

## Supporting Material

### **Asymmetry in the *N*-Inversion of Heteroarene Imines: Pyrimidin-4(3*H*)-Imine, Pyridin-2(1*H*)-Imine, and 1*H*- Purine-6(9*H*)-Imine**

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## **CARTESIAN COORDINATES OF STATIONARY STRUCTURES**

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# CARTESIAN COORDINATES OF STATIONARY STRUCTURES

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## Coordinates in Angstrom & Energies in Hartree

### (E)-Isomer of Pyrimidin-4(3H)-Imine

#### MP2

MP2(full)/6-31G\* -318.722047

C	1.22979100	0.27112000	0.00000000
C	1.19734300	-1.08803000	0.00000000
C	0.00000000	1.04000700	0.00000000
N	-0.21909400	2.31115300	0.00000000
N	0.03943800	-1.84947100	0.00000000
C	-1.06247300	-1.15536900	0.00000000
N	-1.12279200	0.19976700	0.00000000
H	-2.02103100	-1.66983700	0.00000000
H	-2.01934800	0.67995900	0.00000000
H	2.17677400	0.80217900	0.00000000
H	2.12086400	-1.66128400	0.00000000
H	0.67190800	2.81247300	0.00000000

#### CC-L1

CCSD/6-31G\* -318.725385

C	1.23807700	0.26415000	0.00000000
C	1.19558500	-1.09024400	0.00000000
C	0.00000000	1.04226300	0.00000000
N	-0.19963400	2.31097200	0.00000000
N	0.02403000	-1.85044000	0.00000000
C	-1.06838500	-1.15333400	0.00000000
N	-1.12940200	0.20776900	0.00000000
H	-2.03018300	-1.66507900	0.00000000
H	-2.02496800	0.68571800	0.00000000
H	2.18637500	0.79648100	0.00000000
H	2.11415500	-1.67424400	0.00000000
H	0.69799600	2.80200700	0.00000000

#### CC-L2

CCSD/6-31+G\*\* -318.788523

C	1.23842100	0.26324300	0.00000000
C	1.19497200	-1.09304400	0.00000000
C	0.00000000	1.04017000	0.00000000
N	-0.19049100	2.31308700	0.00000000
N	0.02140100	-1.85089800	0.00000000
C	-1.07188500	-1.15206600	0.00000000

N	-1.13192900	0.21058900	0.00000000
H	-2.02891800	-1.65914000	0.00000000
H	-2.02571900	0.68112500	0.00000000
H	2.18119200	0.79329600	0.00000000
H	2.10826700	-1.67355200	0.00000000
H	0.70326100	2.79900800	0.00000000

### **(Z)-Isomer of Pyrimidin-4(3H)-Imine**

#### **MP2**

MP2(full)/6-31G\* -318.717093

C	1.22922400	0.27662000	0.00000000
C	1.21120100	-1.08012700	0.00000000
C	0.00000000	1.04273100	0.00000000
N	-0.01248500	2.33237800	0.00000000
N	0.05287600	-1.84979100	0.00000000
C	-1.05146400	-1.16908100	0.00000000
N	-1.12672300	0.19611500	0.00000000
H	-2.00705400	-1.68978400	0.00000000
H	-2.04539000	0.62968300	0.00000000
H	-0.97059100	2.69941600	0.00000000
H	2.15680400	0.83778800	0.00000000
H	2.13678800	-1.64887300	0.00000000

#### **CC-L1**

CCSD/6-31G\* -318.720709

C	1.23994900	0.27296700	0.00000000
C	1.21497500	-1.07897000	0.00000000
C	0.00000000	1.04463000	0.00000000
N	-0.01266200	2.32882200	0.00000000
N	0.04415300	-1.85037200	0.00000000
C	-1.05194400	-1.16927500	0.00000000
N	-1.13055600	0.20198500	0.00000000
H	-2.00990100	-1.68875800	0.00000000
H	-2.04812500	0.63404100	0.00000000
H	-0.97142000	2.69584900	0.00000000
H	2.16812000	0.83616300	0.00000000
H	2.13690500	-1.65645500	0.00000000

#### **CC-L2**

CCSD/6-31+G\*\* -318.783723

C	1.24163000	0.27529400	0.00000000
C	1.21741600	-1.07881300	0.00000000
C	0.00000000	1.04304500	0.00000000
N	-0.01870600	2.32977700	0.00000000

N	0.04680500	-1.85081500	0.00000000
C	-1.05171400	-1.17018200	0.00000000
N	-1.13152700	0.20178100	0.00000000
H	-2.00416300	-1.68655600	0.00000000
H	-2.04552000	0.62928100	0.00000000
H	-0.97214200	2.69369700	0.00000000
H	2.16647800	0.83323600	0.00000000
H	2.13536000	-1.65091700	0.00000000

## ITS(PMI) - Inversion Transition State Structure

### MP2

MP2(full)/6-31G\* -318.678401

C	0.19752200	1.24109800	0.02116500
C	-1.16279500	1.13552500	0.00312400
C	1.05710200	0.07148700	0.02008900
N	2.30943600	0.01024700	-0.11081200
N	-1.85979000	-0.05483900	-0.01753100
C	-1.11115700	-1.12348400	-0.00601800
N	0.24504700	-1.10523700	0.03663800
H	-1.57974600	-2.10571600	-0.02777600
H	0.76881600	-1.97764700	0.01699200
H	3.16524800	-0.05486800	0.39818800
H	0.68309900	2.21117700	0.02256600
H	-1.78429500	2.02811000	0.00180500

### CC-L1

CCSD/6-31G\* -318.679135

C	0.19515500	1.25042800	0.02171700
C	-1.15786400	1.14260200	0.00226400
C	1.05644800	0.06393200	0.01868500
N	2.30212100	0.01063900	-0.09530400
N	-1.86105100	-0.06005700	-0.01976200
C	-1.11454700	-1.12012200	-0.00632900
N	0.24900400	-1.11245400	0.03790900
H	-1.58324900	-2.10406700	-0.02593100
H	0.76269800	-1.98805900	0.01804100
H	3.21192300	-0.04671000	0.30226000
H	0.68838200	2.21838100	0.02653900
H	-1.78542800	2.03252300	0.00117300

### CC-L2

CCSD/6-31+G\*\* -318.745161

C	0.19606700	1.24983400	0.02659200
C	-1.16020300	1.14212500	0.00237500

C	1.04951200	0.06329300	0.02379100
N	2.30548300	0.01326100	-0.11552700
N	-1.85950200	-0.06068500	-0.02399800
C	-1.11157200	-1.12224800	-0.00777600
N	0.25296000	-1.11095100	0.04529900
H	-1.57426500	-2.10171400	-0.02926600
H	0.76352800	-1.98301000	0.01829600
H	3.17106800	-0.04411800	0.37044200
H	0.68768300	2.21207800	0.03016900
H	-1.78343300	2.02736200	0.00004600

## SOSP (PMI) - In-Plane N-Inversion

### MP2

MP2(full)/6-31G\* -318.677034

H	0.75641000	-1.98942400	0.00009300
N	0.24201200	-1.11253600	0.00009900
C	-1.11581400	-1.12031100	-0.00001300
H	-1.58671500	-2.10214700	-0.00003600
N	-1.86368000	-0.05360000	-0.00007500
C	-1.16000000	1.13906600	-0.00001700
H	-1.78000200	2.03266300	-0.00006800
C	0.19663400	1.24502100	0.00009600
H	0.68191100	2.21536600	0.00013600
C	1.06037700	0.06893600	0.00003600
N	2.30051200	0.00740800	-0.00014000
H	3.28931000	-0.04164100	0.00006800

### CC-L1

CCSD/6-31G\* -318.678753

H	-2.03796700	0.63432800	0.00000000
N	-1.13075900	0.17980700	0.00000000
C	-1.05058600	-1.18202000	0.00000000
H	-2.00426100	-1.71062300	0.00000000
N	0.05108100	-1.86397100	0.00000000
C	1.21134000	-1.08642200	0.00000000
H	2.13733400	-1.65949600	0.00000000
C	1.23925800	0.26858900	0.00000000
H	2.17659800	0.81811900	0.00000000
C	0.00000000	1.06143600	0.00000000
N	-0.12505100	2.29423000	0.00000000
H	-0.23867700	3.27771600	0.00000000

### CC-L2

CCSD/6-31+G\*\* -318.743961

H	-2.03611100	0.63250100	0.00000000
N	-1.13172200	0.18322900	0.00000000
C	-1.05312200	-1.18024200	0.00000000
H	-2.00263900	-1.70281000	0.00000000
N	0.04926800	-1.86398900	0.00000000
C	1.21136800	-1.08912700	0.00000000
H	2.13220100	-1.65835900	0.00000000
C	1.24008700	0.26805400	0.00000000
H	2.17247200	0.81452300	0.00000000
C	0.00000000	1.05655000	0.00000000
N	-0.12108100	2.29580200	0.00000000
H	-0.23117200	3.27743900	0.00000000

**(E)-Isomer of Pyridin-2(1H)-Imine**

**MP2**

MP2(full)/6-31G\* -302.688281

C	1.23972700	0.29018900	0.00000000
C	1.25312500	-1.07364100	0.00000000
C	0.00000000	1.04572900	0.00000000
N	-0.20496900	2.32530600	0.00000000
C	-1.13373600	-1.13369400	0.00000000
N	-1.13510000	0.22907200	0.00000000
H	-2.11027100	-1.60692000	0.00000000
H	-2.01027700	0.74509200	0.00000000
H	2.16860500	0.85410400	0.00000000
H	2.20609300	-1.59765200	0.00000000
C	0.03987800	-1.82525000	0.00000000
H	0.03881400	-2.90805400	0.00000000
H	0.69355400	2.81278000	0.00000000

**CC-L1**

CCSD/6-31G\* -302.695850

C	1.24899500	0.28047800	0.00000000
C	1.25141700	-1.07714700	0.00000000
C	0.00000000	1.04743000	0.00000000
N	-0.17758100	2.32473400	0.00000000
C	-1.14317100	-1.12985600	0.00000000
N	-1.14307600	0.24231500	0.00000000
H	-2.12416400	-1.59758600	0.00000000
H	-2.01651500	0.75719300	0.00000000
H	2.17935800	0.84521300	0.00000000
H	2.19968700	-1.61331400	0.00000000
C	0.01940300	-1.82831900	0.00000000
H	0.01641800	-2.91307300	0.00000000
H	0.72994900	2.79671700	0.00000000

**CC-L2**

CCSD/6-31+G\*\* -302.766813

C	1.24939400	0.27972600	0.00000000
C	1.25049400	-1.08001200	0.00000000
C	0.00000000	1.04493500	0.00000000
N	-0.16884500	2.32687000	0.00000000
C	-1.14611500	-1.12809800	0.00000000
N	-1.14525800	0.24485100	0.00000000
H	-2.12183700	-1.59304800	0.00000000
H	-2.01690500	0.75320100	0.00000000
H	2.17407200	0.84213800	0.00000000
H	2.19353400	-1.61304100	0.00000000
C	0.01717900	-1.82952000	0.00000000
H	0.01010800	-2.90845000	0.00000000
H	0.73403600	2.79496600	0.00000000

**(Z)-Isomer of Pyridin-2(1H)-Imine****MP2**

MP2(full)/6-31G\* -302.683717

C	1.23995000	0.29596600	0.00000000
C	1.26665700	-1.06490200	0.00000000
C	0.00000000	1.04771800	0.00000000
N	0.00081500	2.34338900	0.00000000
C	-1.12330600	-1.14758100	0.00000000
N	-1.13861200	0.22562300	0.00000000
H	-2.09592000	-1.62875000	0.00000000
H	-2.03772500	0.69559100	0.00000000
H	-0.95597200	2.71512700	0.00000000
H	2.14736000	0.89036700	0.00000000
H	2.22251300	-1.58262500	0.00000000
C	0.05411900	-1.82526800	0.00000000
H	0.05980400	-2.90840000	0.00000000

**CC-L1**

CCSD/6-31G\* -302.691781

C	1.25172000	0.28962000	0.00000000
C	1.27092900	-1.06503900	0.00000000
C	0.00000000	1.04907900	0.00000000
N	0.00770800	2.33848100	0.00000000
C	-1.12733500	-1.14640100	0.00000000
N	-1.14413600	0.23647100	0.00000000
H	-2.10360400	-1.62376700	0.00000000
H	-2.04126400	0.70662700	0.00000000

H	-0.94755300	2.71569400	0.00000000
H	2.15964800	0.88604700	0.00000000
H	2.22317700	-1.59319000	0.00000000
C	0.04087200	-1.82779000	0.00000000
H	0.04747900	-2.91289000	0.00000000

### CC-L2

CCSD/6-31+G\*\* -302.762516

C	1.25352000	0.29214400	0.00000000
C	1.27296800	-1.06487400	0.00000000
C	0.00000000	1.04714900	0.00000000
N	0.00100400	2.33971400	0.00000000
C	-1.12658900	-1.14700100	0.00000000
N	-1.14488700	0.23589600	0.00000000
H	-2.09692700	-1.62312000	0.00000000
H	-2.03825000	0.70243200	0.00000000
H	-0.94864600	2.71418600	0.00000000
H	2.15839100	0.88286800	0.00000000
H	2.22106300	-1.58809000	0.00000000
C	0.04388600	-1.82896400	0.00000000
H	0.04884100	-2.90826600	0.00000000

## ITS (PYI) - Inversion Transition State Structure

### MP2

MP2(full)/6-31G\* -302.646233

C	0.22118000	1.25026100	0.02178400
C	-1.14882500	1.19557000	0.00456500
C	1.06027700	0.06937900	0.01994600
N	2.32806800	0.01213600	-0.13089700
C	-1.08641300	-1.19071100	-0.00377100
N	0.27224600	-1.11030900	0.03715700
H	-1.51317500	-2.18875700	-0.02559200
H	0.83585900	-1.95706700	0.00776300
H	3.09155600	-0.05608600	0.51520100
H	0.74525600	2.20069700	0.02031600
H	-1.72154500	2.12061300	0.00189900
C	-1.83367800	-0.04631300	-0.01264200
H	-2.91539900	-0.10131100	-0.04270200

### CC-L1

CCSD/6-31G\* -302.650522

C	0.21893600	1.25882100	0.02364000
C	-1.14276500	1.20408400	0.00470300
C	1.05727500	0.05903100	0.01965000

N	2.32204300	0.01386400	-0.12875900
C	-1.09027600	-1.18821700	-0.00441100
N	0.27981100	-1.11686700	0.04159700
H	-1.51578300	-2.18830300	-0.02551900
H	0.83422500	-1.96671400	0.00924700
H	3.11538700	-0.04299000	0.47813100
H	0.75299300	2.20533400	0.02436800
H	-1.72069900	2.12792100	0.00290900
C	-1.83634500	-0.05238200	-0.01544800
H	-2.92005800	-0.10223700	-0.04780100

## CC-L2

CCSD/6-31+G\*\* -302.725082

C	0.22012700	1.25862500	0.02278700
C	-1.14467400	1.20359400	0.00459900
C	1.05017600	0.05825400	0.02358100
N	2.32560100	0.01631300	-0.13377500
C	-1.08739900	-1.18918900	-0.00403600
N	0.28266900	-1.11629600	0.03998300
H	-1.50877000	-2.18449400	-0.02441100
H	0.83240800	-1.96373200	0.00351100
H	3.08895500	-0.04234500	0.50869400
H	0.75182300	2.19962800	0.02184400
H	-1.71820700	2.12292400	0.00133100
C	-1.83653600	-0.05235500	-0.01490800
H	-2.91427300	-0.10566400	-0.04656800

## SOSP (PYI) - In-Plane N-Inversion

### MP2

MP2(full)/6-31G\* -302.642297

H	-2.02476000	0.69593100	0.00000000
N	-1.13835300	0.20044300	0.00000000
C	-1.11874300	-1.16398600	0.00000000
H	-2.08685400	-1.65620900	0.00000000
C	1.26724400	-1.06978400	0.00000000
H	2.22680900	-1.58291600	0.00000000
C	1.24080900	0.29488400	0.00000000
H	2.15812600	0.87529700	0.00000000
C	0.00000000	1.06703600	0.00000000
N	-0.12511600	2.30759600	0.00000000
H	-0.23839000	3.29036100	0.00000000
C	0.06561100	-1.83779400	0.00000000
H	0.07982400	-2.92086800	0.00000000

### CC-L1

CCSD/6-31G\* -302.6483469

H	-2.02925900	0.71009100	0.00000000
N	-1.14452500	0.21585000	0.00000000
C	-1.12682800	-1.15842600	0.00000000
H	-2.10047600	-1.64299500	0.00000000
C	1.26725400	-1.07412200	0.00000000
H	2.22147600	-1.60076800	0.00000000
C	1.25139300	0.28355200	0.00000000
H	2.16924000	0.86633100	0.00000000
C	0.00000000	1.06568100	0.00000000
N	-0.10391700	2.30519700	0.00000000
H	-0.19869800	3.28975200	0.00000000
C	0.04500200	-1.84067700	0.00000000
H	0.05588700	-2.92578100	0.00000000

### CC-L2

CCSD/6-31+G\*\* -302.7216429

H	-2.02724900	0.70828000	0.00000000
N	-1.14519900	0.21886200	0.00000000
C	-1.12867300	-1.15613700	0.00000000
H	-2.09774200	-1.63629000	0.00000000
C	1.26687700	-1.07673900	0.00000000
H	2.21609500	-1.59966000	0.00000000
C	1.25221700	0.28328800	0.00000000
H	2.16502800	0.86288300	0.00000000
C	0.00000000	1.06045100	0.00000000
N	-0.10035400	2.30695200	0.00000000
H	-0.19231800	3.28972600	0.00000000
C	0.04371200	-1.84164400	0.00000000
H	0.05025200	-2.92095200	0.00000000

### (E)-Isomer of 1H-Purine-6(9H)-Imine

#### MP2

MP2(full)/6-31G\* -465.971644

C	-2.35364800	0.62487900	0.00000700
N	-1.29079100	1.41990900	0.00000100
C	-0.23007000	0.55045300	0.00000100
C	-0.65120300	-0.77209400	0.00000000
N	-2.02007700	-0.70287200	-0.00000800
C	1.18261800	0.84763900	-0.00000200
N	1.84295400	1.95013000	-0.00000400
N	0.10823600	-1.91301200	-0.00000100
C	1.38271100	-1.62315000	0.00000200

N	1.90907000	-0.36503900	0.00000400
H	-3.38251100	0.95930100	0.00000900
H	-2.64859800	-1.49812100	-0.00000700
H	2.10915300	-2.43185200	0.00000200
H	2.91911300	-0.24553900	0.00000100
H	1.17464400	2.72605100	-0.00000300

### CC-L1

CCSD/6-31G\* -465.955358

C	2.36053700	0.61329700	0.00002300
N	1.31471600	1.40956700	-0.00001000
C	0.23566500	0.54578500	-0.00000200
C	0.64570000	-0.76952500	-0.00000100
N	2.01657000	-0.71857100	-0.00001400
C	-1.18277000	0.85589800	-0.00000100
N	-1.82584500	1.96241700	-0.00000200
N	-0.12836800	-1.91197100	0.00000100
C	-1.39501000	-1.61491400	0.00000500
N	-1.92118600	-0.35332200	0.00000200
H	3.39408000	0.93815600	0.00003400
H	2.63719700	-1.51763600	-0.00002800
H	-2.12621500	-2.42145300	0.00000500
H	-2.92914300	-0.23267100	0.00000400
H	-1.15186200	2.73351200	-0.00000400

### CC-L2

CCSD/6-31+G\*\* -466.027965

C	2.36373900	0.61332500	0.00001400
N	1.31628500	1.40987500	-0.00000900
C	0.23531200	0.54679800	-0.00000400
C	0.64671000	-0.76928400	0.00000000
N	2.01836600	-0.71971300	-0.00000700
C	-1.18386800	0.85433100	0.00000000
N	-1.82610200	1.96402400	0.00000200
N	-0.12837000	-1.91156600	0.00000100
C	-1.39700200	-1.61595800	0.00000300
N	-1.92395900	-0.35346100	-0.00000100
H	3.39168300	0.93589700	0.00002300
H	2.63805200	-1.51313800	-0.00001600
H	-2.12402600	-2.41789500	0.00000300
H	-2.92765400	-0.23928100	0.00000200
H	-1.16093100	2.73503700	0.00000000

**(Z)-Isomer of 1H-Purine-6(9H)-Imine**

## MP2

MP2(full)/6-31G\* -465.9605124

C	-1.93514200	1.48868300	0.00000000
N	-0.65015600	1.81646300	0.00000000
C	0.00000000	0.60887700	0.00000000
C	-0.90050200	-0.45014700	0.00000000
N	-2.13887100	0.13532600	0.00000000
C	1.41972800	0.33702300	0.00000000
N	2.34701500	1.22620000	0.00000000
N	-0.64958300	-1.79846600	0.00000000
C	0.63171900	-2.03381400	0.00000000
N	1.61223700	-1.07528800	0.00000000
H	-2.75638100	2.19313100	0.00000000
H	-3.02265500	-0.36050200	0.00000000
H	0.98612800	-3.06183400	0.00000000
H	2.57557100	-1.39806500	0.00000000
H	3.27802000	0.79390000	0.00000000

## CC-L1

CCSD/6-31G\* -465.944416

C	-1.92652100	1.50945700	0.00000000
N	-0.65189300	1.82655300	0.00000000
C	0.00000000	0.60786500	0.00000000
C	-0.90181700	-0.43554400	0.00000000
N	-2.14094700	0.15101700	0.00000000
C	1.42622100	0.32478500	0.00000000
N	2.35974200	1.20032000	0.00000000
N	-0.65600500	-1.79527700	0.00000000
C	0.61695700	-2.03840400	0.00000000
N	1.61236600	-1.09021800	0.00000000
H	-2.74577700	2.21854800	0.00000000
H	-3.02593800	-0.33879600	0.00000000
H	0.96281300	-3.07096100	0.00000000
H	2.57061200	-1.42254800	0.00000000
H	3.28640500	0.75804100	0.00000000

## CC-L2

CCSD/6-31+G\*\* 466.017008

C	-1.93073900	1.51025600	0.00000000
N	-0.65494300	1.82800400	0.00000000
C	0.00000000	0.60963700	0.00000000
C	-0.90268700	-0.43494300	0.00000000
N	-2.14323000	0.14966600	0.00000000
C	1.42559200	0.32444100	0.00000000
N	2.36424600	1.19769100	0.00000000
N	-0.65488700	-1.79484000	0.00000000
C	0.61953800	-2.03930500	0.00000000

N	1.61506600	-1.09028800	0.00000000
H	-2.74655200	2.21406200	0.00000000
H	-3.02474800	-0.33608800	0.00000000
H	0.96419200	-3.06573000	0.00000000
H	2.56806800	-1.42187700	0.00000000
H	3.28505900	0.75748800	0.00000000

## ITS (PUI) - Inversion Transition State Structure

### MP2

MP2(full)/6-31G\* -465.924304

C	2.33506200	-0.70812900	0.00879700
N	1.25007200	-1.46802700	0.01636000
C	0.21177300	-0.56775800	0.00502900
C	0.68277400	0.74554800	-0.00916000
N	2.04882800	0.63090300	-0.00532800
C	-1.21281700	-0.83389700	0.01306900
N	-1.84452000	-1.90513900	-0.09959100
N	-0.01733300	1.91795300	-0.01614400
C	-1.30594100	1.69298800	0.00331200
N	-1.87943700	0.45706700	0.03712300
H	3.35279600	-1.07629700	0.01381400
H	2.70160500	1.40595700	-0.01781600
H	-1.99019800	2.53872800	-0.00321100
H	-2.89424400	0.38622300	0.02534900
H	-2.33833700	-2.65641800	0.32864200

### CC-L1

CCSD/6-31G\* -465.905876

C	2.34458700	-0.70064000	-0.00046400
N	1.27349100	-1.46001200	-0.00099200
C	0.22017600	-0.56178100	-0.00023700
C	0.68041400	0.74069800	0.00071500
N	2.04879200	0.64298100	0.00088300
C	-1.21587800	-0.83771400	0.00006300
N	-1.83512400	-1.90401200	0.00062500
N	-0.03507100	1.91977400	0.00045500
C	-1.31462400	1.68529500	-0.00024400
N	-1.89555100	0.44866700	-0.00087800
H	3.36674800	-1.06046300	-0.00042400
H	2.69419600	1.42182600	-0.00053800
H	-2.00413200	2.52893300	-0.00035100
H	-2.90824400	0.38300800	-0.00205700
H	-2.33238900	-2.76023900	0.00372600

## CC-L2

CCSD/6-31+G\*\* -465.981121

C	2.34560900	-0.69773500	0.01039500
N	1.27457100	-1.45831800	0.01715900
C	0.21825100	-0.56220800	0.00129200
C	0.68036500	0.74371300	-0.01034700
N	2.04833300	0.64821800	-0.00462800
C	-1.21205500	-0.83209600	0.01649000
N	-1.83038000	-1.91463600	-0.09999900
N	-0.03958800	1.91671800	-0.01978400
C	-1.32104700	1.68125000	0.00340100
N	-1.89474300	0.44011200	0.04149400
H	3.36255300	-1.05409700	0.01785700
H	2.69317800	1.42109100	-0.01889900
H	-2.01014600	2.51668000	-0.00224500
H	-2.90287200	0.37175500	0.02858200
H	-2.31680900	-2.67763800	0.30762100

## SOSP (PUI) - In-Plane N-Inversion

### MP2

MP2(full)/6-31G\* -465.923667

C	-1.93751100	1.48719200	0.00000000
N	-0.65330900	1.81486100	0.00000000
C	0.00000000	0.60656800	0.00000000
C	-0.90121200	-0.45531900	0.00000000
N	-2.13967400	0.13330400	0.00000000
C	1.43193800	0.35302100	0.00000000
N	2.39201800	1.13035400	0.00000000
N	-0.66159400	-1.80287900	0.00000000
C	0.62257600	-2.04615700	0.00000000
N	1.60023500	-1.09613800	0.00000000
H	-2.76011000	2.19035000	0.00000000
H	-3.02292600	-0.36333800	0.00000000
H	0.96350000	-3.07952400	0.00000000
H	2.57217900	-1.39431700	0.00000000
H	3.18888500	1.71848600	0.00000000

### CC-L1

CCSD/6-31G\* -465.905744

C	-1.92820900	1.50632600	0.00000000
N	-0.65400800	1.82365400	0.00000000
C	0.00000000	0.60388700	0.00000000
C	-0.90292200	-0.44188600	0.00000000
N	-2.14183400	0.14745100	0.00000000

C	1.43774600	0.33765400	0.00000000
N	2.39910900	1.10975700	0.00000000
N	-0.66697900	-1.80057700	0.00000000
C	0.61000300	-2.04898900	0.00000000
N	1.60165800	-1.10930400	0.00000000
H	-2.74891000	2.21394000	0.00000000
H	-3.02644200	-0.34310400	0.00000000
H	0.94405500	-3.08607300	0.00000000
H	2.56816000	-1.41868700	0.00000000
H	3.19781100	1.69511700	0.00000000

## CC-L2

CCSD/6-31+G\*\* -465.980525

C	-1.93087900	1.50657600	0.00000000
N	-0.65488600	1.82323900	0.00000000
C	0.00000000	0.60349000	0.00000000
C	-0.90443100	-0.44241000	0.00000000
N	-2.14423300	0.14591000	0.00000000
C	1.43604500	0.33358300	0.00000000
N	2.39778000	1.11366800	0.00000000
N	-0.66469700	-1.80101800	0.00000000
C	0.61371400	-2.04949500	0.00000000
N	1.60585700	-1.10794000	0.00000000
H	-2.74695300	2.21015400	0.00000000
H	-3.02621100	-0.33919400	0.00000000
H	0.94840000	-3.07969800	0.00000000
H	2.56669900	-1.41902800	0.00000000
H	3.19261800	1.70028600	0.00000000