

Electronic Supplementary Information

Oxygen Atom Transfer: A Mild and Efficient Method for Generating Iminyl Radicals

Youngsuk Kim,^a Christopher W. Bielawski^{c,d,e}, and Eunsung Lee^{*,a,b,f}

^a Department of Chemistry, Pohang University of Science and Technology (POSTECH), Pohang, 37673, Republic of Korea

^b Center for Self-assembly and Complexity (CSC), Institute for Basic Science (IBS), Pohang, 37673, Republic of Korea

^c Center for Multidimensional Carbon Materials (CMCM), Institute for Basic Science (IBS), Ulsan, 44919, Republic of Korea

^d Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST), Ulsan, 44919, Republic of Korea

^e Department of Energy Engineering, Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919, Republic of Korea

^f Division of Advanced Materials Science, Pohang University of Science and Technology (POSTECH), Pohang, 37673, Republic of Korea

*E-mail: eslee@postech.ac.kr

Table of contents

Materials and Methods	S3
Experimental Details	S4
Synthesis of 2 using PPh ₃	S4
Synthesis of 2 using DAC	S5
NMR	S6
General information	S6
¹ H, ¹³ C NMR spectra of 2	S6
¹ H, ³¹ P NMR spectra of the crude reaction mixture (1 + PPh ₃)	S8
¹ H NMR spectrum of the crude reaction mixture (1 + 3)	S9
X-ray Crystallography	S10
General information	S10
Crystal data and structure refinements	S10
Selected structural data	S11
DFT Calculation	S12
General information	S12
Energy profile	S12
Metric comparison between DFT optimized and X-ray determined structures	S13
Wiberg bond index	S13
Molecular orbitals	S14
Coordinates of optimized structures	S14
References	S32

Materials and Methods

1. General methods

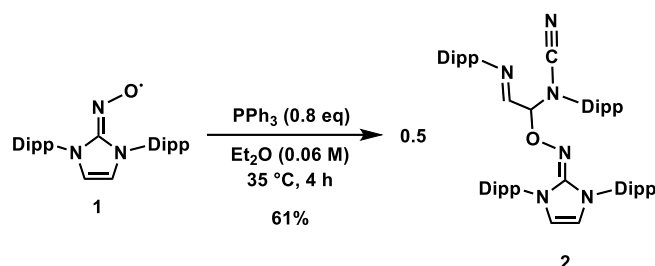
All air- and moisture-insensitive reactions were carried out under an ambient atmosphere, magnetically stirred. All air- and moisture-sensitive manipulations were performed using oven-dried glassware, including standard Schlenk and glovebox techniques under an atmosphere of nitrogen.

2. Reagents

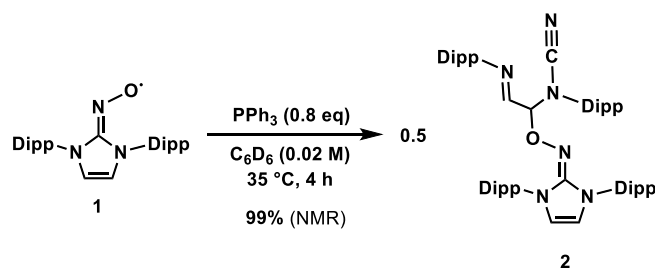
*i*PrNO (**1**), and *N,N'*-dimesityl-4,6-diketo-5,5-dimethylpyrimidin-2-ylidene (DAC, **3**) was synthesized according to a reference.¹ Triphenylphosphine (PPh₃) and all other chemicals were purchased from commercial sources and used as received unless otherwise specified. 3 Å molecular sieves were activated at 240 °C under dynamic vacuum for overnight prior to use. Diethyl ether was distilled from deep purple sodium benzophenone ketyl and stored over 3 Å molecular sieves. Benzene-*d*₆ (C₆D₆) was dried using activated 3 Å molecular sieves.

Experimental Details

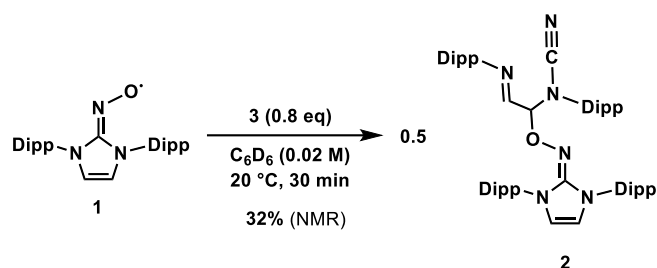
Synthesis of **2** using PPh₃



In a N₂ atmosphere glovebox, *i*PrNO (**1**, 50 mg, 0.12 mmol) and triphenylphosphine (PPh₃, 25 mg, 0.10 mmol) were placed in a 4 mL vial and subsequently dry diethyl ether (2 mL) was added to the vial. The solution was stirred at 35 °C for 4 hours. White precipitate was formed during the reaction. All volatiles in reaction mixture was removed *in vacuo*, and the resulting solid was subsequently washed with acetone:methanol (1:2) solution (2 × 1 mL) pentane (1 × 1 mL) to afford 30 mg of the product (61%). Single crystals suitable for X-ray crystallography were obtained when the same reaction was carried out without stirring. ¹H NMR (500 MHz, Benzene-*d*₆) δ 7.20 – 7.16 (m, 1H), 7.14 – 7.05 (m, 5H), 7.04 – 7.00 (m, 2H), 6.95 – 6.92 (m, 2H), 6.85 – 6.79 (m, 2H), 6.27 (d, *J* = 2.8 Hz, 1H), 5.74 (d, *J* = 2.5 Hz, 1H), 5.64 (d, *J* = 2.5 Hz, 1H), 5.23 (d, *J* = 2.8 Hz, 1H), 3.88 – 3.79 (m, 2H), 3.60 – 3.52 (m, 1H), 3.21 – 3.14 (m, 1H), 3.12 – 3.03 (m, 2H), 2.89 – 2.80 (m, 2H), 1.56 (d, *J* = 6.8 Hz, 3H), 1.47 (d, *J* = 6.9 Hz, 3H), 1.25 (d, *J* = 6.9 Hz, 3H), 1.23 – 1.15 (m, 24H), 1.14 – 1.10 (m, 6H), 1.06 (d, *J* = 6.9 Hz, 3H), 1.00 (d, *J* = 6.9 Hz, 3H), 0.75 (d, *J* = 6.7 Hz, 3H) ppm. ¹³C NMR (126 MHz, Benzene-*d*₆) δ 160.41, 151.27, 148.59, 147.86, 147.54, 147.45, 147.32, 146.90, 145.52, 137.93 (2C), 137.39, 135.62, 133.44, 129.67, 129.16, 128.87, 125.25, 125.17, 124.61, 124.59, 124.24, 124.06, 123.24 (3C), 116.55, 115.56, 114.17, 96.53, 29.32, 28.99, 28.93, 28.80, 28.33, 28.00, 27.64 (2C), 25.53 (2C), 24.99, 24.41, 24.29 (2C), 24.27 (2C), 24.21, 24.16, 23.84, 23.65, 23.58, 23.36, 23.23, 23.12 ppm. Anal. Calcd for C₅₄H₇₂N₆O: C, 78.98; H, 8.84; N, 10.23. Found: C, 78.90; H, 8.66; N, 9.95.



In a N₂ atmosphere glovebox, *i*PrNO (**1**, 5.0 mg, 0.012 mmol) and triphenylphosphine (PPh₃, 2.5 mg, 9.6 μmol) were placed in a 4 mL vial and subsequently dry *d*₆-benzene (C₆D₆, 0.5 mL) was added to the vial. The solution was heated to 35 °C for 4 hours. The reaction mixture was moved to a screw-capped NMR tube, and 1,3,5-trimethoxybenzene (2.4 mg) was added as an internal standard. The sample was analyzed with ¹H and ³¹P NMR.

Synthesis of **2** using DAC

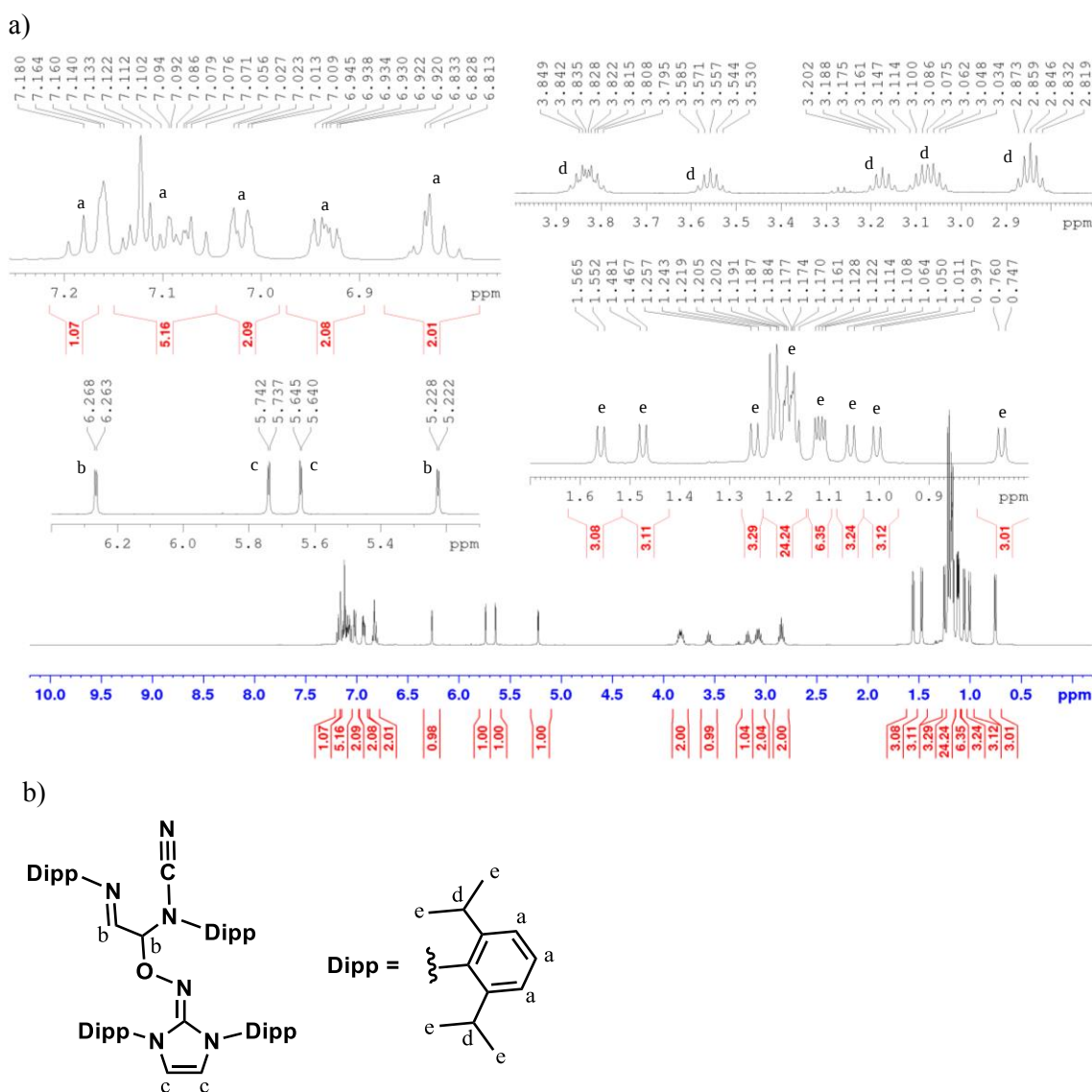
In a N_2 atmosphere glovebox, *i*PrNO (**1**, 5.0 mg, 0.012 mmol) and *N,N'*-dimesityl-4,6-diketo-5,5-dimethylpyrimidin-2-ylidene (**3**, 3.6 mg, 9.6 μ mol) were placed in a 4 mL vial and subsequently dry benzene-*d*₆ (C_6D_6 , 0.5 mL) was added to the vial. After 30 minutes, the reaction mixture was moved to a screw-capped NMR tube, and 1,3,5-trimethoxybenzene (2.9 mg) was added as an internal standard. The sample was analyzed with 1H NMR.

NMR

General information

^1H NMR spectra, proton decoupled ^{13}C NMR spectra ($^{13}\text{C}\{^1\text{H}\}$), ^1H - ^{13}C polarization transfer experiments (DEPT90 and DEPT135), and proton decoupled ^{31}P NMR spectra ($^{31}\text{P}\{^1\text{H}\}$) were recorded using a Bruker DRX 500 spectrometer operating at 500 MHz (for ^1H acquisitions), 126 MHz (for ^{13}C acquisitions), or 202 MHz (for ^{31}P acquisitions). Chemical shifts of ^1H and ^{13}C acquisitions were referenced to the residual solvent peaks (^1H : C_6D_6 , $\delta = 7.16$ ppm; ^{13}C : C_6D_6 , $\delta = 128.06$ ppm).² Chemical shifts of ^{31}P acquisitions were referenced to the residual peak from PPh_3 ($\delta = -6.00$ ppm).

^1H , ^{13}C NMR spectra of **2**



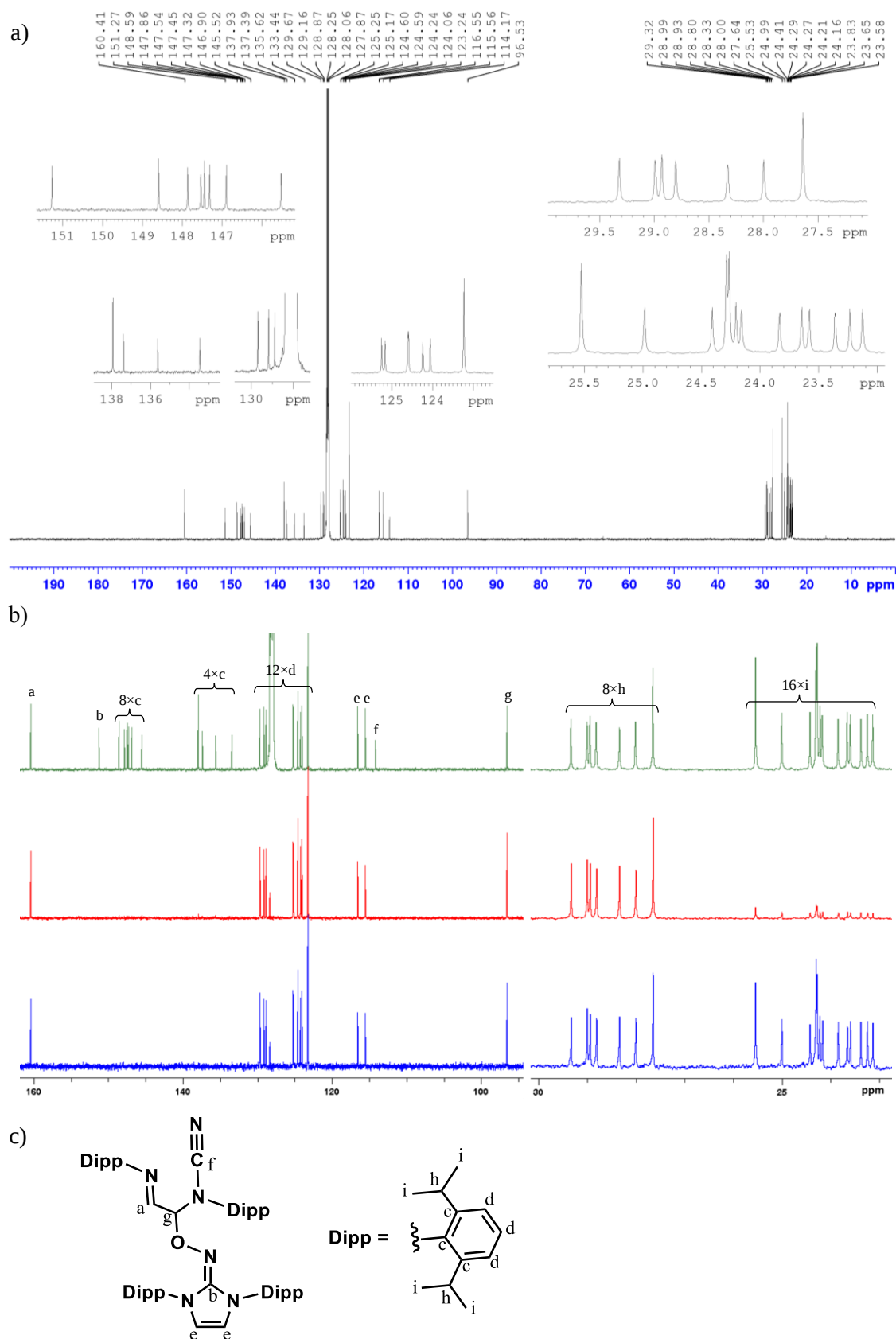
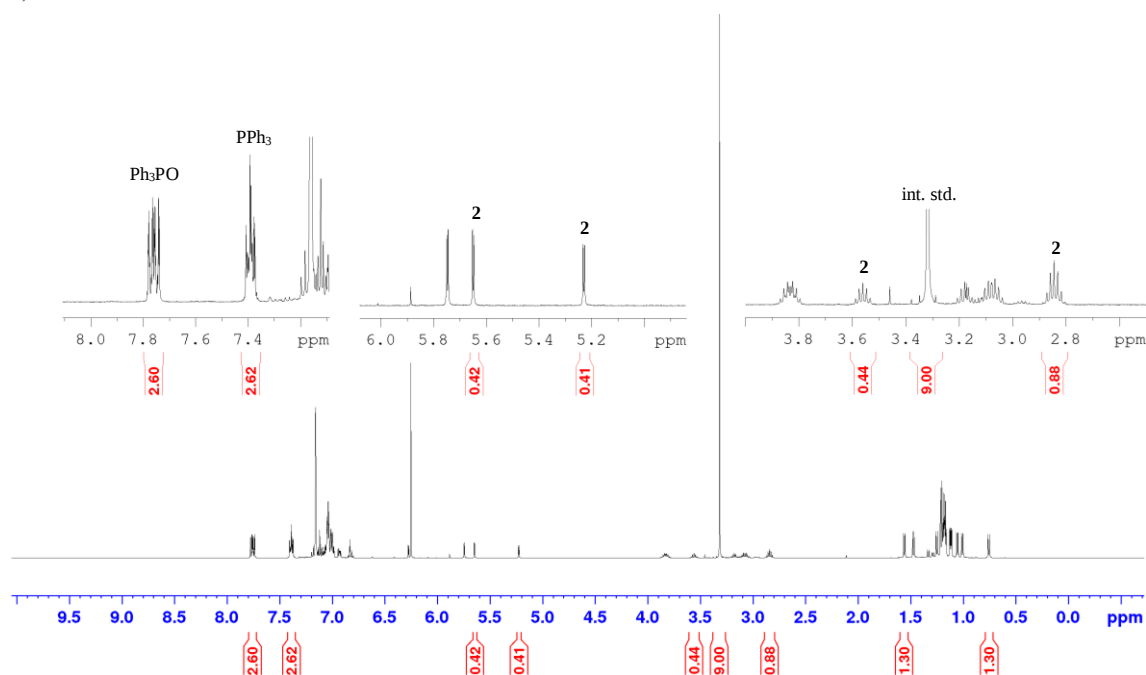


Figure S2. a) Proton decoupled ^{13}C NMR spectrum for the compound **2**. b) Comparison of the proton decoupled ^{13}C NMR (top, green), DEPT90 ^{13}C NMR (middle, red), DEPT135 ^{13}C NMR (bottom, blue) spectra of **2** and c) assignment of the signals.

^1H , ^{31}P NMR spectra of the crude reaction mixture (1** + PPh_3)**

a)



b)

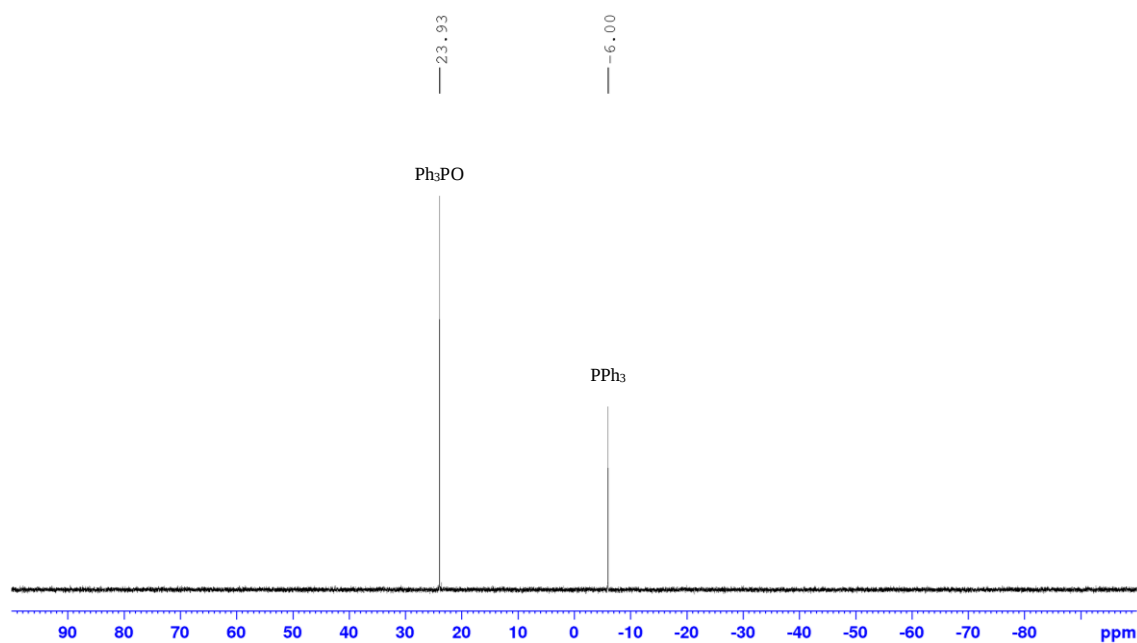


Figure S3. a) ^1H NMR spectrum and b) ^{31}P NMR spectrum of the crude reaction mixture (**1** + PPh_3) with 1,3,5- trimethoxybenzene as an internal standard.

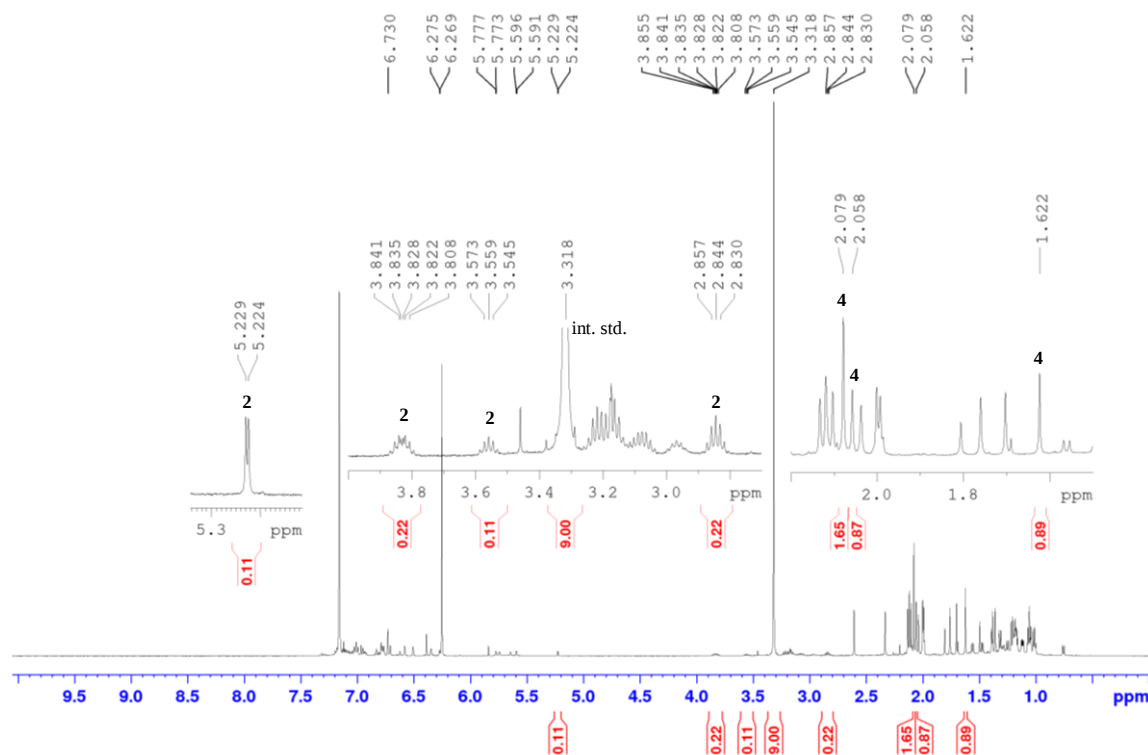
^1H NMR spectrum of the crude reaction mixture (1 + 3)

Figure S4. ^1H NMR spectrum of the crude reaction mixture (1 + 3) with 1,3,5- trimethoxybenzene as an internal standard.

X-ray Crystallography

CCDC 1905718 contains the supplementary crystallographic data for **2**. These data can be obtained free of charge via <https://www.ccdc.cam.ac.uk/> (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB21EZ, UK; fax (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

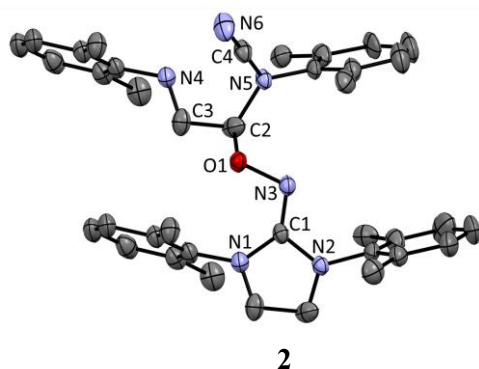
General information

A suitable crystal was coated with paratone-*N* oil and the diffraction data measured at 100 K with synchrotron radiation on a 2D beamline at the Pohang Accelerator Laboratory, Korea. Using Olex2³, The structure was solved by ShelXT⁴ using Intrinsic Phasing and refined by ShelXL⁵ using Least Squares minimization. All the non-hydrogen atoms were refined anisotropically. All hydrogen atoms were added to their geometrically ideal positions.

Crystal data and structure refinements

Table S1. Crystal data and structure refinements for **2**.

	2
Empirical formula	C ₂₇ H ₃₆ N ₃ O _{0.5}
Formula weight	410.59
Temperature/K	100
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	23.496(5)
b/Å	5.6560(11)
c/Å	19.914(4)
α/°	90
β/°	112.55(3)
γ/°	90
Volume/Å ³	2444.1(10)
Z	4
ρ _{calc} /cm ³	1.432
μ/mm ⁻¹	0.125
F(000)	1078.0
Crystal size/mm ³	0.04 × 0.02 × 0.01
Radiation	synchrotron (λ = 0.700)
2θ range for data collection/°	5.59 to 59.078
Index ranges	-33 ≤ h ≤ 33, -7 ≤ k ≤ 7, -28 ≤ l ≤ 28
Reflections collected	20101
Independent reflections	6816 [R _{int} = 0.0331, R _{sigma} = 0.0285]
Data/restraints/parameters	6816/0/418
Goodness-of-fit on F ²	1.039
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0627, wR ₂ = 0.1700
Final R indexes [all data]	R ₁ = 0.0686, wR ₂ = 0.1749
Largest diff. peak/hole / e Å ⁻³	0.26/-0.29

Selected structural data**Table S2.** Selected bond lengths (Å) and angles (°) for **2**.

2		2	
C1–N1	1.336(2)	N1–C1–N2	106.0(2)
C1–N2	1.383(2)	N2–C1–N3	121.7(2)
C1–N3	1.310(2)	N3–C1–N1	132.2(2)
N3–O1	1.462(2)	C1–N3–O1	108.0(2)
O1–C2	1.464(2)	N3–O1–C2	111.9(1)
C2–C3	1.428(2)	O1–C2–C3	104.3(1)
C3–N4	1.316(2)	C2–C3–N4	114.9(1)
C2–N5	1.587(2)	C3–C2–N5	117.5(1)
N5–C4	1.333(2)	C2–N5–C4	117.3(1)
C4–N6	1.154(3)	N5–C4–N6	179.0(2)

The thermal ellipsoids are set at a 50% probability level. Hydrogen atoms methyl groups were omitted for clarity.

DFT Calculation

General information

Geometry optimizations, frequency calculations, and intrinsic reaction coordinate (IRC) calculations were performed using Gaussian09⁶ with M06-2X⁷ functional and Def2-SVP⁸ basis set. In the geometry optimization, the default tight convergence in the SCF cycle was used without any orbital symmetry constraints. IRC calculations were performed using local quadratic approximation (LQA) algorithm⁹ with recomputing the Hessian analytically for every predictor step. Multiwfn¹⁰ and IBOview¹¹ programs were used to visualize Molecular orbitals. Wiberg bond indices (WBIs) were calculated from the optimized geometry with Löwdin orthogonalization method using Multiwfn.

Energy profile

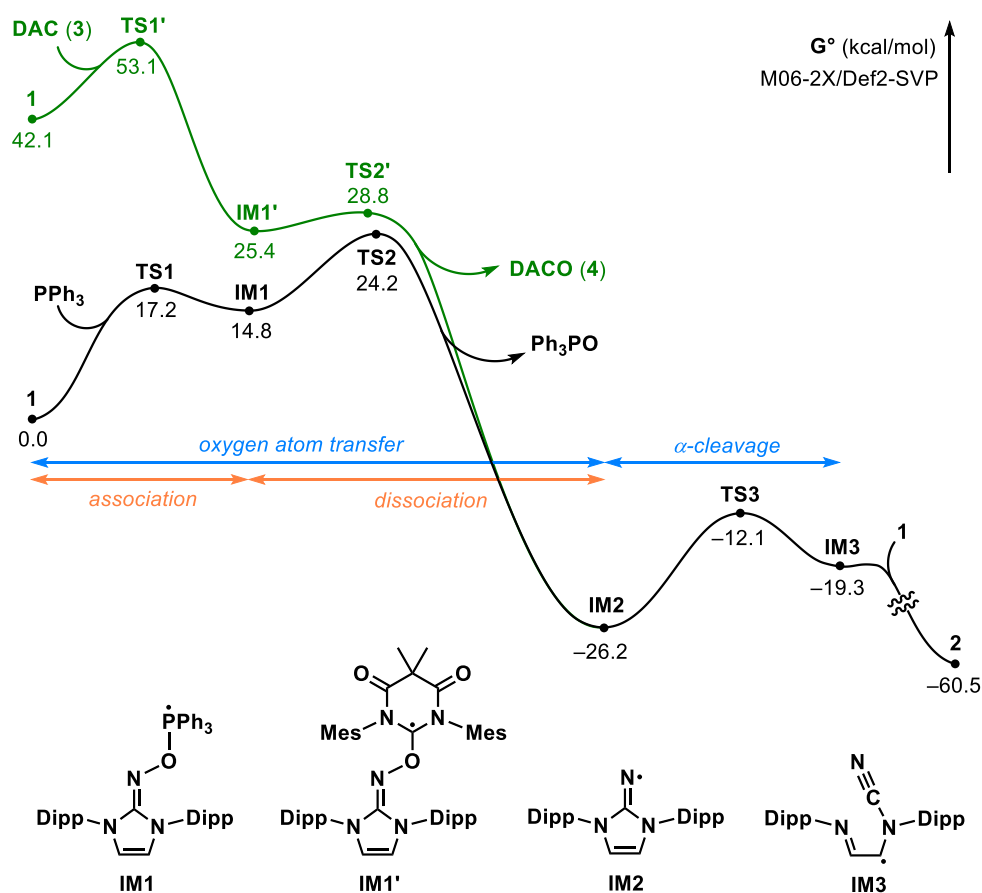
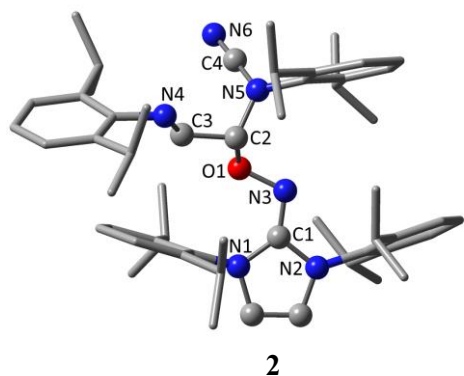


Figure S5. DFT calculated free energy diagram for the reaction between **1** and PPh_3 (black) or **3** (green)

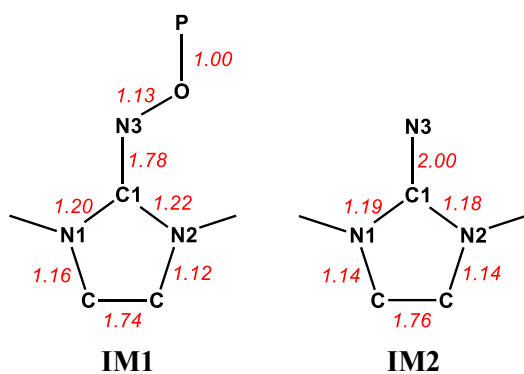
Metric comparison between DFT optimized and X-ray determined structures

**Table S3.** Selected bond lengths (Å) and angles (°) comparison for **2**.

	2 (X-ray)	2 (DFT)		2 (X-ray)	2 (DFT)
C1–N1	1.34	1.38	N1–C1–N2	106	106
C1–N2	1.38	1.38	N2–C1–N3	122	122
C1–N3	1.31	1.30	N3–C1–N1	132	132
N3–O1	1.46	1.41	C1–N3–O1	108	109
O1–C2	1.46	1.39	N3–O1–C2	112	113
C2–C3	1.43	1.52	O1–C2–C3	104	104
C3–N4	1.32	1.26	C2–C3–N4	115	123
C2–N5	1.59	1.46	C3–C2–N5	118	112
N5–C4	1.33	1.33	C2–N5–C4	117	118
C4–N6	1.15	1.16	N5–C4–N6	179	178

Wiberg bond index

Selected WBIs are shown below:



Molecular orbitals

Selected MOs for **IM2** are shown below:

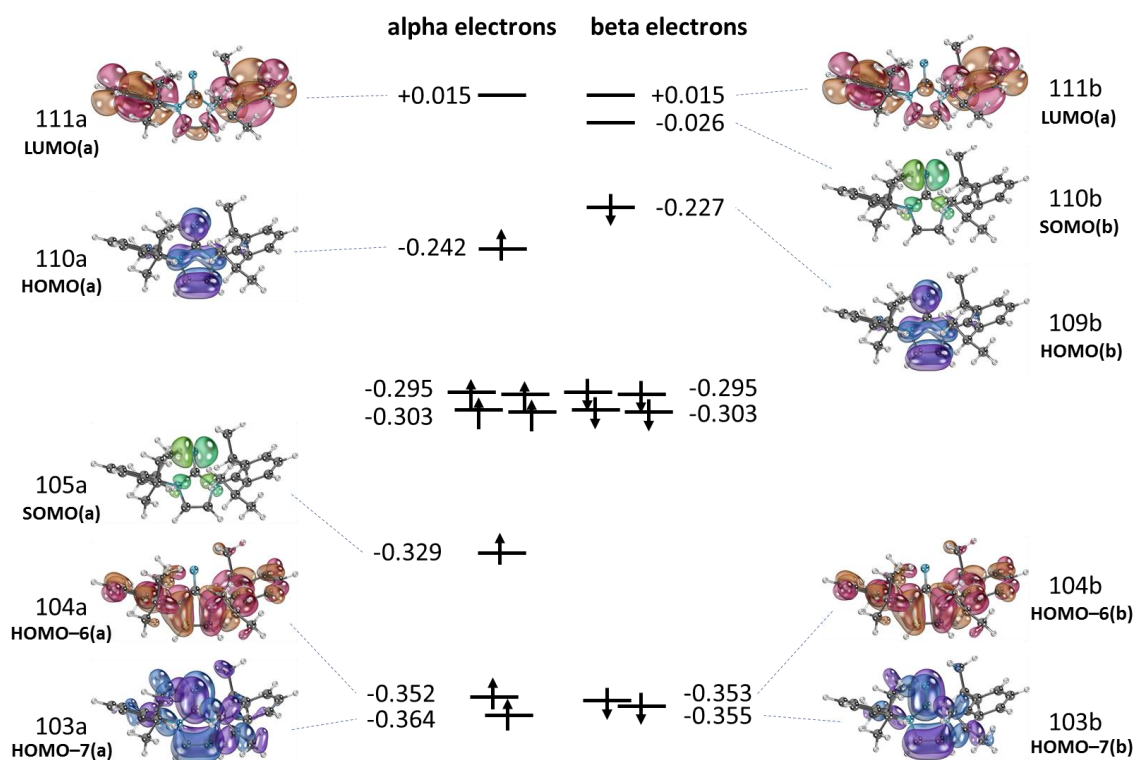
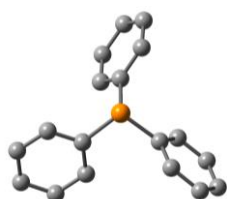


Figure S6. Selected MOs for **IM2**. (Energy in eV; not to scale)

Coordinates of optimized structures

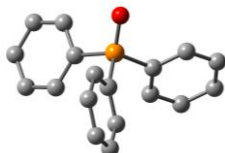
The following optimized geometries were displayed in Cartesian coordinates (atomic unit). E° represents the electronic energy of the optimized structure, and G° represents the sum of electronic and thermal free energies in Hartree unit. For transition states, ν_{im} represents the only one imaginary (negative) frequency.

PPh₃ [$E^\circ = -1035.3747249$; $G^\circ = -1035.144289$]



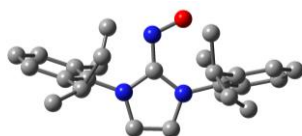
Charge = 0; Multiplicity = 1;

C	-0.7112606209	1.5877224396	0.2680937671	C	-0.7485902724	-1.2697771536	-3.1437327343
P	1.00424103	1.0702290572	-0.178381951	C	-0.5973218955	-0.4322366402	-2.0378862489
C	-1.2139077506	2.7337615395	-0.3630414061	H	-0.5801294111	3.2849778008	-1.062740952
C	-2.5105443974	3.1757255613	-0.1081717909	H	-2.8894413487	4.0672322762	-0.6106798571
C	-3.317126913	2.485600449	0.7967097533	H	-4.3304774201	2.8336621192	1.0032563174
C	0.6769998782	-0.0171648409	-1.6343427442	H	1.9532303196	1.3667784592	2.4997068509
C	1.3350359342	-0.1882111691	1.1320251733	H	2.3875664025	-0.1882627387	4.3813318544
C	1.7924641234	0.2935253643	2.3667403358	H	2.0462792977	-2.6377849204	4.0790661818
C	2.0379717625	-0.579027884	3.4242258209	H	2.791460741	-0.1142679712	-2.0699504643
C	1.8478757385	-1.9509279423	3.2547220242	H	2.5212357358	-1.623517004	-4.0182562379
C	1.7929309259	-0.4464732828	-2.3665113659	H	0.2472974693	-2.3640511219	-4.7160872665
C	1.6422137854	-1.2930519141	-3.4622864507	H	-3.4459398909	0.8111650225	2.1526614581
C	0.3683530248	-1.7059487697	-3.8541863923	H	-1.1500150851	0.0134447927	1.6851844499
C	-2.8210295864	1.3532884629	1.4409570242	H	1.263024079	-3.5135230371	1.8861612537
C	-1.5264366964	0.9045459908	1.1784321143	H	0.7994635341	-1.9602765723	0.0139672006
C	1.409835553	-2.4411461386	2.0258514333	H	-1.7476131752	-1.5860261846	-3.4486045998
C	1.1514948334	-1.5661485841	0.9695823854	H	-1.4791377049	-0.1038354661	-1.4838159369

Ph₃PO [$E^\circ = -1110.5380719$; $G^\circ = -1110.303298$]

Charge = 0; Multiplicity = 1;

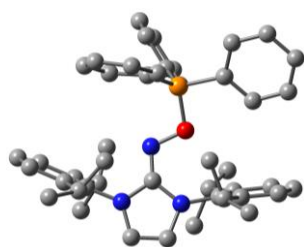
C	-0.8908509093	-0.2185099801	-1.3095174274	C	-0.540442208	3.7472454178	1.6336730847
P	0.599608904	0.6498972982	-0.7274031821	C	-0.1452322584	2.9548327483	0.5573941778
C	-0.9736499656	-0.4311776027	-2.689579707	H	-0.176662208	-0.0483104946	-3.330844626
C	-2.0707196741	-1.103645827	-3.2240063229	H	-2.1357238607	-1.2679638799	-4.3006493521
C	-3.0881798841	-1.5577851563	-2.3847237552	H	-3.9485806034	-2.0806342464	-2.8056187109
C	0.1023530077	1.5917727881	0.7495174428	H	0.2607047711	-2.0793831598	0.5261909749
C	1.739512951	-0.6420491441	-0.1376607963	H	1.9504726807	-3.7094836207	1.3280210533
C	1.3252826492	-1.8477780694	0.4380742351	H	4.3745239043	-3.2153632999	1.0834768687
C	2.2741604349	-2.7684879408	0.8804548887	H	-3.8196869852	-1.672196587	-0.356126151
C	3.634063827	-2.4917681462	0.7384403543	H	-1.8793007475	-0.4590024976	0.6028294046
C	-3.0153947442	-1.3320597607	-1.0100797326	H	5.1118966034	-1.0905316974	0.0219521742
C	-1.9202568289	-0.6581385166	-0.4709805949	H	3.4042573764	0.5565719745	-0.7808736476
C	4.0480949048	-1.2986768382	0.1461803545	H	0.2097365305	-0.0247688978	2.1879843328
C	3.1032017616	-0.3743528917	-0.2952092945	H	-0.5176873323	1.3890483169	4.092699237
O	1.2094993808	1.5175187344	-1.7846262456	H	-0.988969163	3.8046240984	3.7439116231
C	-0.0225559883	1.0305935191	2.0248262346	H	-0.7307879103	4.8111490867	1.4842134089
C	-0.42142357	1.8262577479	3.0976888345	H	-0.0069287904	3.3794029042	-0.4394985305
C	-0.6828390559	3.1824086203	2.9013123924				

IPrNO (1) [$E^\circ = -1288.4478017$; $G^\circ = -1287.927927$]

Charge = 0; Multiplicity = 2;

C	-2.3812987608	-0.9374793195	-1.3730750263	H	-0.7229721651	3.9787654499	-4.7281617952
C	-2.1308973684	-1.8620855729	-0.4160666697	H	-2.3919924492	4.2009649256	-2.9196665448
N	-0.9737342816	-1.4804178125	0.2524403779	H	1.281522872	-4.9873133611	2.167797209
C	-0.5219009575	-0.3066953686	-0.2843981683	H	0.7383573684	-4.2021027073	4.447176254
N	-1.3906488821	0.0281221974	-1.2841446555	H	-0.568694256	-2.1270492965	4.7801149818
C	-1.1942999461	1.1097748807	-2.2044745218	H	0.2797889825	-1.0296777079	-2.6221009669
C	-0.4639023249	-2.1859139154	1.3966390006	H	1.1351056094	-1.8303237579	-4.7748091466
N	0.5242620439	0.4606244371	0.0463488159	H	-0.497120541	-1.1473931023	-4.9986441176
C	-0.2385900256	0.9576250025	-3.2194947669	H	0.9381688103	-0.22661234	-5.508058556
C	-0.0826767243	2.0170720445	-4.1197168535	H	2.7139593805	-0.8377007665	-3.0076351622
C	-0.8560832673	3.1662650845	-4.0121464423	H	2.1376993141	0.4971236329	-1.9680913139
C	-1.7980152256	3.2896912194	-2.9925239418	H	2.5008640206	0.7929071648	-3.6911751784
C	-1.9809563647	2.266328481	-2.0601564718	H	-3.3533132871	1.4214966186	-0.6662175977
C	0.2810057375	-3.3568598194	1.1747041895	H	-2.7843351864	2.8648236968	1.2501854363
C	0.7025390961	-4.0726030315	2.2965861343	H	-1.2764413527	2.1936596231	0.5530637637
C	0.3967762159	-3.6309939002	3.5824290051	H	-1.7384847047	3.87000852	0.2120039573
C	-0.3402489955	-2.4675818964	3.76807631	H	-4.7978600244	3.3355009069	-0.3059553714
C	-0.7951758454	-1.7217099897	2.6759375414	H	-4.633996457	3.0992919185	-2.0646373211
C	0.6367321094	-0.2777260742	-3.3426646241	H	-3.7455756393	4.4064630523	-1.2415815821
C	0.5427911965	-0.9042824572	-4.7364865972	H	-0.1756856784	-3.5350038289	-0.8989898516
C	2.0855113102	0.0646594384	-2.9768539474	H	2.0959174048	-3.1429505613	-1.7640723591
C	-2.9261576661	2.4143410457	-0.8787876699	H	1.6969279806	-1.8543345096	-0.5804220019
C	-2.1349245293	2.853925735	0.3615488006	H	2.7605429901	-3.1825134596	-0.107849597
C	-4.0903576336	3.3659016569	-1.146632384	H	1.1245845393	-5.5082292719	-1.4374950861
C	0.6731313222	-3.7671590421	-0.2356198843	H	0.1390890374	-5.8769595074	0.0010728035
C	1.8715848421	-2.9318517216	-0.706908589	H	1.8819843147	-5.5420810708	0.161231655
C	0.9658780131	-5.2591730045	-0.3785752352	H	-1.9249824555	-0.0731405847	1.9196142217
C	-1.570753792	-0.4349179671	2.8974591456	H	-3.3791951653	0.2741595065	3.8684536614
C	-2.8065770511	-0.6601267969	3.7721433145	H	-3.4679847616	-1.4282815858	3.3456800506
C	-0.655406424	0.6452958647	3.4856852001	H	-2.5243130563	-0.9807090312	4.7862897641
O	1.2832407436	-0.0638496941	0.9347882607	H	-1.1986592711	1.597583597	3.5802038401
H	-3.1688792847	-0.8701669725	-2.1166407748	H	0.225598757	0.7960455902	2.8471891486
H	-2.6666420716	-2.7630184037	-0.1342198659	H	-0.3092287693	0.3505660678	4.4888997936
H	0.65899663	1.9352048516	-4.9166279977				

IM1 [$E^\circ = -2323.8265097$; $G^\circ = -2323.048662$]

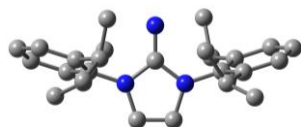


Charge = 0; Multiplicity = 2;

C	-3.3927048052	-1.058656538	-1.421686873	C	-1.243802175	0.528616446	-3.6900854065
C	-3.1455566219	-1.8754730677	-0.3799507032	C	-1.0551861913	1.57383559	-4.6006497346
N	-1.8364402164	-1.6243463208	0.067980361	C	-1.6819569596	2.8001720738	-4.4168516508
C	-1.290596134	-0.6237094423	-0.7076825354	C	-2.5096280313	3.0099669719	-3.3155037342
N	-2.2575869349	-0.2791290188	-1.6293470686	C	-2.7208084154	2.001094251	-2.372885303
C	-2.0795083893	0.7650220306	-2.5881240801	C	-0.2046390614	-3.3779357368	0.601274158
C	-1.183671552	-2.4608636333	1.0314979159	C	0.3352963183	-4.2400969158	1.5611347287
N	-0.1347734904	-0.0401807056	-0.6905207202	C	-0.0864354277	-4.194966878	2.8878746409

C	-1.0279139096	-3.2551874702	3.2928587614	H	-0.5386634317	-2.4503864863	-5.3297572643
C	-1.5861409963	-2.358997979	2.3744683492	H	-2.1063032552	-1.6088012692	-5.2130934595
C	-0.5478393154	-0.8028671473	-3.9088884064	H	-0.7503368599	-0.8553102401	-6.0839215344
C	-1.015894668	-1.4661932011	-5.2074323938	H	1.4685842578	-1.6199237403	-3.9311031738
C	0.973793171	-0.6369287756	-3.8751935184	H	1.2846027299	-0.1430671296	-2.9443284669
C	-3.5645320752	2.2302911793	-1.1283314185	H	1.327337429	-0.0373905438	-4.7289861285
C	-2.6705149229	2.4816490103	0.0939434691	H	-4.1328354134	1.3058757418	-0.9408113282
C	-4.5803875303	3.3602744111	-1.2845413516	H	-3.2770492184	2.5160798656	1.0119564626
C	0.2648865263	-3.409091548	-0.8469960628	H	-1.8984406246	1.7079292138	0.211001007
C	1.6056868607	-4.1210038903	-1.0279891588	H	-2.1424709628	3.4418338401	-0.0049568789
C	-0.7840872793	-4.0315868815	-1.7784879636	H	-5.2390258081	3.390763676	-0.4050011836
C	-2.5053434621	-1.2336643905	2.8245075975	H	-5.2056976052	3.2307057289	-2.1801250045
C	-3.249443971	-1.5348725035	4.1237978077	H	-4.0825990897	4.3393588801	-1.3498264841
C	-1.6912903697	0.0619507882	2.9518249968	H	0.4155790188	-2.3619775306	-1.1586486156
O	0.5943956523	-0.4359648156	0.4513031882	H	1.9719955365	-3.9625813852	-2.0529280945
P	1.6494082127	0.8348726341	0.8383178082	H	2.3677954563	-3.7451043779	-0.3292380632
C	2.1307851099	0.2172017599	2.4654617433	H	1.5117522307	-5.2074723989	-0.8769633191
C	2.9121274219	1.0386013874	3.2916586097	H	-0.4182759423	-4.0230870359	-2.8168424438
C	3.3328756736	0.57930563	4.5357659655	H	-1.7389248243	-3.4881382393	-1.7557225808
C	2.9977759345	-0.7100937803	4.9562842471	H	-0.9778149597	-5.0773923795	-1.4936913132
C	2.237158489	-1.5352482449	4.1298589447	H	-3.2598918303	-1.0741881939	2.0393014412
C	1.8000894631	-1.0782038554	2.8867985653	H	-3.9855215787	-0.743204727	4.3226356795
C	1.0462522559	2.4516011273	0.9034504656	H	-3.7820107501	-2.4961328954	4.0773587986
C	0.4867888456	3.0010629242	2.1050680636	H	-2.5636144611	-1.5628547164	4.9837961733
C	-0.0491151553	4.2749173403	2.1083364858	H	-2.3408953073	0.908712744	3.2191086124
C	-0.0943846128	5.0543860389	0.9391018888	H	-1.1732339988	0.3065787524	2.0130711762
C	0.3746929118	4.4938350713	-0.2622493802	H	-0.9232787934	-0.050199944	3.7344288143
C	0.9040994061	3.2186110484	-0.302415026	H	3.1796428764	2.0424874774	2.9533828425
C	2.9030523549	0.623996857	-0.4365905121	H	3.9315787859	1.2270117563	5.1779207676
C	3.7478601808	1.681657872	-0.8077027693	H	3.3354408509	-1.0707318062	5.929334027
C	4.7757417024	1.4654309228	-1.7190749609	H	1.9690638587	-2.5439903653	4.4495868582
C	4.9953653546	0.1889467826	-2.2459394707	H	1.1895898523	-1.7199355431	2.2509501783
C	4.1752729707	-0.8697281867	-1.8595166215	H	0.4938882692	2.4152390057	3.0265350473
C	3.1289413475	-0.6564274459	-0.9642576044	H	-0.4470436943	4.6766885667	3.0428254612
H	-4.2699954409	-0.9554915352	-2.0519199151	H	-0.5163498798	6.0590771981	0.9577151934
H	-3.7509432247	-2.647651105	0.0833075078	H	0.2978838423	5.0602495199	-1.1931198101
H	-0.4063384589	1.4199997085	-5.465703625	H	1.2037320003	2.7848341828	-1.2583243772
H	-1.5253319458	3.6041581592	-5.1379572035	H	3.5914633425	2.6737291504	-0.3788774303
H	-2.9912922972	3.9792840953	-3.1861180934	H	5.4181461553	2.2967176962	-2.0134896076
H	1.0985226322	-4.9614819479	1.2704893418	H	5.8079357349	0.0226152123	-2.9546855739
H	0.3373124972	-4.8899576501	3.6151920002	H	4.3414559498	-1.8692318862	-2.2660863095
H	-1.3228582881	-3.2076450293	4.3413262786	H	2.4664817808	-1.4753720202	-0.6804680985
H	-0.8257726328	-1.4695218252	-3.0804296219				

IM2 [$E^\circ = -1213.3263274$; $G^\circ = -1212.810607$]

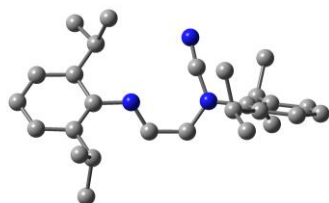


Charge = 0; Multiplicity = 2;

N	0.5825398434	0.2341432018	1.0180990051	C	-0.1262658954	1.7371041268	-0.452730428
C	0.5306160032	1.5996680299	0.7146539294	N	-0.5158163977	0.46129473	-0.8773456759

C	-0.0727405502	-0.4843849586	0.0322043162	H	-2.8181688855	-0.667855397	-5.4974206369
C	1.0955210539	-0.3403496952	2.2192086255	H	-4.1765725355	0.2175309101	-3.6333909153
C	-1.1355634946	0.1436785888	-2.1229918267	H	4.0489978566	-1.1679392174	3.6789626188
N	-0.2360316367	-1.7610145875	-0.025783231	H	-1.498805621	-0.0325667814	2.1325272308
C	0.1971135691	-0.7204065784	3.2284775623	H	1.4514020336	-0.219076785	-2.0236543441
C	0.7303965112	-1.2729374325	4.3987104169	H	-2.7391754032	1.5284418853	-0.4966350896
C	2.1024533064	-1.4232459899	4.5565609188	H	3.0006639745	0.7323428054	0.6882082241
C	-0.3438379569	-0.3580903663	-3.1678718642	H	1.746115352	1.2221907936	-4.047073315
C	-0.9784916658	-0.6530620982	-4.3801185347	H	1.7387792139	-0.2278144339	-5.0787760354
C	-2.341794108	-0.4404049239	-4.542327998	H	3.0357672747	0.0012639836	-3.8890855291
C	-3.1073411515	0.0599536982	-3.4902498162	H	1.1584018179	-2.5485129795	-3.9965496224
C	-2.5222646657	0.3514959593	-2.257176969	H	0.8910637515	-2.6208170577	-2.2291277233
C	2.975430592	-1.0379407045	3.5402289886	H	2.5201869767	-2.2876497509	-2.8789382136
C	2.4894183193	-0.4995768417	2.3478167751	H	-5.3636223637	0.7939478345	-1.9010633716
C	-1.3061231475	-0.569157117	3.0736488475	H	-4.4806749742	2.3190973537	-2.1641258035
C	1.1461026037	-0.6054384386	-3.0077220521	H	-5.1310529747	1.9183843737	-0.554452056
C	-3.3461632049	0.8052454078	-1.0632904381	H	-2.6976361658	-0.9131685534	0.1447129352
C	3.4069841845	-0.1630763793	1.1836727285	H	-4.2688947677	-1.1187871502	-0.6531854163
C	1.9595467501	0.1437369171	-4.0665374975	H	-4.1374162691	-0.0592691316	0.775502414
C	1.4447722014	-2.1083996532	-3.0283467787	H	-1.4264023835	1.2488362876	4.2831053777
C	-4.6501165122	1.5000529457	-1.450094695	H	-1.7975811298	-0.2424773967	5.1795362437
C	-3.6225533176	-0.389998514	-0.1399501126	H	-2.9842009787	0.4176689782	4.0365272265
C	-1.9086673111	0.2634891818	4.2083857922	H	-1.8207330024	-2.522205189	3.8929689745
C	-1.9758246178	-1.9434554504	2.968857937	H	-1.5610073904	-2.5091976503	2.1230283652
C	4.839821257	0.153214554	1.6068643487	H	-3.0598639403	-1.8307626835	2.8165944544
C	3.384580497	-1.3083320877	0.1610638481	H	5.3513637896	-0.7409210045	1.9937620099
H	0.9714483629	2.3363267133	1.3785434618	H	4.8746413388	0.9311114119	2.38325997
H	-0.3649073202	2.6185252874	-1.0392858323	H	5.4164572379	0.5057700342	0.7399184408
H	0.0562344329	-1.5856754584	5.1987654881	H	2.3602366391	-1.564727102	-0.1475194222
H	2.5002352898	-1.8484843149	5.479535143	H	3.8325535151	-2.2127835222	0.6011393618
H	-0.3896711239	-1.0507040236	-5.209424837	H	3.9659623138	-1.0377795938	-0.7341278991

IM3 [$E^\circ = -1213.312596$; $G^\circ = -1212.799646$]



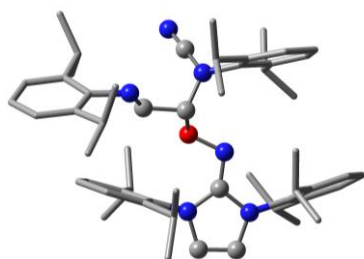
Charge = 0; Multiplicity = 2;

N	0.2100819561	-0.2440848222	1.4945371244	C	-0.9654704431	0.5304215407	-4.8893381473
C	0.4732277749	0.7913114852	0.6156740111	C	-2.3006247617	0.2098810645	-5.0894672336
C	-0.0172149619	0.8596580015	-0.6953692758	C	-3.0602726132	-0.2795114413	-4.0265747202
N	-0.6964855186	-0.1169267217	-1.2300425806	C	-2.5096436004	-0.4220615767	-2.7561338967
C	-0.8473071805	-1.0685613129	1.392986841	C	3.0400457653	-1.1275028933	3.7275894297
C	1.0174942605	-0.3777205583	2.6895749263	C	2.2633064062	-1.0219450319	2.5722081637
C	-1.1643841933	-0.0142062351	-2.5425612816	C	-0.8249155102	0.8158159527	4.008687556
N	-1.7415337265	-1.8022700614	1.4537663347	C	1.1338248896	0.6775761213	-3.5249667565
C	0.533374212	0.1444351181	3.8975036567	C	-3.2918766813	-1.0451213742	-1.6126196793
C	1.3440963823	-0.0013774591	5.0291017349	C	2.6975952451	-1.6411805085	1.2531307136
C	2.5827029626	-0.6255130738	4.9449611575	C	1.4838423596	2.1485210527	-3.7715185703
C	-0.3649562874	0.4218182321	-3.6286528903	C	1.9140875277	-0.2282538261	-4.4849787154

C	-4.8067936217	-0.9600496608	-1.7823811976
C	-2.8480808647	-2.5031483519	-1.4378700809
C	-0.7388600338	2.1636315958	4.7290993845
C	-1.8271604811	-0.1181846056	4.6976402022
C	4.2130406886	-1.7763439499	1.1191273732
C	2.0172834078	-3.004858275	1.0644322698
H	1.1307731907	1.5601009386	1.0207859034
H	0.1927876699	1.7953062398	-1.2371039625
H	0.9980162221	0.3849734538	5.9895987974
H	3.2023707627	-0.7231213241	5.8377263582
H	-0.3633101098	0.8675540353	-5.7362721752
H	-2.7480897411	0.3191445577	-6.0786325864
H	-4.1011504542	-0.5561635294	-4.1964334597
H	4.0142581088	-1.6144295479	3.6804834587
H	-1.1942885721	1.0103118119	2.9910155886
H	1.4633132516	0.4129159067	-2.5113696664
H	-3.020763965	-0.5115149589	-0.6902133219
H	2.3495366624	-0.9823355115	0.4422051054
H	0.9606892943	2.8175106622	-3.0725898459
H	1.1950159062	2.4510435764	-4.7898969129
H	2.5664400577	2.3148484075	-3.6660803088

H	1.6849669501	0.0048910186	-5.5354374243
H	1.6712065083	-1.2860936466	-4.3128383787
H	2.9968196563	-0.0925303088	-4.3426938035
H	-5.1576126565	-1.5906411384	-2.6139986643
H	-5.1412891071	0.0711164247	-1.9696555356
H	-5.3018954129	-1.3218821321	-0.8700749049
H	-1.7660005653	-2.5559619441	-1.258075309
H	-3.0896273063	-3.0825031556	-2.343324151
H	-3.3534138818	-2.9592985036	-0.5748315859
H	0.0068867025	2.8232637379	4.2627099262
H	-0.4679323847	2.038007488	5.7879759434
H	-1.7143593838	2.6696464462	4.6983293134
H	-1.4918188091	-0.3557288678	5.7191753587
H	-1.9411378358	-1.0587982251	4.1417065183
H	-2.813691579	0.3632312954	4.7651876416
H	4.6129251218	-2.5328489371	1.8110004652
H	4.7272135389	-0.8244211699	1.3154860984
H	4.4681602743	-2.1016791465	0.1008869681
H	0.9214016203	-2.9296961452	1.0922539875
H	2.330352627	-3.6959184051	1.8619702197
H	2.30299128	-3.442496828	0.0969374915

2 [$E^\circ = -2501.8593792$; $G^\circ = -2500.793236$]



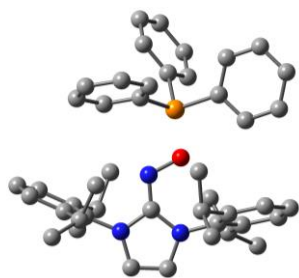
Charge = 0; Multiplicity = 1;

N	-12.0614642703	-2.7492730508	-10.0406741424
C	-9.8714153581	-1.9372430289	-10.6399661395
O	-13.548978916	-5.7770816664	-9.11187485
C	-10.8454198108	-2.1421207338	-9.6342860684
C	-8.615347347	-1.4640473759	-10.2667123115
C	-16.0592616295	-3.2799468164	-11.579438828
C	-10.6073929254	-1.7517024046	-8.3012280561
C	-11.6839895927	-1.7644154904	-7.2281587054
C	-12.4132502439	-3.8073800191	-9.4443366557
C	-14.2474752231	-3.0384313809	-13.3028669982
N	-14.8838693295	-3.8399319764	-9.5109880359
C	-14.9690448704	-3.2770242835	-8.3040449071
C	-9.3318357564	-1.2681054387	-7.9779664559
C	-11.4118438934	-2.8109345437	-6.14644295
C	-13.6668084439	-4.5817371026	-9.8191344493
C	-11.0684156659	-1.0011317923	-12.611335145
C	-17.9897075008	-4.6540371621	-7.546582455
C	-14.8945359841	-2.4290778822	-12.0551594348
C	-17.1841751721	-3.4188203258	-12.398219777
C	-10.2358182605	-2.1811417459	-12.0938534118

C	-8.3342460391	-1.1508185634	-8.9356444252
C	-11.8667246503	-0.3770370887	-6.6044733748
C	-18.2605133307	-4.8100876554	-10.7540328501
C	-17.6737744825	-6.8767130376	-8.7000772722
C	-9.0369470403	-2.4366978678	-13.0035357602
N	-15.0042690461	-2.7861097452	-7.2531241999
C	-17.1492637329	-4.7264682056	-9.9091255553
C	-15.3292589836	-0.9834132793	-12.3128340712
C	-16.0570439252	-3.9488458292	-10.3415308822
C	-18.2795895316	-4.1697822264	-11.9888018204
C	-17.1622613359	-5.4423083882	-8.569890017
H	-7.8415388088	-1.3294987123	-11.0233570902
H	-12.6404866909	-2.0175315891	-7.6982159816
H	-11.8201056451	-4.2704945841	-8.6366409505
H	-13.9785074014	-4.0926399347	-13.1402373639
H	-13.3338631208	-2.4865830012	-13.5700836542
H	-14.9327011336	-3.0032477224	-14.1648122321
H	-9.1269546771	-0.97374576	-6.9461170842
H	-11.2884970868	-3.8120294056	-6.5818723845
H	-12.2508324432	-2.8499452252	-5.4360506413

H	-10.4926690483	-2.5717693167	-5.5870473731	C	-11.1028292128	-6.7869673942	-11.957909369
H	-13.6991107287	-4.7814162383	-10.9043513023	C	-12.0849810182	-6.5162435538	-6.0256764384
H	-11.9825149475	-0.8832362557	-12.011768135	C	-10.0879409118	-7.7495855862	-12.5866750461
H	-11.3542831476	-1.1565346162	-13.6633053699	C	-17.4838952657	-10.3390763565	-9.6506188597
H	-10.4878970695	-0.0678809793	-12.5488872745	C	-11.332208992	-5.5812874059	-12.8668805564
H	-19.0365212362	-4.5765201073	-7.8803589145	C	-15.4392693443	-10.5171678571	-8.1387409924
H	-17.5961611915	-3.6390382495	-7.4004904544	C	-18.1171851788	-9.8645047881	-10.798154938
H	-17.9786690003	-5.1662458127	-6.5731271589	C	-15.8544665379	-6.7230930821	-12.8539862566
H	-14.1333429038	-2.4030907116	-11.2647553425	C	-16.0954712725	-11.7222087471	-7.4674970266
H	-17.2041757413	-2.914252924	-13.3665156569	C	-15.4263876645	-9.360944302	-10.4069761958
H	-10.878657057	-3.0703840895	-12.1223536727	H	-9.2933840526	-4.8562124957	-11.2014598504
H	-7.3441346657	-0.7876940085	-8.6557869575	H	-12.032502846	-8.2397826882	-7.2876989839
H	-10.9840972396	-0.0740597016	-6.0201822995	H	-10.8442197093	-9.7570042153	-9.8386173096
H	-12.7335767337	-0.3883739491	-5.927945791	H	-13.1905765932	-11.049614543	-10.5742125729
H	-12.042703767	0.384952164	-7.376750255	H	-9.7020693387	-8.9647904363	-6.7542266381
H	-19.1233673465	-5.4007433996	-10.4419827578	H	-10.6898088362	-8.7814637648	-5.2809557422
H	-17.5744484487	-7.3950091861	-7.7353977809	H	-9.4935547341	-7.5403333177	-5.7091042311
H	-17.0923109923	-7.4289252291	-9.4512605643	H	-9.3927095055	-5.5476093116	-6.9651582449
H	-18.7382334811	-6.9111135723	-8.9795393726	H	-14.948569832	-8.4316268981	-7.6416980373
H	-8.4167513511	-1.5347791896	-13.1202584862	H	-14.7131419833	-9.5957644696	-6.3015089123
H	-9.3820169429	-2.7246459683	-14.0075681061	H	-16.3520886746	-9.0900804942	-6.7794095651
H	-8.3890270807	-3.2402556568	-12.6196264432	H	-14.2381249831	-8.0005104163	-12.292290504
H	-16.0744187193	-0.9250084963	-13.1211363356	H	-14.7818084322	-9.9116341861	-13.8021462159
H	-14.463267356	-0.3735164799	-12.6105382778	H	-14.6352285419	-8.3809012637	-14.7060189243
H	-15.7706579974	-0.5370253149	-11.4107805509	H	-16.2406876033	-9.0605403623	-14.3608077386
H	-19.1542070364	-4.2567348912	-12.635849658	H	-8.5160307515	-4.3015228578	-8.9247303865
H	-16.1243608913	-5.5075059154	-8.2129092643	H	-17.9093151326	-8.7742239068	-12.6414406613
N	-12.1800678896	-8.0646486623	-9.6215531202	H	-12.0614690483	-7.3209157156	-11.8725778233
C	-10.6589012063	-6.4014027997	-10.5558346344	H	-11.4008788846	-5.7959679003	-5.5511956879
N	-14.0391388612	-9.095583871	-10.1918898377	H	-12.6066434861	-7.0580479458	-5.2226976961
C	-11.1739735779	-7.0606709312	-9.4253516169	H	-12.8292063143	-5.9545413969	-6.6092613311
C	-9.69412844	-5.4095929823	-10.3493056017	H	-9.1052975486	-7.261201989	-12.6770177501
C	-16.0388262815	-8.883288262	-11.5754344926	H	-10.4149654627	-8.0547837461	-13.5917611212
C	-13.5356293012	-7.8716412042	-9.8049442406	H	-9.9621702672	-8.6553676962	-11.9774902926
C	-11.3137921627	-7.4947213527	-6.9165974107	H	-18.0597229603	-10.9030417445	-8.9167291581
N	-14.2997454194	-6.8229592916	-9.6819917627	H	-12.0067827951	-4.8488330124	-12.4003203262
C	-11.8646059132	-9.3974885098	-9.9203950604	H	-11.7804771239	-5.9037033925	-13.8185060519
C	-10.7273890555	-6.7855944224	-8.1239659086	H	-10.388297512	-5.0666848212	-13.1042723215
C	-13.0019632954	-10.0233335215	-10.2766139484	H	-14.4095583581	-10.8084439884	-8.3947484923
C	-10.2363266409	-8.2392131162	-6.1237499247	H	-19.179798598	-10.0606525616	-10.9503996916
C	-9.7483886932	-5.7964545747	-7.9678008447	H	-16.8842502752	-6.7705497239	-13.2416474926
C	-15.3497212434	-9.3367069342	-7.1610820003	H	-15.2520837471	-6.1642464924	-13.5870424185
C	-15.2726479237	-8.1224371708	-12.6424836816	H	-15.8713582219	-6.161868414	-11.9082464539
C	-15.2288754216	-8.9178723638	-13.9512252924	H	-15.4803121593	-12.0572686608	-6.620260835
C	-9.2460254573	-5.1023058721	-9.0659376582	H	-16.2106454786	-12.5643616973	-8.1651519575
C	-16.1292345662	-10.0882880258	-9.4249422561	H	-17.0886515425	-11.4701276222	-7.066543949
C	-17.403583496	-9.1420997728	-11.7462277165				

TS1 [$E^\circ = -2323.8194588$; $G^\circ = -2323.044830$; $\nu_{\text{im}} = -290.41 \text{ cm}^{-1}$]

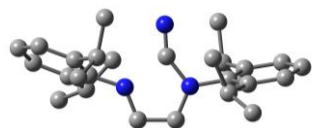


Charge = 0; Multiplicity = 2;

C	-2.4703176988	-1.0736117299	-1.1469018195	C	1.9859322305	3.042507676	-0.314546763
C	-2.1556148392	-1.9910569842	-0.206612693	C	4.7294069895	1.046101048	0.0751702465
N	-1.0057100894	-1.5502135867	0.4598899282	C	5.2702144915	2.3081948855	-0.2017108187
C	-0.6249411354	-0.3374150736	-0.0708682219	C	6.5290768918	2.4219860715	-0.7958240338
N	-1.5313704119	-0.0510436274	-1.065786155	C	7.2601572902	1.2816675971	-1.1229860437
C	-1.3849366192	1.085979835	-1.917427497	C	6.7263602686	0.0192681226	-0.8580475718
C	-0.4883860796	-2.1639427824	1.6455751627	C	5.4679640945	-0.0937482528	-0.2740779964
N	0.3188834001	0.4976030362	0.2464306852	H	-3.2751297201	-1.0462144304	-1.8742231572
C	-0.4955391308	1.0021862568	-3.0010943462	H	-2.6379878676	-2.9227538278	0.070718873
C	-0.3330275093	2.1402365368	-3.7974251059	H	0.3524713657	2.1085276149	-4.6469084577
C	-1.0314374284	3.3113149728	-3.5198114885	H	-0.8954374384	4.1882368644	-4.1553172648
C	-1.8975862734	3.3722795541	-2.4312804639	H	-2.4266465647	4.3017724963	-2.2147932449
C	-2.0840675816	2.2634830093	-1.6014989699	H	1.3654915789	-4.841911217	2.6039563842
C	0.3055769744	-3.3171640662	1.5069220683	H	0.7875902268	-3.9307520173	4.8281259911
C	0.7534843589	-3.9425205022	2.6726255002	H	-0.5627559187	-1.8633644944	5.0216179293
C	0.4316136923	-3.427093529	3.9274134374	H	-0.0662909153	-1.0570331292	-2.6366067195
C	-0.3319147615	-2.2705893462	4.0348367726	H	0.7054074672	-1.660176512	-4.8897180213
C	-0.8140205746	-1.6161077606	2.8952182787	H	-0.8923153107	-0.8750857654	-4.9973766366
C	0.314729473	-0.2519239604	-3.2836545477	H	0.5798889384	0.0219055184	-5.43681923
C	0.1634000498	-0.7158284537	-4.7344780873	H	2.3752455511	-0.9397752883	-3.0947877302
C	1.7867659997	-0.0265243759	-2.9197278598	H	1.8864519993	0.2495490268	-1.8591558005
C	-2.9317272684	2.3583849268	-0.3451548105	H	2.2204661588	0.7798147003	-3.5326745544
C	-2.0942979634	2.9636848744	0.79106475	H	-3.2059692309	1.3338256889	-0.050052884
C	-4.2278338715	3.1415104491	-0.5551099988	H	-2.6649682526	2.95763253	1.733065182
C	0.7215969072	-3.797768726	0.12568809	H	-1.15246524	2.4102555743	0.932541111
C	1.8403801767	-2.8989936522	-0.4202297786	H	-1.8339065593	4.0077461697	0.5542790381
C	1.1462917725	-5.2640537445	0.0931660166	H	-4.8475531373	3.0939306067	0.3519119821
C	-1.6255749111	-0.3400529726	3.0415054138	H	-4.8134217469	2.7397492616	-1.3947773565
C	-2.8998219957	-0.5801203537	3.8565745364	H	-4.0288409935	4.2050046748	-0.7554197783
C	-0.7702630437	0.7778942376	3.6497612612	H	-0.1481220385	-3.6883878516	-0.5417199232
O	1.1680745765	0.0298745055	1.172735709	H	2.1329683902	-3.2183956931	-1.4323723737
P	3.0327525184	0.7270792359	0.813797969	H	1.5414954276	-1.8417143934	-0.4550175818
C	3.5284608932	0.2644876179	2.5216635203	H	2.7255387781	-2.9642711167	0.2330781854
C	4.6015328378	0.9101635067	3.1515062931	H	1.3115761325	-5.5821330138	-0.9459183287
C	4.9928606348	0.5440612024	4.4379478923	H	0.3838283657	-5.9208584023	0.5368131291
C	4.3256168323	-0.4827257943	5.1055524998	H	2.091407388	-5.4202290565	0.6348859161
C	3.2653492606	-1.1379060693	4.4811652238	H	-1.9354476551	-0.0095789911	2.0387003037
C	2.8636156994	-0.7681609941	3.1980607904	H	-3.501284822	0.3399037725	3.9021943798
C	2.3568488836	2.4258332946	0.8887761681	H	-3.5164984142	-1.3742420971	3.4109584956
C	2.0688921498	3.0640026036	2.098164327	H	-2.6622806398	-0.8747898396	4.8902192083
C	1.4420824045	4.3119617497	2.1039044515	H	-1.3495801639	1.7113130771	3.7127477312
C	1.0910321996	4.9257183592	0.9035619626	H	0.1241934983	0.9593756932	3.0368119589
C	1.3604993006	4.2860836118	-0.3078426999	H	-0.4455159236	0.5106083602	4.6682236382

H	-2.6171205214	3.4824526986	0.6301057617	H	-0.6382394203	1.130888838	2.012268945
H	-1.2223805958	2.5382741518	0.0363100043	H	-0.4100096488	1.1358888888	3.7671980219
H	-1.5784533012	4.131246231	-0.6695770056	H	5.0445335919	-0.79580978	2.0774426597
H	-4.73160753	3.6587592684	-0.8077213411	H	5.7482204163	-2.2963492781	3.8992132971
H	-4.7165000507	3.075868808	-2.4911856414	H	4.567823009	-2.2668365512	6.097446185
H	-3.7318231919	4.4823181992	-2.0139664584	H	2.6408822106	-0.7125638828	6.4326067864
H	1.5037085009	-1.5750220708	-0.625981274	H	1.88254972	0.7506611128	4.6037795618
H	3.5196653404	-2.7615724395	-1.223818024	H	3.4377109729	2.6948360833	4.1310715103
H	3.691569456	-2.1774119245	0.451262834	H	2.6975990402	4.970492965	4.7761001779
H	3.3502130798	-3.8987560017	0.1280491894	H	1.0553770836	6.1994345833	3.3660078685
H	1.236398353	-3.6138309787	-2.0277796879	H	0.1649487869	5.1417575126	1.2945029254
H	-0.2175909853	-3.3374728085	-1.039214302	H	0.8970464314	2.850885616	0.6475475171
H	0.9535326255	-4.5941764268	-0.5657040956	H	5.3219537129	2.3327397023	1.8827443537
H	-2.4131602608	-0.6297483791	2.266089041	H	7.1415485799	2.5253143132	0.2012331315
H	-3.265905396	-0.0572043508	4.4613488933	H	6.8894116622	1.4655515002	-2.035220309
H	-2.7244459413	-1.7546101143	4.5145764995	H	4.8101726933	0.2122704838	-2.5910019387
H	-1.7350167871	-0.46789861	5.249553494	H	2.9873878871	0.0218411903	-0.8952404436
H	-1.9677266605	1.6666151498	3.0811371561				

TS3 [$E^\circ = -1213.3008282$; $G^\circ = -1212.788171$; $\nu_{\text{im}} = -216.16 \text{ cm}^{-1}$]

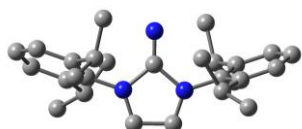


Charge = 0; Multiplicity = 2;

N	0.565229506	0.0778801203	1.078566257	C	-1.7975395926	-2.1196427301	3.0343692256
C	0.4187304334	1.3873846217	0.7688729308	C	4.8160086291	0.3565154358	1.6669623916
C	-0.2059374719	1.5926443618	-0.4717058722	C	3.5317625704	-1.378684744	0.3662060337
N	-0.5024101385	0.4606149776	-1.0449009945	H	0.7801465428	2.1403851741	1.4642197714
C	0.0669667322	-0.8872121533	0.1956412067	H	-0.4001623044	2.5824515011	-0.8989314406
C	1.1249869108	-0.3655275864	2.3270152163	H	0.1606561573	-1.4259850386	5.3963972297
C	-1.1513957955	0.2154535734	-2.260050457	H	2.6151301078	-1.5268552684	5.6795549075
N	-0.0918389675	-2.0424511606	0.0129678481	H	-0.5284415779	-1.1640592047	-5.3034456968
C	0.2464179012	-0.7150249757	3.3627972695	H	-2.9313550796	-0.6350205431	-5.589262833
C	0.8129266995	-1.1378604041	4.5700807946	H	-4.2100664183	0.3851125062	-3.7393765026
C	2.192425622	-1.1974869364	4.728956378	H	4.1194916446	-0.9051552282	3.8216049461
C	-0.4168759933	-0.3988569376	-3.2921170216	H	-1.4858160864	-0.1544544221	2.2498445617
C	-1.0816451123	-0.694117607	-4.4870701406	H	1.3790232402	-0.3706166719	-2.149368816
C	-2.4294152966	-0.4017708044	-4.6490935712	H	-2.7316150091	1.7753443257	-0.6986142659
C	-3.1481435746	0.1789510896	-3.6043052414	H	2.9527734708	0.6624376815	0.6720171408
C	-2.5344817491	0.487698732	-2.3910063396	H	1.7526686473	1.0683590693	-4.1641305153
C	3.0400940763	-0.8465073912	3.6802331308	H	1.6547142947	-0.3679557594	-5.2074113436
C	2.524497565	-0.430890036	2.4505750581	H	2.9745327449	-0.2239777069	-4.028014797
C	-1.2617716817	-0.6905485803	3.1842184808	H	0.9620414409	-2.6766371299	-4.1250166699
C	1.0568459563	-0.7327641834	-3.1366511968	H	0.7128159073	-2.7301870145	-2.3544098282
C	-3.3299339389	0.9988395801	-1.1992982846	H	2.3484888291	-2.4783564897	-3.0271286674
C	3.4273196832	-0.136290829	1.2633019413	H	-5.3682412103	0.8905180749	-1.9731342064
C	1.9060955785	-0.0202074509	-4.193624205	H	-4.5385709008	2.424596738	-2.3368971321
C	1.2806203388	-2.2475465126	-3.1617914074	H	-5.130267447	2.0867609212	-0.6901109519
C	-4.6637235859	1.6379713936	-1.5786504247	H	-2.6004967565	-0.6341253285	0.0770191358
C	-3.5460364122	-0.1416746561	-0.1934732173	H	-4.1991346379	-0.9091954437	-0.6359915404
C	-1.9661737343	0.05596545	4.3196716159	H	-4.0272937292	0.2334044497	0.7232390952

H	-1.573258605	1.0763891614	4.436326971	H	5.402719642	-0.4417374401	2.1457508739
H	-1.8471984936	-0.4656167333	5.2812395494	H	4.7619245773	1.2064728368	2.3625503197
H	-3.044489204	0.1221034886	4.1140602755	H	5.3728812071	0.6751977992	0.7745581235
H	-1.6103944925	-2.6985110353	3.952597428	H	2.543904869	-1.7421605842	0.049431962
H	-1.3105382053	-2.6293900455	2.1913331106	H	4.0282136279	-2.1946738422	0.9135794039
H	-2.8831809824	-2.1036232831	2.8559538549	H	4.1283940315	-1.1537781713	-0.5308808587

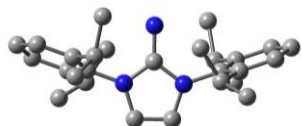
IM2⁺(singlet) [$E^\circ = -1213.063767$; $G^\circ = -1212.548529$]



Charge = +1; Multiplicity = 1;

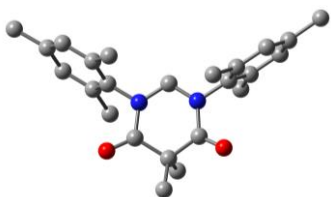
N	0.5452660457	0.2779914456	1.07603862	H	2.5644402282	-1.8876496626	5.4327258835
C	0.4980268538	1.5350083948	0.7795818201	H	-0.4714583888	-1.2064786566	-5.176773684
C	-0.1516672131	1.673658646	-0.5111467333	H	-2.882406432	-0.7353312253	-5.4514072156
N	-0.4766020049	0.4944811253	-0.9295814692	H	-4.1833659787	0.290045235	-3.6246767608
C	-0.0735928109	-0.5512424987	0.0283854093	H	4.0813151159	-1.0937147103	3.6566426824
C	1.105281364	-0.3074360324	2.2693638485	H	-1.5342894876	-0.0538199553	2.2047238472
C	-1.1395349109	0.1686864514	-2.1674178166	H	1.4739032474	-0.2841738052	-2.0741418578
N	-0.216439608	-1.765642372	-0.0289751911	H	-2.7164020937	1.678650011	-0.5324264475
C	0.2050971112	-0.7615845298	3.2428259106	H	2.9862237323	0.8384831396	0.6849802104
C	0.7689494153	-1.3326988476	4.3879058087	H	1.7492715454	1.017659149	-4.2072023261
C	2.1472248528	-1.4401217336	4.5298560511	H	1.6897454107	-0.5047658712	-5.1232445373
C	-0.3643585207	-0.4267800213	-3.1719584852	H	3.0073594917	-0.2242464465	-3.9735596873
C	-1.0294584046	-0.7448440103	-4.3605226371	H	1.0427010109	-2.714742604	-3.890296604
C	-2.3845889274	-0.4807577241	-4.514953442	H	0.8138879326	-2.6842246051	-2.1246578024
C	-3.1193891205	0.102843619	-3.4834944631	H	2.4403214066	-2.4325649275	-2.8287311977
C	-2.5174056594	0.4405953943	-2.2716340879	H	-5.339175033	1.0098722546	-1.949318509
C	3.0044004991	-0.9875640376	3.5278419209	H	-4.3910550894	2.4900978715	-2.2441658284
C	2.5057863398	-0.4103350378	2.359757155	H	-5.0702164636	2.1561068507	-0.6317221026
C	-1.3042134773	-0.6630227973	3.0949943149	H	-2.7766075805	-0.7720576229	0.1586287997
C	1.1199049014	-0.7178265254	-3.0242761083	H	-4.3364545585	-0.919563497	-0.6622964247
C	-3.3318618507	0.9563889905	-1.094168594	H	-4.1856440309	0.1587534049	0.7478217965
C	3.4218040536	-0.0302506631	1.2059929316	H	-1.5017664504	1.0288402383	4.4743814602
C	1.9337431564	-0.064275539	-4.1459357477	H	-1.8316194561	-0.5544277087	5.2135905223
C	1.3675971758	-2.2286729275	-2.957976126	H	-3.0239208841	0.1687816395	4.1225661606
C	-4.6009060256	1.6973723806	-1.5125704364	H	-1.7162405193	-2.7027135142	3.7342196449
C	-3.6699375746	-0.2093491003	-0.1513441086	H	-1.4734700727	-2.5322605367	1.9784798306
C	-1.9462898867	0.0393997548	4.2955374589	H	-2.9982353051	-1.9778961905	2.7366495458
C	-1.9089688505	-2.0529917216	2.8672437404	H	5.3824477371	-0.4706133344	2.0583478653
C	4.8211304993	0.3854527985	1.6578568156	H	4.7858007403	1.1672516284	2.4294095522
C	3.4943994278	-1.1928306577	0.2033998511	H	5.3898290033	0.7707861242	0.8007185663
H	0.8888016715	2.3232481736	1.4243560298	H	2.4982260005	-1.5177958117	-0.1323440395
H	-0.3447659813	2.5894917543	-1.0713195082	H	3.9768270927	-2.0613969785	0.6753404994
H	0.1129139009	-1.6983051283	5.1793399951	H	4.0895066877	-0.9069079058	-0.6765865694

IM2⁺(triplet) [$E^\circ = -1213.0884382$; $G^\circ = -1212.576350$]



Charge = +1; Multiplicity = 3;

N	0.5413888624	0.2693746375	1.0436319168	H	2.5076604837	-1.9206461743	5.4239566769
C	0.5059795021	1.5902279874	0.7402347044	H	-0.3789724089	-1.080910543	-5.210408769
C	-0.127540223	1.7219750363	-0.4828554348	H	-2.8155845598	-0.7535082713	-5.4672713189
N	-0.4803518851	0.4805631432	-0.8983574045	H	-4.1740775336	0.1251252091	-3.6039183863
C	-0.0704798495	-0.4293777133	0.0382238678	H	4.0370714504	-1.2388620462	3.6116527391
C	1.0817267711	-0.3349862321	2.2425873483	H	-1.542343137	0.0305950607	2.200444622
C	-1.1245751249	0.1326889003	-2.1469955856	H	1.5077862039	-0.1756858901	-2.0645389114
N	-0.2360795351	-1.7345064972	-0.0152730821	H	-2.7373974646	1.4561577794	-0.447238153
C	0.1785888739	-0.7092130261	3.246986477	H	2.970667467	0.7119777109	0.6361338877
C	0.7282798982	-1.2896328688	4.3951083963	H	1.7350873162	1.2221088067	-4.1328751576
C	2.1006438815	-1.4707308825	4.5175206216	H	1.7407239125	-0.2577280702	-5.1191846608
C	-0.3169939874	-0.3673889408	-3.1781250651	H	3.0459764905	0.0271035567	-3.9549004171
C	-0.9632003975	-0.6869134084	-4.3771088768	H	1.2051483055	-2.5477051167	-3.9861152022
C	-2.3332757348	-0.503898956	-4.5213142734	H	0.9646162556	-2.6140887362	-2.2261594863
C	-3.1006408179	-0.006331464	-3.4690726362	H	2.5785347455	-2.2500675252	-2.8968590792
C	-2.5149003421	0.3205246337	-2.2456341702	H	-5.3444022058	0.8649145439	-1.9382766081
C	2.9647410389	-1.0844956567	3.4936833031	H	-4.3911637095	2.3567788348	-2.1433625048
C	2.4755269695	-0.5084524573	2.3209195445	H	-5.096170237	1.9443954905	-0.5609474268
C	-1.3254862277	-0.5260901109	3.1276082641	H	-2.8073915845	-1.0000993663	0.1441662444
C	1.179920752	-0.5883485381	-3.0335697193	H	-4.3324348517	-1.1446473655	-0.7464751811
C	-3.3484183309	0.7694352312	-1.0554299002	H	-4.2551004537	-0.1270473262	0.7137480533
C	3.3917614352	-0.1636409661	1.1566597112	H	-1.3782934268	1.2750210365	4.3722893712
C	1.9664697992	0.1477640303	-4.1223988275	H	-1.7621037869	-0.2245449206	5.2465743233
C	1.4994611166	-2.087972999	-3.0308810997	H	-2.9578848803	0.4806303193	4.1445544565
C	-4.6128956641	1.5287913902	-1.45565642	H	-1.8575915234	-2.475908108	3.9401750959
C	-3.7000832088	-0.4441027104	-0.1813564418	H	-1.6499362898	-2.4726842287	2.174800798
C	-1.8830790966	0.3022749828	4.2890784854	H	-3.1096270673	-1.7514058026	2.906907721
C	-2.0251355646	-1.8864634104	3.0265086644	H	5.3474857413	-0.655560896	1.9950572672
C	4.8062581156	0.2137918931	1.5950922464	H	4.7985180542	0.9994837031	2.3632496169
C	3.428977872	-1.3299185951	0.1578002217	H	5.3782110334	0.5807624879	0.7320779961
H	0.9265370112	2.3402798775	1.4057188879	H	2.4255992493	-1.6148332242	-0.1941401622
H	-0.3468168941	2.606510351	-1.0761183378	H	3.8736209957	-2.2179478313	0.6307976784
H	0.0675175277	-1.6003541644	5.2060265296	H	4.0397658728	-1.0664865938	-0.718479039

DAC (3) [$E^\circ = -1189.9888733$; $G^\circ = -1189.577896$]

Charge = 0; Multiplicity = 1;

N	-0.3635113225	-2.290121138	1.3588883153	O	-3.8431207208	-0.8844881187	2.6731089093
C	-1.489667689	-3.0635797994	1.0008125888	H	-4.9152290716	-2.7755870506	1.2894474011
C	-2.8181503168	-2.3351893589	1.0710341361	H	-3.8559008025	-3.846491731	2.236941205
C	-2.8369502456	-1.2539948606	2.1348789728	H	-3.9587015241	-4.0621722509	0.4730365624
N	-1.5892791484	-0.63429829	2.3800930503	H	-3.9286808258	-1.0706829916	-0.3066792013
C	-0.3659262639	-1.1061619612	2.025918314	H	-2.9412894161	-2.3373358803	-1.0988489605
C	-3.9632338282	-3.3193092475	1.2792033073	H	-2.1561297852	-0.8711333884	-0.4376100877
C	-2.9656204688	-1.5996045419	-0.2847629711	C	0.9349979943	-2.8605026478	1.0718019088
O	-1.3834178236	-4.1887738326	0.5974868927	C	1.4619514914	-3.8257688613	1.9371551599

C	1.6223615474	-2.42393706	-0.0622823943	H	-1.5337953674	-1.6312612717	4.944464425
C	2.7206614718	-4.3483739383	1.6421772791	H	0.1590329201	-1.1648080835	4.6731771182
C	2.8812311013	-2.9738264269	-0.3189565383	H	-0.645893548	-0.7521499209	6.2137219968
C	3.4464520858	-3.934387834	0.5208091466	C	0.6852529019	-4.2842602535	3.1408297624
H	3.1473147833	-5.1017623484	2.3096609763	H	0.3474964187	-3.428079182	3.743746784
H	3.4329739402	-2.6411606983	-1.2018256172	H	-0.2055431621	-4.8511714892	2.8302813336
C	-1.6125571635	0.5587280101	3.1983326685	H	1.2998295606	-4.9326309581	3.7776347161
C	-1.2311735267	0.4687162076	4.539127584	C	1.0172185472	-1.3864115198	-0.9683703178
C	-2.0238265977	1.7661777106	2.6229053055	H	0.0619620522	-1.7392298395	-1.3884518185
C	-1.2586237434	1.6359356245	5.3077679459	H	0.8139454579	-0.4583890551	-0.4117515942
C	-2.038168144	2.9052969202	3.4271933365	H	1.6908935384	-1.1539805258	-1.8023269423
C	-1.6603437696	2.8599366436	4.772466851	C	4.8143344218	-4.5020337434	0.2452358908
H	-0.9587415273	1.5818968342	6.3572938782	H	4.8158354971	-5.5967696663	0.3424915523
H	-2.352767826	3.8566114028	2.9897291209	H	5.1564964598	-4.2458197059	-0.7659118188
C	-2.4302711815	1.8245896859	1.1758955715	H	5.5518824143	-4.1070349354	0.9604965311
H	-1.6342021511	1.4285753518	0.5270660271	C	-1.7068967521	4.1052119932	5.619238311
H	-3.3389894073	1.2276995665	0.9995808341	H	-1.212720063	4.9463657344	5.1125742508
H	-2.6408091162	2.8573176025	0.871487898	H	-2.7477053902	4.404717603	5.8152893506
C	-0.7892009996	-0.8417430269	5.1297836011	H	-1.2132809161	3.9490725429	6.5871444912

DACO (4) [$E^\circ = -1035.3747249$; $G^\circ = -1264.803970$]

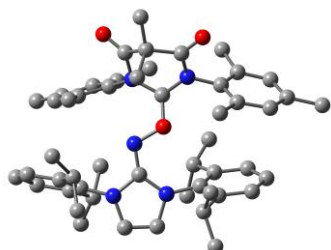


Charge = 0; Multiplicity = 1;

N	-0.3470366016	-2.2847268482	1.282225032	C	-1.1590468314	0.5013699871	4.4990554484
C	-1.481642185	-3.0337999306	0.9689825407	C	-2.1115896003	1.8070893139	2.6614952463
C	-2.8043685552	-2.2886076583	1.0273507695	C	-1.1922404942	1.6475701525	5.2977356586
C	-2.8290657364	-1.210923834	2.0985947401	C	-2.1307115944	2.9240903551	3.4952624021
N	-1.6140597614	-0.5681255936	2.3455241564	C	-1.6760223025	2.8642248987	4.8161582324
C	-3.9522433709	-3.2687909239	1.2385089944	H	-0.8314873014	1.5824904485	6.3271217597
C	-2.9513490542	-1.5599965127	-0.3298692884	H	-2.5096289765	3.8706858735	3.1007350469
O	-1.3988426274	-4.1720297212	0.5897203664	C	-2.6031498704	1.8812001756	1.2421890764
O	-3.845613054	-0.8602084258	2.6362420235	H	-1.8418405918	1.5088027532	0.5400908629
H	-4.9023482679	-2.7221715276	1.2434635766	H	-3.511038079	1.2713095724	1.1159612074
H	-3.8488428379	-3.7907734552	2.1993813792	H	-2.8460893905	2.9150557813	0.967410851
H	-3.9457116832	-4.0161320252	0.4367564055	C	-0.6224500956	-0.7998912161	5.0283705508
H	-3.9096596933	-1.0226318995	-0.3528371251	H	-1.3037483589	-1.6331562875	4.7987975182
H	-2.9358091732	-2.3006304075	-1.1415394146	H	0.3545785363	-1.0220590306	4.5709794388
H	-2.1369785875	-0.8386144531	-0.4913246211	H	-0.4895855542	-0.7552004391	6.116223594
C	0.9491413307	-2.8683812576	1.0336383772	C	0.6360801712	-4.2482692084	3.1234405067
C	1.4425195746	-3.8228818162	1.9274172823	H	0.2654195169	-3.3782798378	3.6856562643
C	1.6638580449	-2.4681576209	-0.0997851859	H	-0.2359082886	-4.8385345198	2.8035113006
C	2.69532545	-4.3799603823	1.6619492567	H	1.2394226071	-4.8632767499	3.8025062279
C	2.9117807141	-3.0491679918	-0.3249059207	C	1.0908547832	-1.4432301798	-1.0400287508
C	3.4449375768	-4.0043009792	0.5455123293	H	0.1210755508	-1.7763162604	-1.4414461436
H	3.0944317341	-5.1294581058	2.3499355869	H	0.9354287283	-0.4865534588	-0.5185266171
H	3.483343258	-2.748656846	-1.2068585313	H	1.7674329697	-1.2679668941	-1.88539924
C	-1.6227375941	0.6042906641	3.1851198217	C	4.8102441856	-4.5892834836	0.2956145595

H	4.9303190513	-5.5556167933	0.8025882742	C	-1.7252568513	4.0882030391	5.6928492623
H	4.9883633389	-4.7373993142	-0.7782319466	H	-1.2440939547	4.9451700381	5.2000611142
H	5.5953142121	-3.9144488477	0.6704932692	H	-2.7665750558	4.3732929856	5.9057706794
C	-0.3672465557	-1.0253621098	1.8977232035	H	-1.2191519106	3.9146913064	6.6511206753
O	0.6383015263	-0.3937390579	2.0750663957				

IM1' [$E^\circ = -2478.4995677$; $G^\circ = -2477.532448$]

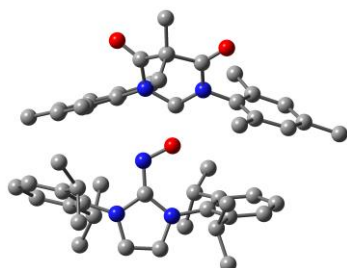


Charge = 0; Multiplicity = 2;

N	-0.2129424736	-2.133100485	1.2138666249	C	-2.5424443507	5.2460947974	0.5496237772
C	-1.3420338362	-2.8236062833	0.7910107772	C	-1.0849624863	5.7009836787	2.4237534534
C	-2.6151039636	-1.9881477143	0.7430309845	C	-2.2923714915	5.8903045868	1.760508397
C	-2.6634338868	-1.0698331214	1.9570818163	H	-3.5028331848	5.3933254859	0.0545424675
N	-1.4880482276	-0.3559164257	2.1926703206	H	-0.9080112802	6.1976056293	3.3799891909
C	-0.2760033649	-0.7788058641	1.6154586594	H	-3.0534684147	6.5421492223	2.193214815
C	-3.8335186425	-2.8992910057	0.7250534599	C	1.047115355	-2.8179892571	1.0545325087
C	-2.5660419587	-1.1064082472	-0.5255465277	C	1.6534322407	-3.4572325005	2.1450170461
O	-1.3056083894	-3.9849638603	0.4665029596	C	1.5570414394	-2.9722121713	-0.2450368695
O	-3.6515637175	-0.9332014603	2.6343407213	C	2.8433994446	-4.1592164458	1.9251507029
O	0.3854287968	0.0304697194	0.718697416	C	2.7178004848	-3.7220938637	-0.422717222
N	0.0009654778	1.3730351036	0.7455564444	C	3.3943848559	-4.2995414714	0.6526364662
C	0.9036127392	2.1340344356	0.1966911489	H	3.3252645511	-4.6511056112	2.7751102159
N	2.1584602659	1.9028668539	-0.3341365209	H	3.1113324508	-3.8471020936	-1.4346342228
C	2.7013317728	3.1222726111	-0.7698321073	C	-1.573882489	0.7081307628	3.1661533875
C	1.7994923181	4.0878145677	-0.5343877763	C	-0.960508119	0.5775209913	4.418194238
N	0.6800993001	3.4910267649	0.0417053017	C	-2.3985423971	1.8107465603	2.8806476905
H	-4.7475223916	-2.2945096401	0.6815972	C	-1.1531548398	1.5839314541	5.3706894608
H	-3.8726047491	-3.5141611241	1.6333165348	C	-2.5582675606	2.7915165592	3.8588305535
H	-3.7791028171	-3.5679669115	-0.1424586867	C	-1.9469545186	2.6982820363	5.1111196318
H	-3.4787807787	-0.4949137152	-0.5774722136	H	-0.6714409974	1.4795543011	6.3464972345
H	-2.5248054192	-1.7505483782	-1.4156945066	H	-3.1862806898	3.6564060525	3.6280864708
H	-1.6974008023	-0.4319924084	-0.5323411803	C	3.1615035514	0.7176408623	2.0951176893
H	3.6950639683	3.1583046745	-1.2025884835	H	2.1056074372	1.0305087084	2.1036832326
H	1.8326049646	5.1586449478	-0.7076161286	C	2.7457962163	0.9027292076	-3.0005485909
C	2.9353834599	0.702703628	-0.4415826576	H	2.0358343943	1.6917326093	-2.7155237168
C	3.467307545	0.1242538908	0.729024734	C	1.2039907347	4.6281676527	2.6323071905
C	3.2683158372	0.2474182813	-1.7280779422	H	1.9114406681	4.1415172594	1.9458245115
C	4.3511615001	-0.9433586583	0.5785736913	C	-1.8210041736	3.6912576049	-1.3473592058
C	4.1760813206	-0.8151872564	-1.8251997827	H	-1.3743076	2.6883334147	-1.2403261115
C	4.7147065381	-1.3990677909	-0.6877403183	C	-3.1430012881	1.9195953384	1.5828491185
H	4.770575321	-1.4288948025	1.4605099119	H	-2.4722473434	1.6984948176	0.7404283348
H	4.4661869422	-1.183145835	-2.812047016	H	-3.9827879997	1.2079645137	1.5675797011
H	5.4171430563	-2.229237903	-0.7826766556	H	-3.5455541653	2.9326861987	1.4640920815
C	-0.3658674401	4.2509747016	0.6544624682	C	-0.1529040874	-0.63956118	4.7570575102
C	-1.585735584	4.4070847796	-0.0261510003	H	-0.7576583124	-1.547203463	4.6177335561
C	-0.0933695894	4.8770940617	1.8815942755	H	0.7224954096	-0.7301509755	4.1002448925

H	0.1890204089	-0.6072873732	5.7998301195	C	3.8920739486	1.5565766407	-3.7820653869
C	-2.1504830063	3.7774634381	6.1420707137	H	3.5029276108	2.0934405142	-4.6595209709
H	-2.0257566621	4.7755440161	5.6951393816	H	4.45696535	2.2699438287	-3.1652051209
H	-3.1666717923	3.7342209654	6.5630702103	H	4.6027927246	0.7962297091	-4.1402815642
H	-1.4373765926	3.6794750635	6.9714605719	C	1.9882452127	-0.0781619778	-3.8995434721
C	1.034864096	-3.4817022019	3.5153439993	H	1.6651890063	0.4295234396	-4.820371062
H	1.5178627673	-2.7652397185	4.1970252457	H	2.6232675882	-0.9284538957	-4.1933322656
H	-0.0340440966	-3.2436183253	3.4735561458	H	1.0975660957	-0.475474749	-3.3972609209
H	1.1496462466	-4.4813957894	3.955591525	C	3.3389160258	-0.2816760814	3.2362091935
C	0.834007522	-2.3984674377	-1.4294290551	H	4.3990155788	-0.5322084699	3.3963794709
H	-0.1007051486	-2.9548726324	-1.6058739599	H	2.9600994416	0.1530231905	4.1728570319
H	0.5817149455	-1.3417647013	-1.2586155784	H	2.7914156009	-1.2141088993	3.0329681342
H	1.4564476842	-2.4736809054	-2.330110625	C	4.0324887522	1.9597602791	2.3320819538
C	4.6854908856	-5.0476195805	0.4489573593	H	5.0977515538	1.6810697819	2.3290413734
H	4.7247970211	-5.9529589305	1.0707511996	H	3.8810278129	2.7243531513	1.5557715028
H	4.8143077111	-5.3440487016	-0.6006395773	H	3.8008855845	2.413189594	3.3074480748
H	5.5485534462	-4.4220170433	0.7296599663	C	0.9480573642	3.6529314623	3.7828303923
C	-3.3002294725	3.509730641	-1.6852814061	H	1.8890592933	3.3891097224	4.2897667028
H	-3.779567799	4.4728566855	-1.9186077564	H	0.2756908636	4.1025754036	4.5293085058
H	-3.4012657323	2.8719678836	-2.5749941991	H	0.4661764793	2.732853365	3.4172350309
H	-3.8547717758	3.0380464247	-0.8622968783	C	1.8598019392	5.9197690148	3.1219077073
C	-1.1129762049	4.4157753931	-2.500472852	H	2.0287065025	6.6259869823	2.2958962833
H	-1.5129661637	5.4356464088	-2.6093474906	H	1.2422265371	6.4251710093	3.879698911
H	-0.0288885284	4.4872622994	-2.3403744801	H	2.8307636625	5.6959393084	3.5877719294
H	-1.2805917154	3.8818046641	-3.4477048272				

TS1' [$E^\circ = -2478.4506873$; $G^\circ = -2477.488327$; $\nu_{\text{im}} = -423.36 \text{ cm}^{-1}$]

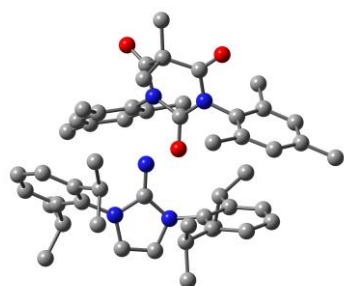


Charge = 0; Multiplicity = 2;

N	-0.3589153469	-2.2982593505	1.414055601	C	1.7821717264	4.0724761183	-0.4951470262
C	-1.4779366341	-2.9943006609	0.9340124896	N	0.6508698924	3.4745712256	0.0376097865
C	-2.7596028846	-2.1861896947	0.8725109285	H	-4.8872248631	-2.5097987873	0.7686177805
C	-2.8418827639	-1.2380692678	2.0511954171	H	-4.026056309	-3.7115913493	1.7558787675
N	-1.6346998202	-0.5918481583	2.3761365221	H	-3.8910064779	-3.7858843424	-0.0168585612
C	-0.3794076809	-1.0605404499	2.0368225068	H	-3.591380988	-0.701832868	-0.4795421449
C	-3.9705298263	-3.1074509778	0.8406476596	H	-2.6377947222	-1.9808154369	-1.2852350107
C	-2.6849493725	-1.320048166	-0.4077778468	H	-1.8013954979	-0.6659153795	-0.397418775
O	-1.413237456	-4.1362741894	0.5583216552	H	3.6796054473	3.1266565835	-1.1622068928
O	-3.8680284104	-1.0163852998	2.6388276729	H	1.8420967211	5.1481990834	-0.6256271973
O	0.2156068531	0.0506571349	0.5243983071	C	2.8457089668	0.651960892	-0.4480321499
N	-0.1062082019	1.3064819326	0.5631363993	C	3.3228985766	0.0731980384	0.7454562554
C	0.848838834	2.1214768081	0.1216991371	C	3.1704823366	0.1594819568	-1.7187189746
N	2.1054145032	1.882030087	-0.3690614175	C	4.1610561554	-1.0332981142	0.6281508546
C	2.6764072691	3.0927122519	-0.7495520585	C	4.0313280236	-0.944622103	-1.7812566097

C	4.52669818	-1.5271348691	-0.6239812538	H	-3.5045849417	3.7797470547	6.387790335
H	4.5297147065	-1.5277409225	1.5275838659	H	-1.8250281788	3.6681904384	6.9587546505
H	4.3129595269	-1.348991602	-2.7562377088	C	0.9508314845	-3.5619313069	3.7031359566
H	5.1894903044	-2.3918351611	-0.6906280205	H	1.2493397777	-2.6515216225	4.2414441202
C	-0.3793517182	4.2117868938	0.7125251815	H	-0.1468577877	-3.5809271667	3.6723856518
C	-1.5898900281	4.4720360841	0.0499284145	H	1.2972832958	-4.4266013781	4.2838621346
C	-0.0861831856	4.6951455834	1.9964928539	C	0.6918722141	-2.5477992715	-1.2598431906
C	-2.5130693351	5.2903880541	0.7046579729	H	-0.2513389087	-3.084325744	-1.4477833975
C	-1.0402297917	5.513026347	2.609526397	H	0.4652575452	-1.486044045	-1.0854748007
C	-2.2347283158	5.8164098167	1.9657907715	H	1.3180001497	-2.6375589411	-2.1572572258
H	-3.4674835309	5.5166452126	0.2282787183	C	4.5525863083	-5.18963188	0.6005455275
H	-0.8450028748	5.9084373981	3.6086652736	H	4.5715466679	-6.1274656696	1.1738257525
H	-2.9686682684	6.4581413137	2.456602286	H	4.7053280548	-5.4323810959	-0.4596166426
C	0.9023261658	-2.9804739619	1.230385561	H	5.4125431371	-4.5871826736	0.9359118466
C	1.5358593995	-3.5968388847	2.3191550689	C	-3.3371305306	3.7498036758	-1.6556248809
C	1.4011812107	-3.1337647498	-0.0722342203	H	-3.8173958436	4.7323491915	-1.7808886224
C	2.7258916409	-4.2939644603	2.09204326	H	-3.4591172382	3.2059379177	-2.6029912409
C	2.5678761006	-3.8767303187	-0.2558817394	H	-3.8754217579	3.1976253408	-0.8730266942
C	3.2602574989	-4.4449570566	0.812187867	C	-1.1538104189	4.7227455857	-2.4137447242
H	3.2262035038	-4.7676798877	2.9414810759	H	-1.5548206642	5.7478688915	-2.4211018112
H	2.9530047493	-3.9984361146	-1.2716235984	H	-0.0687175588	4.7817079479	-2.2529328562
C	-1.7665497177	0.528201217	3.2829395046	H	-1.3251175266	4.2805659052	-3.4062921058
C	-1.2642123553	0.4363359255	4.5892275267	C	3.8086748405	1.3618626187	-3.8367119766
C	-2.51576509	1.6503001767	2.8807001915	H	3.4244108632	1.8633601389	-4.7369548824
C	-1.4889867319	1.4964201106	5.473289954	H	4.4008244993	2.0901381964	-3.2635670934
C	-2.7067271769	2.6850805936	3.7978053082	H	4.4923120219	0.5632791888	-4.1623504117
C	-2.2073568567	2.6290098304	5.0991940137	C	1.8337312089	-0.2050584673	-3.832607492
H	-1.0945290393	1.4205595539	6.4900360353	H	1.4779283665	0.2728506895	-4.75724073
H	-3.2788141847	3.5604704705	3.4791546229	H	2.4356038551	-1.0813518273	-4.1186128302
C	3.0048133892	0.6930338752	2.0966190343	H	0.9619179733	-0.5619858685	-3.2688315893
H	1.9634624482	1.0494064526	2.0684413124	C	3.0781090841	-0.3042479434	3.2489279
C	2.6558696934	0.7876243455	-3.006017418	H	4.109489407	-0.6414897166	3.4367426155
H	1.9844594049	1.617388711	-2.7418749881	H	2.7157924255	0.1758803901	4.170340923
C	1.1834651937	4.3027858458	2.7329218729	H	2.444671517	-1.1765611957	3.0374425681
H	1.8437993471	3.772872515	2.0317683719	C	3.9400118413	1.8835646449	2.3552232314
C	-1.851304513	3.8905802199	-1.3296823872	H	4.9843764988	1.539658895	2.4112324482
H	-1.4129128328	2.8789367452	-1.330334015	H	3.8786179949	2.6430409709	1.5614328414
C	-3.1664443092	1.7447947347	1.5293791385	H	3.6897876548	2.3702532359	3.3100072568
H	-2.4708037303	1.432255036	0.7386045784	C	0.8400695845	3.3218677781	3.8567957207
H	-4.0659983712	1.1116382638	1.4957311019	H	1.7548005416	2.9551271487	4.348013708
H	-3.469008097	2.7825516819	1.3395135885	H	0.2175300513	3.8097785577	4.6223346896
C	-0.5082890217	-0.76946092	5.0646576723	H	0.2751596387	2.459375585	3.4696783144
H	-1.0021351812	-1.6983981714	4.7477990902	C	1.9546277558	5.5163731865	3.2536339857
H	0.5004801577	-0.7806007972	4.6308377321	H	2.202253838	6.2162481441	2.442013833
H	-0.431488912	-0.7689970858	6.1598610998	H	1.3745104437	6.065247585	4.0108840402
C	-2.453108804	3.7604285749	6.0625900266	H	2.8926227707	5.1920347534	3.7279259989
H	-2.2416260934	4.7322836597	5.5911443171				

TS2' [$E^\circ = -2478.4946912$; $G^\circ = -2477.526985$; $\nu_{\text{im}} = -722.55 \text{ cm}^{-1}$]



Charge = 0; Multiplicity = 2;

N	-0.2128417537	-2.4120767138	0.9250543377	C	1.0177328102	-2.995123312	0.4547865818
C	-1.3757311865	-3.1371269386	0.6969993146	C	1.7111394661	-3.8984931423	1.2691716425
C	-2.6590714317	-2.3646911508	0.960266339	C	1.3966552977	-2.7538244581	-0.8674619947
C	-2.5323837504	-1.5464634981	2.2377963111	C	2.8509934182	-4.511102369	0.7462900872
N	-1.3157502879	-0.881863458	2.3937010908	C	2.5242059168	-3.411880677	-1.3611931682
C	-0.1913289294	-1.2050647671	1.6322643402	C	3.2711961815	-4.280838811	-0.5662471844
C	-3.8366668714	-3.3222740161	1.0656594253	H	3.4064830756	-5.2144298297	1.3731085791
C	-2.8500563017	-1.3748553849	-0.2118208915	H	2.8292395598	-3.2303477901	-2.3947624795
O	-1.3542849896	-4.2652635377	0.2671968071	C	-1.2535608303	0.1536980535	3.3913058782
O	-3.4377912009	-1.4203735231	3.0250254298	C	-0.4663362472	-0.0336439339	4.5363883139
O	0.7022643528	-0.3110745903	1.3779272239	C	-2.067503734	1.2849036278	3.2399300202
N	0.0756416579	0.9557971301	0.5929021921	C	-0.5064085862	0.9368283848	5.537268262
C	1.0087865832	1.8557763763	0.5431270999	C	-2.0957917455	2.2151465515	4.2816973233
N	2.3922107658	1.7391834309	0.5938244409	C	-1.3300952779	2.0604864658	5.4376864535
C	2.9548743884	3.0187643477	0.4657953964	H	0.099270675	0.7916410016	6.4358795019
C	1.960429224	3.9072963745	0.3105731515	H	-2.7407223685	3.092035221	4.1753103477
N	0.7489517772	3.2139853548	0.3697476413	C	3.5846415904	-0.1157354642	2.4781248493
H	-4.7577223416	-2.7547968043	1.2453280841	H	2.5559402882	0.2338855128	2.6467719011
H	-3.6960246938	-4.0219933617	1.8998265161	C	2.7355536051	1.5499209107	-2.2880472578
H	-3.9219386566	-3.9031896489	0.1394289136	H	2.0061434294	2.1736106701	-1.7529732595
H	-3.767678686	-0.7906462361	-0.0502961298	C	0.2005945906	5.2129103501	2.4675545048
H	-2.9531104833	-1.9391708323	-1.1501492589	H	1.0517357256	4.5194232843	2.4411117021
H	-2.0017943179	-0.6786877516	-0.3046515794	C	-1.0719218002	2.7002250493	-1.8016049009
H	4.0318667437	3.1515861934	0.4669911799	H	-0.4004463752	1.8985053872	-1.4663232931
H	1.9861395386	4.9824408692	0.1742925243	C	-2.9201825825	1.4896642578	2.0209652668
C	3.1378966843	0.615838773	0.0812335101	H	-2.3664048597	1.1995492371	1.117043859
C	3.7534275696	-0.2774812824	0.9771414782	H	-3.8372127407	0.8835865221	2.0935515409
C	3.3267566351	0.5381935007	-1.3121544808	H	-3.2041207621	2.5465246769	1.926848835
C	4.5870147963	-1.2610848279	0.4404562116	C	0.3613803723	-1.2752347959	4.7057852869
C	4.1868519391	-0.4533852598	-1.7970823659	H	-0.2627279485	-2.1724807886	4.575488082
C	4.8154299041	-1.3371303848	-0.9311718601	H	1.1675243349	-1.3220159507	3.958589554
H	5.0703712133	-1.9814111163	1.1012851613	H	0.8139852437	-1.3103467748	5.704992955
H	4.3731192684	-0.524082483	-2.8710625887	C	-1.3797655866	3.0710102705	6.5542123031
H	5.47962374	-2.1073834801	-1.328239177	H	-2.0907960325	3.8777934912	6.3317423832
C	-0.5425486776	3.8251929857	0.424422966	H	-1.6870687179	2.5966932348	7.4979175152
C	-1.4771537283	3.5195799921	-0.5867264338	H	-0.3911346899	3.5251334505	6.7219810989
C	-0.8367504127	4.7367166821	1.4592556064	C	1.185019236	-4.2613366224	2.6292981095
C	-2.7464628508	4.0946825317	-0.5036859802	H	0.9556255099	-3.3696868042	3.2262003333
C	-2.1182148169	5.2996252516	1.4851923069	H	0.2526097806	-4.8378459143	2.520200396
C	-3.0698917831	4.9727855857	0.5271943555	H	1.9085210526	-4.8754113399	3.180657061
H	-3.492754045	3.864567009	-1.264077193	C	0.5635363107	-1.8555837588	-1.7344877595
H	-2.3705947713	6.0123878363	2.2723561783	H	-0.4404172646	-2.2867996072	-1.8781360855
H	-4.0662167279	5.4152668404	0.5744087611	H	0.4394594938	-0.8641262352	-1.2678030742

H	1.0281304692	-1.7347588704	-2.7207358253	H	2.5964541142	0.1328209823	-3.9577966412
C	4.5114136305	-4.9518510622	-1.0958774293	H	1.0529803629	0.4326227816	-3.1223586453
H	4.4833217827	-6.0365975965	-0.9186284431	C	3.7720249992	-1.4252898954	3.242352397
H	4.6271601351	-4.7841108322	-2.1748905846	H	4.8180084031	-1.7677205569	3.2118247959
H	5.4113331495	-4.5638096692	-0.5922065725	H	3.5092190073	-1.283489161	4.3006461844
C	-2.2471859206	2.0203604485	-2.5007615381	H	3.1391090005	-2.2238272714	2.8269633519
H	-2.9027575746	2.7465312656	-3.0052531861	C	4.5472794368	0.9530730172	3.0106919741
H	-1.8719013983	1.3304715633	-3.2707779854	H	5.5917377904	0.6565796482	2.8270464734
H	-2.8540884626	1.4422515727	-1.788734953	H	4.3771164976	1.9267695926	2.5305379075
C	-0.3043810447	3.6034041773	-2.7768198193	H	4.4134613805	1.0843114042	4.0949127185
H	-0.9455333111	4.4308979151	-3.1180289118	C	-0.3067801585	5.2274153188	3.9091910586
H	0.5885788098	4.0405641671	-2.303386747	H	0.4970495852	5.5607855251	4.5822535726
H	0.0192749525	3.0332607084	-3.6597822429	H	-1.1518339738	5.919963423	4.0421960726
C	3.8398740536	2.4733186151	-2.8191272908	H	-0.6223555556	4.2258488001	4.2195824541
H	3.4064665997	3.2726135978	-3.4389545146	C	0.6939326878	6.6140793631	2.0789606495
H	4.4066760006	2.9395015112	-2.0017405769	H	1.0425828721	6.6649463078	1.0376230066
H	4.5495914603	1.9063797847	-3.441470756	H	-0.1243419533	7.3437780235	2.1791308361
C	1.9878831383	0.9006570345	-3.4564893195	H	1.5153352404	6.9328486016	2.7375273225
H	1.7386304025	1.6625144445	-4.209413379				

References

-
- ¹ a) J. Park, H. Song, Y. Kim, B. Eun, Y. Kim, D. Y. Bae, S. Park, Y. M. Rhee, W. J. Kim, K. Kim, E. Lee, *J. Am. Chem. Soc.* **2015**, *137*, 4642–4645. b) T. W. Hudnall, J. P. Moerdyk, C. W. Bielawski, *Chem. Commun.* **2010**, *46*, 4288–4290.
- ² G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw and K. I. Goldberg, *Organometallics*, 2010, **29**, 2176.
- ³ O.V. Dolomanov, L.J. Bourhis, R.J. Gildea, J.A.K. Howard, H. Puschmann, *J. Appl. Cryst.* **2009**, *42*, 339–341.
- ⁴ G.M. Sheldrick, *Acta Cryst.* **2015**, *A71*, 3–8.
- ⁵ G.M. Sheldrick, *Acta Cryst.* **2015**, *C71*, 3–8.
- ⁶ M. J. Frisch *et al.*, Gaussian 09, Revision B.01 (Gaussian, Inc., Wallingford CT, 2010).
- ⁷ Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215–241.
- ⁸ F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297–3305.
- ⁹ M. Page, C. Doubleday Jr., J. W. McIver Jr., *J. Chem. Phys.* **1990**, *93*, 5634–5642.
- ¹⁰ T. Lu, F. Chen, *J. Comp. Chem.* **2012**, *33*, 580–592.
- ¹¹ a) G. Knizia, *J. Chem. Theory Comput.* **2013**, *9*, 4834–4843. b) G. Knizia, J.E.M.N. Klein, *Angew. Chem. Int. Ed.* **2015**, *54*, 5518–5522.