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**Supporting Information**

(72 pages including the cover page)

***Cooperative Ruthenium Catalyst for Deaminative Coupling of  
Primary Amines to Symmetrical Secondary Amines***

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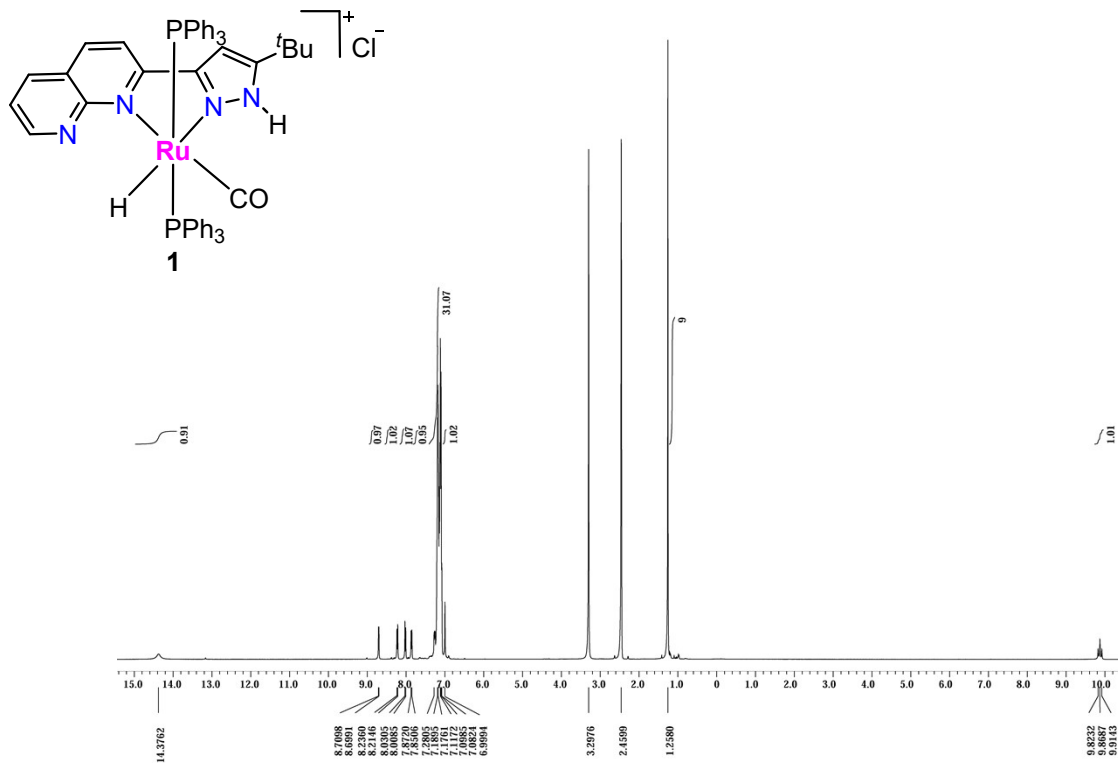
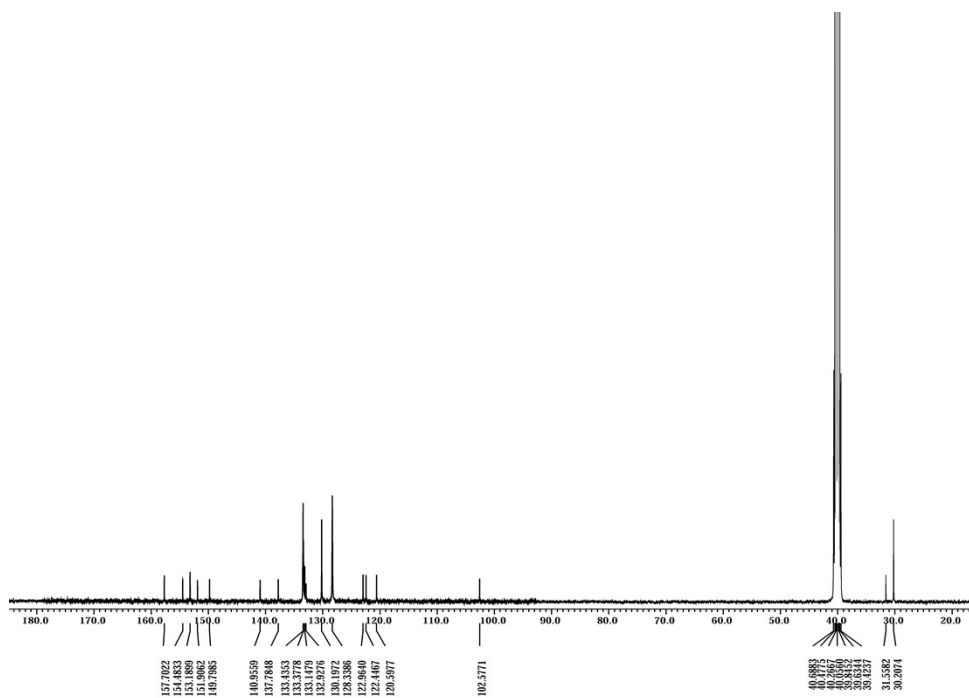
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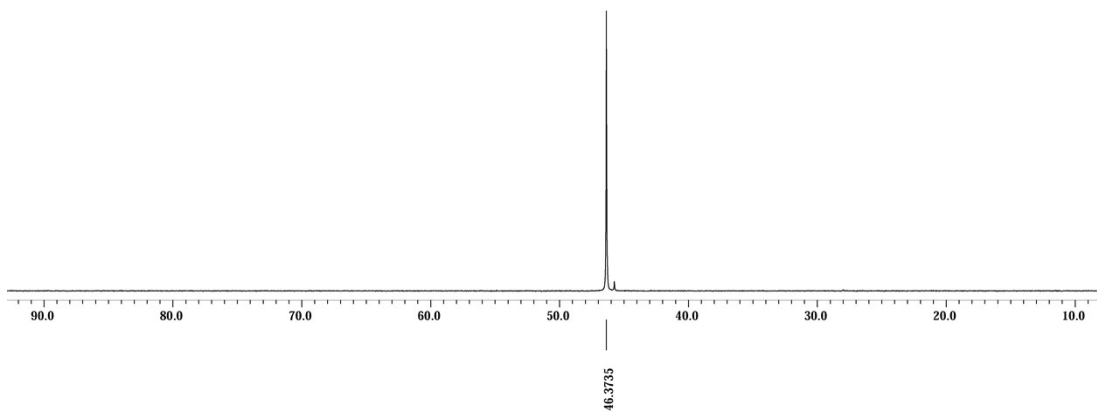
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## 1. X-Ray Data Collection and Refinements Parameters for Complexes 1, 2, 3 and 4.

Table S1. Crystallographic Data and Refinement Parameters for Complexes 1, 2, 3 and 4.				
	1.CH <sub>2</sub> Cl <sub>2</sub>	2.Et <sub>2</sub> O	3	4.CH <sub>2</sub> Cl <sub>2</sub>
Empirical formula	C <sub>53</sub> H <sub>49</sub> N <sub>4</sub> OP <sub>2</sub> Cl <sub>3</sub> Ru	C <sub>56</sub> H <sub>53</sub> N <sub>4</sub> O <sub>2</sub> P <sub>2</sub> Ru	C <sub>53</sub> H <sub>49</sub> N <sub>4</sub> OP <sub>2</sub> ClRu	C <sub>50</sub> H <sub>48</sub> N <sub>3</sub> OP <sub>2</sub> Cl <sub>3</sub> Ru
Formula Weight	1027.32	977.03	956.42	974.50
Crystal System	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space Group	<i>P2<sub>1</sub>/n</i>	<i>C2/c</i>	<i>P2<sub>1</sub>/n</i>	<i>P<sub>1</sub></i>
a (Å)	13.990(2)	40.571(2)	16.1059(9)	10.3020(2)
b (Å)	20.087(3)	11.2694(5)	15.2451(7)	14.3537(3)
c (Å)	19.489(3)	24.0395(11)	21.8945(11)	17.0125(4)
α (deg)	90.00	90.00	90.00	93.451(10)
β (deg)	102.038(3)	116.642(2)	103.724(2)	104.760(10)
γ (deg)	90.00	90.00	90.00	109.298(10)
V (Å <sup>3</sup> )	5356.3(15)	9824.2(8)	5222.4(5)	2267.05(9)
Z	4	8	4	2
ρ <sub>calcd</sub> (g cm <sup>-3</sup> )	1.274	1.322	1.216	1.428
μ (mm <sup>-1</sup> )	0.541	0.430	0.451	0.631
F(000)	2112	4060	1976	1002
Reflections Collected	50434	56524	41318	38910
Independent	13290	8373	9228	11227
Observed [I > 2σ(I)]	10072	6554	5834	10285
No. of variables	584	589	590	574
GooF	1.044	1.035	1.032	1.039
R <sub>int</sub>	0.0843	0.0665	0.0905	0.0271
Final R indices	R1 = 0.0677	R1 = 0.0414	R1 = 0.0575	R1 = 0.0308
[I > 2σ(I)] <sup>a</sup>	wR2 = 0.1671	wR2 = 0.0965	wR2 = 0.1135	wR2 = 0.0768
R indices (all data) <sup>a</sup>	R1 = 0.0891	R1 = 0.0613	R1 = 0.1062	R1 = 0.0347
	wR2 = 0.1780	wR2 = 0.1042	wR2 = 0.1283	wR2 = 0.0790
<sup>a</sup> R <sub>1</sub> = Σ   F <sub>o</sub> -  F <sub>c</sub>    / Σ  F <sub>o</sub>   with F <sub>o</sub> <sup>2</sup> > 2σ(F <sub>o</sub> <sup>2</sup> ). wR <sub>2</sub> = [Σw( F <sub>o</sub> <sup>2</sup> -  F <sub>c</sub> <sup>2</sup>   ) <sup>2</sup> / Σ F <sub>o</sub> <sup>2</sup>   <sup>2</sup> ] <sup>1/2</sup>				

## 2. NMR Spectra of Metal Complexes.

Figure S1. <sup>1</sup>H NMR spectrum for **1** in DMSO-*d*<sub>6</sub>Figure S2. <sup>13</sup>C NMR spectrum for **1** in DMSO-*d*<sub>6</sub>



**Figure S3.**  $^{31}\text{P}\{\text{H}\}$  NMR spectrum for **1** in  $\text{DMSO-}d_6$

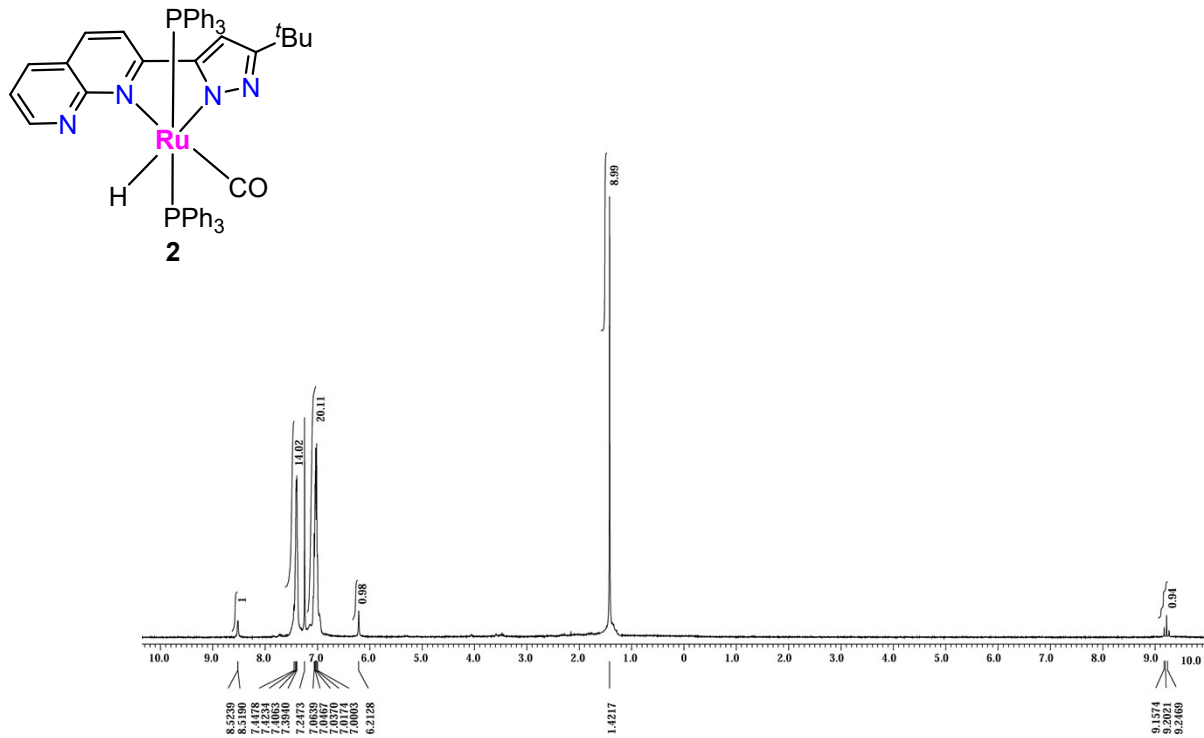


Figure S4.  $^1\text{H}$  NMR spectrum for **2** in  $\text{CDCl}_3$

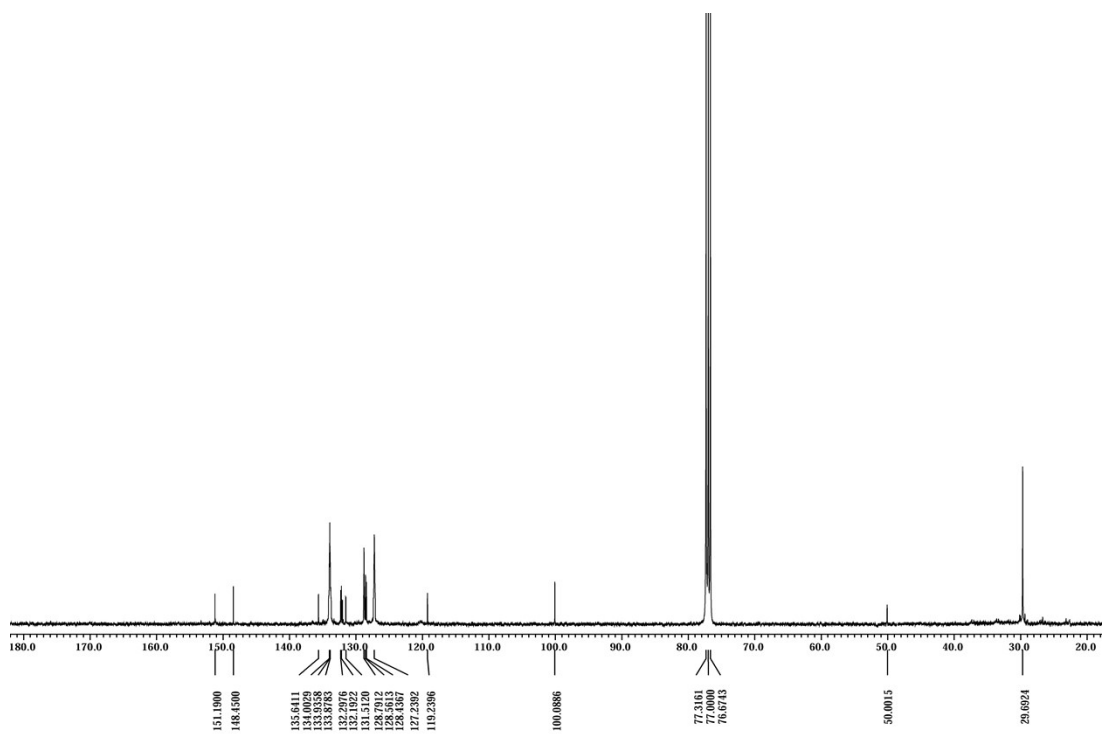
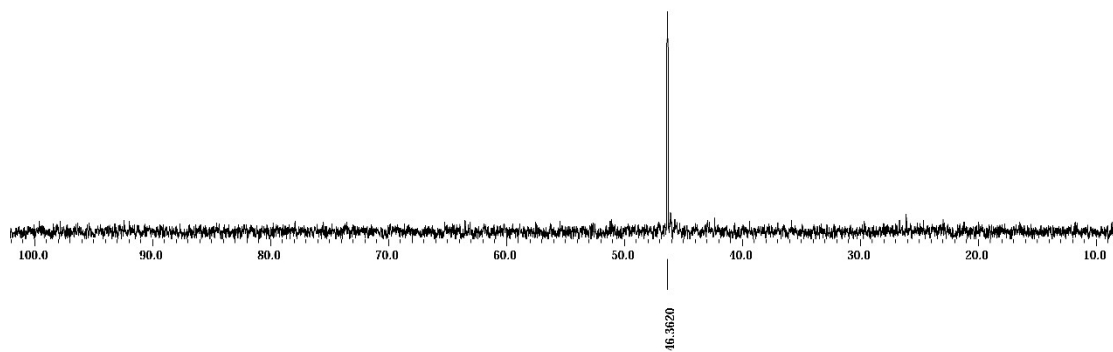


Figure S5.  $^{13}\text{C}$  NMR spectrum for **2** in  $\text{CDCl}_3$



**Figure S6.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum for **2** in  $\text{CDCl}_3$

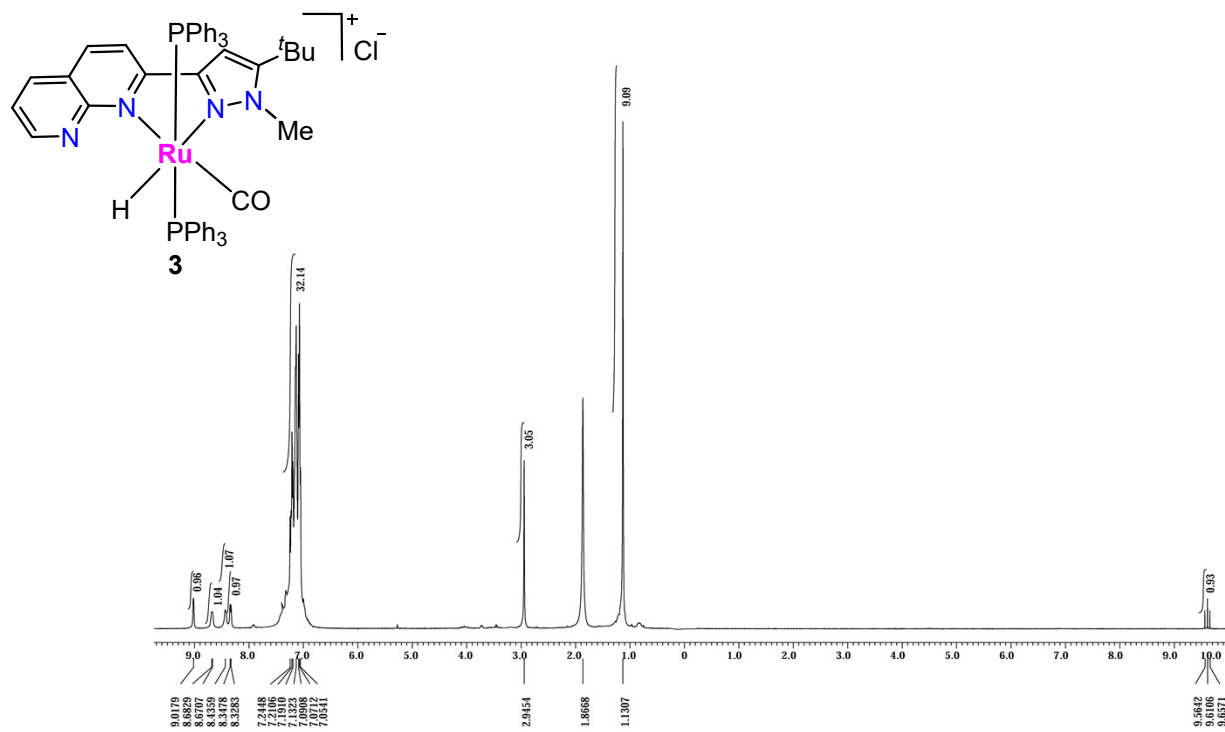


Figure S7.  $^1\text{H}$  NMR spectrum for **3** in  $\text{CDCl}_3$

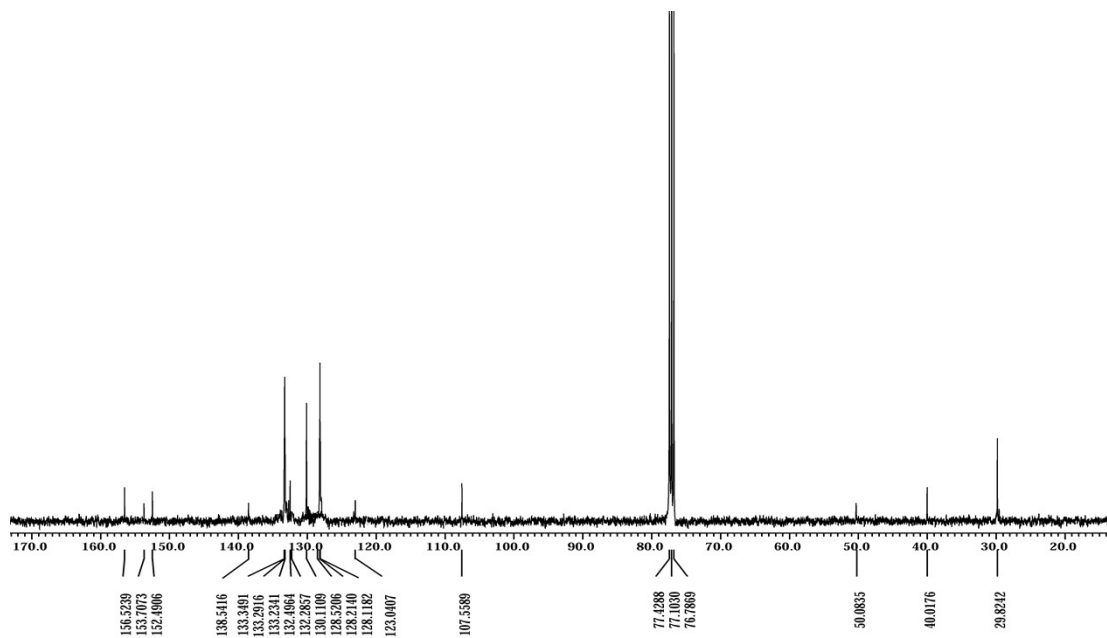
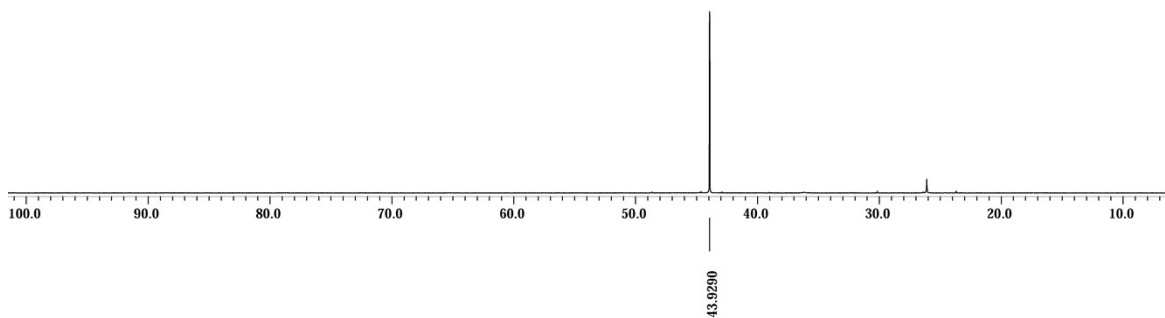


Figure S8.  $^{13}\text{C}$  NMR spectrum for **3** in  $\text{CDCl}_3$



**Figure S9.**  $^{31}\text{P}\{\text{H}\}$  NMR spectrum for **3** in  $\text{CDCl}_3$

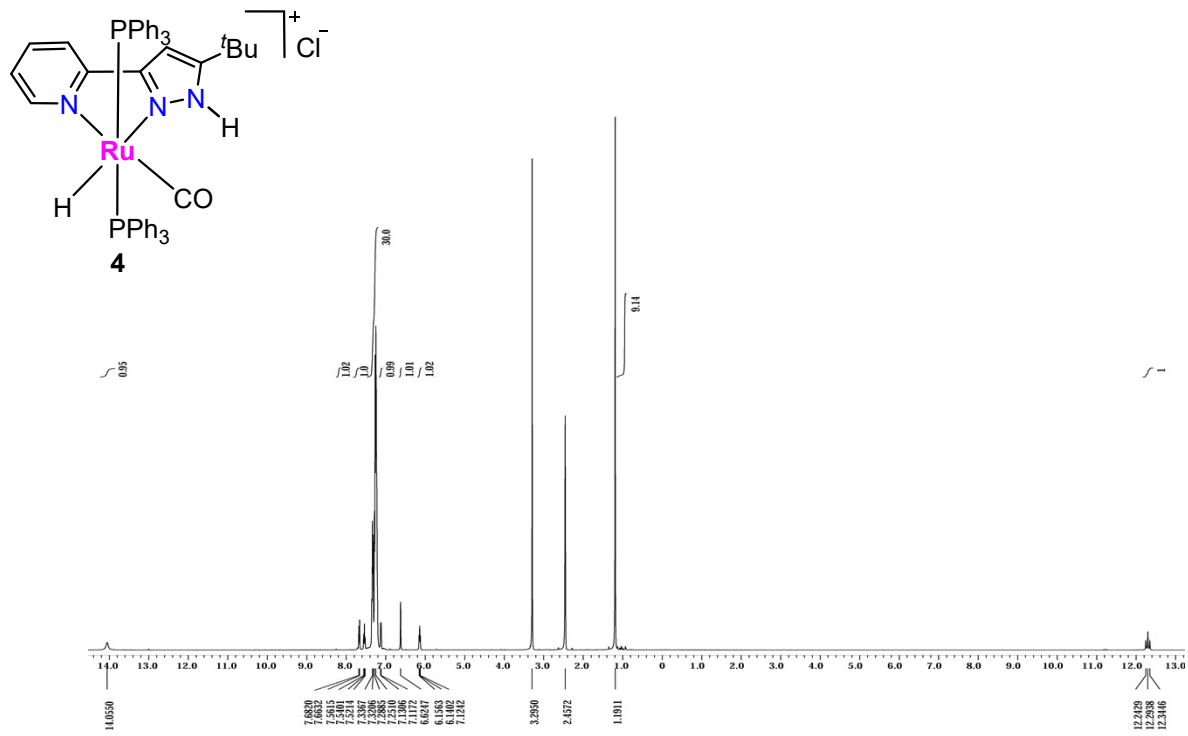


Figure S10.  $^1\text{H}$  NMR spectrum for **4** in  $\text{DMSO-}d_6$

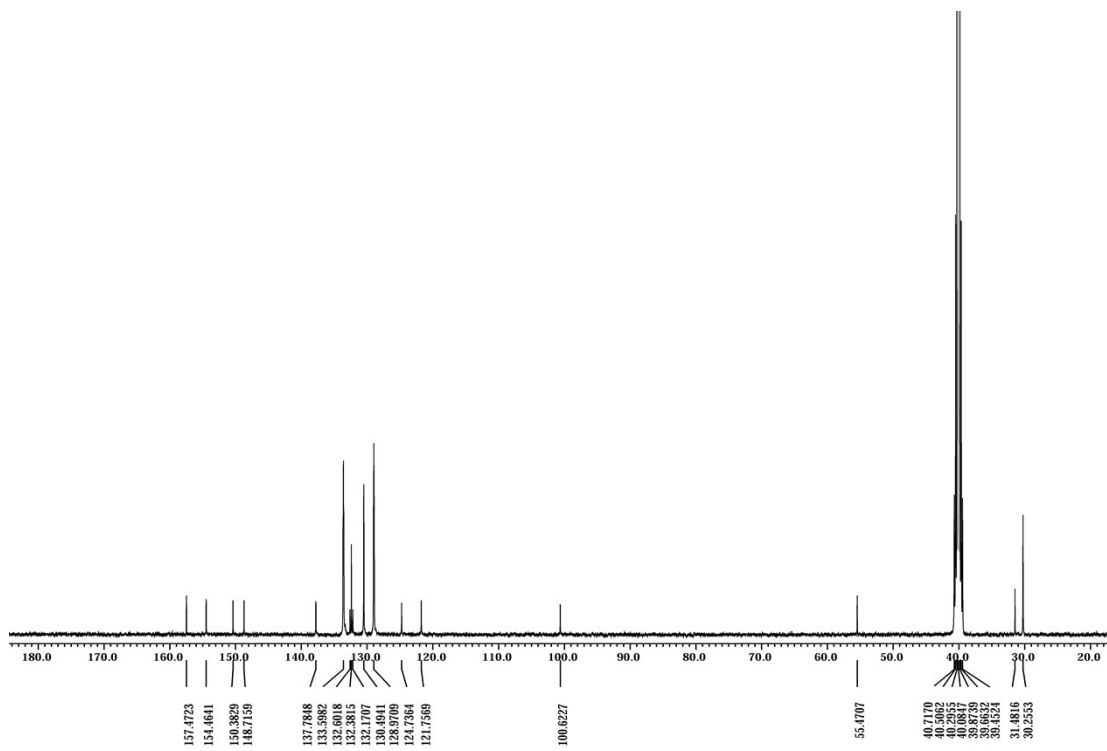
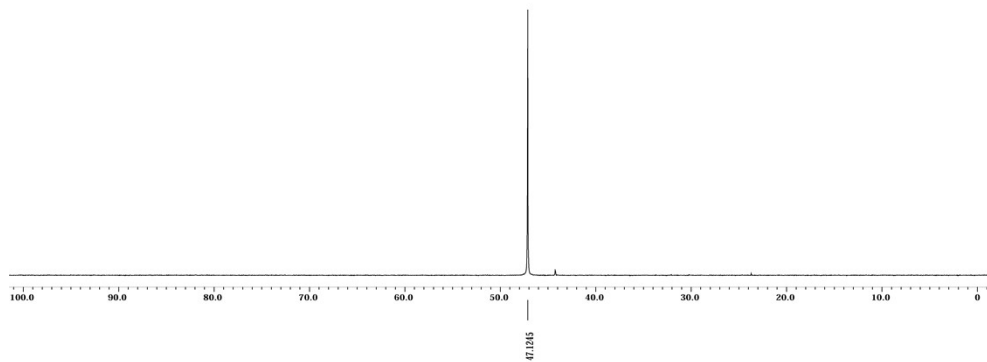
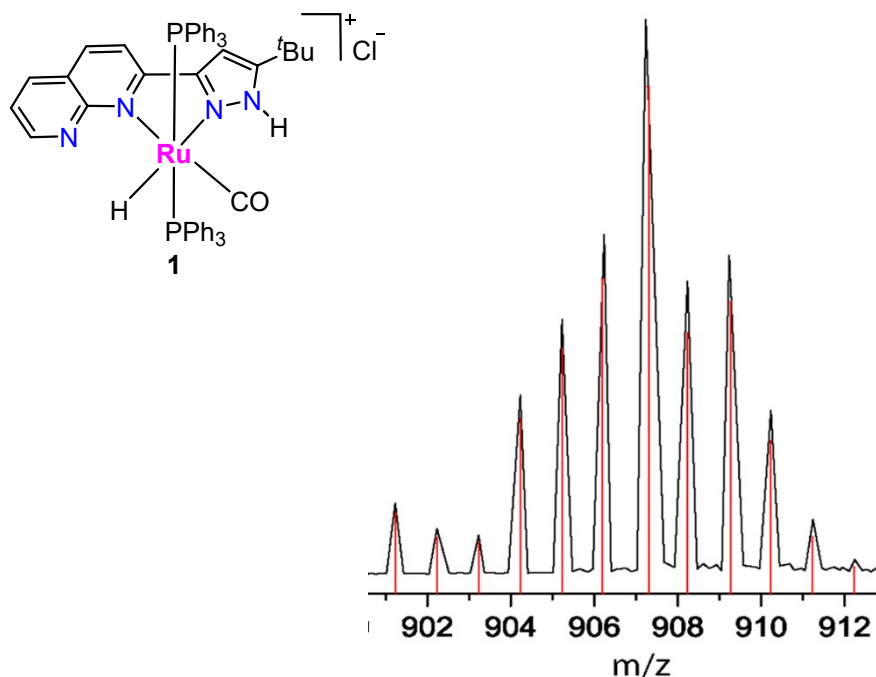


Figure S11.  $^{13}\text{C}$  NMR spectrum for **4** in  $\text{DMSO-}d_6$

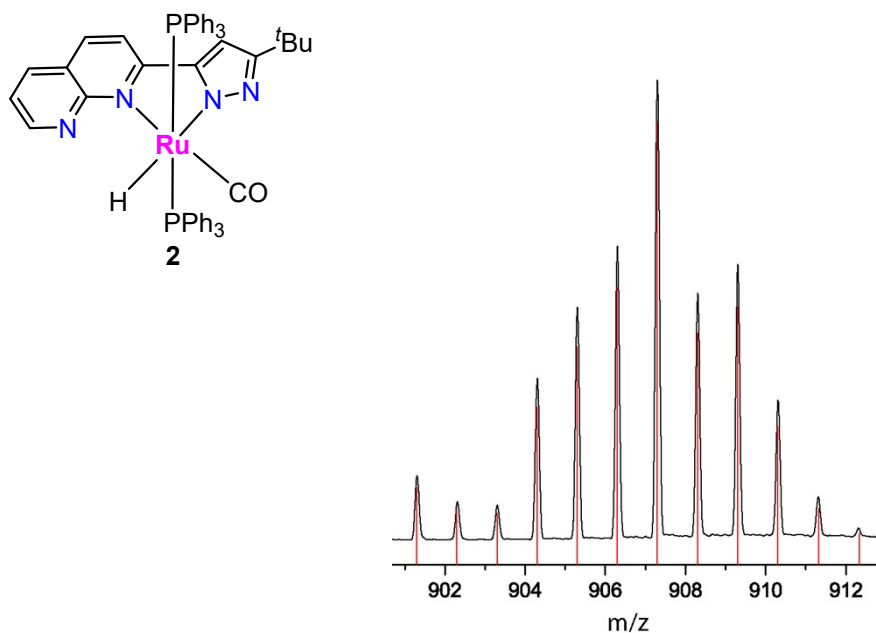


**Figure S12.**  $^{31}\text{P}\{\text{H}\}$  NMR spectrum for **4** in  $\text{DMSO-}d_6$

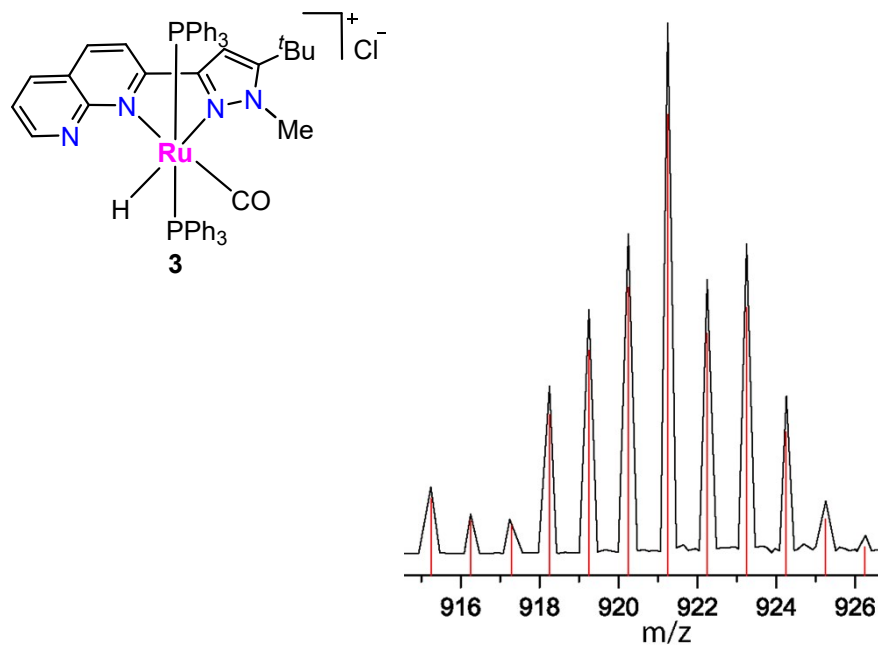
### 3. ESI-MS of Metal Complexes



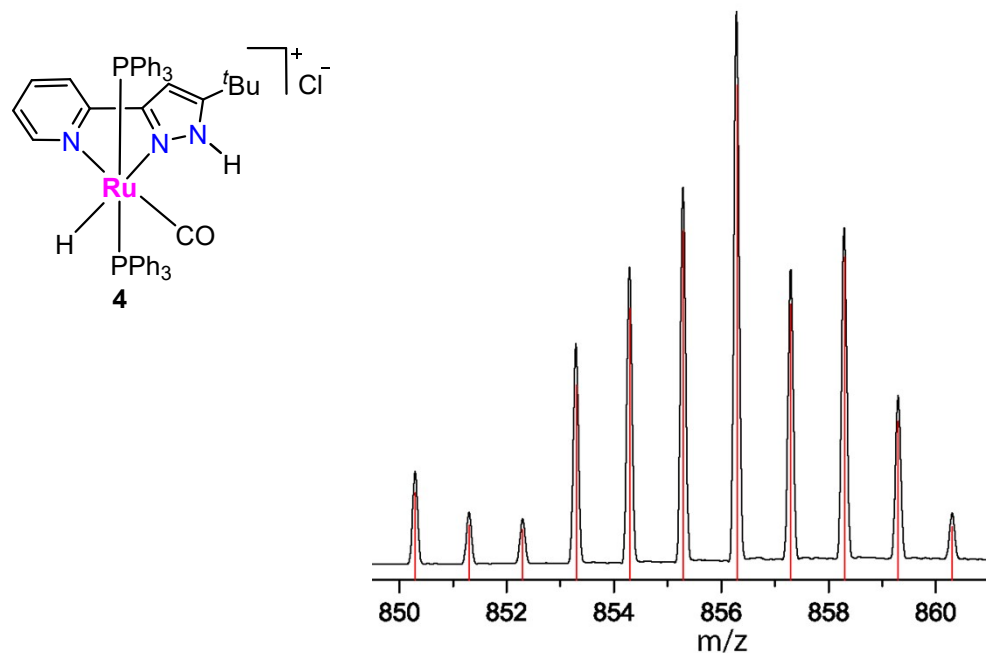
**Figure S13.** Experimental (black) and simulated (red) ESI-MS Spectrum for molecular ion at  $m/z = 907.2305$  ( $z=1$ ) in complex 1.



**Figure S14.** Experimental (black) and simulated (red) ESI-MS Spectrum for molecular ion at  $m/z = 907.2291$  ( $z=1$ ) in complex 2.

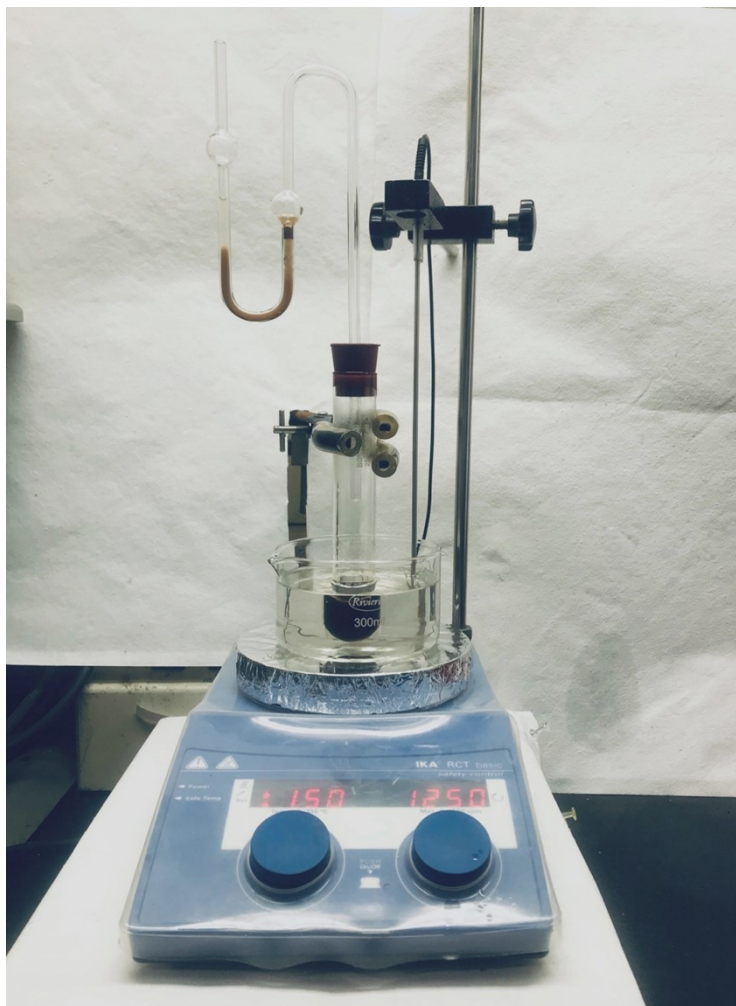


**Figure S15.** Experimental (black) and simulated (red) ESI-MS Spectrum for molecular ion at  $m/z = 921.2469$  ( $z=1$ ) in complex 3.

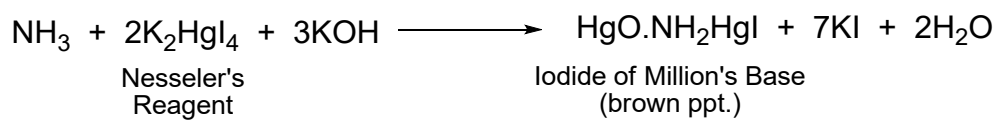


**Figure S16.** Experimental (black) and simulated (red) ESI-MS Spectrum for molecular ion at  $m/z = 856.2159$  ( $z=1$ ) in complex 4.

#### 4. Qualitative Analysis of Ammonia Gas.

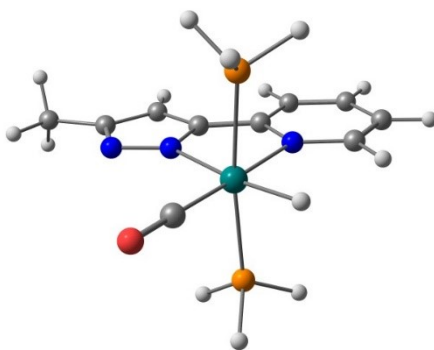


**Figure S17.** Qualitative  $\text{NH}_3$  gas detection using Nessler's reagent



## 5. Coordinates of DFT Optimized Structures

	Product - Reactant	$\Delta E = E_{\text{product}} - E_{\text{reactant}}$ (energies in Hartree)	$\Delta E$ (Kcal mole <sup>-1</sup> )
<b>A</b>			0 0.0
<b>TSAC</b>	(TSAC) – (A+I)	(-1391.1476) – (-1391.17954)	20.0
<b>C</b>	(C+II) – (A+I)	(-1065.17) – (-1065.4375)	4.1
<b>TSCA</b>	(TSCA) – (A+III+H <sub>2</sub> )	(-1661.4972) – (-1661.5268)	18.6
<b>A+V</b>	(A+V) – (A+III+H <sub>2</sub> )	(-1661.5338) – (-1661.52689)	-4.4
<b>TSBC</b>	(TSBC+CO) – (A+I)	(-1391.1217) – (-1391.1795)	36.29
<b>TSAB</b>	(TSAB) – (A+2*I)	(-1718.0626) – (-1718.1026)	25.09
<b>B</b>	B – (A+I)	(-1391.14570) – (-1391.1795)	21.23
<b>TS1</b>	(TS1) – (A+II)	(-1389.9281) – (-1389.985354)	34.58
<b>TS2</b>	(TS2) – (A+I+II)	(-1716.850262) – (-1716.908406)	36.49
<b>Energy Details of Intermediates and Transition states (EE+E<sub>Thermal free energy correction</sub>) in Hartree</b>			
<b>A</b>	-1064.2565	<b>TSAB</b>	-1718.063
<b>B</b>	-1391.1457	<b>TSBC</b>	-1277.745
<b>C</b>	-1065.4310	<b>TSCA</b>	-1661.4972
<b>I</b>	-326.9230	<b>TSAC</b>	-1391.148
<b>II</b>	-325.742	<b>H<sub>2</sub></b>	-1.181
<b>III</b>	-596.0893	<b>CO</b>	-113.376
<b>IV</b>	-56.5695	<b>TS1</b>	-1389.928
<b>V</b>	-597.2773	<b>TS2</b>	-1716.850



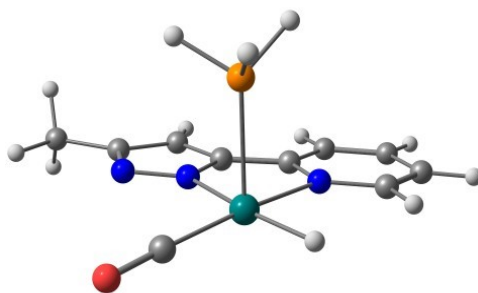
1

	Energy (in Hartree)
EE	-1407.6185
Thermal free energy corrections	0.1811
EE+E <sub>thermal free energy correction</sub>	-1407.4374

O 1

Ru	0.89668400	-0.79101100	-0.00000300
O	3.88262500	-0.49036500	-0.00012500
N	-1.29182300	-0.94228800	0.00014500
N	0.21178200	1.25364200	0.00045700
N	0.82176500	2.43157200	-0.00031700
C	-1.99110000	-2.08734800	0.00008400
C	-1.95750900	0.24900100	0.00020100
C	-3.37131300	-2.12668000	0.00000900
C	-3.36206800	0.26789200	0.00016300
H	-3.87201700	1.22091500	0.00024200
C	-1.13790600	1.42574700	0.00034300
C	-4.06688200	-0.91599100	0.00003500
H	-5.14961400	-0.90541900	-0.00001700
C	-0.13916600	3.38829800	-0.00079200
C	-1.40284800	2.80230100	-0.00058300
H	-2.36013500	3.29758200	-0.00102700
H	1.09971600	-2.40876900	-0.00033900
C	2.73733200	-0.59367400	-0.00009800
C	0.23635900	4.83562900	0.00019100
H	-0.17237200	5.36095500	-0.86687400
H	-0.12935900	5.34888700	0.89351700
H	1.32159500	4.93071600	-0.02494400
P	0.90545200	-0.95292600	2.31659800
H	2.02794600	-1.51229100	2.95574400

H	0.76540500	0.19589100	3.12700600
H	-0.08727500	-1.74572100	2.93078000
P	0.90524900	-0.95320500	-2.31653500
H	0.76660900	0.19534800	-3.12756600
H	2.02719200	-1.51414600	-2.95525800
H	-0.08833700	-1.74516300	-2.93040500
H	-1.40131600	-2.99352500	0.00007200
H	-3.88510000	-3.07741000	-0.00007500



A

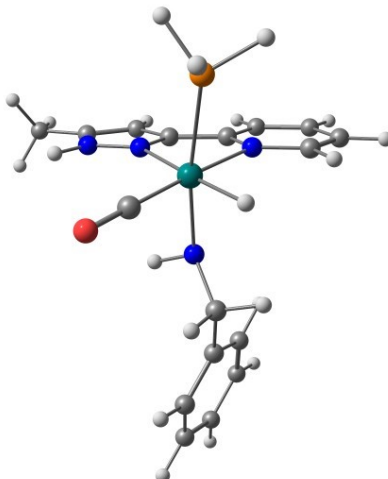
	Energy (in Hartree)
EE	-1064.4121
Thermal free energy corrections	0.1557
EE+E <sub>thermal free energy correction</sub>	-1064.2565

0 1

Ru	-0.40927	-1.18912	-0.39994
O	-3.26417	-1.82424	-1.11689
N	1.606292	-0.42509	-0.21476
N	-0.72497	0.760862	-0.1614
N	-1.84356	1.451751	-0.08835
C	2.750316	-1.11621	-0.27519
C	1.650401	0.930358	-0.08755
C	3.994423	-0.51958	-0.20951

---

C	2.88246	1.593729	-0.01371
H	2.896155	2.67008	0.085354
C	0.367394	1.566873	-0.04158
C	4.054175	0.868222	-0.07504
H	5.010578	1.372582	-0.02194
C	-1.49194	2.750307	0.081573
C	-0.10383	2.87547	0.116775
H	0.474991	3.776142	0.238776
H	-0.2366	-0.92152	-1.98102
C	-2.18156	-1.59687	-0.81448
C	-2.54409	3.804655	0.204737
H	-2.5294	4.277675	1.190266
H	-2.41082	4.594117	-0.53868
H	-3.52752	3.359877	0.056941
P	-0.68233	-1.56213	1.998814
H	-1.622	-0.73882	2.655131
H	-1.14249	-2.79325	2.519905
H	0.371014	-1.39067	2.929437
H	2.653028	-2.18997	-0.38375
H	4.888705	-1.12365	-0.26458

**B**

	Energy (in Hartree)
EE	-1391.4352
Thermal free energy corrections	0.2895
EE+E <sub>thermal free energy correction</sub>	-1391.1457

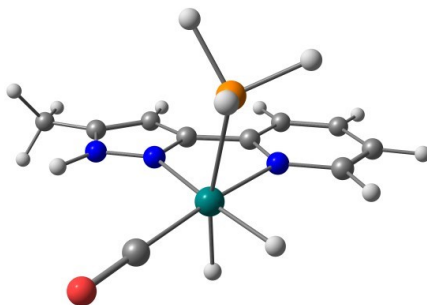
O 1

Ru	-0.85987200	-1.13797800	0.51043400
O	-0.31235000	-3.83090100	-0.65350600
N	-1.13593400	0.92348700	1.30335200
N	-1.46676000	0.10253600	-1.19149100
N	-1.65904100	-0.07113600	-2.50430400
C	-0.95467900	1.28030700	2.57667900
C	-1.36780800	1.88675600	0.38397200
C	-1.00108100	2.59906200	3.00217000
C	-1.43650600	3.23232300	0.74012600
H	-1.62696600	3.98054000	-0.01674100
C	-1.54677900	1.41723100	-0.98259900
C	-1.24878800	3.59291000	2.06356500
H	-1.29093700	4.63349700	2.35831600
C	-1.86803500	1.10186500	-3.16148800

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C	-1.80561000	2.08664300	-2.20051100
H	-1.92282800	3.14323000	-2.36669500
H	-0.29190800	-1.72457400	1.88907100
C	-0.53245700	-2.78902300	-0.20012200
C	-2.09917100	1.16506500	-4.63185900
H	-2.24951500	2.19822100	-4.93949100
H	-1.24587800	0.77001400	-5.18837700
H	-2.98358600	0.59451000	-4.92539900
P	-2.91322700	-1.81749100	1.31526500
H	-4.13678800	-1.76794900	0.59143700
H	-3.05939800	-3.15408700	1.74630700
H	-3.43602100	-1.21889400	2.49047600
H	-0.75549700	0.47233300	3.26665300
H	-0.84031300	2.83433000	4.04503700
H	-1.61533600	-1.00253600	-2.88411100
N	1.06840000	-0.41342900	0.06763400
H	1.20789900	-0.47606400	-0.93926600
C	2.23388900	-1.03388200	0.68904600
H	2.13659900	-0.92274500	1.77423000
H	2.32432900	-2.11762700	0.50938600
C	3.52792800	-0.38064700	0.24276200
C	4.54913800	-1.12453000	-0.34678200
C	3.72460100	0.99371600	0.40705800
C	5.73675400	-0.52197400	-0.75552100
H	4.41179400	-2.19126900	-0.48591000

C	4.90661200	1.60012400	0.00412600
H	2.92817900	1.58248400	0.84500100
C	5.92028200	0.84330000	-0.57987300
H	6.51624800	-1.12057000	-1.21190700
H	5.04259900	2.66601200	0.14630700
H	6.84251400	1.31605600	-0.89516400



C

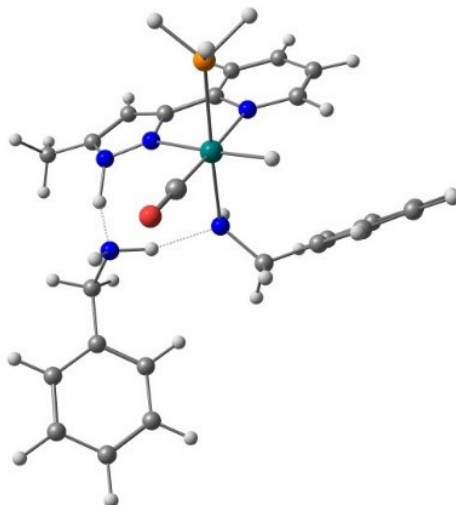
	Energy (in Hartree)
EE	-1065.6065
Thermal free energy corrections	0.1755
EE+E <sub>thermal free energy correction</sub>	-1065.4310

O 1

Ru	-1.13428500	-0.57333000	-0.37958000
O	-3.84483900	0.52620100	-1.00566300
N	0.94211400	-1.25159400	-0.24035600
N	0.05083600	1.19929200	-0.03808800
N	-0.17964500	2.51374200	0.04883200
C	1.33954000	-2.52578600	-0.36496400
C	1.88889400	-0.29552800	-0.05764500
C	2.66797200	-2.90913800	-0.30842200
C	3.24515200	-0.61424400	0.01028500
H	3.97223100	0.17260300	0.15720100

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C	1.37832400	1.05704900	0.04201300
C	3.64116900	-1.93322100	-0.11570900
H	4.68933400	-2.19836600	-0.06802800
C	0.96686000	3.23973400	0.17926500
C	1.99372500	2.32378900	0.18278800
H	3.04301000	2.54679200	0.26802800
H	-1.68926200	-2.02070100	-0.81489100
C	-2.80382500	0.09279600	-0.74440800
C	0.96257600	4.72562300	0.28503400
H	1.98279500	5.09384300	0.37704500
H	0.51642100	5.18963600	-0.59804800
H	0.40244400	5.06562700	1.15965300
P	-1.69379200	-1.29578700	1.79043800
H	-1.60751100	-0.57632900	3.01803700
H	-3.01421800	-1.74760400	2.00103900
H	-1.05522300	-2.45697500	2.29498000
H	0.54901800	-3.24516200	-0.52284500
H	2.92951700	-3.95241700	-0.41811100
H	-0.89204000	-0.45855700	-1.98594400
H	-1.12785800	2.84479600	-0.01998000



TSAB

	Energy (in Hartree)
EE	-1717.6394
Thermal free energy corrections	0.4232
EE+E <sub>thermal free energy correction</sub>	-1718.0626
Imaginary frequency	-1005.7 cm <sup>-1</sup>

0 1

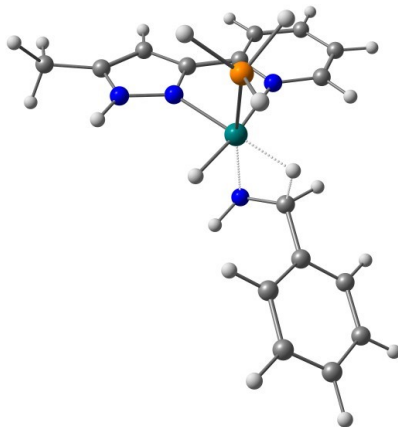
Ru	-0.99811100	-0.20596500	0.98341900
O	1.63402400	-0.29875800	2.37893100
N	-2.99740100	-0.19056600	-0.01520400
N	-1.06252400	-1.94590300	-0.37122100
N	-0.14757400	-2.82170400	-0.80098400
C	-3.92051500	0.76160800	0.16138400
C	-3.30841600	-1.27471100	-0.77027800
C	-5.19360700	0.68323600	-0.37933100
C	-4.57672800	-1.41980500	-1.33473000
H	-4.79975200	-2.29817900	-1.92440900
C	-2.22315500	-2.21735600	-0.97855700
C	-5.52758300	-0.43449900	-1.13551300

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H	-6.51481500	-0.53270200	-1.56890900
C	-0.72054500	-3.67790300	-1.68660400
C	-2.05633000	-3.33551900	-1.81940800
H	-2.78722900	-3.81497600	-2.44856800
H	-1.22561300	1.19142300	1.73539200
C	0.60956400	-0.26399000	1.83618500
C	0.05761200	-4.77265800	-2.33881200
H	-0.55286800	-5.28065800	-3.08448300
H	0.94880900	-4.38839300	-2.84102600
H	0.38782800	-5.51674600	-1.60994500
P	-1.99926200	-1.13540700	2.82353700
H	-2.17436500	-2.53290700	3.01098300
H	-1.46812000	-0.87349800	4.10444000
H	-3.33852900	-0.78206200	3.12208400
H	-3.60937900	1.61349400	0.74917000
H	-5.89806600	1.48562800	-0.21191500
H	0.97676700	-2.26933200	-0.77229800
N	-0.07760400	0.74429300	-0.71492900
H	1.34428400	-0.45576100	-0.83111600
C	0.21168300	2.17993200	-0.70713300
H	0.81654500	2.40380100	0.17390800
H	-0.68871900	0.56006000	-1.50818100
N	1.93974400	-1.33470400	-0.82839400
H	0.83162600	2.43560900	-1.58243300
C	-0.98513500	3.11339700	-0.72964300

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C	-1.39264500	3.81280000	0.40686900
C	-1.71741400	3.29167300	-1.90620100
C	-2.50149300	4.65313600	0.37479000
H	-0.83589200	3.69191800	1.32782100
C	-2.82831600	4.12573300	-1.94573300
H	-1.40804200	2.77310400	-2.80782900
C	-3.22676300	4.81021800	-0.80140600
H	-2.79605200	5.18998500	1.26884500
H	-3.37710500	4.25124600	-2.87155200
H	-4.08626100	5.46872300	-0.83018400
H	2.51158600	-1.32828600	0.01175900
C	2.77783400	-1.44462200	-2.03847300
H	3.12969400	-2.47501900	-2.12886500
H	2.12468300	-1.25206700	-2.89286100
C	3.96553100	-0.51047800	-2.06812100
C	3.78650700	0.87102100	-2.16742300
C	5.26338100	-1.01245900	-1.98759200
C	4.87945300	1.72680400	-2.18354600
H	2.78405800	1.27797400	-2.22431900
C	6.36121600	-0.15765000	-2.00464800
H	5.41864100	-2.08293600	-1.91231500
C	6.17115200	1.21455100	-2.10253700
H	4.72369500	2.79561100	-2.25988900
H	7.36245600	-0.56513700	-1.94096600
H	7.02294300	1.88274000	-2.11525000



TSBC

	Energy (in Hartree)
EE	-1,278.028179
Thermal free energy corrections	0.283064
EE+E <sub>thermal free energy correction</sub>	-1277.745115
Imaginary frequency	-507.30 cm <sup>-1</sup>

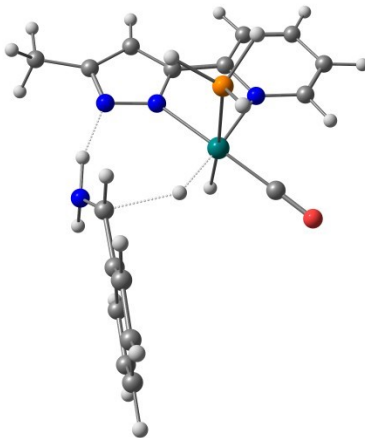
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Ru	-1.01879	-2.07209	-0.49478
N	-0.50343	-0.57525	1.064093
N	-1.33724	-0.23488	-1.38709
N	-1.72766	0.156676	-2.60822
C	-0.12487	-0.79999	2.32949
C	-0.55635	0.715545	0.637526
C	0.222389	0.207286	3.212717
C	-0.2202	1.781077	1.473534
H	-0.27343	2.79363	1.096777
C	-1.00771	0.884084	-0.72794
C	0.177958	1.528203	2.773223
H	0.445713	2.341817	3.434651
C	-1.65744	1.508883	-2.76574

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C	-1.20141	2.007427	-1.56686
H	-1.02937	3.044367	-1.33588
H	-0.57685	-3.48413	0.288943
C	-2.03054	2.183271	-4.04038
H	-3.07576	2.000485	-4.30263
H	-1.8923	3.258884	-3.94498
H	-1.41258	1.838384	-4.87336
P	-3.14341	-2.54385	0.066369
H	-4.24926	-2.01607	-0.65813
H	-3.56509	-3.89062	-0.00052
H	-3.71027	-2.28553	1.346335
H	-0.10671	-1.83784	2.635778
H	0.522262	-0.04137	4.221553
H	-1.97652	-0.55232	-3.27800
N	1.046892	-2.27365	-1.05302
C	0.866254	-3.25949	-0.12046
H	-1.37993	-2.97821	-1.78776
C	1.186882	-4.69657	-0.43797
C	2.150892	-5.35679	0.32267
C	0.591544	-5.37489	-1.50291
C	2.523646	-6.66354	0.02315
H	2.620577	-4.83984	1.151883
C	0.961334	-6.67886	-1.80252
H	-0.18087	-4.87544	-2.07428
C	1.92976	-7.32866	-1.04177

H	3.277577	-7.1594	0.622258
H	0.485475	-7.19555	-2.62724
H	2.214105	-8.34711	-1.27556
H	1.079181	-2.68907	-1.98030
H	1.215274	-2.98975	0.876757



TSAC

	Energy (in Hartree)
EE	-1390.86184
Thermal free energy corrections	0.2858
EE+E <sub>thermal free energy correction</sub>	-1391.148
Imaginary frequency	-166.5 cm <sup>-1</sup>

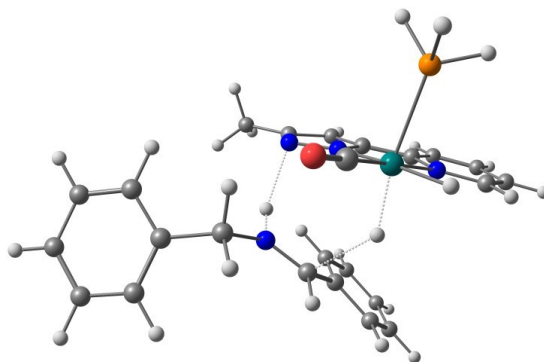
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Ru	0.051567	-0.51528	0.304762
O	-1.55457	-3.04146	0.221825
N	2.04869	-1.30717	-0.08725
N	1.298014	1.229427	0.07790
N	1.086365	2.550801	0.103917
C	2.367733	-2.60427	-0.19435
C	3.028181	-0.38006	-0.25746
C	3.649141	-3.04910	-0.46465
C	4.344313	-0.76579	-0.53141

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H	5.100182	-0.00396	-0.66294
C	2.60502	0.997418	-0.15191
C	4.659784	-2.10651	-0.63566
H	5.674857	-2.41635	-0.84911
C	2.268166	3.176587	-0.11069
C	3.269036	2.22821	-0.27534
H	4.314966	2.408859	-0.45936
H	-0.21421	-0.42746	-1.29745
C	-0.93066	-2.0670	0.27439
C	2.361231	4.66808	-0.15235
H	3.402345	4.985336	-0.21139
H	1.839087	5.081476	-1.01990
H	1.921042	5.11974	0.739602
P	0.279042	-0.45169	2.669747
H	-0.74901	-0.96078	3.497863
H	1.337092	-1.07935	3.38167
H	0.401688	0.79001	3.345387
H	1.553822	-3.30296	-0.05891
H	3.844313	-4.10984	-0.53975
H	-1.82616	1.983174	1.454281
H	-0.45880	2.881715	-0.17705
N	-1.51800	2.761905	-0.38318
H	-1.82245	2.822521	-1.34454
C	-2.19214	2.009989	0.43807
H	-1.39917	0.274155	0.35110

C	-3.5551	1.533432	0.203802
C	-4.09571	1.409665	-1.07987
C	-4.34648	1.214694	1.310713
C	-5.40525	0.990863	-1.24766
H	-3.48511	1.602334	-1.95303
C	-5.66006	0.802718	1.141785
H	-3.92563	1.290442	2.305839
C	-6.19169	0.6917	-0.13784
H	-5.8127	0.885497	-2.24465
H	-6.2654	0.560953	2.005603
H	-7.21352	0.361132	-0.27323



TSCA

	Energy (in Hartree)
EE	-1661.0936
Thermal free energy corrections	0.3866
EE+E <sub>thermal free energy correction</sub>	-1661.497
Imaginary frequency	-309.8 cm <sup>-1</sup>

0 1

Ru	-2.37665200	-2.21861200	1.79103300
O	-0.85951300	-4.72613900	2.35450200
N	-3.61629400	-0.46007800	1.32958900
N	-1.25143000	-0.47563600	2.55225900

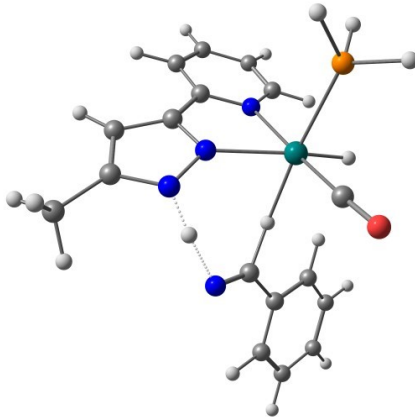
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N	-0.12389000	-0.28869700	3.25943400
C	-4.83491500	-0.51307700	0.77540000
C	-3.04453800	0.75292400	1.54860700
C	-5.54452700	0.61443400	0.40346200
C	-3.70752300	1.93107600	1.18355500
H	-3.22730700	2.88339000	1.36035600
C	-1.75602300	0.72829600	2.19827000
C	-4.96096200	1.86286800	0.60863400
H	-5.48182800	2.76842500	0.32372100
C	0.10652500	1.04707100	3.32965200
C	-0.90236700	1.73789700	2.66831100
H	-1.00244400	2.80511200	2.55598500
H	-3.52054600	-3.22638100	1.26770700
C	-1.42134100	-3.73072700	2.15293400
C	1.32356900	1.58187000	4.01555600
H	1.55013100	1.01155800	4.91841800
H	2.20327700	1.52485800	3.36799400
H	1.18828900	2.62714500	4.29679400
P	-1.61043200	-2.22720400	-0.39727900
H	-0.48005600	-1.50296600	-0.86272300
H	-1.25065600	-3.46311400	-0.97393900
H	-2.48562500	-1.80935600	-1.42916000
H	-5.23692900	-1.50617000	0.63320600
H	-6.52668700	0.51281400	-0.03662300
H	-0.74872600	-1.19136500	4.84019700

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C	-2.51779800	-2.10794000	5.17984700
N	-1.21715200	-2.03244500	5.21572300
C	-0.33343200	-3.19989100	5.26526100
H	-0.94813600	-4.08507000	5.42549100
H	-3.15863300	-2.46293800	3.25842300
H	-2.94223300	-3.09135700	5.33849300
C	-3.42431000	-0.97534000	5.33405400
C	-4.78807700	-1.25054700	5.49785800
C	-2.98520000	0.35111100	5.39285700
C	-5.69328100	-0.22611700	5.71594700
H	-5.13374900	-2.27515400	5.43581700
C	-3.89604400	1.37481100	5.60659400
H	-1.93922000	0.59286600	5.26436200
C	-5.24820700	1.09185800	5.77004300
H	-6.74437700	-0.45207800	5.84053800
H	-3.54714800	2.39855300	5.64534500
H	-5.95348600	1.89572300	5.93902300
C	0.70723700	-3.05543300	6.35209600
C	0.41301300	-3.39825200	7.67181800
C	1.97693900	-2.56717400	6.04807400
C	1.36891500	-3.25707900	8.66964100
H	-0.56897300	-3.78474100	7.92057500
C	2.93518500	-2.42287300	7.04557600
H	2.21248600	-2.29747400	5.02560000
C	2.63324800	-2.76773000	8.35762000

H	1.12975700	-3.53325900	9.68892500
H	3.91870000	-2.04517400	6.79587000
H	3.38034500	-2.66005700	9.13385300
H	0.14697500	-3.29831000	4.29277400



TS1

	Energy (in Hartrees)
EE	-1390.1911
Thermal free energy corrections	0.2630
EE+E <sub>thermal free energy correction</sub>	-1389.928
Imaginary frequency	-619.25 cm <sup>-1</sup>

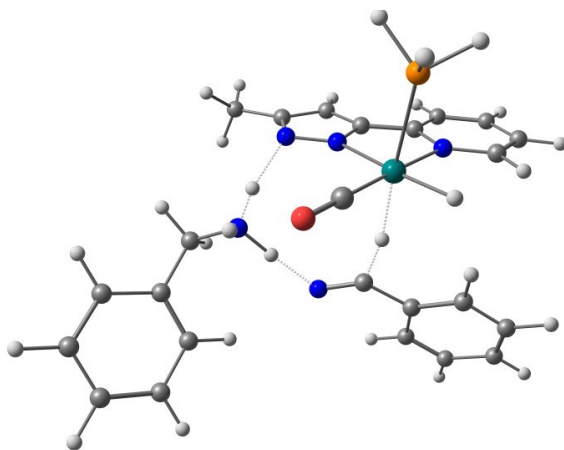
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Ru	-0.50512400	-0.68950500	-0.64069100
O	0.16593200	0.28202500	-3.39234600
N	-1.09720900	-1.48258600	1.33483400
N	-1.62313400	0.87392100	0.33855500
N	-1.68123600	2.19808600	0.13459500
C	-0.77542200	-2.69846400	1.79983000
C	-1.96937400	-0.72057900	2.05000400
C	-1.29274400	-3.21753000	2.97287400
C	-2.53907800	-1.19441600	3.23369400
H	-3.23734800	-0.56928100	3.77276800

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C	-2.18027300	0.61212200	1.52576600
C	-2.19843600	-2.44985600	3.70040200
H	-2.62854200	-2.82753000	4.61903000
C	-2.29025400	2.79890200	1.19698700
C	-2.65294600	1.81376400	2.09457300
H	-3.15093900	1.95272700	3.03910500
H	0.51826900	-1.90045000	-0.94450400
C	-0.08607300	-0.06259900	-2.32384100
C	-2.45429100	4.27906300	1.25651000
H	-3.17253400	4.62965000	0.51163600
H	-2.80846600	4.58417000	2.24029200
H	-1.50543100	4.78243700	1.06021200
P	-2.04162000	-2.06214200	-1.56378100
H	-3.40985300	-1.70436800	-1.67291700
H	-1.85956500	-2.47869600	-2.89729600
H	-2.24671700	-3.33814000	-0.98797500
H	-0.07206200	-3.25667400	1.19818200
H	-0.98856600	-4.19985500	3.30595600
H	-0.70234000	2.56569600	-0.29884700
C	1.42975600	1.65656100	-0.19967800
H	0.82991200	0.49695400	-0.08590700
C	2.87240400	1.33928300	-0.08464300
C	3.33135700	0.02899000	0.00827200
C	3.79203900	2.39418500	-0.07019600
C	4.69288800	-0.23100100	0.11472800

H	2.61295600	-0.78157600	-0.01757100
C	5.14849600	2.13170300	0.03905600
H	3.42160700	3.40771200	-0.14702700
C	5.60378400	0.81808800	0.13221300
H	5.04178200	-1.25404600	0.18125000
H	5.85539400	2.95215300	0.04956200
H	6.66450500	0.61607000	0.21544300
N	0.79562800	2.67129300	-0.36167400



TS2

	Energy (in Hartrees)
EE	-1717.2491
Thermal free energy corrections	0.3988
EE+E <sub>thermal free energy correction</sub>	-1716.850
Imaginary frequency	-290.25 cm <sup>-1</sup>

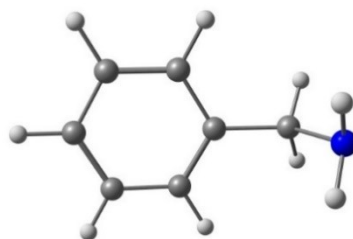
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Ru	-0.61927600	-0.04407800	1.06746900
O	-1.44921600	-2.74638200	2.02579000
N	0.03179700	1.88359400	0.23451600
N	-1.88933100	0.28658000	-0.67865500
N	-2.87110800	-0.39538300	-1.27851100
C	1.02850500	2.63506900	0.72184600

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C	-0.66469200	2.33135400	-0.84408800
C	1.38850600	3.85473200	0.17939000
C	-0.34874700	3.55932000	-1.43678300
H	-0.91601600	3.89205900	-2.29461500
C	-1.71318400	1.46099900	-1.31883700
C	0.68073200	4.32361100	-0.92481600
H	0.93377600	5.27347800	-1.37852600
C	-3.33453400	0.34834100	-2.31236100
C	-2.63174200	1.54423400	-2.37656700
H	-2.76643300	2.34413900	-3.08543900
H	0.53204500	-0.03209800	2.20520500
C	-1.12426900	-1.68652500	1.67675400
C	-4.43038700	-0.15296300	-3.19725800
H	-5.26909500	-0.53407700	-2.61084500
H	-4.80273600	0.64545600	-3.83915400
H	-4.08728100	-0.96329100	-3.84756100
P	-1.92445600	1.01546200	2.61992300
H	-2.11703000	0.40738300	3.87716200
H	-1.51873000	2.28516700	3.09454100
H	-3.28089800	1.35530500	2.38343000
H	1.54528700	2.22628800	1.57831700
H	2.20404000	4.41733900	0.61133200
H	-2.54548200	-2.02815300	-1.13186800
H	0.50396800	-0.92213800	-0.00385000
C	1.14506200	-1.70983200	-0.99057800

N	0.50343300	-2.51678800	-1.59116000
C	2.54477800	-1.24347900	-0.95009000
C	3.07065800	-0.54990900	0.13535200
C	3.37054400	-1.55566400	-2.03658100
C	4.40951500	-0.17606000	0.14198200
H	2.42097600	-0.32148500	0.97069200
C	4.70156500	-1.16772500	-2.03158000
H	2.95195000	-2.10191300	-2.87113000
C	5.22626400	-0.47855600	-0.94098000
H	4.81566000	0.35137100	0.99626400
H	5.33344500	-1.40594000	-2.87820600
H	6.26766800	-0.18138400	-0.93689000
H	-1.00398800	-2.84678700	-1.31214100
N	-2.07018000	-2.99460300	-1.06426300
H	-2.49109900	-3.65154000	-1.71352300
H	-2.14711300	-3.35301600	-0.11447700



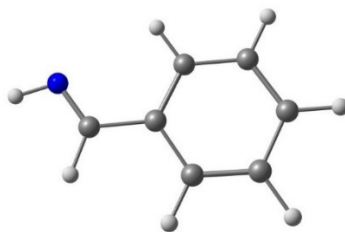
I

	Energy (in Hartrees)
EE	-327.0366
Thermal free energy corrections	0.1136
EE+E <sub>thermal free energy correction</sub>	-326.923

O 1

N	2.77669300	0.00009200	0.65895200
C	1.94528800	-0.00013900	-0.55284600

H	2.22371600	-0.87665100	-1.14240700
H	2.22379300	0.87607400	-1.14281900
C	0.44946900	-0.00005800	-0.31688800
C	-0.25379600	-1.19847300	-0.18303200
C	-0.25370700	1.19842800	-0.18311100
C	-1.61711000	-1.20167200	0.08844600
H	0.27149700	-2.14045800	-0.29897600
C	-1.61700800	1.20174200	0.08836000
H	0.27167800	2.14035500	-0.29912100
C	-2.30290400	0.00006100	0.22728800
H	-2.14584800	-2.14199700	0.18492200
H	-2.14569900	2.14210000	0.18476400
H	-3.36550000	0.00012800	0.43495900
H	2.56402100	-0.81200300	1.22854400
H	2.56410000	0.81246900	1.22816900



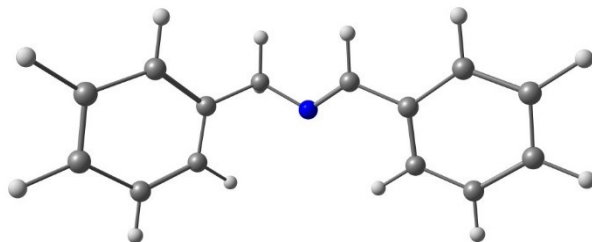
II

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Thermal free energy corrections	0.0915
EE+E <sub>thermal free energy correction</sub>	-325.742

0 1

N	-2.84018300	0.44536200	-0.00010300
C	-1.96755300	-0.47843300	0.00004300

H	-2.23198100	-1.54328300	-0.00009700
C	-0.52024500	-0.20899200	0.00008000
C	-0.02116100	1.09830600	0.00006500
C	0.37596400	-1.27959600	0.00007200
C	1.34585300	1.32164800	0.00000600
H	-0.72296000	1.92156700	0.00006400
C	1.74744500	-1.05497500	-0.00007200
H	-0.00620100	-2.29429800	0.00007900
C	2.23381000	0.24647900	-0.00004500
H	1.72651400	2.33540500	-0.00001300
H	2.43364000	-1.89237800	-0.00010700
H	3.30171000	0.42598400	-0.00006200
H	-3.78411700	0.06285200	-0.00004500



III

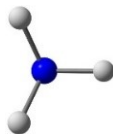
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Thermal free energy corrections	0.1890
EE+E <sub>thermal free energy correction</sub>	-596.09

0 1

N	-0.02206500	-0.29155900	-0.87673900
C	-1.00146600	-0.94368000	-0.40978600
H	-0.92497400	-2.02282500	-0.20778100
C	-2.30642200	-0.34128100	-0.09911800

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C	-2.55459600	1.02178000	-0.29714600
C	-3.32663600	-1.14940600	0.40764100
C	-3.79574200	1.55648400	0.00684300
H	-1.76045000	1.64274400	-0.68908900
C	-4.57170400	-0.61242500	0.71205700
H	-3.14068400	-2.20601400	0.56376900
C	-4.80824900	0.74188400	0.51204300
H	-3.98000900	2.61223000	-0.14841300
H	-5.35432200	-1.24936800	1.10443400
H	-5.77689000	1.16432200	0.74819900
C	1.21582400	-1.00190000	-1.14572000
H	1.38783200	-0.95139000	-2.22722300
H	1.14955100	-2.06565400	-0.87671500
C	2.39504700	-0.37150700	-0.43443800
C	3.23430400	-1.14328900	0.36501300
C	2.67157300	0.98900500	-0.58051300
C	4.33359000	-0.57443400	1.00200500
H	3.02781200	-2.19976100	0.49303700
C	3.76492600	1.56006800	0.05640400
H	2.01665200	1.59971600	-1.18887100
C	4.60175200	0.77936100	0.84912400
H	4.97576700	-1.18997300	1.61973400
H	3.96647000	2.61723100	-0.06553400
H	5.45448600	1.22569000	1.34517500

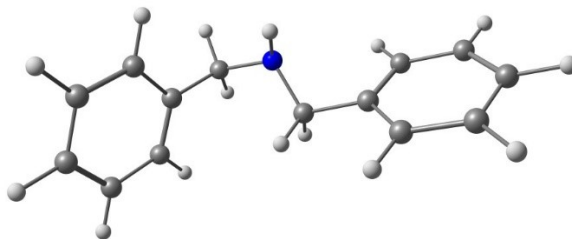


IV

	Energy (in Hartrees)
EE	-56.5857
Thermal free energy corrections	0.0161
EE+E <sub>thermal free energy correction</sub>	-56.5695

0 1

N	0.00000000	0.00000000	0.11161700
H	0.00000000	0.94298400	-0.26044100
H	-0.81664800	-0.47149200	-0.26044100
H	0.81664800	-0.47149200	-0.26044100



V

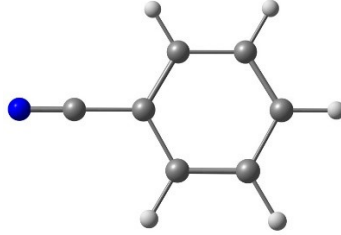
	Energy (in Hartrees)
EE	-597.4896
Thermal free energy corrections	0.2122
EE+E <sub>thermal free energy correction</sub>	-597.28

0 1

N	-0.11304000	-1.33249100	0.27077700
C	1.24614800	-1.78525100	-0.03085900
H	1.22891800	-2.24418400	-1.02314300
H	1.48627900	-2.57898600	0.68104900
C	2.33277000	-0.72555300	0.01358800
C	2.85367400	-0.16962700	-1.15429300
C	2.81835900	-0.26446200	1.23941500

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C	3.82690400	0.82359700	-1.10316300
H	2.49714400	-0.52123600	-2.11602100
C	3.78960200	0.72671500	1.29768000
H	2.43746900	-0.69333900	2.16038500
C	4.29652500	1.27576900	0.12374300
H	4.21925000	1.24175200	-2.02198100
H	4.15741000	1.06632600	2.25809100
H	5.05578200	2.04645800	0.16656900
H	-0.16193500	-0.97031400	1.21676800
C	-0.66632400	-0.35355200	-0.66174000
H	-0.06961200	0.56666300	-0.73338300
H	-0.64550500	-0.81219500	-1.65763300
C	-2.08884500	0.01175900	-0.30553100
C	-3.04752000	-0.98073600	-0.08816800
C	-2.47598800	1.34654600	-0.20290900
C	-4.35901700	-0.64367200	0.21881200
H	-2.75126100	-2.02013300	-0.15127100
C	-3.79033600	1.68821400	0.10214100
H	-1.74105500	2.12738900	-0.36234100
C	-4.73590200	0.69321000	0.31343300
H	-5.09104900	-1.42494600	0.38315000
H	-4.07194300	2.73120200	0.17843700
H	-5.75891100	0.95524000	0.55298600



VI

	Energy (in Hartrees)
EE	-324.6145
Thermal free energy corrections	0.0687
EE+E <sub>thermal free energy correction</sub>	-324.5458

0 1

C	-1.47778600	-1.20568200	-0.00000100
C	-0.09077700	-1.21207100	0.00001600
C	0.60842400	-0.00005000	-0.00000300
C	-0.09073500	1.21205200	0.00000700
C	-1.47770400	1.20573200	0.00000700
C	-2.17168700	0.00002500	-0.00001300
H	-2.01799300	-2.14334100	-0.00001300
H	0.45678700	-2.14462400	0.00001100
H	0.45693500	2.14454300	0.00000300
H	-2.01791400	2.14338900	0.00000100
H	-3.25412300	0.00008000	-0.00001200
C	2.03920100	-0.00002900	-0.00000700
N	3.19181400	0.00001300	-0.00000400



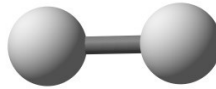
CO

	Energy (in Hartrees)
EE	-113.362526
Thermal free energy corrections	-0.014072
EE+E <sub>thermal free energy correction</sub>	-113.376598

0 1

C 0.51227600 -0.52414500 -1.28080800

O 1.63716600 -0.52414500 -1.28080800



H2

	Energy (in Hartrees)
EE	-1.179649
Thermal free energy corrections	-0.001416
EE+E <sub>thermal free energy correction</sub>	-1.181065

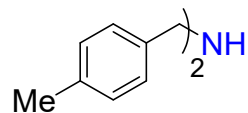
0 1

H 3.42905997 0.38461538 0.00000000

H 2.82905997 0.38461538 0.00000000

## 6. Analytical Data of Secondary Amines

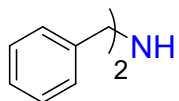
### *Bis-(4-methylbenzyl)amine, (2a)*



$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 7.28 (d,  $J = 7.7$  Hz, 2H), 7.11 (d,  $J = 7.7$  Hz, 1H), 3.50 (s, 4H), 2.32 (s, 6H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm)

136.99, 136.57, 129.18, 129.03, 57.73, 21.43.

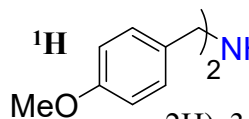
### *Dibenzylamine, (2b)*



$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 7.35–7.25 (m, 10H), 3.82 (s, 4H).  $^{13}\text{C}\{^1\text{H}\}$

NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 140.43, 128.50, 128.25, 127.04, 53.28.

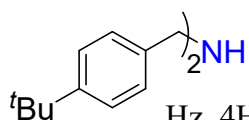
### *Bis-(4-methoxybenzyl)amine, (2c)*



$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 7.21 (d,  $J = 8.6$  Hz, 2H), 6.86 (d,  $J = 8.6$  Hz, 2H), 3.50 (s, 4H), 2.32 (s, 6H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 158.59, 135.58,

128.36, 114.00, 55.37, 45.97.

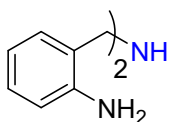
### *Bis-(4-*t*-butylbenzyl)amine, (2d)*



$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 7.36 (d,  $J = 8.56$  Hz, 4H), 7.23 (d,  $J = 8.56$  Hz, 4H), 3.82 (s, 4H), 1.31 (s, 18H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 149.81,

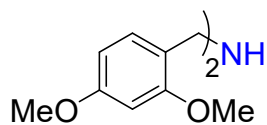
140.43, 126.88, 125.53, 46.21, 43.97, 31.30.

### *Bis-(2-aminobenzyl)amine, (2e)*

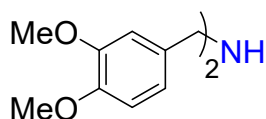


$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 8.61 (d,  $J = 7.96$  Hz, 2H), 7.67–7.63 (m, 4H), 7.41 (t,  $J = 7.96$  Hz, 2H), 1.24 (s, 4H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm)

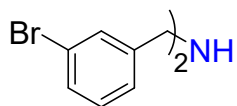
134.65, 127.59, 126.73, 126.57, 29.78.ppm.

**Bis-(2,4-dimethoxybenzyl)amine, (2f)**

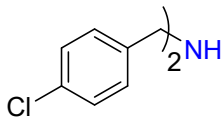
$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 7.08 (d,  $J = 8.0$  Hz, 2H), 6.44–6.39 (m, 4H), 3.80 (s, 6H), 3.78 (s, 6H), 3.72 (s, 4H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 159.93, 158.37, 129.00, 124.37, 103.64, 98.58, 55.31, 55.13, 42.08.

**Bis-(3,4-dimethoxybenzyl)amine, (2g)**

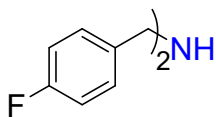
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 6.92 (s, 2H), 6.89–6.87 (m, 2H), 6.80–6.78 (m, 2H), 3.86 (s, 6H), 3.84 (s, 6H), 3.49 (s, 4H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 148.92, 148.03, 132.28, 120.87, 111.93, 110.96, 57.32, 55.99, 55.84.

**Bis-(3-bromobenzyl)amine, (2h)**

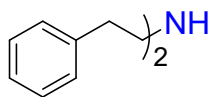
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 7.46 (s, 2H), 7.35 (d,  $J = 7.32$  Hz, 2H), 7.25–7.15 (m, 4H), 3.83 (s, 4H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 145.59, 130.26, 130.19, 129.94, 125.77, 122.72, 46.00.

**Bis-(4-chlorobenzyl)amine, (2i)**

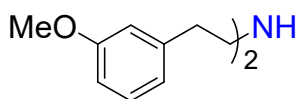
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 7.30–7.24 (m, 8H), 3.74 (s, 4H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 138.63, 137.79, 129.55, 128.64, 52.38.

**Bis-(4-fluorobenzyl)amine, (2j)**

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 7.21–7.19 (m, 4H), 6.92 (t, 4H), 3.67 (s, 4H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 135.86, 132.03, 129.58, 128.43, 52.33.

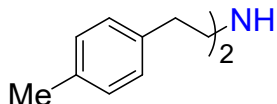
**Bis-(phenethyl)amine, (2k)**

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 7.30–7.24 (m, 4H), 7.21–7.17 (m, 6H), 2.95 (t,  $J = 6.72$  Hz, 4H), 2.74 (t,  $J = 6.72$ , 4H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 139.89, 128.92, 128.54, 126.25, 43.64, 40.18.

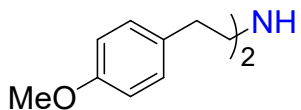
**Bis-(3-methoxyphenethyl)amine, (2l)**

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 7.21–7.17 (m, 2H), 6.77–6.72 (m, 6H), 3.77 (s, 6H), 2.93 (t,  $J = 6.72$  Hz, 4H), 2.69 (t,  $J = 6.72$  Hz, 4H).

$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 159.78, 141.51, 129.41, 121.29, 114.68, 111.47, 55.19, 43.47, 40.17.

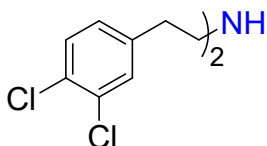
**Bis-(4-methylphenethyl)amine, (2m)**

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 7.10–7.05 (m, 8H), 2.94–2.90 (m, 4H), 2.69 (t,  $J = 6.72$  Hz, 4H), 2.30 (s, 6H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 136.80, 135.67, 129.21, 128.78, 43.74, 39.77, 21.07.

**Bis-(4-methoxyphenethyl)amine, (2n)**

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 7.11 (d,  $J = 8.6$  Hz 4H), 6.84 (d,  $J = 8.75$  Hz 4H), 3.78 (s, 6H), 2.92 (t,  $J = 6.85$  Hz, 4H), 2.68 (t,  $J = 6.9$  Hz 4H).

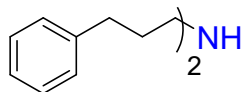
$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 158.39, 132.24, 130.08, 114.23, 55.60, 44.10, 39.56.

**Bis-(3,4-dichlorophenethyl)amine, (2o)**

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm) 7.28 (d,  $J = 8.05$  Hz, 2H), 7.21 (d,  $J = 2.3$  Hz, 2H), 6.96–6.95 (m, 2H), 2.87 (t,  $J = 6.95$  Hz, 4H) 2.63 (t,  $J = 6.95$

Hz, 4H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta(\text{ppm})$  140.01, 132.38, 130.66, 130.30, 130.14, 128.22, 43.00, 38.89.

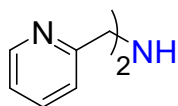
***Bis-(3-phenylpropyl)amine, (2p)***



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta(\text{ppm})$  7.28–7.24 (m, 4H), 7.18–7.14 (m, 6H), 2.71 (t,  $J = 7.32$  Hz, 4H), 2.63 (t,  $J = 7.32$  Hz, 4H), 1.79–1.72 (m, 4H).  $^{13}\text{C}\{^1\text{H}\}$

NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta(\text{ppm})$  142.19, 128.42, 125.83, 41.83, 35.46, 33.32.

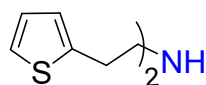
***Bis-(2-picolyl)amine, (2q)***



$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta(\text{ppm})$  8.54 (d,  $J = 3.85$  Hz, 2H), 7.56–7.53 (m, 2H), 7.12–7.08 (m, 4H), 3.22 (s, 4H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta(\text{ppm})$

162.27, 149.61, 136.86, 122.11, 121.52, 48.15.

***Bis-(2-thiophenethyl)amine, (2r)***



$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta(\text{ppm})$  7.14–7.13 (m, 2H), 6.94–6.92 (m, 2H), 6.82 (d,  $J = 2.9$  Hz, 2H), 2.99–2.94 (m, 8H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):

$\delta(\text{ppm})$  142.67, 127.23, 125.41, 123.89, 44.07, 34.53.

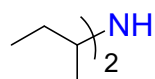
***Bis-(cyclohexyl)amine, (2s)***



$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta(\text{ppm})$  2.56–2.51 (m, 2H), 1.85–1.83 (m, 4H), 1.72–1.69 (m, 4H), 1.61–1.58 (m, 2H), 1.28–1.20 (m, 4H), 1.16–1.09 (m, 2H),

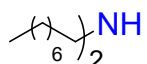
1.04–0.97 (m, 4H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta(\text{ppm})$  53.42, 34.70, 26.56, 25.67.

***Bis-(sec-butyl)amine, (2t)***

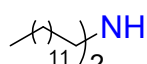


$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta(\text{ppm})$  2.38–2.37 (m, 4H), 1.77–1.69 (m, 2H), 0.89–0.87 (m, 12H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta(\text{ppm})$  58.33, 28.57, 21.00.

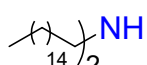
**Bis-(n-octyl)amine, (2u)**

 **<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>): δ(ppm) 2.59–2.56 (m, 4H), 1.32–1.26 (m, 24H), 0.88–0.85 (m, 6H). **<sup>13</sup>C{<sup>1</sup>H} NMR** (125 MHz, CDCl<sub>3</sub>): δ(ppm) 50.48, 32.17, 30.48, 29.89, 29.61, 27.77, 22.99, 14.43.

**Bis-(tridecyl)amine, (2v)**

 **<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>): δ(ppm) 2.63 (t, *J* = 7.0 Hz, 4H), 1.26–1.22 (m, 44H), 0.85–0.83 (m, 6H). **<sup>13</sup>C{<sup>1</sup>H} NMR** (125 MHz, CDCl<sub>3</sub>): δ(ppm) 42.62, 34.24, 32.25, 29.98, 29.85, 28.68, 27.24, 23.02, 14.43.

**Bis-(hexadecyl)amine, (2w)**

 **<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>): δ(ppm) 2.66 (t, *J* = 7.0 Hz, 4H), 1.30–1.22 (m, 56H), 0.88–0.85 (m, 6H). **<sup>13</sup>C{<sup>1</sup>H} NMR** (125 MHz, CDCl<sub>3</sub>): δ(ppm) 42.66, 34.27, 32.77, 30.04, 29.87, 29.71, 27.25, 23.03, 14.45.

7.  $^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra of Secondary Amines