Electronic Supporting Information for

Reactivity of NHC Au(I)-C σ-Bonds with Carbon Dioxide and Other Electrophiles. An investigation of their possible involvement in catalytic C–C bond formation

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Contents

1. Experimental section

General procedures and materials. All experiments were carried out under an atmosphere of argon or nitrogen using standard Schlenk or high vacuum line techniques[i] unless otherwise noted. All solvents were distilled under vacuum directly to the reaction vessel from sodium/benzophenone ketyl radical, except THF and dichloromethane which were dried over calcium hydride. Stirbars and J. Young NMR-tubes were washed in aqua regia prior to use. Dry carbon dioxide was obtained by passing it through a P_2O_5 column and a -78 °C trap on the high vacuum line. Carbon dioxide was purchased from AGA Gas AB. NMR experiments were carried out using J. Young NMR tubes. All chemicals were purchased from either Acros or Sigma-Aldrich. ^{1}H-, ^{13}C- and ^{31}P-NMR experiments were recorded on a Varian Unity INOVA 500 spectrometer operating at 499.77 MHz (^{1}H). Complex **1**[ii] and IPrAuPh[iii] were prepared according to literature procedures. Chemical shifts are given in ppm downfield from TMS using residual solvent peaks (^{1}H- and ^{13}C-NMR) or H_3PO_4 as reference. Multiplicities are abbreviated as follows: (s) singlet, (d) doublet, (t) triplet, (q) quartet, (m) multiplet, (b) broad, (v) virtual. Elemental analyses were performed by H. Kolbe Microanalytisches Laboratorium, Mülheim an der Ruhr, Germany. GC-MS was performed on an Agilent Technologies 6890 N gas cromatograph, with a HP5 column; 30 m, ID 0, 32mm, film 0.25 μm. Program 80 °C 2 min, + 10°/min → 285 °C, hold 30 min. Detector: Waters GCT, EI+. ICP-MS was performed on a Perkin-Elmer Elan 6000 by Tommy Olsson at the Department of Ecology, Lund University.

Synthesis of IMesAuOtBu (2).

1 (240 mg, 0.45 mmol) was placed in a Strauss flask to which 10 ml benzene was distilled. Sodium tert-butoxide (43 mg, 0.45 mmol) was added. The solution was stirred at room temperature for 2 h while covered in aluminum foil. Filtration through Celite® and subsequent evaporation left **2** (ImesAuOtBu) as a white solid. Yield 236 mg (92%). ^{1}H NMR (C_6D_6) δ 6.71 (s, 4H), 5.96 (s, 2H), 2.11 (s, 6H), 1.96 (s, 12H), 1.45 (s, 9H). ^{13}C{^{1}H} NMR (C_6D_6) δ 139.29 (s), 135.67 (s), 134.91 (s), 129.57 (s), 121.13 (s), 36.72 (s), 31.41 (s), 21.13 (s), 17.80 (s).

Synthesis of IMesAuPh (3).

In a Strauss flask, to **2** (200 mg, 0.35 mmol) was distilled 10 ml toluene. To the colorless solution $PhB(OH)_2$ (42 mg, 0.35 mmol) was added. The solution was stirred in the dark at room temperature for 1h whereafter it was filtered and the filtrate volatiles were evaporated. The remaining solids were washed with pentane (3 x 3 ml) to yield 89 mg (44 %) of **3**. ^{1}H NMR (C_6D_6) δ 7.66 (dd, J = 7.9, 1.5 Hz, 2H), 7.21 (m, 2H), 7.00 (tt, J = 7.4, 1.5 Hz, 1H), 6.70 (s, 4H), 6.02 (s, 2H), 2.06 (s, 5H), 2.05 (s, 10H). ^{13}C{^{1}H} NMR (C_6D_6) δ 178.07 (s), 163.23 (s), 141.32 (s), 139.13 (s), 135.83 (s), 134.94 (s), 129.49 (s), 127.13 (s), 124.82 (s), 121.42 (s), 21.10 (s), 17.96 (s). This compound was previously synthesised through a different route. The published structure is identical to the one we have obtained but since our data is significantly better we have included our structure in the ESI.[iv]

Synthesis of IMesAuMe (4).

Toluene (5 ml) was distilled to a Strauss flask with **1** (30 mg, 56 µmol). Methyl lithium (150 µl, 240 µmol, 1.6 M in diethyl ether) was added. The mixture was stirred for 8 h at 28°C. After filtration through Celite, the solvent was evaporated to yield (10 mg, 19 µmol), (34 %) as a white solid.

^{1}H NMR (C_6D_6) δ 6.68 (s, 4H), 6.02 (s, 2H), 2.06 (s, 12H), 2.05 (s, 6H), 0.83 (s, 3H). ^{13}C{^{1}H} NMR (C_6D_6) δ 201.7 (s), 138.9 (s), 136.1 (s), 134.9 (s), 129.5 (s), 121.1 (s), 21.1 (s), 18.0 (s), 1.0 (s). Anal. found: C, 51.77; H, 5.70; N, 5.23 $C_{25}H_{33}AuN_2O$ requires C, 51.17; H, 5.27; N, 5.42;

Separate of IMesAuI (5).

In a round bottom flask, **1** (10.0 mg, 18.6 µmol) was dissolved in acetone (5 ml). Sodium iodide (18.0 mg, 120 µmol) was added. The solution was stirred for 48 hours at room temperature. Evaporation of the solvent left a pale yellow solid. The iodide (**5**) was extracted with toluene (3 x 3 ml), evaporation resulted in a white solid (10.7 mg, 92 %). X-ray diffraction quality crystals were obtained from benzene recrystallization. ^{1}H NMR (C_6D_6) δ 6.62 (s, 4H), 5.90 (s, 2H), 2.02 (s, 6H), 1.91 (s, 12H) ^{13}C{^{1}H} NMR (C_6D_6) δ 139.7 (s), 135.0 (s), 134.6 (s), 129.6 (s), 121.3 (s), 21.1 (s), 17.6 (s).

Synthesis of IMesAu-*p*-PhMe (6).

The synthesis was analogous to that of **3** except the use of *p*-tolyl boronic acid instead of phenyl boronic acid. Yield 89 %. ^{1}H NMR (C_6D_6) δ 7.58 (d, 2H), 7.03 (d, 2H), 6.71 (s, 4H), 6.05 (s, 2H), 2.15 (s, 3H), 2.07 (s, 6H), 2.05 (s, 12H). ^{13}C{^{1}H} NMR (C_6D_6) δ 197.1 (s), 166.5 (s), 141.09 (s), 139.1 (s), 135.9 (s), 135.0 (s), 133.07 (s),

129.5 (s), 128.4 (s), 121.4 (s), 21.5 (s), 21.1 (s), 18.0 (s). Anal. found: C, 58.12; H, 4.77; N, 4.37 $C_{25}H_{33}AuN_2O$ requires C, 56.76; H, 5.27; N, 4.73.

Typical conditions for reaction of the gold nucleophile with electrophiles.

The gold complex (3 mg) was mixed with an equimolar amount of electrophile (except with CO_2) in C_6D_6 or THF-d_8 (0.5 ml) in a J. Young NMR tube. The reaction was followed by ^{1}H-NMR until complete consumption of the starting material. Product distribution was determined by GC-MS or ^{1}H-NMR.

Typical conditions for reactivity studies with CO_2.

The gold complex (3 mg) was dissolved in dry C_6D_6 or THF-d_8 (0.5 ml) in a J. Young NMR tube. The solution was degassed by three consecutive freeze-pump-thaw cycles. A CO_2 pressure corresponding to 3-5 bar was applied to the tube whereafter it was sealed and heated to the indicated temperature.

2. Crystal structure X-ray diffraction data

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

Empirical formula	$C_{29}H_{41}AuN_2O_2$ (incl THF)	
Formula weight	646.60	
Collection temperature	112 K	
Wavelength	0.71069 Å	
Crystal size	0.30 x 0.25 x 0.20 mm^3	
Crystal habit	colorless plate	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 13.323(2) Å	α = 90°
	b = 13.5457(19) Å	β = 98.623(17)°
	c = 18.023(4) Å	γ = 90°
Volume	3215.8(10) $Å^3$	
Z	4	
Density, ρ_{calc}	1.336 g/cm^3	
Absorption coefficient	4.598 mm^{-1}	
F(000)	1296e^-	
Diffractometer	Xcalibur, Sapphire3, Oxford Diffraction	
Detector distance	50.00 mm	
Detector resolution	16.1829 pixels/mm	
θ_{min}	2.55°	
θ_{max}	33.36°	
Index ranges	$-19 \le h \le 20$, $-20 \le k \le 20$, $-26 \le l \le 20$	
Reflections collected	32111	
Independent reflections	11441	
Observed reflections, I>2σ(I)	4467	
$R[F^2 > 2\sigma(F^2)]$[a]	0.0988	
$wR(F^2)$[b]	0.2437	
R_{int}	0.1167	
GOOF[c]	0.861	
Largest diff. peak and hole	7.378 and -2.836 $e^-/Å^3$	

[a] $R = \Sigma(|F_O|-|F_C|)/\Sigma|F_O|$. [b] $wR = [\Sigma w(|F_O|-|F_C|)^2/\Sigma|F_O|^2]^{1/2}$. [c] $S = [\Sigma w(|F_O|-|F_C|)^2/(m-n)]^{1/2}$.

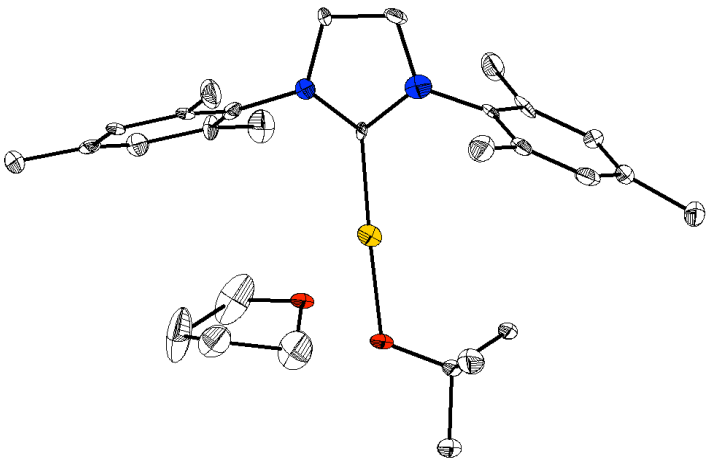


Table S2. Crystal data for structure **3**.

Empirical formula	$C_{27}H_{29}AuN_2$	
Formula weight	578.49	
Collection temperature	293 K	
Wavelength	0.71069 Å	
Crystal size	0.2 x 0.2 x 0.2 mm^3	
Crystal habit	colorless plate	
Crystal system	Triclinic	
Space group	P–1	
Unit cell dimensions	a = 9.9639(5) Å	α = 79.470(4)°
	b = 15.6363(8) Å	β = 83.978(4)°
	c = 16.4516(8) Å	γ = 77.020(4)°
Volume	2445.2(2) $Å^3$	
Z	4	
Density, ρ_{calc}	1.571 g/cm^3	
Absorption coefficient	6.031 mm^{-1}	
F(000)	1136e^-	
Diffractometer	Xcalibur, Sapphire3, Oxford Diffraction	
Detector distance	50.00 mm	
Detector resolution	16.1829 pixels/mm	
θ_{min}	2.25°	
θ_{max}	33.16°	
Index ranges	$-11 \le h \le 14$, $-23 \le k \le 19$, $-24 \le l \le 23$	
Reflections collected	24817	
Independent reflections	15799	
Observed reflections, I>2σ(I)	6460	
$R[F^2 > 2\sigma(F^2)]$[a]	0.0370	
$wR(F^2)$[b]	0.1025	
R_{int}	0.0287	
GOOF[c]	0.924	
Largest diff. peak and hole	1.038 and -0.908 $e^-/Å^3$	

[a] $R = \Sigma(|F_O|-|F_C|)/\Sigma|F_O|$. [b] $wR = [\Sigma w(|F_O|-|F_C|)^2/\Sigma|F_O|^2]^{1/2}$. [c] $S = [\Sigma w(|F_O|-|F_C|)^2/(m-n)]^{1/2}$.

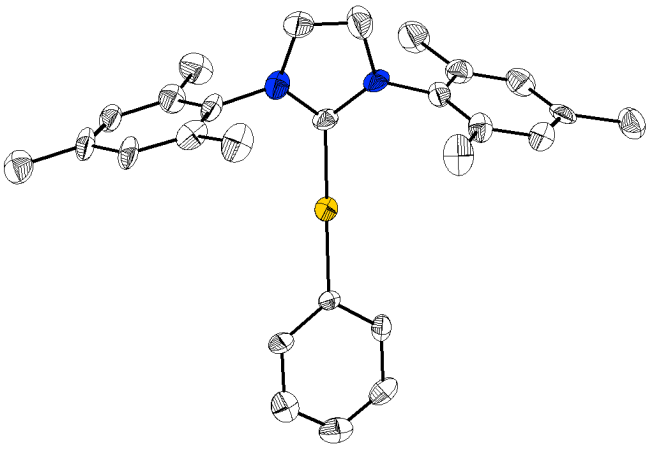


Table S3. Crystal data for structure **4**.

Empirical formula	$C_{22}H_{27}AuN_2$	
Formula weight	516.42	
Collection temperature	293 K	
Wavelength	0.71069 Å	
Crystal size	0.48 x 0.25 x 0.08 mm^3	
Crystal habit	colorless plate	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 8.327(2) Å	α = 90°
	b = 29.402(4) Å	β = 98.648(5)°
	c = 8.849(1) Å	γ = 90°
Volume	2141.9(7) $Å^3$	
Z	4	
Density, ρ_{calc}	1.601 g/cm^3	
Absorption coefficient	6.874 mm^{-1}	
F(000)	$1008e^-$	
Diffractometer	Xcalibur, Sapphire3, Oxford Diffraction	
Detector distance	50.00 mm	
Detector resolution	16.1829 pixels/mm	
θ_{min}	2.43°	
θ_{max}	26°	
Index ranges	$-10 \le h \le 10$, $-36 \le k \le 21$, $-10 \le l \le 10$	
Reflections collected	13994	
Independent reflections	4149	
Observed reflections, I>2σ(I)	2236	
$R[F^2 > 2\sigma(F^2)]$[a]	0.0612	
$wR(F^2)$[b]	0.151	
R_{int}	0.1155	
GOOF[c]	0.875	

[a] $R = \Sigma(|F_O|-|F_C|)/\Sigma|F_O|$. [b] $wR = [\Sigma w(|F_O|-|F_C|)^2/\Sigma|F_O|^2]^{1/2}$. [c] $S = [\Sigma w(|F_O|-|F_C|)^2/(m-n)]^{1/2}$.

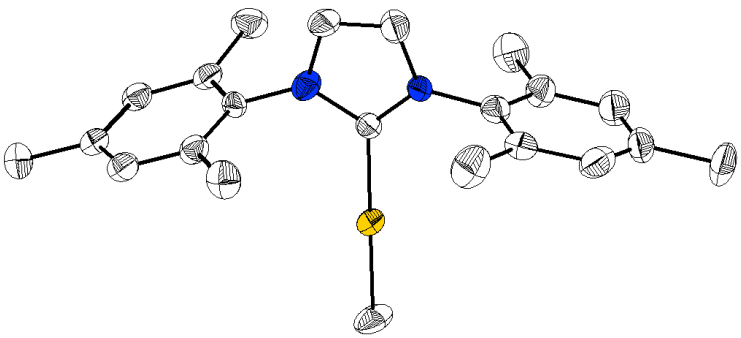
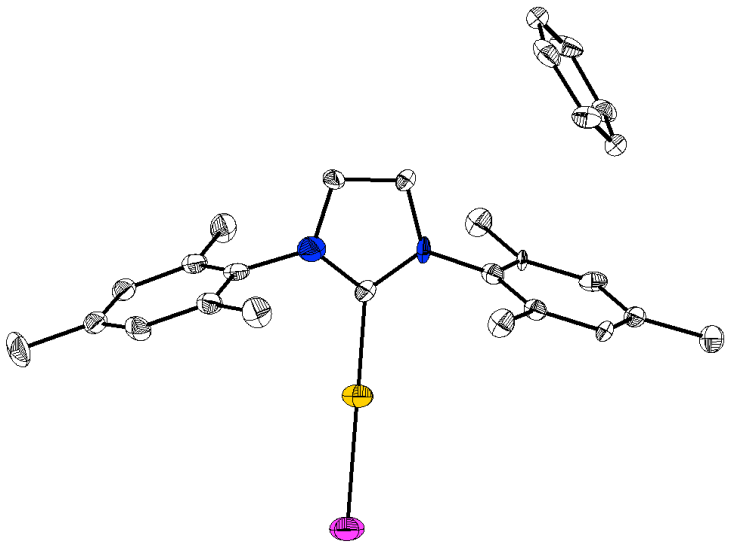


Table S4. Crystal data for structure **5**.

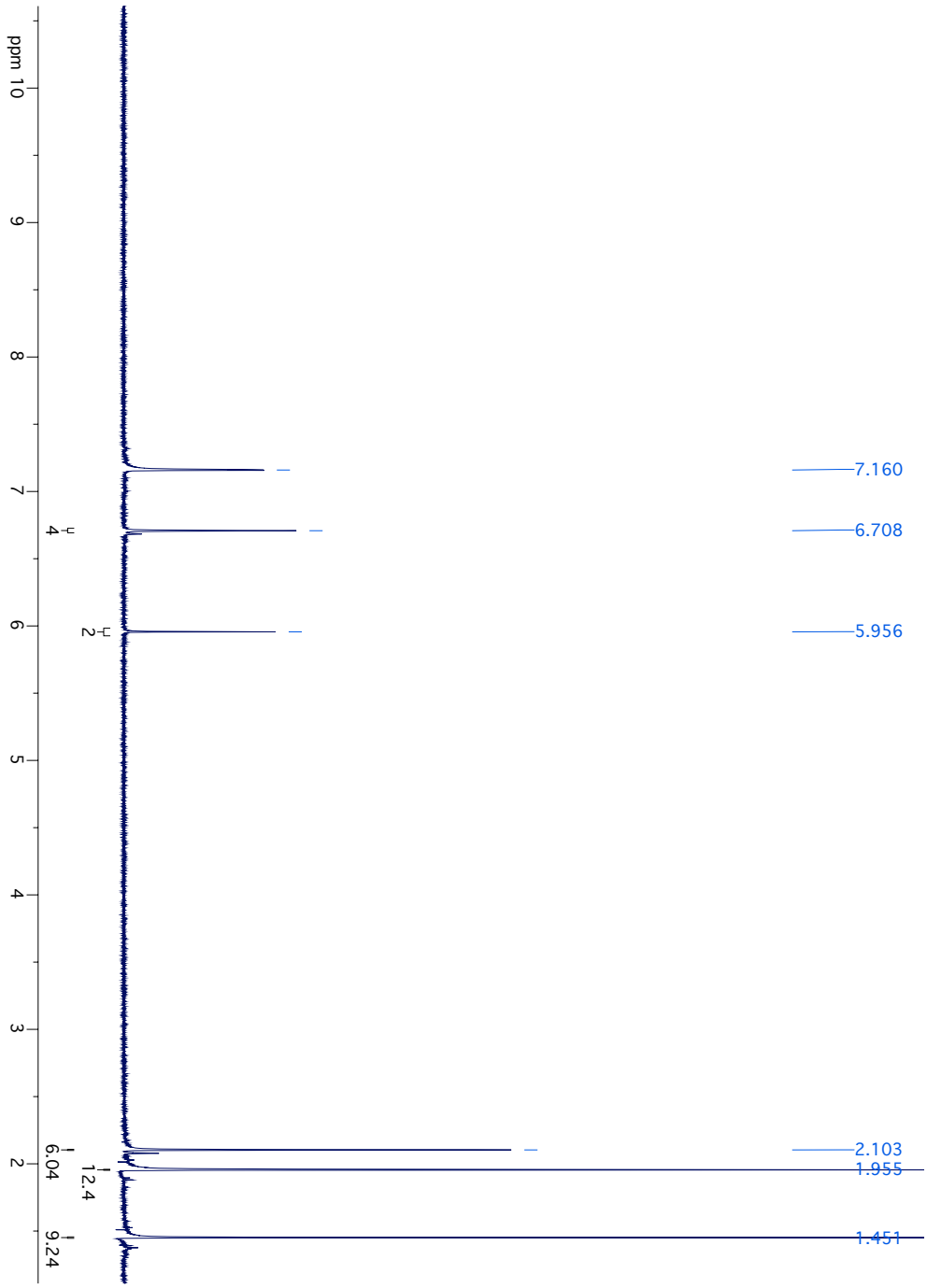
Empirical formula	$C_{27}H_{30}AuN_2I$ (incl. C_6H_6)	
Formula weight	706.40	
Collection temperature	116 K	
Wavelength	0.71069 Å	
Crystal size	0.25 x 0.20 x 0.15 mm^3	
Crystal habit	colorless block	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 9.1235 (14) Å	α = 90°
	b = 7.999(2) Å	β = 94.1810(18)°
	c = 34.742(12) Å	γ = 90°
Volume	2528.7(11) $Å^3$	
Z	4	
Density, ρ_{calc}	1.856 g/cm^3	
Absorption coefficient	7.055 mm^{-1}	
F(000)	$1352e^-$	
Diffractometer	Xcalibur, Sapphire3, Oxford Diffraction	
Detector resolution	16.1829 pixels/mm	
θ_{min}	2.54°	
θ_{max}	33°	
Index ranges	$-11 \le h \le 13$, $-11 \le k \le 11$, $-51 \le l \le 52$	
Reflections collected	23826	
Independent reflections	8886	
Observed reflections, I>2σ(I)	5887	
$R[F^2 > 2\sigma(F^2)]$[a]	0.1069	
$wR(F^2)$[b]	0.2665	
R_{int}	0.0797	
GOOF[c]	1.206	

[a] $R = \Sigma(|F_O|-|F_C|)/\Sigma|F_O|$. [b] $wR = [\Sigma w(|F_O|-|F_C|)^2/\Sigma|F_O|^2]^{1/2}$. [c] $S = [\Sigma w(|F_O|-|F_C|)^2/(m-n)]^{1/2}$.

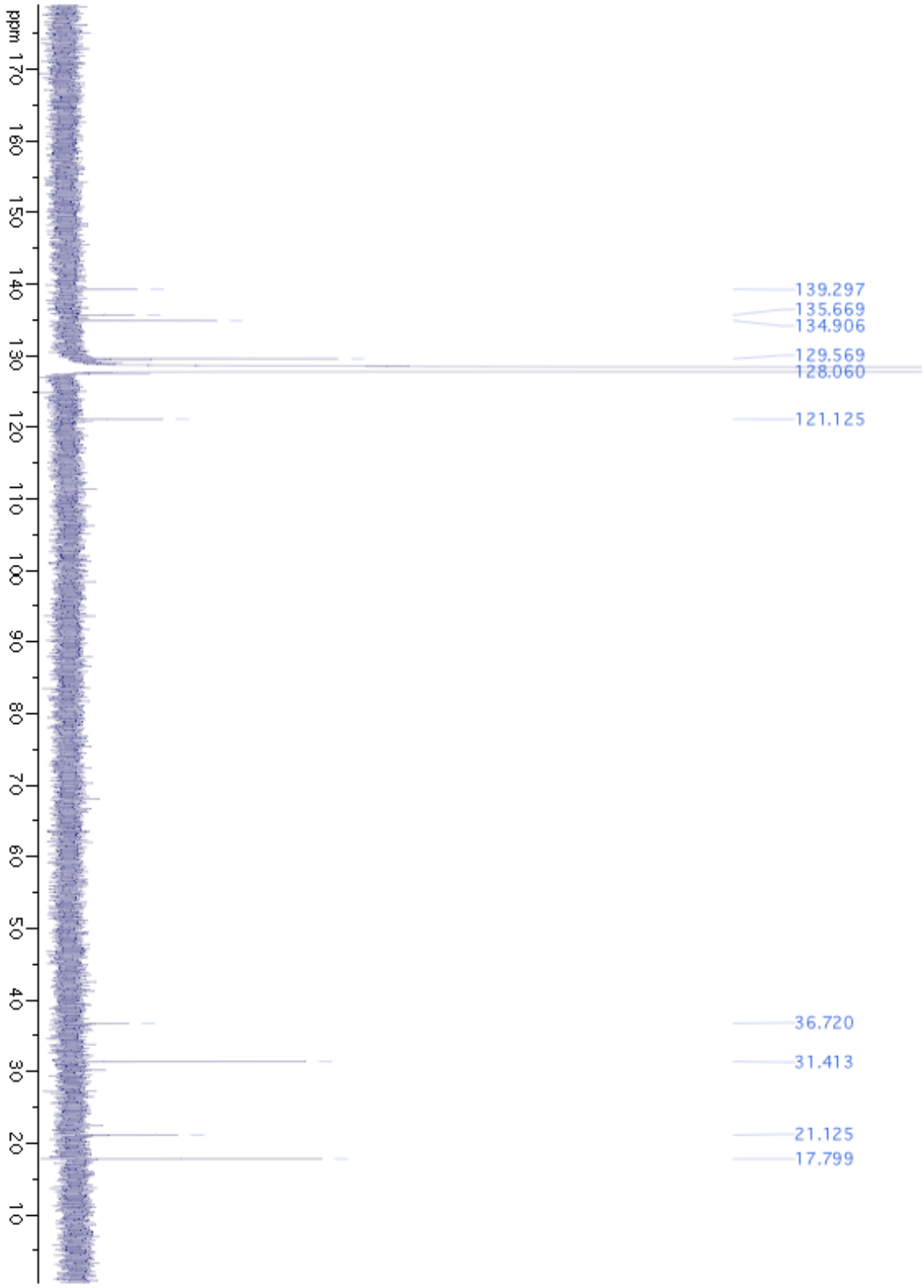


3. NMR-spectra

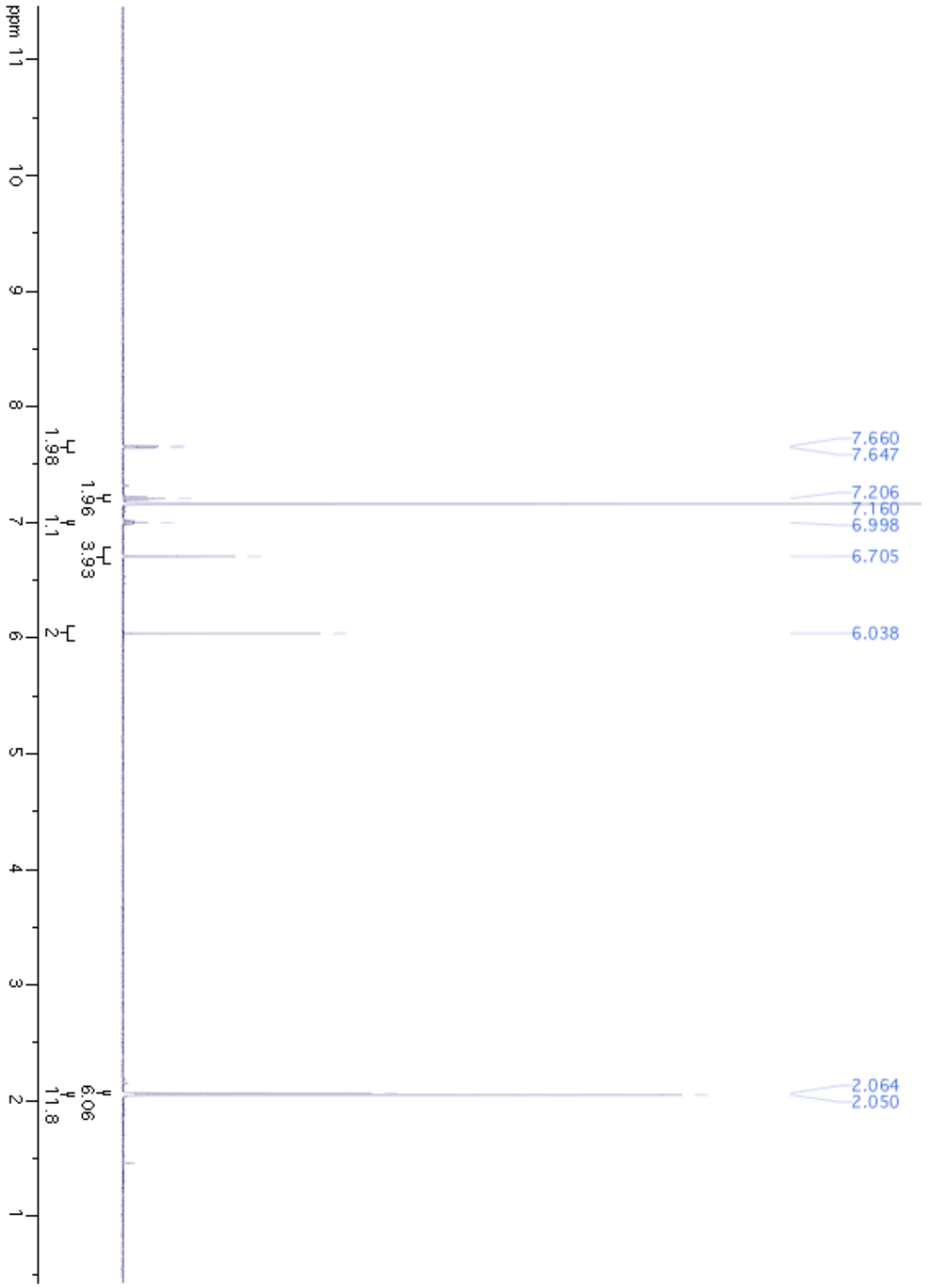
^{1}H-NMR (C_6D_6) compound **2**



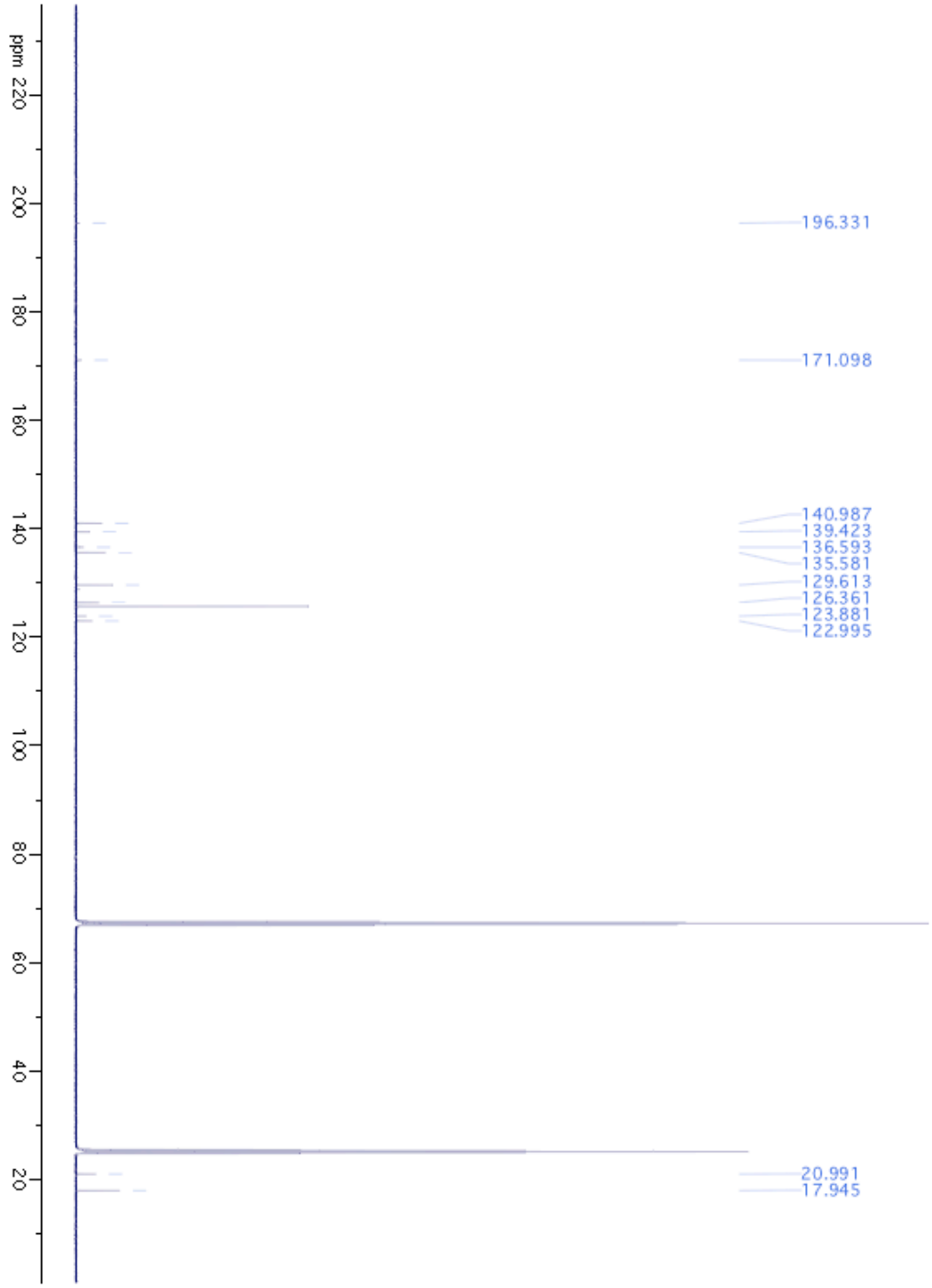
^{13}C-NMR (C_6D_6) compound **2**



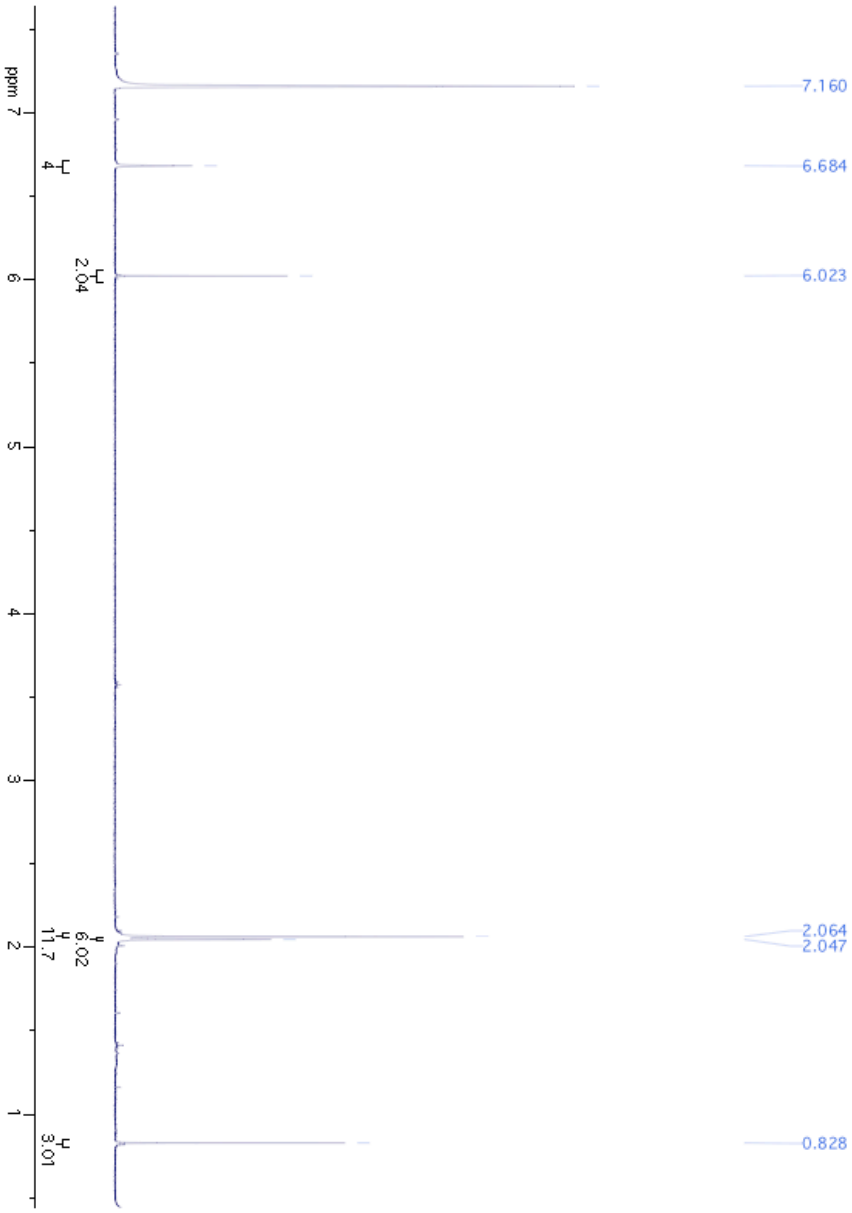
^{1}H-NMR (C_6D_6) compound **3**



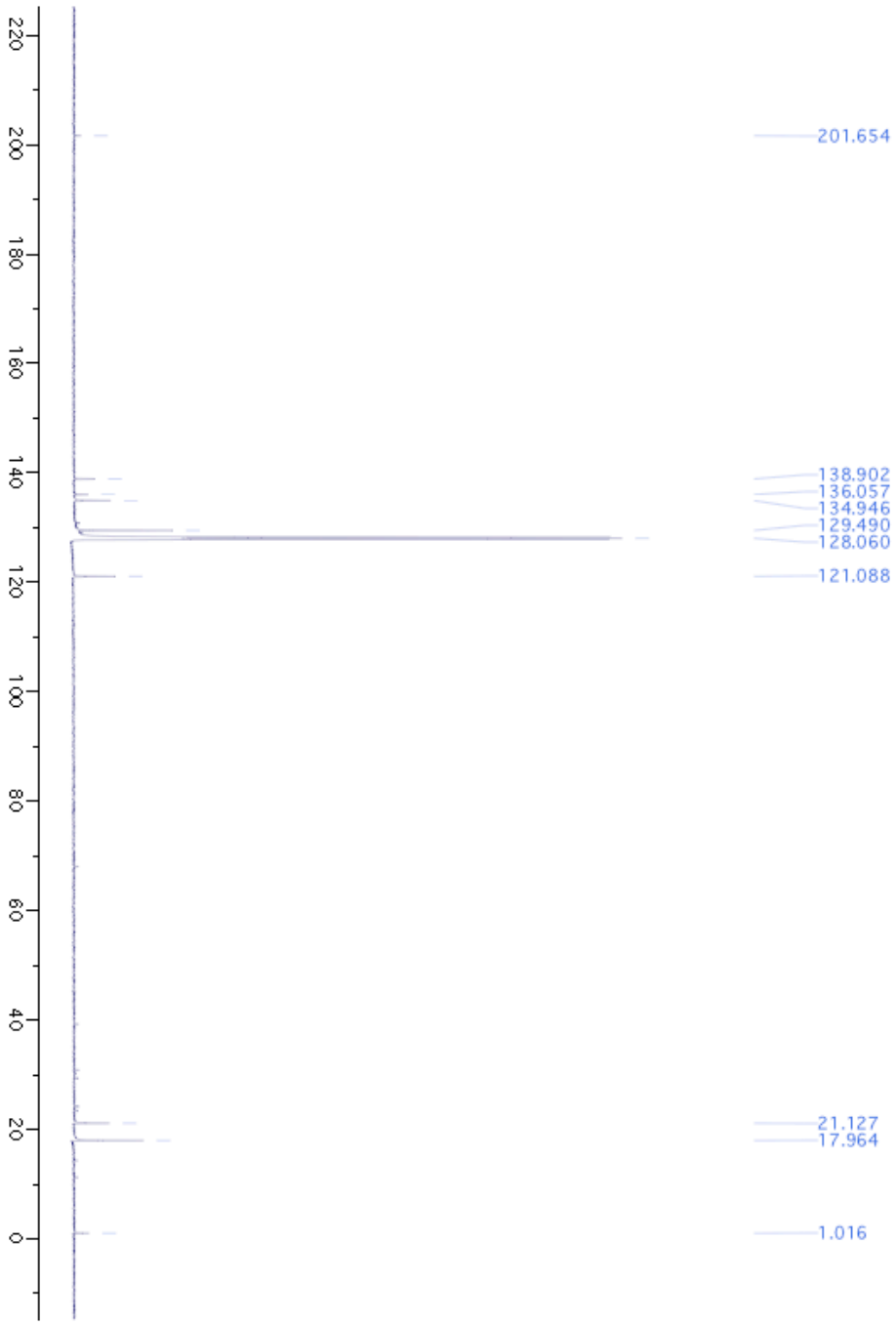
^{13}C-NMR (THF-d_8) compound **3**



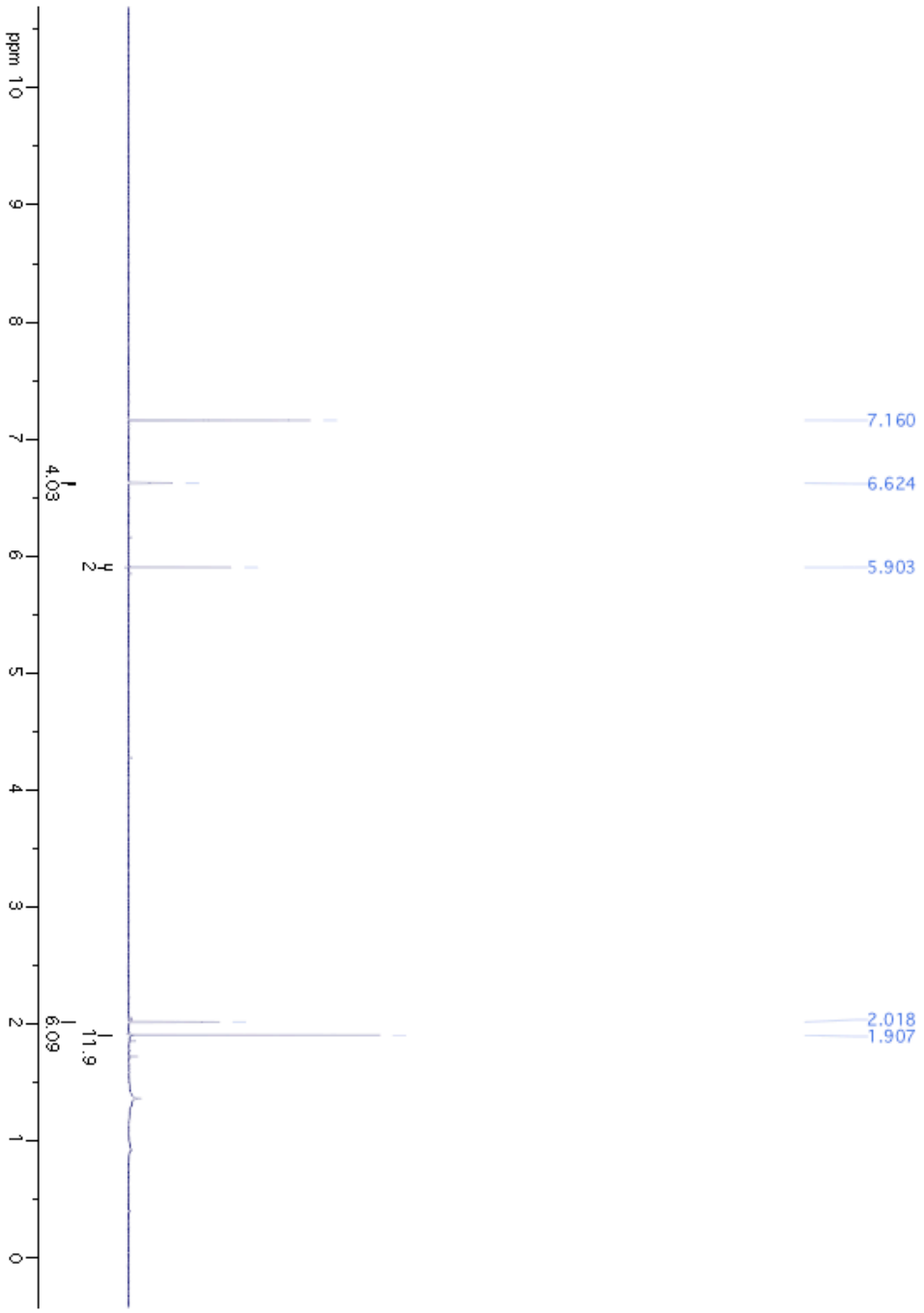
^{1}H-NMR (C_6D_6) compound **4**



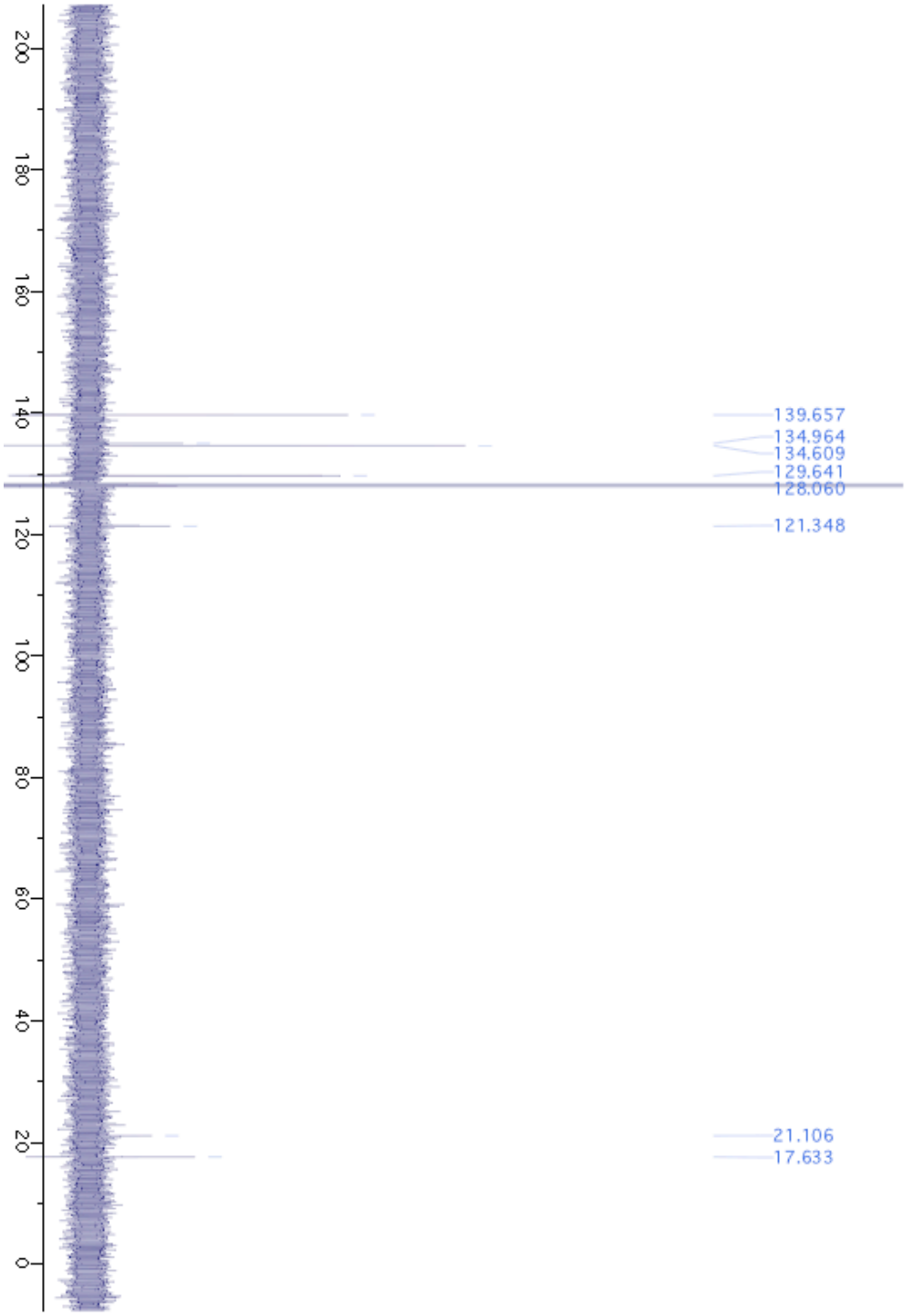
^{13}C-NMR (C_6D_6) compound **4**



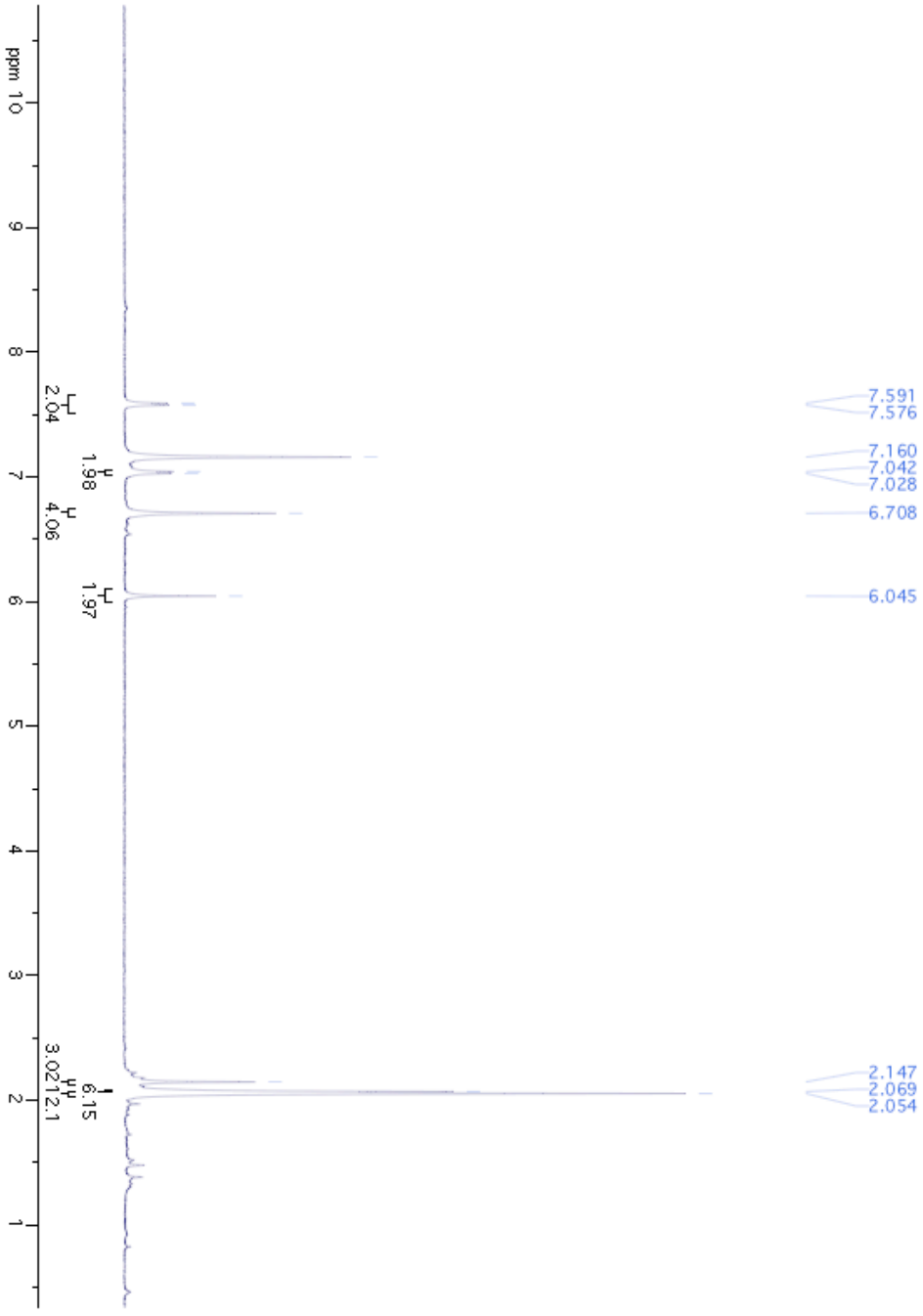
^{1}H-NMR (C_6D_6) compound **5**



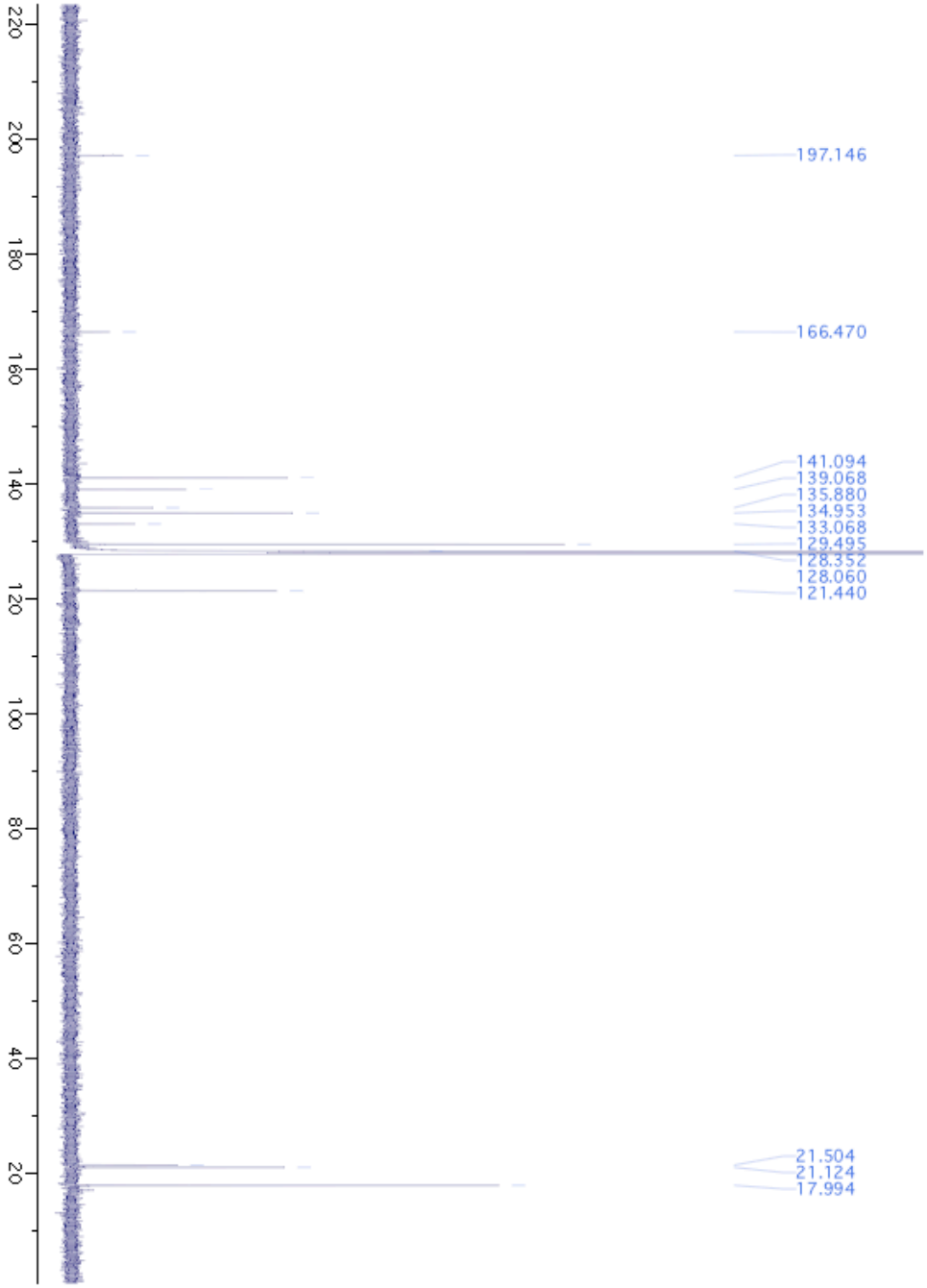
^{13}C-NMR (C_6D_6) compound **5**



^{1}H-NMR (C_6D_6) compound **6**



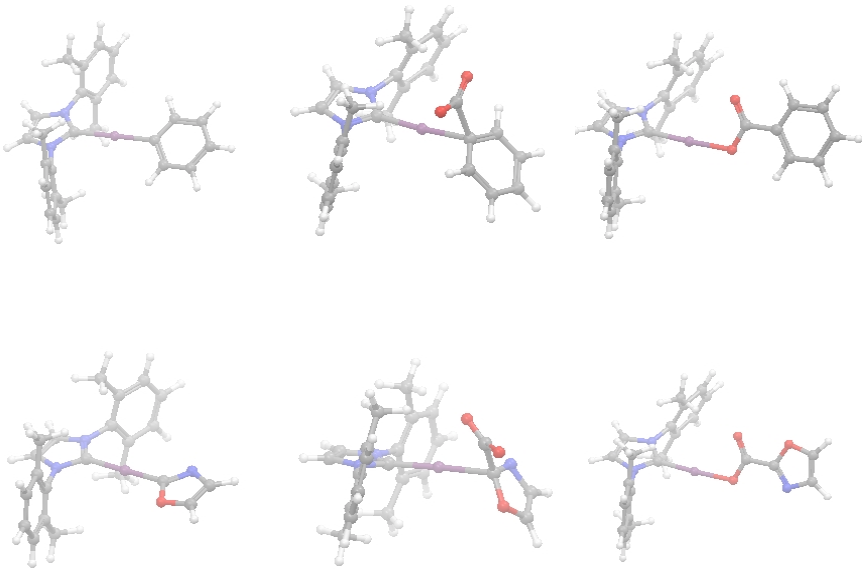
^{13}C-NMR (C_6D_6) compound **6**

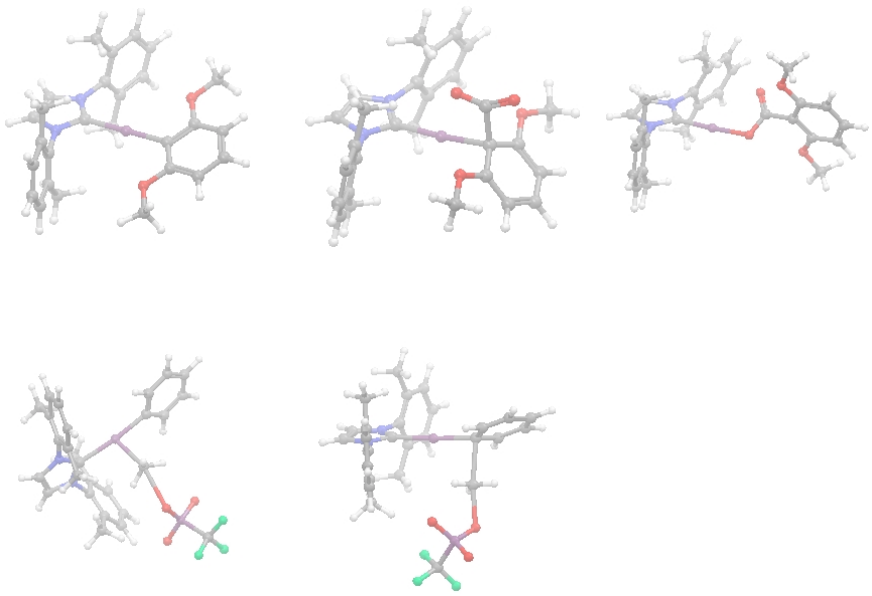


4. Computational details

All calculations were performed using the B3LYP flavor of density functional theory as implemented in Jaguar 7.5 except the final energy corrections, which were performed with M06. For geometry optimizations, solvation energy, and frequency calculations the LACVP** core potential and basis set was used, while for single point energy corrections LACV3P**++ augmented with two f-functions on Au as suggested by Martin was used. All geometries were fully optimized using the Poisson Boltzmann self consistent reaction field (PBF) to simulate the effect solvent implicitly. The dielectric constant was set to 2.284 and the probe radius to 2.60 to simulate benzene. All transition states were confirmed to be first-order saddle points by analytical frequency calculations. The Gibbs free energies were calculated as the sum G = E(M06/LACV3P**++(2f)) + Gsolv + ZPE + H298 + S298.

Figures of the optimized geometries of selected complexes and transition states.





Cartesian coordinates in Å and energies in atomic units unless stated otherwise of the calculated geometries. Numbered as in article.

3’

E (M06/LACV3P**++ 2f(Au)) = -1212.12737843477

ZPE (kcal mol 1) = 272.740

Gsolv = -0.009781

DH298 (kcal mol 1)= 17.707

DS298 (cal K 1 mol-1)= 182.2625035

Au1	-2.5256125777	1.4312785689	-0.0008619081
C2	-4.6095222687	1.3652537250	0.0013173959
N3	-5.4113811885	0.2644756909	-0.0486518860
C4	-6.7581018695	0.6172982334	-0.0325059688
C5	-6.8021739968	1.9715169836	0.0302079399
N6	-5.4812899354	2.4113980969	0.0507550640
H7	-7.5444717760	-0.1209471056	-0.0655825211

H8	-7.6350156706	2.6566207312	0.0603494807
C9	-4.3839118502	6.4694165135	0.2421345859
C10	-4.5818147490	5.7482284045	1.4181716727
C11	-4.9400219218	4.3960651429	1.3788828284
C12	-5.0929943953	3.7999793681	0.1161256451
C13	-4.8983398545	4.5010574794	-1.0854396638
C14	-4.5406232962	5.8512460904	-0.9970277439
H15	-4.1048536732	7.5187617866	0.2915941322
H16	-4.4539020415	6.2341934030	2.3819879188
H17	-4.3809417109	6.4173697595	-1.9111352487
C18	-4.0512410064	-3.7132006241	-0.2290800132
C19	-4.2889826059	-3.0074218486	-1.4070933943
C20	-4.7352389877	-1.6815079520	-1.3715056667
C21	-4.9341429177	-1.0959401928	-0.1101815821
C22	-4.7015499601	-1.7820438298	1.0931683676
C23	-4.2558288828	-3.1059005178	1.0083881004
H24	-3.7034973909	-4.7419695744	-0.2758870715
H25	-4.1237068831	-3.4845257490	-2.3696479300
H26	-4.0649965530	-3.6599331013	1.9239050192
C27	-5.1288448453	3.6077526728	2.6534824663
H28	-6.1158893176	3.1341976766	2.7005416767
H29	-4.3833566660	2.8083645464	2.7326368587
H30	-5.0237854080	4.2561918336	3.5271371673
C31	-5.0426251894	3.8247465321	-2.4283792697
H32	-4.9483834602	4.5521276813	-3.2388295837

H33	-4.2674743003	3.0619076524	-2.5649925548
H34	-6.0111759295	3.3236637980	-2.5335566086
C35	-4.8976635042	-1.1152637886	2.4341821859
H36	-4.7599510032	-1.8337282933	3.2463205559
H37	-4.1754478258	-0.3026670426	2.5737665733
H38	-5.8976622258	-0.6790343794	2.5333597819
C39	-4.9684148252	-0.9081350685	-2.6480323023
H40	-5.9837099523	-0.4992746774	-2.7002421267
H41	-4.2756281445	-0.0624156681	-2.7249169173
H42	-4.8175860106	-1.5494071401	-3.5202733517
C43	2.3799188422	1.5829550100	-0.0142917445
C44	1.6388290929	2.7044615498	0.3638151594
C45	0.2417827373	2.6555116061	0.3656412593
C46	-0.4709147003	1.4951260537	-0.0056952182
C47	0.3096650336	0.3807835826	-0.3812990625
C48	1.7069305181	0.4179502379	-0.3880339420
H49	3.4672112638	1.6164684661	-0.0177222806
H50	2.1498670361	3.6196852455	0.6581192909
H51	-0.3066857806	3.5468518080	0.6645429389
H52	-0.1846974749	-0.5424471370	-0.6775917929
H53	2.2714423705	-0.4640537761	-0.6857841929

4’

E (M06/LACV3P**++ 2f(Au)) = -1020.49527422293

ZPE (kcal mol 1) = 238.617

Gsolv = -0.0079525

DH298 (kcal mol 1)= 15.890

DS298 (cal K 1 mol-1)= 169.4172798

Au1	1.8241747207	-0.1771985673	1.4265402926
C2	3.6408036513	0.1335863827	0.4428057065
N3	4.4348851144	1.2418383492	0.4603086992
C4	5.5718948907	1.0655530920	-0.3253124614
C5	5.4895158483	-0.1825981558	-0.8491647740
N6	4.3048532905	-0.7365127084	-0.3702066938
H7	6.3196058099	1.8361798281	-0.4333211527
H8	6.1506650928	-0.7244600509	-1.5078179852
C9	2.9863966340	-4.6074163707	-1.3640910305
C10	3.7775505264	-4.4134133156	-0.2335590249
C11	4.2207718275	-3.1342541066	0.1212668184
C12	3.8418396430	-2.0620192015	-0.7029402866
C13	3.0407139667	-2.2271734549	-1.8448919947
C14	2.6212686781	-3.5241266019	-2.1611325695
H15	2.6494727255	-5.6076918625	-1.6235294995
H16	4.0535148382	-5.2606759487	0.3888519386
H17	1.9976911500	-3.6797098055	-3.0377365976
C18	3.6240190164	4.7893410907	2.5748008216
C19	3.1594683084	4.6380977464	1.2697184353

C20	3.4084738589	3.4636654399	0.5506931690
C21	4.1419680671	2.4512892102	1.1912448705
C22	4.6177920597	2.5740647385	2.5074383019
C23	4.3450887450	3.7663686687	3.1875789368
H24	3.4207557309	5.7083983599	3.1182222850
H25	2.5918680632	5.4365776663	0.7988273339
H26	4.6997292411	3.8868343446	4.2080425269
C27	5.0528636420	-2.9188905260	1.3629918854
H28	5.9900842319	-2.3957682800	1.1430243140
H29	4.5079201191	-2.3113320459	2.0944281360
H30	5.3002467419	-3.8743586253	1.8326922180
C31	2.6198948726	-1.0491327687	-2.6912163633
H32	2.0390579179	-1.3825411104	-3.5551059741
H33	2.0001614146	-0.3558216661	-2.1115225610
H34	3.4808511461	-0.4808934945	-3.0606509204
C35	5.3762786500	1.4547816033	3.1800945059
H36	5.6981631048	1.7535516630	4.1808277648
H37	4.7478726475	0.5627193278	3.2769032241
H38	6.2656094477	1.1628971409	2.6110094593
C39	2.8826605129	3.2889781748	-0.8544017179
H40	3.6819058672	3.0481110706	-1.5641953099
H41	2.1546100666	2.4710832411	-0.8979657625
H42	2.3888388264	4.2015276112	-1.1981524524
C54	0.0141385623	-0.4985151921	2.4028096740
H55	-0.7633336368	-0.8227825732	1.6994800445

H56	0.1115910967	-1.2777641154	3.1694522381
H57	-0.3402282340	0.4147191491	2.8971857716

8

E (M06/LACV3P**++ 2f(Au)) = -2213.45841193912

ZPE (kcal mol 1) = 314.891

Gsolv = -0.0139341

DH298 (kcal mol 1)= 23.523

DS298 (cal K 1 mol-1)= 233.4569777

C46	-0.2964051349	-0.8068774386	2.4419277684
Au1	1.6270327922	-0.5016419596	1.7510166567
C2	3.6670863487	-0.1706098667	1.0843111487
N3	4.3923676697	0.9710585414	1.2265912871
C4	5.6688315908	0.8204511554	0.6937365172
C5	5.7426269871	-0.4469033337	0.2160374359
N6	4.5080839474	-1.0406889918	0.4665233129
H7	6.3907000353	1.6224112331	0.7038518968
H8	6.5425975206	-0.9796146166	-0.2746877525
C9	3.5481419689	-4.9721537744	-0.7040747717
C10	4.0364959641	-4.7318092835	0.5782052978
C11	4.3646051878	-3.4348272089	0.9900934761
C12	4.1738321465	-2.3913081599	0.0686358406
C13	3.7097044669	-2.6069693650	-1.2413151851
C14	3.3945658511	-3.9212100796	-1.6053006723

H15	3.2962288964	-5.9852184598	-1.0065783143
H16	4.1727813456	-5.5572468195	1.2722481789
H17	3.0250177145	-4.1154238104	-2.6087670175
C18	2.9457718310	4.5145758113	2.9830626335
C19	2.6577340181	4.2331081265	1.6494268086
C20	3.1368942939	3.0683555936	1.0385505482
C21	3.9044282982	2.1927280066	1.8276182302
C22	4.2423704844	2.4682761726	3.1637041691
C23	3.7376353533	3.6447984906	3.7297331422
H24	2.5581886141	5.4213395356	3.4400836350
H25	2.0543251822	4.9230787464	1.0657629262
H26	3.9733573977	3.8766939455	4.7653115748
C27	4.9027348998	-3.1900643592	2.3804707170
H28	5.7610896003	-2.5104791671	2.3750347177
H29	4.1409289471	-2.7460289031	3.0300704629
H30	5.2197327022	-4.1305599230	2.8384371607
C31	3.5381310796	-1.4767995003	-2.2263784538
H32	3.3308322793	-1.8701310009	-3.2246596523
H33	2.7023212043	-0.8356501815	-1.9349633714
H34	4.4336658782	-0.8494122001	-2.2887230222
C35	5.1509507423	1.5667873336	3.9675684688
H36	5.0466635746	1.7702332102	5.0364744265
H37	4.9399100698	0.5074901757	3.8008746317
H38	6.2038669902	1.7285139065	3.7038468214
C39	2.8518243444	2.7883319092	-0.4164552552

H40	3.7807124235	2.6500515123	-0.9828035525
H41	2.2510218296	1.8857531182	-0.5469945914
H42	2.3045241952	3.6207938955	-0.8641810662
C43	-2.9467235645	-1.2006835031	3.2762398894
C44	-2.1694509160	-2.2869078079	2.8693351636
C45	-0.8469373869	-2.0924831287	2.4594200258
C47	-1.0724158924	0.2784481006	2.8615316292
C48	-2.3947315965	0.0815357945	3.2715787531
H49	-3.9761244967	-1.3520639139	3.5911180482
H50	-2.5929312234	-3.2886496116	2.8632372437
H51	-0.2595555845	-2.9480786751	2.1354012628
H52	-0.6649798094	1.2852218030	2.8457471091
H53	-2.9939668170	0.9354236758	3.5794350456
C54	2.1208238175	-0.8205727085	3.7455895372
H55	1.7110444137	-1.7833771626	4.0488694776
H56	3.2048009508	-0.8040377026	3.8330198126
H57	1.6673887156	-0.0147115630	4.3221032168
O58	1.0043302587	-0.1750144022	-0.3819006430
S59	-0.3784022408	0.2692292936	-0.7835173901
O60	-0.7330941711	1.5644092002	-0.2469146058
O62	-1.3650609627	-0.7832325372	-0.7522749915
C62	-0.0667829431	0.5643995022	-2.5759613637
F63	0.3442995090	-0.5612064311	-3.1842115472
F64	-1.1910579974	0.9817006369	-3.1745159982
F65	0.8796888588	1.5031882609	-2.7574505535

9

E (M06/LACV3P**++ 2f(Au)) = -1400.69692197602

ZPE (kcal mol 1) = 282.460

Gsolv = -0.0233636

DH298 (kcal mol 1)= 19.339

DS298 (cal K 1 mol-1)= 202.086

C32	0.2352355132	-0.3017815229	0.1811998722
Au1	1.8560157808	-1.5010185713	2.1817088869
C2	3.2511993446	-1.4140502268	3.5985552139
N3	4.4440969354	-2.0663463127	3.6593509873
C4	5.1888987632	-1.6364711088	4.7530890971
C5	4.4436477369	-0.6974101301	5.3864999060
N6	3.2590437466	-0.5720178194	4.6687774872
H7	6.1667142642	-2.0367639732	4.9677443917
H8	4.6398948174	-0.1045268543	6.2652784260
C9	0.1937930143	2.0825594506	5.7943252577
C10	1.0604027532	2.4300575393	4.7639126416
C11	2.0804659428	1.5630280564	4.3498696138
C12	2.1936843016	0.3378327131	5.0265290962
C13	1.3213972029	-0.0480106172	6.0607328290
C14	0.3202564716	0.8509297111	6.4348555898
H15	-0.5904246138	2.7710138491	6.0965203207
H16	0.9475476754	3.3842098513	4.2569174971
H17	-0.3692033398	0.5760232643	7.2282601886
C18	5.7995410371	-4.9208799160	0.8863998234

C19	5.0497812926	-5.3273572314	1.9875924622
C20	4.5817682640	-4.3957086860	2.9198643713
C21	4.8989471819	-3.0457625953	2.7020229013
C22	5.6482766384	-2.6045457607	1.5989717490
C23	6.0952171180	-3.5733687405	0.6944828394
H24	6.1527459139	-5.6583289879	0.1711470402
H25	4.8159375037	-6.3790038354	2.1280334622
H26	6.6734719773	-3.2611543801	-0.1706763003
C27	2.9587418971	1.9384372130	3.1812787960
H28	3.9671049360	1.5240580728	3.2661564139
H29	2.5125390254	1.5648308780	2.2500182092
H30	3.0418254068	3.0261930191	3.1007074887
C31	1.4316886848	-1.4010610910	6.7240606171
H32	0.6385409857	-1.5297106384	7.4646616306
H33	1.3407476450	-2.2080686260	5.9884945653
H34	2.3916563899	-1.5378712916	7.2347878818
C35	5.9380626239	-1.1396058641	1.3726382214
H36	6.5936415398	-1.0065674264	0.5085019544
H37	5.0132645229	-0.5824194960	1.1838186257
H38	6.4238545894	-0.6775545504	2.2392691684
C39	3.7404989546	-4.8300039498	4.0962591165
H40	4.1417850659	-4.4621629514	5.0468782348
H41	2.7177240645	-4.4463452438	4.0065320422
H42	3.6883906862	-5.9202381151	4.1505005378
O31	0.4220142807	-1.4963523667	0.6791096143

O33	0.8405932311	0.7204815017	0.5271254695
C46	-2.7506913476	-0.0219958066	-2.9093020325
C47	-2.4808050095	-1.2601803841	-2.3226345277
C48	-1.5165362949	-1.3650056697	-1.3207913385
C49	-0.8139827285	-0.2301938972	-0.8987099483
C50	-1.0885053168	1.0088507905	-1.4905910893
C51	-2.0523659464	1.1134022941	-2.4910909922
H52	-3.5031172115	0.0583317576	-3.6900757195
H53	-3.0234109113	-2.1445050851	-2.6471108890
H54	-1.2955296773	-2.3190481015	-0.8548773437
H55	-0.5313682574	1.8744159907	-1.1469955220
H56	-2.2607660638	2.0785403161	-2.9460450874

10

E (M06/LACV3P**++ 2f(Au)) = -1226.00420561510

ZPE (kcal mol 1) = 246.393

Gsolv = -0.0241725

DH298 (kcal mol 1)= 16.635

DS298 (cal K 1 mol-1)= 180.888

Au1	-2.5086733738	1.4372361527	-0.0010969310
C2	-4.5761743028	1.3641765380	-0.0022256199
N3	-5.3698661459	0.2579648396	-0.0491038243
C4	-6.7179578866	0.6027286445	-0.0320445774
C5	-6.7702210139	1.9564790467	0.0269104085

N6	-5.4532428221	2.4053972534	0.0446980713
H7	-7.4977004754	-0.1416406978	-0.0623067748
H8	-7.6052413030	2.6382223223	0.0573117133
C9	-4.4385909944	6.4829863470	0.2299803086
C10	-4.6285128912	5.7617114302	1.4061044900
C11	-4.9534245176	4.4020717985	1.3691734874
C12	-5.0836648006	3.7996407693	0.1074504145
C13	-4.8926967420	4.4994430984	-1.0946844540
C14	-4.5681789366	5.8573040980	-1.0074013850
H15	-4.1836111453	7.5378692644	0.2780690966
H16	-4.5168816529	6.2524626628	2.3689015897
H17	-4.4105485827	6.4225098980	-1.9217584789
C18	-4.0195368495	-3.7208975201	-0.2277284000
C19	-4.2701545231	-3.0203671419	-1.4052408775
C20	-4.7085391333	-1.6927526654	-1.3704607402
C21	-4.8883232422	-1.1012402892	-0.1097941082
C22	-4.6381087027	-1.7801080431	1.0934541275
C23	-4.2003637666	-3.1058011648	1.0086986302
H24	-3.6776811779	-4.7510732194	-0.2740235336
H25	-4.1190364265	-3.5022155443	-2.3672508947
H26	-3.9958717719	-3.6542106304	1.9240546242
C27	-5.1264376936	3.6116313207	2.6442964917
H28	-6.0943141658	3.0996081656	2.6838160905
H29	-4.3493667466	2.8443457897	2.7348851909
H30	-5.0558451533	4.2673411390	3.5156436131

C31	-5.0037455260	3.8135086065	-2.4354429649
H32	-4.9283240437	4.5411808410	-3.2473206668
H33	-4.2006107081	3.0789101321	-2.5636263621
H34	-5.9536731851	3.2791033365	-2.5460382935
C35	-4.8046604831	-1.1027186497	2.4324274087
H36	-4.6641679483	-1.8182340020	3.2464523029
H37	-4.0689495101	-0.2998480770	2.5558801458
H38	-5.7971696702	-0.6529971683	2.5435185767
C39	-4.9476749298	-0.9207162601	-2.6461662756
H40	-5.9567435023	-0.4957432584	-2.6873759368
H41	-4.2414571866	-0.0874598604	-2.7347251789
H42	-4.8180416031	-1.5674338062	-3.5175236258
C43	-0.4849502907	1.5509780747	0.0082253667
N44	0.2760360233	2.6113455850	0.1338736744
C45	1.5850830143	2.1531355483	0.0783107627
C46	1.5785685590	0.8075335656	-0.0817535379
O47	0.2758883942	0.3976210907	-0.1295057100
H49	2.4289462241	2.8244284182	0.1574579645
H50	2.3367625805	0.0457875887	-0.1731174179

11

E (M06/LACV3P**++ 2f(Au)) = -1414.55986294824

ZPE (kcal mol 1) = 255.941

Gsolv = -0.0320425

DH298 (kcal mol 1)= 18.817

DS298 (cal K 1 mol-1)= 199.109

C43	-0.8051627791	-0.2075138752	-0.8962036281
C32	0.2427205394	-0.2494678926	0.1772089698
Au1	1.8577761999	-1.4747139223	2.1700201823
C2	3.2459360637	-1.4194295513	3.5948923127
N3	4.4305782007	-2.0861746362	3.6558672231
C4	5.1729425751	-1.6760793494	4.7587279787
C5	4.4340022289	-0.7356432462	5.3976653558
N6	3.2555702971	-0.5894508537	4.6741164836
H7	6.1446002929	-2.0901498093	4.9753895939
H8	4.6309789158	-0.1548778667	6.2843052558
C9	0.2039292677	2.0746939860	5.8139609784
C10	1.0795643248	2.4281795775	4.7931602220
C11	2.0959289784	1.5588782664	4.3756962046
C12	2.1957041866	0.3246991763	5.0373997076
C13	1.3146447680	-0.0672463944	6.0616907407
C14	0.3178466377	0.8347779767	6.4406761906
H15	-0.5773117929	2.7650470966	6.1195266983
H16	0.9768605802	3.3890300208	4.2968916051
H17	-0.3781534653	0.5556305798	7.2268576667
C18	5.7784768940	-4.9349928180	0.8730325113
C19	5.0169457657	-5.3416290540	1.9659754143
C20	4.5501417694	-4.4117702789	2.9008100262
C21	4.8810830506	-3.0632950648	2.6936002672

C22	5.6428616602	-2.6219802942	1.5990963791
C23	6.0876504124	-3.5891314690	0.6918533854
H24	6.1302107532	-5.6711547631	0.1558077155
H25	4.7726881481	-6.3919602928	2.0979394447
H26	6.6753359988	-3.2769836730	-0.1668748445
C27	2.9870666803	1.9433097998	3.2201173243
H28	3.9907157047	1.5191469955	3.3092133794
H29	2.5475275957	1.5877654482	2.2789840072
H30	3.0798977030	3.0312125236	3.1553394690
C31	1.4113639277	-1.4285736872	6.7098426879
H32	0.6137053295	-1.5596318220	7.4451616358
H33	1.3177194533	-2.2265493866	5.9648331046
H34	2.3677350225	-1.5784845051	7.2236044636
C35	5.9496196032	-1.1586649843	1.3851583253
H36	6.6105508013	-1.0265771086	0.5250278767
H37	5.0322343223	-0.5894188032	1.1963835457
H38	6.4367872078	-0.7086899132	2.2573611980
C39	3.6972241952	-4.8465745742	4.0686605301
H40	4.0920848725	-4.4838569456	5.0239201549
H41	2.6765510163	-4.4590086719	3.9717719681
H42	3.6402318350	-5.9367266147	4.1184689604
O31	0.4305881483	-1.4387680393	0.6614580223
O33	0.8143743926	0.7942791496	0.4975053527
N44	-1.5252096786	-1.1707537826	-1.3986000516
C45	-2.3187564990	-0.5550003829	-2.3486772427

C46	-2.0338424482	0.7745960522	-2.3735835938
O47	-1.0657287758	1.0137036605	-1.4488329048
H49	-3.0329866379	-1.1075180223	-2.9424148526
H50	-2.3914567915	1.6226789169	-2.9355267723

12

E (M06/LACV3P**++ 2f(Au)) = -2405.08955841395

ZPE (kcal mol 1) = 348.445

Gsolv = -0.0139714

DH298 (kcal mol 1)= 25.915

DS298 (cal K 1 mol-1)= 245.6410058

C1	-0.3091273085	-0.8364679262	2.4024385273
Au2	1.6242415686	-0.4923706091	1.7494131129
C3	3.6754405735	-0.1720282327	1.0625315325
N4	4.3925162591	0.9818503988	1.1081786542
C5	5.6366464017	0.8223709191	0.5067669540
C6	5.6995116234	-0.4636656862	0.0822341121
N7	4.4911825180	-1.0593242938	0.4326275581
H8	6.3454594482	1.6332301720	0.4379236416
H9	6.4762205044	-1.0073011471	-0.4327807778
C10	3.6369465001	-5.1271778404	-0.2475526848
C11	4.3025650080	-4.7401448376	0.9148243998
C12	4.6033959456	-3.3948125759	1.1538623741
C13	4.1915751963	-2.4539773396	0.1913375678

C14	3.5557589404	-2.8176036714	-1.0073818364
C15	3.2791456898	-4.1776077173	-1.2010372721
H16	3.4102508802	-6.1765874915	-0.4176414767
H17	4.6034043064	-5.4876253596	1.6444790280
H18	2.7809693288	-4.4874493713	-2.1159881643
C19	3.1095332877	4.5753758262	2.8849278134
C20	2.8102870601	4.3180303472	1.5491171014
C21	3.2347412345	3.1354866981	0.9306386544
C22	3.9514512299	2.2177402749	1.7159047983
C23	4.3004939047	2.4644365301	3.0557964012
C24	3.8564607994	3.6621421879	3.6279573407
H25	2.7674958972	5.4975900843	3.3476736459
H26	2.2409066252	5.0399534358	0.9698917675
H27	4.1051045465	3.8773252765	4.6641382115
C28	5.3661026567	-2.9846788138	2.3924412678
H29	6.3115489933	-2.4918746753	2.1379952223
H30	4.7914364736	-2.2884167955	3.0103966890
H31	5.5994278479	-3.8597451152	3.0046034964
C32	3.1851732771	-1.8026622215	-2.0606066145
H33	2.8990021904	-2.3060828271	-2.9875694917
H34	2.3445127505	-1.1834185270	-1.7366025994
H35	4.0204894193	-1.1303226404	-2.2846665996
C36	5.1364257868	1.4908647476	3.8535920083
H37	5.2944640345	1.8651463855	4.8684006710
H38	4.6509927500	0.5135501165	3.9305084492

H39	6.1201562215	1.3345329209	3.3959389974
C40	2.9492884387	2.8771629487	-0.5276142400
H41	3.8782014142	2.8355135697	-1.1103283564
H42	2.4248110142	1.9313463893	-0.6751039057
H43	2.3276984239	3.6729549359	-0.9433106672
C44	-2.9726458198	-1.2929522189	3.1300395060
C45	-2.1801930763	-2.3482265031	2.6754659235
C46	-0.8481149740	-2.1226532950	2.3200140525
C47	-1.0959321274	0.2163789330	2.8744849145
C48	-2.4285278806	-0.0119896905	3.2299287912
H49	-4.0098305583	-1.4685658219	3.4049037070
H50	-2.5979889414	-3.3489717862	2.5933341694
H51	-0.2442198560	-2.9537135293	1.9646422890
H52	-0.6911414207	1.2218640163	2.9430500322
H53	-3.0406384880	0.8160244128	3.5797652373
O54	0.9898382463	0.0344525104	-0.3411000886
S55	-0.3994394020	0.4954698160	-0.7096465187
O56	-0.7565395579	1.7554700322	-0.0978782891
O57	-1.3784146107	-0.5639967429	-0.7297534433
C58	-0.1173640505	0.8872990733	-2.4896243563
F59	0.3380993841	-0.1901604752	-3.1519026483
F60	-1.2702382219	1.2725932544	-3.0541606830
F61	0.7762527078	1.8796587643	-2.6429612944
C62	2.5519110859	-1.6851751029	6.3475066203
C63	2.3009503688	-0.3561603435	6.0003059419

C64	2.0395637705	-0.0077108561	4.6704419988
C65	2.0399928075	-0.9974458178	3.6846513651
C66	2.2783422110	-2.3308731359	4.0245036552
C67	2.5401639472	-2.6690879332	5.3573319159
H68	2.7445764939	-1.9530314833	7.3828936348
H69	2.2946512487	0.4168730366	6.7651541307
H70	1.8302505628	1.0268941711	4.4172945638
H71	2.2522638297	-3.1092977757	3.2682567915
H72	2.7228850935	-3.7088405384	5.6181860465

TS1

E (M06/LACV3P**++ 2f(Au)) = -2213.41819812328

ZPE (kcal mol 1) = 314.110

Gsolv = -0.0182615

DH298 (kcal mol 1)= 24.664

DS298 (cal K 1 mol-1)= 234.0172017

O58	0.0000000000	0.0000000000	0.0000000000
C54	0.0000000000	0.0000000000	2.6260664534
Au1	0.6211491827	0.0000000000	4.7146329267
C46	-1.3789333499	0.0239981502	5.1149024280
C2	2.7465563393	-0.0215755913	4.5305264919
N3	3.5550619436	-1.0546199933	4.1810160494
C4	4.8873124901	-0.6654911989	4.1960827811
C5	4.9094562465	0.6426715929	4.5655792168

N6	3.5871590054	1.0196525354	4.7643013352
H7	5.6843391287	-1.3470194356	3.9415572406
H8	5.7290310927	1.3316013006	4.7007494506
C9	2.2553171884	4.8660621449	5.8291709872
C10	2.4706195640	4.5534316351	4.4880369253
C11	2.9204508609	3.2832320195	4.1087645442
C12	3.1427745022	2.3446540120	5.1322548967
C13	2.9431910126	2.6326381181	6.4931381753
C14	2.4916549170	3.9162090112	6.8215727070
H15	1.9032669846	5.8572040156	6.1024591837
H16	2.2858210274	5.2993899424	3.7196520652
H17	2.3257423435	4.1680624634	7.8657541814
C18	2.0712208834	-4.7957104185	2.9522147327
C19	2.2205335520	-4.5237008973	4.3127131643
C20	2.7205982684	-3.2923163193	4.7467316652
C21	3.0737570674	-2.3533641125	3.7604086700
C22	2.9616686461	-2.6080996703	2.3831712459
C23	2.4355608269	-3.8496380747	1.9990270942
H24	1.6616823127	-5.7507022183	2.6338840126
H25	1.9398421456	-5.2709065209	5.0507070664
H26	2.2908983849	-4.0513176451	0.9423098975
C27	3.1457052117	2.9472634907	2.6526089837
H28	4.1844826942	2.6590860539	2.4552527069
H29	2.5141113215	2.1133536429	2.3269991723
H30	2.9120752126	3.8064784423	2.0193275387

C31	3.1974778313	1.6023315335	7.5696650549
H32	3.0705885998	2.0433238707	8.5614210107
H33	2.5050266995	0.7558603416	7.4904004955
H34	4.2113711401	1.1916403739	7.5092988829
C35	3.3930348901	-1.6210629962	1.3232642080
H36	2.7488662251	-1.7134272515	0.4453731720
H37	3.3544866401	-0.5848329728	1.6690313266
H38	4.4264636044	-1.8185025681	1.0098380050
C39	2.8660186330	-2.9949007743	6.2215741965
H40	3.8626553779	-2.6117076409	6.4667950086
H41	2.1412414939	-2.2420247471	6.5546935600
H42	2.6977249625	-3.8988882154	6.8122007922
C43	-4.0351725183	0.0269099107	6.0328479133
C44	-3.3008186031	1.2149040830	6.0126138277
C45	-1.9839910266	1.2173348443	5.5447333215
C47	-2.1383004702	-1.1576503316	5.1045160589
C48	-3.4542206160	-1.1574335992	5.5732744434
H49	-5.0627752976	0.0276370095	6.3870681894
H50	-3.7539896980	2.1424250656	6.3538337281
H51	-1.4292993440	2.1523273958	5.5279838178
H52	-1.7065481452	-2.0849248032	4.7371617548
H53	-4.0277580695	-2.0808511715	5.5694493383
H55	-0.9153970768	-0.5728648878	2.5437535185
H56	-0.0963760968	1.0601324319	2.4150594283
H57	0.8823482015	-0.4804855788	2.2243966277

S59	-0.3716105972	-1.3696337000	-0.3742410719
O60	-1.4259969153	-1.9486830570	0.4465542229
O62	0.7572881023	-2.2472716482	-0.6577865482
C62	-1.1602995497	-1.1370947843	-2.0190858005
F63	-0.2967436401	-0.5886402158	-2.8928404058
F64	-1.5737145548	-2.3118868965	-2.5259646244
F65	-2.2288577660	-0.3254182146	-1.9364311379

TS2

E (M06/LACV3P**++ 2f(Au)) = -2213.41526166809

ZPE (kcal mol 1) = 314.232

Gsolv = -0.0160419

DH298 (kcal mol 1)= 23.498

DS298 (cal K 1 mol-1)= 233.8627694

O58	0.0000000000	0.0000000000	0.0000000000
C54	0.0000000000	0.0000000000	2.0698476038
C46	0.2603755747	0.0000000000	4.3299952179
Au1	-1.6770653295	0.7815533885	4.5379199394
C2	-3.5763671182	1.5301115917	4.8375598615
N3	-3.9330936775	2.7164302185	5.4018088136
C4	-5.3172750482	2.8575304007	5.4344348542
C5	-5.8346299329	1.7331045918	4.8779468249
N6	-4.7557967564	0.9332800702	4.5172136394
H7	-5.7933691007	3.7347787921	5.8446881806

H8	-6.8545583246	1.4302269456	4.6981095428
C9	-5.1368275327	-2.8284953410	2.6661287610
C10	-5.0258144156	-1.6852317018	1.8841768466
C11	-4.8999903511	-0.4175978579	2.4710306952
C12	-4.8808743522	-0.3544725513	3.8718671616
C13	-4.9923724131	-1.4959300445	4.6903425263
C14	-5.1227453922	-2.7346959304	4.0592834418
H15	-5.2303332586	-3.8011833811	2.1903125014
H16	-5.0148037596	-1.7643517150	0.8012987503
H17	-5.2097057035	-3.6325410184	4.6659885223
C18	-1.2613103465	5.6355111220	6.8317841818
C19	-1.6950761592	4.6185768511	7.6802501478
C20	-2.5790853619	3.6328966965	7.2264087933
C21	-3.0064894059	3.7099484970	5.8904176399
C22	-2.5881217985	4.7242029793	5.0122536299
C23	-1.7041377381	5.6876226207	5.5113506153
H24	-0.5754567374	6.3930497585	7.2021396745
H25	-1.3463879283	4.5833630344	8.7091226580
H26	-1.3628194280	6.4832920227	4.8541904873
C27	-4.7813845863	0.7961454726	1.5799956198
H28	-4.7408336079	1.7314847646	2.1402983786
H29	-3.8804150909	0.7212677628	0.9642959352
H30	-5.6354954431	0.8510882209	0.8952201438
C31	-4.9569662636	-1.3953881339	6.1980194006
H32	-5.1130357907	-2.3774795681	6.6518868018

H33	-3.9914915527	-1.0117985305	6.5479758480
H34	-5.7295582609	-0.7204246030	6.5836220904
C35	-3.0617214054	4.7774571370	3.5782441681
H36	-2.6292991349	5.6381130753	3.0617173809
H37	-2.7730780575	3.8738428123	3.0296491150
H38	-4.1527472828	4.8590225682	3.5116741982
C39	-3.0391305821	2.5237906112	8.1432487361
H40	-4.1319005934	2.4627826942	8.1945035104
H41	-2.6777109299	1.5496136588	7.7945782202
H42	-2.6617541822	2.6803337067	9.1569883280
C43	2.8341967237	-1.0059608766	5.0019843106
C44	1.7482371115	-1.8801549882	4.8862443211
C45	0.4891801811	-1.3834355700	4.5528428126
C47	1.3889416491	0.8528024593	4.4554182708
C48	2.6513203678	0.3645368247	4.7874544684
H49	3.8203742936	-1.3916749501	5.2481078025
H50	1.8893852617	-2.9466515337	5.0436360506
H51	-0.3368671845	-2.0820536963	4.4405515248
H52	1.2712901875	1.9187694779	4.2716583343
H53	3.4950555809	1.0453141884	4.8708613259
H55	0.9743940263	-0.4551322493	2.0168223735
H56	-0.8881973911	-0.6112639445	2.0776241417
H57	-0.0922474965	1.0717473597	2.0219521928
S59	-1.0626815745	-0.7597189671	-0.7214484676
O60	-2.1232960133	-1.2325752205	0.1513996023

O62	-0.5432861720	-1.6848779513	-1.7033679471
C62	-1.8538211909	0.5717969965	-1.7118158476
F63	-0.9741863632	1.1489072355	-2.5420715608
F64	-2.8660845157	0.0785068423	-2.4407977833
F65	-2.3515266653	1.5289454150	-0.9008541429

TS3

E (M06/LACV3P**++ 2f(Au)) = -1400.65165929616

ZPE (kcal mol 1) = 280.608

Gsolv = -0.0252226

DH298 (kcal mol 1)= 19.382

DS298 (cal K 1 mol-1)= 199.469

C32	0.0000000000	0.0000000000	0.0000000000
C46	0.0000000000	0.0000000000	1.8774560782
Au1	2.1621539230	0.0000000000	1.5511485693
C2	4.1263668022	-0.0025802087	1.0493369868
N3	4.8965729709	-1.0833496278	0.7517931493
C4	6.1340849309	-0.6860093222	0.2571533371
C5	6.1343904358	0.6704466873	0.2490497230
N6	4.8968726918	1.0742995616	0.7386608558
H7	6.8811454394	-1.4016556792	-0.0463886618
H8	6.8814370980	1.3821934489	-0.0636752918
C9	3.7609490136	5.0996175970	1.1937994079
C10	3.3542115704	4.3935109131	0.0672283836

C11	3.7084234824	3.0495431086	-0.1150716092
C12	4.4905060718	2.4530883730	0.8869093208
C13	4.9121341566	3.1402373794	2.0405412594
C14	4.5341836551	4.4779427599	2.1735404065
H15	3.4736419659	6.1406467446	1.3124429226
H16	2.7456258613	4.8805019359	-0.6895106928
H17	4.8441087418	5.0311691863	3.0558794070
C18	3.7506614755	-5.1006352577	1.2505944347
C19	4.5222125645	-4.4692408540	2.2254175041
C20	4.9046995158	-3.1345290858	2.0774982426
C21	4.4887336113	-2.4599494483	0.9145642882
C22	3.7100754988	-3.0665961267	-0.0839501891
C23	3.3515908951	-4.4076315619	0.1129805006
H24	3.4589477065	-6.1390551681	1.3812697984
H25	4.8271545946	-5.0126199761	3.1154986215
H26	2.7458489861	-4.9025649427	-0.6410503571
C27	3.2130734310	2.3007006903	-1.3285880437
H28	3.8868995836	1.4924992134	-1.6246353881
H29	2.2260697738	1.8627575267	-1.1309836665
H30	3.1058196091	2.9828889283	-2.1770233604
C31	5.7221376338	2.4557498841	3.1171270018
H32	5.9336367172	3.1477764474	3.9360971590
H33	5.1821793048	1.5973041400	3.5323797049
H34	6.6799811616	2.0803838975	2.7393259447
C35	3.2233998381	-2.3310994548	-1.3092608495

H36	3.1151045970	-3.0240183434	-2.1489415494
H37	2.2383900492	-1.8841827618	-1.1214384297
H38	3.9034643723	-1.5313437662	-1.6136261815
C39	5.7133771462	-2.4395736509	3.1481929174
H40	6.6747358032	-2.0745635648	2.7692489309
H41	5.1764742108	-1.5727485462	3.5495931288
H42	5.9185378131	-3.1216833214	3.9769686406
C43	-1.4257009544	-0.0014585457	4.3089362312
C44	-1.0859237491	1.2122721681	3.7033955206
C45	-0.3905945415	1.2102575130	2.4959302385
C47	-0.3866517958	-1.2113779932	2.4969478527
C48	-1.0815256558	-1.2148034492	3.7049398191
H49	-1.9790387843	-0.0019227973	5.2452621001
H50	-1.3787265944	2.1507260801	4.1675533932
H51	-0.1638626373	2.1415549911	1.9841698977
H52	-0.1569859620	-2.1425544561	1.9856560015
H53	-1.3706898501	-2.1539501082	4.1700562814
O31	-0.0163706915	-1.1499101168	-0.4108540142
O33	-0.0211913610	1.1493195246	-0.4108438713

TS4

E (M06/LACV3P**++ 2f(Au)) = -1414.51137494595

ZPE (kcal mol 1) = 254.204

Gsolv = -0.0333249

DH298 (kcal mol 1)= 18.242

DS298 (cal K 1 mol-1)= 191.303

C43	0.0000000000	0.0000000000	0.0000000000
C32	0.0000000000	0.0000000000	1.6968911498
Au1	2.2619341091	0.0000000000	-0.0460033460
C2	4.2703036903	0.1205501918	-0.0330668594
N3	5.0163904276	0.9934816472	0.6952439829
C4	6.3709158489	0.7085819334	0.5659795148
C5	6.4698495647	-0.3618385506	-0.2607276235
N6	5.1719368233	-0.7099998414	-0.6209457714
H7	7.1231727659	1.2868006446	1.0778707374
H8	7.3254884314	-0.9095157762	-0.6217835843
C9	4.2588066502	-3.9227493932	-3.1732135755
C10	4.2642448885	-4.1154534390	-1.7944774371
C11	4.5551576774	-3.0613263830	-0.9211636369
C12	4.8414695841	-1.8115670197	-1.4931981062
C13	4.8380900078	-1.5843272207	-2.8795534531
C14	4.5423942252	-2.6689809897	-3.7107473539
H15	4.0300451470	-4.7542766629	-3.8337776595
H16	4.0351323309	-5.0936017177	-1.3813729351
H17	4.5306781606	-2.5230288169	-4.7873771895
C18	3.5371464004	4.2011661776	2.9788787409
C19	4.0285369936	4.4277012561	1.6938697519
C20	4.5122717931	3.3713317096	0.9197032359
C21	4.4902591177	2.0833050996	1.4867195085

C22	3.9964352138	1.8208517570	2.7742507925
C23	3.5206406565	2.9158250686	3.5087102863
H24	3.1603301556	5.0329437638	3.5672834939
H25	4.0300545041	5.4322509433	1.2799605954
H26	3.1257605975	2.7441381236	4.5058998519
C27	4.5282132353	-3.2664576175	0.5746073369
H28	5.4165852322	-2.8515665062	1.0622514226
H29	3.6533215649	-2.7798529930	1.0214082520
H30	4.4770253077	-4.3312334230	0.8144724292
C31	5.1154232637	-0.2164569139	-3.4572480271
H32	5.1056615883	-0.2512892418	-4.5494985774
H33	4.3572665518	0.5063211541	-3.1348512566
H34	6.0888318923	0.1750786514	-3.1414370639
C35	3.9186620312	0.4312999602	3.3590967221
H36	4.0004943640	0.4742931768	4.4490510898
H37	2.9523771533	-0.0299559864	3.1139736774
H38	4.7097504969	-0.2237447395	2.9839455669
C39	5.0110181360	3.6099199326	-0.4868579923
H40	6.0638032429	3.3301606322	-0.6080626759
H41	4.4371195735	3.0251648073	-1.2145545878
H42	4.9144191040	4.6654267295	-0.7528928897
O31	0.8924209983	-0.7349655633	2.1548409417
O33	-0.8865014609	0.7068863487	2.1382504247
N44	-0.1761501854	-1.1170127696	-0.7108849249
C45	-0.9008918639	-0.7609292136	-1.8189979697

C46	-1.1786393011	0.5755537667	-1.7491809674
O47	-0.6280458182	1.0753212048	-0.6315351395
H49	-1.1845666471	-1.4750436612	-2.5785876295
H50	-1.7167079659	1.2620900934	-2.3854846678

TS5

E (M06/LACV3P**++ 2f(Pd)) = -2213.43335174080

ZPE (kcal mol 1) = 313.606

Gsolv = -0.0152152

DH298 (kcal mol 1)= 23.088

DS298 (cal K 1 mol-1)= 235.8500823

C43	0.0000000000	0.0000000000	0.0000000000
C54	0.0000000000	0.0000000000	2.1308594987
Au1	1.9040089825	0.0000000000	0.8834770205
C2	3.8606671199	-0.0910387161	1.6621229841
N3	4.5989774542	-1.2136582788	1.8705161040
C4	5.8342672732	-0.9009239472	2.4296048814
C5	5.8669735790	0.4478990138	2.5688865807
N6	4.6512899893	0.9274743479	2.0910649257
H7	6.5621012747	-1.6611136467	2.6673854863
H8	6.6304981986	1.1074917498	2.9511111599
C9	3.6105309667	4.9995534198	1.9143775828
C10	4.4099492363	4.4431134338	0.9191980060
C11	4.7728735358	3.0917229086	0.9581873133

C12	4.2961754530	2.3268463555	2.0357109102
C13	3.5120262985	2.8655039887	3.0693240751
C14	3.1705201348	4.2196277936	2.9828576265
H15	4.7545719220	5.0563733376	0.0911104402
H16	2.5611704487	4.6638803688	3.7657359849
C17	3.3462976497	-5.1318562370	0.9777976450
C18	2.9618164214	-4.5380380969	2.1790209687
C19	3.3712685233	-3.2388659012	2.4982441654
C20	4.1685872239	-2.5579800758	1.5616243165
C21	4.5845195806	-3.1351420172	0.3491565255
C22	4.1529653525	-4.4397506382	0.0780715936
H23	2.3422859520	-5.0870941093	2.8835099427
H24	4.4544761381	-4.9100348391	-0.8541831820
C25	5.6288259926	2.4881878579	-0.1270314047
H26	6.5270955280	2.0112823848	0.2811456135
H27	5.0733862893	1.7351531259	-0.6889159378
H28	5.9465828829	3.2581487226	-0.8338427440
C29	3.0640803488	2.0295879449	4.2458003267
H30	2.5962991837	2.6581745956	5.0079666683
H31	2.3408529086	1.2628487466	3.9468792713
H32	3.9051037498	1.5046976995	4.7122334039
C33	5.4481281686	-2.3896238708	-0.6390582247
H34	5.7693756418	-3.0583436372	-1.4418208676
H35	4.8937518708	-1.5587619357	-1.0868104504
H36	6.3451160002	-1.9757347146	-0.1658285376

C37	2.9680965728	-2.6032683304	3.8089175401
H38	3.8397377729	-2.2605224977	4.3781052109
H39	2.3289685870	-1.7276999353	3.6504050454
H40	2.4183844480	-3.3159116996	4.4294037893
H41	3.0203946275	-6.1424315937	0.7450537122
H42	3.3347370713	6.0496009010	1.8612480390
C44	-1.7585505044	-0.0659882084	-2.1557002143
C45	-1.3162284616	1.1607120237	-1.6533681728
C46	-0.4495619822	1.2025580708	-0.5623986575
C47	-0.4567885893	-1.2329212326	-0.4820683924
C48	-1.3253873808	-1.2589848668	-1.5741964885
H49	-2.4360245033	-0.0916225467	-3.0048746787
H50	-1.6386839468	2.0883676865	-2.1182807491
H51	-0.1030422254	2.1563244216	-0.1770877720
H52	-0.1207120313	-2.1616097607	-0.0305160517
H53	-1.6583414039	-2.2135699334	-1.9735827278
H55	-1.0194888856	0.2918978456	1.9115581374
H56	0.0398503268	-1.0289829127	2.4832711496
H57	0.4341215700	0.7035612523	2.8410093483
O58	3.0436582958	-0.2413705439	-1.4169830206
S59	2.7834375789	0.7462358842	-2.4849249882
O60	2.9185846694	2.1266562124	-2.0467084121
O61	1.6532210158	0.4421918125	-3.3406031433
C62	4.2444162681	0.4753112932	-3.5772549453
F63	4.2701501161	-0.7823923288	-4.0519011346

F64	4.2299875348	1.3141261656	-4.6258849884
F65	5.4020314311	0.6761082786	-2.9083333741

TS6

E (M06/LACV3P**++ 2f(Au)) = -2405.07685276302

ZPE (kcal mol 1) = 347.599

Gsolv = -0.015567

DH298 (kcal mol 1)= 25.731

DS298 (cal K 1 mol-1)= 244.1811434

C46	0.0000000000	0.0000000000	0.0000000000
C47	0.0000000000	0.0000000000	2.0968583855
Au1	1.8498340779	0.0000000000	1.0319544265
C2	3.6876526058	-0.0805435868	2.1117364362
N3	4.4159051812	-1.1908867995	2.4033047110
C4	5.5723585760	-0.8602185353	3.1034234703
C5	5.5633220907	0.4878210486	3.2514401177
N6	4.4011433177	0.9479101533	2.6393539047
H7	6.2812659617	-1.6088924120	3.4218409462
H8	6.2620705466	1.1594567839	3.7257436488
C9	3.3041290237	5.0090103283	2.5681915376
C10	4.1218452715	4.4949245951	1.5643001075
C11	4.4981322944	3.1459928119	1.5602180111
C12	4.0132102742	2.3392004791	2.6033420650
C13	3.2014833567	2.8319834871	3.6399702543

C14	2.8524858058	4.1865750531	3.5989168393
H15	4.4761357076	5.1425682167	0.7668019294
H16	2.2254204365	4.5963287822	4.3867220573
C17	3.3143415642	-5.1461148199	1.4797752526
C18	2.8677668280	-4.5582818036	2.6623810906
C19	3.2227215948	-3.2444881968	2.9870906044
C20	4.0346475444	-2.5454456060	2.0755449790
C21	4.5169114513	-3.1169301635	0.8855972450
C22	4.1338476087	-4.4352016389	0.6064337354
H23	2.2417502290	-5.1230476565	3.3485744299
H24	4.4875596015	-4.9025609590	-0.3087965612
C25	5.3916043683	2.5928291123	0.4773014274
H26	6.3152750805	2.1741250445	0.8945829752
H27	4.8915012108	1.7974521524	-0.0826468855
H28	5.6683081567	3.3803924244	-0.2275738887
C29	2.7155412089	1.9433070379	4.7616514804
H30	2.2419355177	2.5409369643	5.5451900686
H31	1.9776666537	1.2175181178	4.4026376547
H32	3.5348889326	1.3770646393	5.2177581229
C33	5.4079777553	-2.3557176782	-0.0654571153
H34	5.7904051939	-3.0222751945	-0.8428237940
H35	4.8620298417	-1.5410169007	-0.5519769789
H36	6.2662657860	-1.9124363252	0.4517832325
C37	2.7456556395	-2.6122350981	4.2746291741
H38	3.5741223543	-2.1843093114	4.8497313056

H39	2.0320637741	-1.8032483364	4.0831412647
H40	2.2480016239	-3.3551356809	4.9037534381
H41	3.0301241687	-6.1682406169	1.2430199646
H42	3.0231444852	6.0589874013	2.5514450605
C43	-1.6623041784	-0.0279006691	-2.2442686432
C44	-1.2589397526	1.1874630196	-1.6866412426
C45	-0.4360874879	1.2069653190	-0.5611068324
C48	-0.4105886586	-1.2217399548	-0.5511304037
C49	-1.2347426813	-1.2303985216	-1.6760586367
H50	-2.3069950466	-0.0383351548	-3.1189314613
H51	-1.5801125303	2.1257648616	-2.1306784231
H52	-0.1301698546	2.1579559037	-0.1376926162
H53	-0.0881613404	-2.1629624065	-0.1153671143
H54	-1.5397887566	-2.1789461138	-2.1105834753
C55	-1.7384260895	0.0312826999	4.2926072048
C56	-1.3117928145	-1.1822593824	3.7490668539
C57	-0.4466943227	-1.2045097385	2.6533783687
C58	-0.4231403009	1.2203307639	2.6381844199
C59	-1.2888835480	1.2295105092	3.7336198905
H60	-2.4194854012	0.0430093820	5.1391121584
H61	-1.6578684244	-2.1222993000	4.1719032011
H62	-0.1357587995	-2.1561965215	2.2347802827
H63	-0.0913070821	2.1602749432	2.2093086584
H64	-1.6162764542	2.1818290637	4.1437955671
O58	3.3526971566	0.1856351180	-0.9060198204

S59	2.8578129162	0.5703462225	-2.2576867030
O60	2.3875566260	1.9388899316	-2.3375604244
O62	2.0577660064	-0.4463173030	-2.9073649678
C62	4.4417786576	0.5689340256	-3.1991891639
F63	5.0369493063	-0.6375359749	-3.1392377582
F64	4.2247732314	0.8609661577	-4.4918233319
F65	5.3059584928	1.4781837578	-2.7091230584

NHC-Au-OH

E (M06/LACV3P**++ 2f(Au)) = -1056.42659458454

ZPE (kcal mol 1) = 224.603

Gsolv = -0.0278613

DH298 (kcal mol 1)= 15.541

DS298 (cal K 1 mol-1)= 169.895

Au1	-2.5496997392	1.5027651883	0.0110403868
C2	-4.5496657431	1.3653591985	-0.0036001024
N3	-5.3238232955	0.2408284978	-0.0453250275
C4	-6.6788324219	0.5616933550	-0.0378466667
C5	-6.7591894547	1.9129576500	0.0093706911
N6	-5.4519389377	2.3907731214	0.0297974166
H7	-7.4426900400	-0.1989444083	-0.0658992714
H8	-7.6081427259	2.5773805011	0.0300392862
C9	-4.5622031970	6.4973201949	0.1888615507

C10	-4.7121732591	5.7747786424	1.3708995500
C11	-4.9927013985	4.4042603982	1.3416073292
C12	-5.1188100812	3.7931759461	0.0835521045
C13	-4.9667263600	4.4948795751	-1.1231386990
C14	-4.6862089576	5.8632823314	-1.0456919684
H15	-4.3450871100	7.5610653402	0.2302297494
H16	-4.6076882202	6.2729889458	2.3307182344
H17	-4.5615932025	6.4302667389	-1.9639643608
C18	-3.9958279519	-3.7467998027	-0.1922117857
C19	-4.2261072181	-3.0486696400	-1.3752790789
C20	-4.6497731181	-1.7160119620	-1.3506521963
C21	-4.8348738955	-1.1157141726	-0.0946140122
C22	-4.6062926200	-1.7929767032	1.1140406784
C23	-4.1821479039	-3.1238663968	1.0395426007
H24	-3.6673839446	-4.7817173141	-0.2304469026
H25	-4.0732828517	-3.5373510174	-2.3335854043
H26	-3.9953102854	-3.6713265351	1.9592740820
C27	-5.1283455039	3.6094392519	2.6183953903
H28	-6.0854268661	3.0787026173	2.6713786393
H29	-4.3363424131	2.8556904610	2.6921898690
H30	-5.0565040726	4.2643364776	3.4902919378
C31	-5.0751034906	3.7970811150	-2.4574844589
H32	-4.9955914923	4.5157961153	-3.2768884048
H33	-4.2757908067	3.0566554685	-2.5745610261
H34	-6.0267706116	3.2652757784	-2.5643994294

C35	-4.7876555848	-1.1098083272	2.4482606119
H36	-4.6514214571	-1.8213808217	3.2665475184
H37	-4.0568857954	-0.3028739242	2.5740956445
H38	-5.7836190023	-0.6642620266	2.5485640000
C39	-4.8760416731	-0.9499143437	-2.6321067971
H40	-5.8845944617	-0.5248208818	-2.6836791692
H41	-4.1686930406	-0.1175769482	-2.7181394671
H42	-4.7398500878	-1.6013580188	-3.4988886343
O43	-0.5480842022	1.5632012702	0.0255774960
H44	-0.2928119881	2.4948267708	0.0620841682

NHC-Au-(Ph-2,4-(OMe)2)

E (M06/LACV3P**++ 2f(Au)) = -1441.11514870904

ZPE (kcal mol 1) = 313.566

Gsolv = -0.0197016

DH298 (kcal mol 1)= 20.45

DS298 (cal K 1 mol-1)= 207.551

Au1	-2.4946448152	1.4335576739	-0.0142267232
C2	-4.5619035943	1.3639073060	0.0051328877
N3	-5.3648330587	0.2619762245	-0.0457415584
C4	-6.7117058437	0.6126514612	-0.0190842468
C5	-6.7577660522	1.9655255167	0.0498578677
N6	-5.4380423118	2.4080739768	0.0645388105
H7	-7.4949258206	-0.1278942059	-0.0521096624
H8	-7.5896750245	2.6504400217	0.0895265423
C9	-4.4359589480	6.4869590675	0.2837010870

C10	-4.6052197053	5.7505091404	1.4538817363
C11	-4.9208140707	4.3886812431	1.4049463362
C12	-5.0657512211	3.7998172047	0.1386830639
C13	-4.8902219998	4.5145329560	-1.0568339837
C14	-4.5737411522	5.8732321749	-0.9588928532
H15	-4.1919135497	7.5442988609	0.3404270547
H16	-4.4868128433	6.2313215012	2.4212013082
H17	-4.4301336151	6.4492910357	-1.8689227186
C18	-4.0798678838	-3.7381061901	-0.2388692451
C19	-4.2933969851	-3.0213917959	-1.4138436947
C20	-4.7041115921	-1.6848726917	-1.3745704526
C21	-4.8974080548	-1.1011717810	-0.1125289781
C22	-4.6798877459	-1.7959123989	1.0883440142
C23	-4.2682299340	-3.1295708194	0.9997055823
H24	-3.7614251817	-4.7757801017	-0.2883790302
H25	-4.1357797804	-3.4976819094	-2.3777342043
H26	-4.0898613150	-3.6894477072	1.9136888256
C27	-5.0631724126	3.5800349521	2.6720170105
H28	-6.0193671330	3.0471229693	2.7161759576
H29	-4.2685547371	2.8282803735	2.7400061632
H30	-4.9948776366	4.2260319664	3.5511050974
C31	-5.0053734772	3.8402784060	-2.4025788154
H32	-4.9269569031	4.5733811420	-3.2094484636
H33	-4.2056891816	3.1024045149	-2.5340727343
H34	-5.9575975195	3.3108639380	-2.5160253075
C35	-4.8493262632	-1.1242843063	2.4300322662

H36	-4.7153022256	-1.8445162391	3.2411934904
H37	-4.1090614889	-0.3262404052	2.5580553435
H38	-5.8398475660	-0.6691630694	2.5405203179
C39	-4.8947470693	-0.8944011337	-2.6466291010
H40	-5.8806603480	-0.4190059913	-2.6929528290
H41	-4.1456756138	-0.0976082348	-2.7197622477
H42	-4.7890012691	-1.5407308427	-3.5217224707
C43	2.3895822973	1.6031933368	-0.0781485448
C44	1.6682872626	2.7287167635	0.3126121755
C45	0.2661491091	2.6622307918	0.3259954600
C46	-0.4389568309	1.5032426808	-0.0399757901
C47	0.3358312286	0.3963145222	-0.4261714862
C48	1.7388704427	0.4294571936	-0.4505064681
H49	3.4761638108	1.6414870293	-0.0928234262
H50	2.1973886510	3.6301098421	0.5988871799
H53	2.3225687642	-0.4323892379	-0.7518690422
O53	-0.5129149522	3.7369999298	0.7033312509
O54	-0.3749636839	-0.7306268191	-0.7848398418
C55	0.3409356727	-1.8852279249	-1.1688314747
H56	-0.4097445775	-2.6463809783	-1.3941870354
H57	0.9557311099	-1.7134542043	-2.0643808840
H58	0.9929353495	-2.2550548982	-0.3643659201
C58	0.1282729652	4.9427205244	1.0614374852
H59	-0.6687914003	5.6491174199	1.3049768501
H60	0.7789507753	4.8218500923	1.9396783958
H61	0.7287231967	5.3533660712	0.2368858164

NHC-Au-(OOC-Ph-2,4-(OMe)2)-CO2extTS

E (M06/LACV3P**++ 2f(Au)) = -1629.63486347955

ZPE (kcal mol 1) = 321.314

Gsolv = -0.032197

DH298 (kcal mol 1)= 22.176

DS298 (cal K 1 mol-1)= 218.501

C32	0.0000000000	0.0000000000	0.0000000000
C46	0.0000000000	0.0000000000	1.8038301687
Au1	2.1853571135	0.0000000000	1.9963231093
C2	4.2074449246	-0.0344422881	1.9451955575
N3	5.0146701467	-1.1307278288	1.9478123060
C4	6.3411724161	-0.7735207644	1.7257739506
C5	6.3628088653	0.5740496926	1.5835045260
N6	5.0492330054	1.0117317293	1.7213234103
H7	7.1282952135	-1.5091099701	1.6827595549
H8	7.1728748304	1.2590584509	1.3910430971
C9	3.9597533531	5.0526775071	1.3325069058
C10	3.8464232638	4.1984176498	0.2394528997
C11	4.1850198575	2.8431299451	0.3417543946
C12	4.6464707119	2.3909150950	1.5887344730
C13	4.7623874906	3.2265328852	2.7126083733
C14	4.4113895518	4.5705598261	2.5599109519
H15	3.6953027880	6.1015360851	1.2281256592
H16	3.4885431101	4.5788951795	-0.7131997776

H17	4.4917849766	5.2397432650	3.4123878062
C18	3.8052356199	-5.1287234496	2.4185766479
C19	4.2865535384	-4.4152741876	3.5151030194
C20	4.6767563236	-3.0800984956	3.3811512250
C21	4.5686980607	-2.4935900584	2.1083134262
C22	4.0757467237	-3.1808275726	0.9869970101
C23	3.6993791894	-4.5174031980	1.1726695068
H24	3.5117823604	-6.1682977593	2.5373861026
H25	4.3602685170	-4.8941014829	4.4877876474
H26	3.3196940858	-5.0772886831	0.3223686718
C27	4.0246573286	1.9204091499	-0.8426097783
H28	4.8715878025	1.2342244767	-0.9448026047
H29	3.1162954818	1.3108197735	-0.7508831579
H30	3.9462252243	2.4994087584	-1.7665587814
C31	5.2245552651	2.6922786678	4.0480029866
H32	5.2443903645	3.4900170321	4.7948889444
H33	4.5536971620	1.9049399324	4.4095520888
H34	6.2294645928	2.2584514293	3.9936285326
C35	3.9179794159	-2.5201125419	-0.3610405173
H36	3.8403727963	-3.2759335798	-1.1472482874
H37	3.0090098479	-1.9050285123	-0.3938665028
H38	4.7648844404	-1.8692679725	-0.6003737069
C39	5.1713868059	-2.2929283151	4.5720902922
H40	6.1892459959	-1.9148880597	4.4234893283
H41	4.5307128159	-1.4244698959	4.7620065942

H42	5.1732996820	-2.9153889592	5.4704690418
C43	-1.8267116002	-0.0148981656	3.9711593320
C44	-1.3897100376	1.2102045009	3.4658055304
C45	-0.5003915598	1.2089067612	2.3880767896
C47	-0.5034613069	-1.2160021517	2.3652938883
C48	-1.4027301593	-1.2308291080	3.4391207428
H49	-2.5232555312	-0.0205714494	4.8059786883
H50	-1.7506488659	2.1314752967	3.9063136869
H53	-1.7762126441	-2.1578076877	3.8561655940
O31	1.0807665401	-0.3122226993	-0.5114619060
O33	-1.1126553034	0.3079752128	-0.3824826667
O56	-0.0679934680	-2.3475618836	1.7556051581
O57	-0.0605180243	2.3439012285	1.7945066631
C58	-0.5399111141	-3.6055753429	2.2121757136
H59	-0.0620618019	-4.3502069046	1.5741606325
H60	-0.2551884558	-3.7892031334	3.2561479737
H61	-1.6294990359	-3.6877765910	2.1135736772
C61	-0.5550491932	3.5966087449	2.2425691365
H62	-0.0900659018	4.3455971799	1.6002989681
H63	-1.6454247037	3.6566745011	2.1413119475
H64	-0.2750589277	3.7915293464	3.2859077705

NHC-Au-(OOC-Ph-2,4-(OMe)2)

E (M06/LACV3P**++ 2f(Au)) = -1629.66875102676

ZPE (kcal mol 1) = 323.020

Gsolv = -0.0294264

DH298 (kcal mol 1)= 22.151

DS298 (cal K 1 mol-1)= 220.203

C32	0.1084542249	-0.2946808815	0.2656427310
Au1	1.9232562474	-1.4787104377	2.0923473666
C2	3.2559763441	-1.4020749105	3.5711121225
N3	4.4481931364	-2.0529761792	3.6676437195
C4	5.1551813946	-1.6326693622	4.7898793993
C5	4.3861951976	-0.7024079233	5.4069302694
N6	3.2254594005	-0.5725883811	4.6518232717
H7	6.1263866719	-2.0328778960	5.0329683986
H8	4.5505764633	-0.1186861030	6.2982424526
C9	0.0920150221	1.9988783381	5.7855314810
C10	0.9525237254	2.3756909686	4.7611760881
C11	1.9950831755	1.5379841669	4.3427782457
C12	2.1361929281	0.3099190139	5.0067716946
C13	1.2684332166	-0.1069141413	6.0339508908
C14	0.2457895238	0.7641408925	6.4144260041
H15	-0.7100783697	2.6650877597	6.0908546241
H16	0.8161169784	3.3295259653	4.2596233194
H17	-0.4395247844	0.4645785728	7.2026391391
C18	5.8865877699	-4.9273542990	0.9576702914
C19	5.1129685050	-5.3261804779	2.0450262085
C20	4.6162906474	-4.3869439496	2.9543471106
C21	4.9303986221	-3.0371036753	2.7293191944

C22	5.7039132152	-2.6042175664	1.6401648094
C23	6.1781656487	-3.5802283769	0.7575616969
H24	6.2613909105	-5.6707519862	0.2597378870
H25	4.8821097667	-6.3776922650	2.1919058626
H26	6.7751231313	-3.2742413466	-0.0970487184
C27	2.8611146212	1.9492309373	3.1781695491
H28	3.8622025310	1.5127029383	3.2231845878
H29	2.3835762345	1.6227814746	2.2453689979
H30	2.9619019068	3.0381105567	3.1422804542
C31	1.4068604149	-1.4637605266	6.6847642909
H32	0.5965281981	-1.6290126876	7.3991586678
H33	1.3671211115	-2.2646782761	5.9381977029
H34	2.3546517342	-1.5737580385	7.2241844386
C35	5.9913194220	-1.1403229321	1.4058483079
H36	6.6746006069	-1.0127835885	0.5625533426
H37	5.0689357154	-0.5930095121	1.1799904587
H38	6.4438186144	-0.6646510669	2.2829983053
C39	3.7484685839	-4.8134687923	4.1143059467
H40	4.1283748068	-4.4399420837	5.0715708640
H41	2.7283009121	-4.4296667145	3.9987931927
H42	3.6943844757	-5.9033967107	4.1741879217
O31	0.5943404445	-1.4827588714	0.4972783137
O33	0.3936421935	0.7384631793	0.8731965175
C46	-2.7546297696	-0.0830085998	-2.9578170776
C47	-3.0801217639	-0.7957006558	-1.8067510558

C48	-2.1410104466	-0.8781210798	-0.7684677474
C49	-0.8892164656	-0.2521677400	-0.8752148764
C50	-0.5925001139	0.4606857425	-2.0478132015
C51	-1.5207712511	0.5476617660	-3.0948488044
H52	-3.4787642755	-0.0174277117	-3.7657362369
H53	-4.0487301569	-1.2728770712	-1.7234708461
H56	-1.2903580129	1.0908841196	-4.0029288870
O56	0.6507125412	1.0257535680	-2.0960126723
O57	-2.3748201301	-1.5332945717	0.4072441054
C58	0.9912129884	1.8082403295	-3.2238188115
H59	1.9965787194	2.1888207677	-3.0332705645
H60	1.0015633568	1.2145385697	-4.1483630758
H61	0.3050225629	2.6559163907	-3.3544790460
C61	-3.6071490725	-2.2087049787	0.5693991736
H62	-3.5665217073	-2.6748256940	1.5556117702
H63	-4.4613941432	-1.5185163663	0.5329834946
H64	-3.7480682736	-2.9886605604	-0.1911562607

HOOC-Ph-2,4-(OMe)2

E (M06/LACV3P**++ 2f(Au)) = -649.63957916134

ZPE (kcal mol 1) = 113.443

Gsolv = -0.0179008

DH298 (kcal mol 1)= 8.425

DS298 (cal K 1 mol-1)= 110.904

C1	0.0254884000	0.2568940739	-0.3092820949

C2	-0.6938048818	1.4595588084	-0.3202355624
C3	-2.0678158824	1.4710705767	-0.0259790528
C4	-2.7176829122	0.2624177663	0.2788529127
C5	-2.0032218762	-0.9431347598	0.2949751431
C6	-0.6420536372	-0.9260453079	-0.0003371030
H7	1.0823750217	0.2369463761	-0.5421579108
H11	-2.4931052731	-1.8775509492	0.5367104431
H12	-0.0868040624	-1.8596386716	0.0094521709
O12	-0.1512052082	2.6683302483	-0.6341772916
O13	-4.0410096480	0.3672191497	0.5746688892
C14	1.2306713337	2.7314621455	-0.9506467328
H15	1.4412578675	3.7813534639	-1.1596675981
H16	1.8532764227	2.3987802168	-0.1105968872
H17	1.4706800812	2.1313366634	-1.8374858813
C17	-4.7704892636	-0.8151499286	0.8627461775
H18	-5.7980962999	-0.4947489291	1.0401774129
H19	-4.7514261124	-1.5164742900	0.0193114467
H20	-4.3884897337	-1.3186789520	1.7600618053
C20	-2.8548134965	2.7456789648	-0.0863297275
O21	-3.7602026910	2.9723676342	-0.8576881396
O22	-2.4473503587	3.6425726249	0.8422310667
H23	-2.9957738693	4.4330053084	0.6992455930

CO2

E (M06/LACV3P**++ 2f(Au)) = -188.55926301192

ZPE (kcal mol 1) = 7.281

Gsolv = - (gas phase)

DH298 (kcal mol 1)= 2.252

DS298 (cal K 1 mol-1)= 51.158

O1	-0.0000000172	-0.0000000534	1.1696369369
C3	0.0000000460	0.0000001422	-0.0000020463
O4	-0.0000000172	-0.0000000534	-1.1696354017

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