.33201300
H	-0.97763800	2.98846200	0.13912400
C	1.78659300	2.89908600	-0.68624500
H	1.14535100	0.86004300	-0.44684900
H	0.21828800	1.76211800	-1.63820900
C	2.73936500	2.67667600	-1.85641900
H	1.33243300	3.89536200	-0.75720100
H	2.33461700	2.84933700	0.25876800
H	3.57101200	3.38362100	-1.83120900
H	3.14942300	1.66507500	-1.81659700
H	2.22579200	2.79336900	-2.81565000
C	-0.36421900	-1.39259800	-1.60331400
C	-0.61713900	-3.04222200	-0.19645300
C	-1.61100700	-3.05959400	-1.14350900
H	0.08091000	-0.52636700	-2.06897400
H	-0.39319400	-3.69290300	0.63267100
H	-2.41431900	-3.77226500	-1.25276300
N	0.17004600	-1.96711200	-0.50244500
N	-1.44782800	-2.01659500	-2.02085100
C	3.01592000	-1.36798000	-2.06282600
H	2.50456700	-1.74546800	-2.91609000
C	3.57821200	-0.96066700	-1.08194700
C	4.37709800	-0.46652800	0.06229300

C	4.82788800	-1.63382300	0.94612300
H	5.47963900	-2.29658800	0.37329200
H	5.38743400	-1.22764100	1.79199400
H	3.97017500	-2.19227400	1.31233600
C	5.60061600	0.27494600	-0.48395200
H	5.28641500	1.13524000	-1.07514300
H	6.20112800	0.62557800	0.35732200
H	6.19927000	-0.39064200	-1.10761700
O	3.67390600	0.52520800	0.80927300
C	2.46874800	0.20961800	1.44878700
O	2.01548600	1.13235600	2.12042500
O	1.99250600	-0.93181700	1.23181900
H	0.99027000	-1.62496700	0.03445900

Sum of electronic and zero-point Energies: -1303.903175;
Sum of electronic and thermal Free Energies: -1303.964346.

[Bu-DBU][Im]-TS$_{23\text{-}24}$

0 1

N	1.76697700	0.05692200	0.69843100
N	-0.05352400	-1.28252300	-0.08759400
C	-0.15334700	-1.86753000	1.24458300
H	-0.78913700	-1.26910300	1.91811800
H	-0.63554900	-2.84226500	1.12869100
C	1.22552900	-2.02190600	1.84996000
H	1.16239100	-2.49037300	2.83483600
H	1.83909900	-2.64940100	1.19780700
C	1.84150300	-0.64178200	1.96866000
H	2.90036600	-0.72250100	2.23081400
H	1.35386100	-0.09347200	2.79270500
C	0.63989100	-0.00551200	-0.18991100
C	1.16102200	0.19991900	-1.62940300
C	2.67606100	1.17492900	0.49941100
C	2.33366400	-0.71359500	-1.99442600
H	1.44462900	1.24855200	-1.74854100
H	0.35641500	0.02600400	-2.34315900
C	3.75117600	0.90880600	-0.59724000
H	3.16626600	1.36351500	1.45613600
H	2.11044500	2.08550800	0.27070200
C	3.63057700	-0.49705600	-1.18527700
H	2.54282200	-0.53938400	-3.05440100
H	2.00921400	-1.75337800	-1.90481500
H	3.66133600	1.65287900	-1.39492900
H	4.74894700	1.03789400	-0.17051600
H	4.49116600	-0.69263600	-1.83075900
H	3.68081000	-1.22102600	-0.36915700
C	-1.32668700	-1.39696700	-0.81056200

C	-2.60339000	-1.00241300	-0.05159400
H	-1.41896600	-2.44293200	-1.12723300
H	-1.27419600	-0.81076100	-1.72829600
C	-3.79499000	-0.88966100	-0.99903600
H	-2.82643100	-1.75356000	0.71436200
H	-2.47397200	-0.05094200	0.47147100
C	-5.08178900	-0.52925800	-0.26157200
H	-3.58057300	-0.12005700	-1.74905900
H	-3.92568100	-1.83326700	-1.54188300
H	-5.92944700	-0.45521400	-0.94556900
H	-5.32264400	-1.28269300	0.49336200
H	-4.97090300	0.43274300	0.24502500
C	-1.14583700	1.78573300	-0.75645300
C	-1.66619200	2.49047900	1.18319500
C	-0.64227100	1.59767400	1.36266900
H	-1.11174100	1.62798600	-1.82320400
H	-2.18566300	3.06419600	1.93447300
H	-0.12491900	1.26986100	2.24659800
N	-1.97472100	2.60086900	-0.14683800
N	-0.30551200	1.14797000	0.10720000

Sum of electronic and zero-point Energies: -1303.863604;
Sum of electronic and thermal Free Energies: -1303.925557.

[Bmim][Im]-23

0 1

C	-1.78163300	-1.88010100	1.76043400
H	-1.30644800	-2.21558300	2.65153700
C	-2.29222000	-1.51697000	0.73514500
C	-3.04341100	-1.13222500	-0.47944400
C	-3.02722400	-2.27186800	-1.50153200
H	-3.51742400	-3.15057100	-1.07826400
H	-3.57817600	-1.94898500	-2.38787200
H	-2.00664200	-2.52546900	-1.77880200
C	-4.48319400	-0.80760200	-0.07197800
H	-4.49373600	0.03631800	0.61842400
H	-5.04950100	-0.53985400	-0.96553900
H	-4.94387200	-1.67153300	0.40883400
O	-2.56382600	0.08822500	-1.04574700
H	0.38563200	-1.31248400	0.16119500
C	2.30957400	-2.18092500	0.32653700
C	1.47787900	-1.06619400	2.01067000
C	2.74264400	-1.51437600	2.30256300
H	2.34787600	-2.66169200	-0.63941400
H	0.76043300	-0.49443200	2.57609000

H	3.30059700	-1.38241000	3.21634800
N	1.21700900	-1.49985700	0.73929300
N	3.25905200	-2.20878300	1.23830500
C	-1.27152200	0.17883800	-1.55266600
O	-1.05705600	1.23149000	-2.16228700
O	-0.47626400	-0.75981400	-1.31340500
C	2.69644900	1.62689500	0.51020200
C	3.46882300	0.72905400	-0.15239600
C	1.69816200	1.16131200	-1.39926600
H	2.81450500	2.07648500	1.48078700
H	4.37364200	0.22176000	0.13578700
H	0.92310100	1.12276500	-2.15982800
N	2.82813800	0.45924900	-1.34350400
C	3.25879500	-0.49129100	-2.36290500
H	3.77492200	0.02799500	-3.16998600
H	3.92851600	-1.21158400	-1.89666900
H	2.37649600	-1.00424000	-2.74529900
N	1.60397700	1.88815500	-0.28975300
C	0.42722100	2.69563600	0.06680600
C	-0.45868300	1.97580900	1.07890400
H	-0.12598300	2.85637800	-0.85844700
H	0.78686800	3.65310700	0.44977700
C	-1.84413600	2.61502700	1.14160000
H	-0.56331300	0.92648500	0.78169400
H	0.01590300	1.98606800	2.06804100
C	-2.70315100	1.98403600	2.23304200
H	-1.74901700	3.69330600	1.31563900
H	-2.32101900	2.47991900	0.16551200
H	-3.71278700	2.39932900	2.23295100
H	-2.77677200	0.90426100	2.08106400
H	-2.27011900	2.15378500	3.22327200

Sum of electronic and zero-point Energies: -1107.52594;
Sum of electronic and thermal Free Energies: -1107.582352.

[Bmim][Im]-TS23-24

0 1

C	-3.18586200	-1.60176100	0.53010500
H	-3.99011900	-2.10367600	1.04345200
C	-3.08595900	-0.39948600	0.18003200
C	-3.60500400	1.00273400	0.05897400
C	-4.34342300	1.19915100	-1.26374900
H	-5.22153700	0.55185400	-1.29701700
H	-4.65732800	2.24078000	-1.35787600
H	-3.69148500	0.94395100	-2.10091300

C	-4.47869000	1.35335400	1.25320700
H	-3.90891500	1.24985000	2.17662500
H	-4.83310000	2.38171400	1.16093600
H	-5.33766200	0.68158600	1.29017400
O	-2.47284500	1.89212900	0.07891800
H	-1.25825400	-1.90598600	1.00890000
C	0.42642100	-3.06789300	1.66059500
C	0.53298400	-0.88369100	1.59603800
C	1.71088000	-1.41600000	2.05931500
H	0.00512700	-4.05917600	1.57804700
H	0.20519400	0.12894700	1.42866700
H	2.59996200	-0.88885200	2.37068700
N	-0.27917400	-1.95497200	1.34500800
N	1.63879100	-2.78547000	2.08953100
C	-1.35284300	1.28482100	-0.38829800
O	-0.32458000	1.92382500	-0.54279700
O	-1.51968900	0.02897400	-0.61078600
C	2.96416000	-1.20887000	-1.00541300
C	2.15165900	-2.29221700	-1.10329400
C	1.00229500	-0.52280000	-1.72311500
H	3.97893900	-1.11989900	-0.65916500
H	2.31829000	-3.32285600	-0.84198600
H	0.19219200	0.11789200	-2.02221900
N	0.93119400	-1.84061800	-1.55308000
C	-0.27443400	-2.64521900	-1.76034400
H	-0.38260300	-2.88164600	-2.81873200
H	-0.16814700	-3.56115900	-1.18279600
H	-1.13662100	-2.08596600	-1.39265700
N	2.22688900	-0.11556800	-1.40584300
C	2.63821900	1.29286300	-1.33126700
C	2.80001400	1.74990300	0.11186500
H	1.84837000	1.87063600	-1.81166800
H	3.56475900	1.40208400	-1.90005300
C	3.07470500	3.24955100	0.18194200
H	1.87099300	1.52580800	0.64049200
H	3.60974300	1.19143100	0.59591600
C	3.23591800	3.72927800	1.62161300
H	3.97534000	3.49190400	-0.39388700
H	2.23946600	3.77628600	-0.29001100
H	3.41972400	4.80408900	1.66318900
H	2.33188100	3.51980200	2.19807200
H	4.07256500	3.22526100	2.11258200

Sum of electronic and zero-point Energies: -1107.48356;
Sum of electronic and thermal Free Energies: -1107.540898.

[Bu-DBU][Im]

0 1

N	1.76697700	0.05692200	0.69843100
N	-0.05352400	-1.28252300	-0.08759400
C	-0.15334700	-1.86753000	1.24458300
H	-0.78913700	-1.26910300	1.91811800
H	-0.63554900	-2.84226500	1.12869100
C	1.22552900	-2.02190600	1.84996000
H	1.16239100	-2.49037300	2.83483600
H	1.83909900	-2.64940100	1.19780700
C	1.84150300	-0.64178200	1.96866000
H	2.90036600	-0.72250100	2.23081400
H	1.35386100	-0.09347200	2.79270500
C	0.63989100	-0.00551200	-0.18991100
C	1.16102200	0.19991900	-1.62940300
C	2.67606100	1.17492900	0.49941100
C	2.33366400	-0.71359500	-1.99442600
H	1.44462900	1.24855200	-1.74854100
H	0.35641500	0.02600400	-2.34315900
C	3.75117600	0.90880600	-0.59724000
H	3.16626600	1.36351500	1.45613600
H	2.11044500	2.08550800	0.27070200
C	3.63057700	-0.49705600	-1.18527700
H	2.54282200	-0.53938400	-3.05440100
H	2.00921400	-1.75337800	-1.90481500
H	3.66133600	1.65287900	-1.39492900
H	4.74894700	1.03789400	-0.17051600
H	4.49116600	-0.69263600	-1.83075900
H	3.68081000	-1.22102600	-0.36915700
C	-1.32668700	-1.39696700	-0.81056200
C	-2.60339000	-1.00241300	-0.05159400
H	-1.41896600	-2.44293200	-1.12723300
H	-1.27419600	-0.81076100	-1.72829600
C	-3.79499000	-0.88966100	-0.99903600
H	-2.82643100	-1.75356000	0.71436200
H	-2.47397200	-0.05094200	0.47147100
C	-5.08178900	-0.52925800	-0.26157200
H	-3.58057300	-0.12005700	-1.74905900
H	-3.92568100	-1.83326700	-1.54188300
H	-5.92944700	-0.45521400	-0.94556900
H	-5.32264400	-1.28269300	0.49336200
H	-4.97090300	0.43274300	0.24502500
C	-1.14583700	1.78573300	-0.75645300

C	-1.66619200	2.49047900	1.18319500
C	-0.64227100	1.59767400	1.36266900
H	-1.11174100	1.62798600	-1.82320400
H	-2.18566300	3.06419600	1.93447300
H	-0.12491900	1.26986100	2.24659800
N	-1.97472100	2.60086900	-0.14683800
N	-0.30551200	1.14797000	0.10720000

Sum of electronic and zero-point Energies: -844.952315;
Sum of electronic and thermal Free Energies: -845.001446.

[Bmim][Im]

0 1

C	-0.82082200	2.97394400	0.03893400
C	0.51909000	3.11119100	-0.13614200
C	0.06686700	0.95027000	-0.06467800
H	-1.60118500	3.70965900	0.13203600
H	1.13250800	3.99124000	-0.22581800
H	0.24881900	-0.15287100	-0.02874900
N	1.04794400	1.84148900	-0.19852800
C	2.46655100	1.48572700	-0.33821800
H	2.54026800	0.48070600	-0.75883100
H	2.93433600	2.20977600	-1.00346800
H	2.94599900	1.48994300	0.63934200
N	-1.07978000	1.61924800	0.07995700
C	-2.39345400	0.99665600	0.30539500
C	-2.40984700	-0.47094700	-0.09823100
H	-3.12156600	1.56609100	-0.27696900
H	-2.64006300	1.10906200	1.36444100
C	-3.78584900	-1.09052600	0.14047200
H	-2.14186900	-0.55720900	-1.15683500
H	-1.65254900	-1.03111000	0.45996600
C	-3.81865200	-2.55894700	-0.27528700
H	-4.04387700	-1.00281200	1.20117800
H	-4.54574400	-0.53006800	-0.41516600
H	-4.79892600	-3.00104600	-0.09049000
H	-3.59502800	-2.66639600	-1.33927600
H	-3.07422000	-3.13451800	0.27892000
C	2.07737200	-1.38401700	1.15596700
C	1.93153900	-1.96976800	-0.88753100
C	3.26650700	-1.89857700	-0.51802500
H	1.78852700	-1.09512400	2.16070100
H	1.49419800	-2.25571400	-1.83431200
H	4.14646100	-2.11833100	-1.10654500
N	1.16200400	-1.63964100	0.19556300

N	3.35384700	-1.51842600	0.7892850

Sum of electronic and zero-point Energies: -648.572715;
Sum of electronic and thermal Free Energies: -648.617775.