Supporting Information

Competitive Benzene C-H Bond Activation versus Olefin Insertion in a Palladium(II) β-Diketiminate Complex

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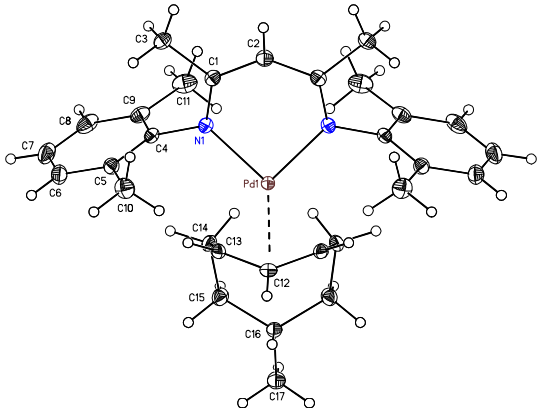
Part I

Crystal Structure Analysis of:

3

(shown below)

Contents



3

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC). The deposition number is 295981.

Table S1. Crystal data and structure refinement for 3 (CCDC 295981).

Empirical formula	$C_{30}H_{40}N_2Pd$
Formula weight	535.04
Crystallization Solvent	Dichloromethane/n-pentane
Crystal Habit	Block
Crystal size	0.32 x 0.28 x 0.19 mm^3
Crystal color	Yellow

Data Collection

Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 24440 reflections used in lattice determination	2.18 to 49.62°
Unit cell dimensions	a = 15.0554(4) Å b = 7.2730(2) Å c = 11.8708(3) Å
Volume	1299.83(6) $Å^3$
Z	2
Crystal system	Orthorhombic
Space group	$Pmn2_1$
Density (calculated)	1.367 Mg/m^3
F(000)	560
Data collection program	Bruker SMART v5.630
θ range for data collection	2.18 to 45.01°
Completeness to θ = 45.01°	96.5 %
Index ranges	$-26 \le h \le 29$, $-14 \le k \le 12$, $-23 \le l \le 22$
Data collection scan type	ω scans at 7 ϕ settings
Data reduction program	Bruker SAINT v6.45A
Reflections collected	36614
Independent reflections	10105 [R_{int}= 0.0629]
Absorption coefficient	0.734 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.8732 and 0.7991

Table S1 (cont.)

Structure solution and Refinement

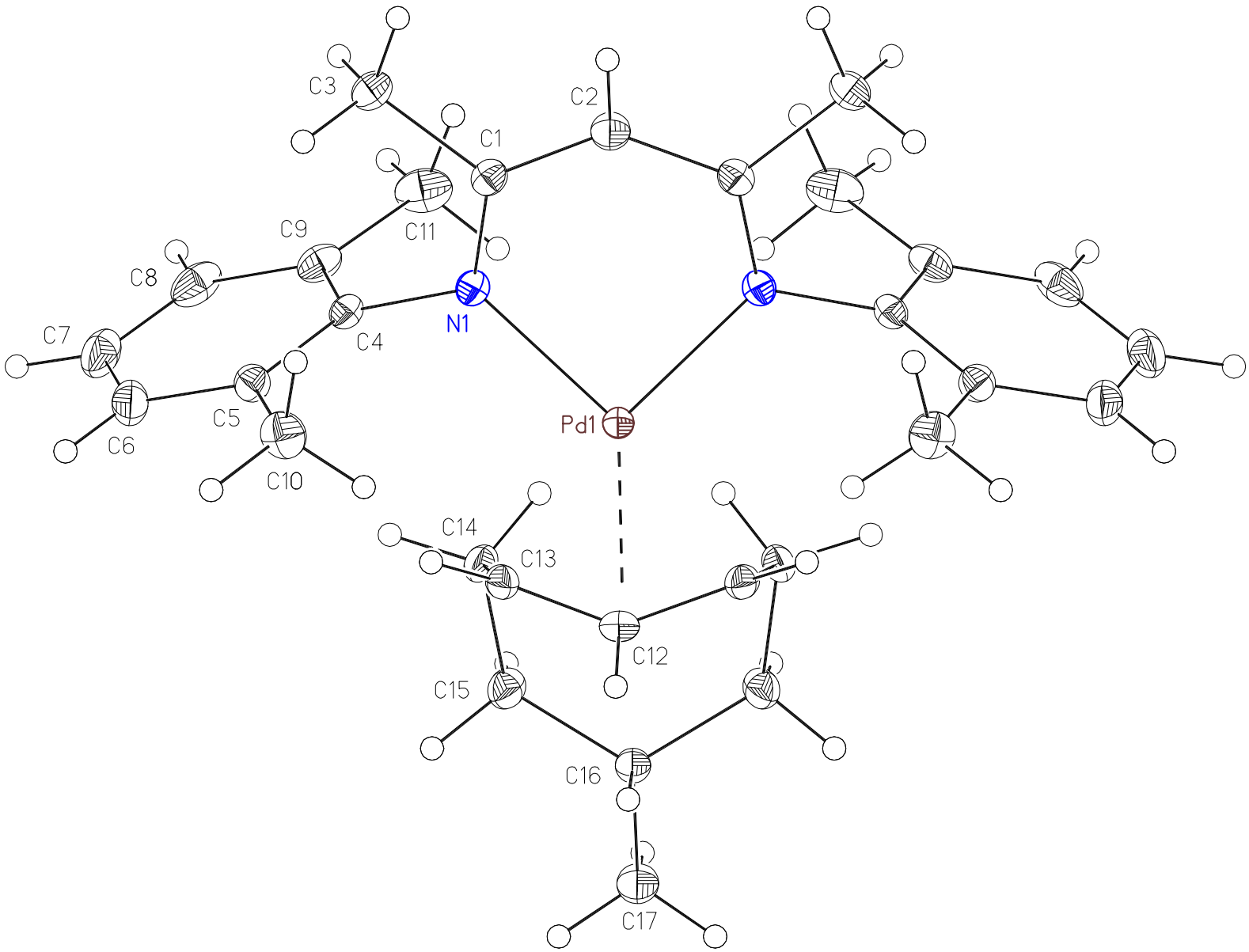
Structure solution program	Bruker XS v6.12
Primary solution method	Patterson method
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	Bruker XL v6.12
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	10105 / 1 / 160
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.370
Final R indices [$I>2\sigma(I)$, 8998 reflections]	R1 = 0.0294, *w*R2 = 0.0589
R indices (all data)	R1 = 0.0363, *w*R2 = 0.0601
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.005
Average shift/error	0.000
Absolute structure determination	Anomalous differences
Absolute structure parameter	-0.008(14)
Largest diff. peak and hole	1.350 and -0.724 e.Å^{-3}

Special Refinement Details

The molecule sits on a crystallographic mirror plane. Hydrogen atomic positions were evident in the difference Fourier map and placed in geometrically calculated positions and treated as riding atoms during least-squares refinement. These calculated position may vary slightly from the actual positions, particularly for hydrogens bonded to C12, C13, C14, C13A and C14A.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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C11
C9
C8
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C4
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C16
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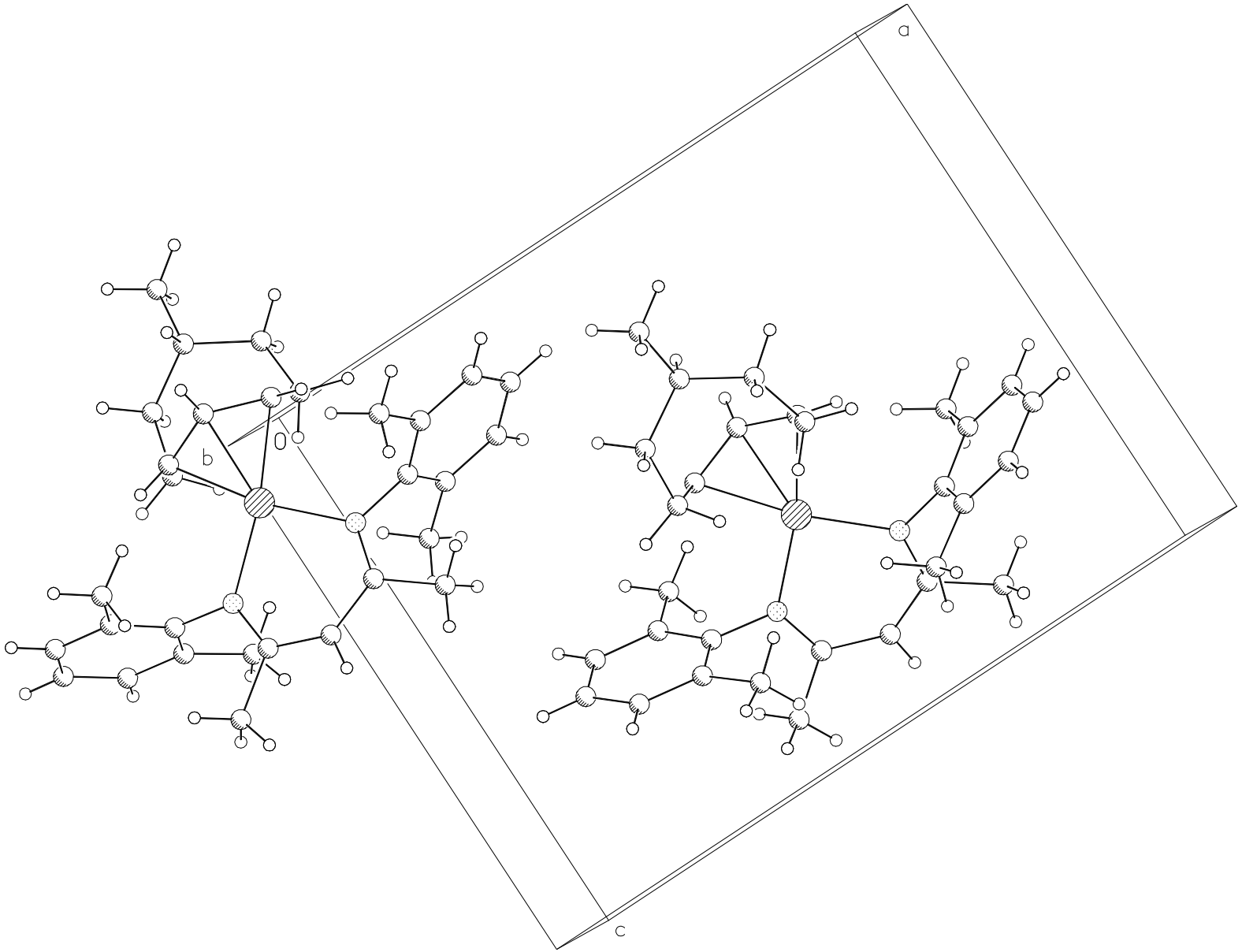
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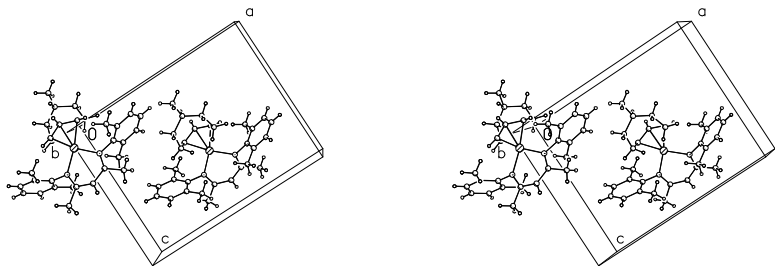
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a
b
c

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 3 (CCDC 295981). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Pd(1)	0	10589(1)	1080(1)	11(1)
N(1)	975(1)	11264(1)	2239(1)	13(1)
C(1)	839(1)	12182(2)	3189(1)	14(1)
C(2)	0	12730(2)	3584(1)	16(1)
C(3)	1627(1)	12642(2)	3935(1)	18(1)
C(4)	1852(1)	10562(2)	2039(1)	13(1)
C(5)	2466(1)	11605(2)	1417(1)	16(1)
C(6)	3315(1)	10884(2)	1250(1)	22(1)
C(7)	3556(1)	9185(2)	1689(1)	25(1)
C(8)	2935(1)	8154(2)	2291(1)	23(1)
C(9)	2079(1)	8819(2)	2470(1)	17(1)
C(10)	2207(1)	13446(2)	957(2)	22(1)
C(11)	1399(1)	7706(2)	3105(1)	25(1)
C(12)	0	10277(2)	-673(1)	15(1)
C(13)	816(1)	9552(2)	-286(1)	15(1)
C(14)	1012(1)	7520(2)	-113(1)	17(1)
C(15)	866(1)	6341(2)	-1184(1)	18(1)
C(16)	0	6614(2)	-1851(1)	14(1)
C(17)	0	5294(2)	-2860(2)	19(1)

Table S3. Selected bond lengths [Å] and angles [°] for 3 (CCDC 295981).

Pd(1)-N(1)	2.0708(10)	C(12)-Pd(1)-C(13)	38.70(4)
Pd(1)-N(1)#1	2.0708(10)	C(12)-Pd(1)-C(13)#1	38.70(4)
Pd(1)-C(12)	2.0932(16)	C(13)-Pd(1)-C(13)#1	69.03(4)
Pd(1)-C(13)	2.1696(11)	N(1)-Pd(1)-N(1)#1	90.23(5)
Pd(1)-C(13)#1	2.1696(11)	N(1)-Pd(1)-C(12)	133.35(3)
		N(1)#1-Pd(1)-C(12)	133.35(3)
		N(1)-Pd(1)-C(13)#1	168.65(4)
		N(1)-Pd(1)-C(13)	100.22(4)
		N(1)#1-Pd(1)-C(13)#1	100.22(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,z

Table S4. Bond lengths [Å] and angles [°] for 3 (CCDC 295981).

Pd(1)-N(1)	2.0708(10)	C(8)-C(9)-C(4)	118.79(12)
Pd(1)-N(1)#1	2.0708(10)	C(8)-C(9)-C(11)	121.21(12)
Pd(1)-C(12)	2.0932(16)	C(4)-C(9)-C(11)	120.00(11)
Pd(1)-C(13)	2.1696(11)	C(13)-C(12)-C(13)#1	120.72(15)
Pd(1)-C(13)#1	2.1696(11)	C(12)-C(13)-C(14)	125.04(11)
N(1)-C(1)	1.3257(15)	C(13)-C(14)-C(15)	113.57(10)
N(1)-C(4)	1.4367(14)	C(16)-C(15)-C(14)	118.09(10)
C(1)-C(2)	1.4057(13)	C(17)-C(16)-C(15)	108.71(9)
C(1)-C(3)	1.5170(16)	C(17)-C(16)-C(15)#1	108.72(9)
C(2)-C(1)#1	1.4057(13)	C(15)-C(16)-C(15)#1	115.97(14)
C(4)-C(5)	1.4046(16)		
C(4)-C(9)	1.4089(16)		
C(5)-C(6)	1.3957(15)		
C(5)-C(10)	1.4980(18)		
C(6)-C(7)	1.389(2)		
C(7)-C(8)	1.395(2)		
C(8)-C(9)	1.3926(18)		
C(9)-C(11)	1.5074(19)		
C(12)-C(13)	1.4144(14)		
C(12)-C(13)#1	1.4144(14)		
C(13)-C(14)	1.5213(17)		
C(14)-C(15)	1.5493(17)		
C(15)-C(16)	1.5380(14)		
C(16)-C(17)	1.535(2)		
C(16)-C(15)#1	1.5380(14)		
C(12)-Pd(1)-C(13)	38.70(4)		
C(12)-Pd(1)-C(13)#1	38.70(4)		
C(13)-Pd(1)-C(13)#1	69.03(4)		
N(1)-Pd(1)-N(1)#1	90.23(5)		
N(1)-Pd(1)-C(12)	133.35(3)		
N(1)#1-Pd(1)-C(12)	133.35(3)		
N(1)-Pd(1)-C(13)#1	168.65(4)		
N(1)-Pd(1)-C(13)	100.22(4)		
N(1)#1-Pd(1)-C(13)#1	100.22(4)		
C(1)-N(1)-C(4)	117.46(9)		
C(1)-N(1)-Pd(1)	125.14(7)		
C(4)-N(1)-Pd(1)	117.23(7)		
N(1)-C(1)-C(2)	124.40(11)		
N(1)-C(1)-C(3)	119.16(10)		
C(2)-C(1)-C(3)	116.41(11)		
C(1)-C(2)-C(1)#1	128.02(15)		
C(5)-C(4)-C(9)	121.14(10)		
C(5)-C(4)-N(1)	120.01(10)		
C(9)-C(4)-N(1)	118.85(10)		
C(6)-C(5)-C(4)	118.28(11)		
C(6)-C(5)-C(10)	121.52(11)		
C(4)-C(5)-C(10)	120.21(10)		
C(7)-C(6)-C(5)	121.35(12)		
C(6)-C(7)-C(8)	119.71(12)		
C(9)-C(8)-C(7)	120.71(12)		

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,z

Table S5. Anisotropic displacement parameters ($Å^2 x 10^4$) for 3 (CCDC 295981). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

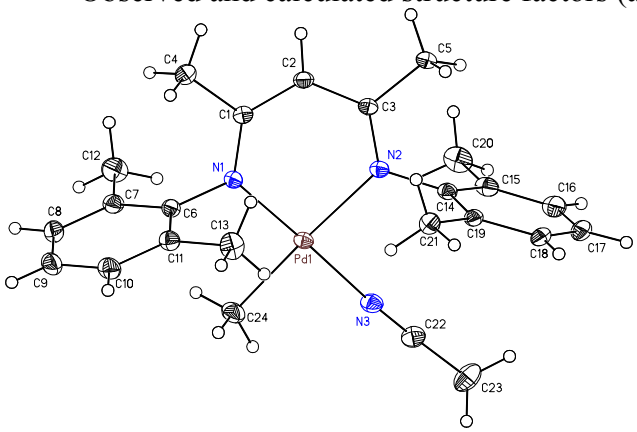
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	106(1)	113(1)	105(1)	3(1)	0	0
N(1)	125(3)	119(4)	138(4)	-2(3)	-9(3)	2(3)
C(1)	149(4)	122(4)	149(4)	1(3)	-16(3)	-17(3)
C(2)	174(6)	153(7)	161(6)	-37(5)	0	0
C(3)	184(4)	173(5)	170(5)	-23(4)	-33(4)	-19(4)
C(4)	128(4)	119(4)	133(4)	-11(3)	-22(3)	2(3)
C(5)	147(4)	163(4)	159(4)	-17(4)	-1(3)	-18(4)
C(6)	145(4)	288(6)	230(9)	-71(5)	0(4)	-9(4)
C(7)	170(5)	323(7)	265(6)	-106(5)	-53(5)	81(5)
C(8)	267(5)	196(5)	226(5)	-51(5)	-98(5)	99(5)
C(9)	217(5)	139(4)	164(5)	-1(4)	-53(4)	22(4)
C(10)	236(4)	174(4)	248(9)	35(5)	18(5)	-37(4)
C(11)	364(7)	167(5)	212(6)	52(4)	-27(5)	-8(5)
C(12)	179(6)	153(6)	105(5)	5(4)	0	0
C(13)	130(4)	182(5)	133(4)	-19(4)	10(3)	-35(4)
C(14)	127(4)	215(5)	156(4)	-29(4)	-27(3)	40(4)
C(15)	155(4)	204(5)	187(5)	-41(4)	-20(4)	47(4)
C(16)	139(5)	145(6)	134(6)	-12(5)	0	0
C(17)	195(7)	184(7)	179(7)	-45(5)	0	0

Crystal Structure Analysis of:

6

(shown below)

Contents



6

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC). The deposition number is 296075.

Table S6. Crystal data and structure refinement for 6 (CCDC 296075).

Empirical formula	$C_{24}H_{31}N_3Pd$
Formula weight	467.92
Crystallization Solvent	Dichloromethane/n-pentane
Crystal Habit	Block
Crystal size	0.30 x 0.26 x 0.26 mm^3
Crystal color	Pale yellow

Data Collection

Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	100(2) K	
θ range for 26590 reflections used in lattice determination	2.72 to 49.62°	
Unit cell dimensions	a = 7.9947(2) Å b = 11.0299(3) Å c = 14.0889(4) Å	α= 72.0190(10)° β= 86.2190(10)° γ = 69.5370(10)°
Volume	1105.90(5) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.405 Mg/m^3	
F(000)	484	
Data collection program	Bruker SMART v5.630	
θ range for data collection	1.52 to 49.65°	
Completeness to θ = 49.65°	83.5 %	
Index ranges	$-15 \le h \le 16$, $-22 \le k \le 22$, $-29 \le l \le 25$	
Data collection scan type	ω scans at 7 ϕ settings	
Data reduction program	Bruker SAINT v6.45A	
Reflections collected	44455	
Independent reflections	19083 [R_{int}= 0.0610]	
Absorption coefficient	0.853 mm^{-1}	
Absorption correction	None	
Max. and min. transmission	0.8088 and 0.7840	

Table S6 (cont.)

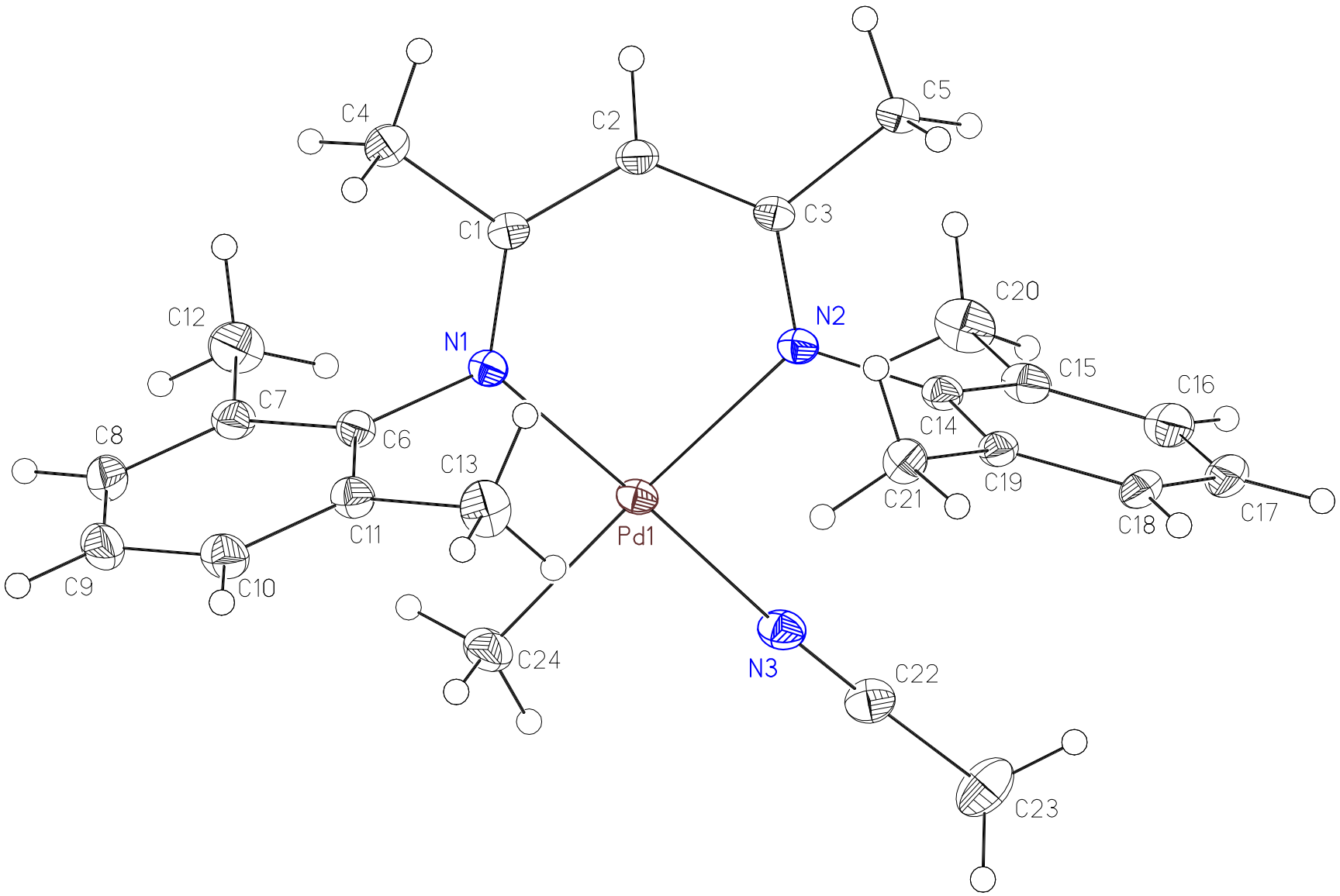
Structure solution and Refinement

Structure solution program	Bruker XS v6.12
Primary solution method	Patterson method
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	Bruker XL v6.12
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	19083 / 0 / 261
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.202
Final R indices [$I>2\sigma(I)$, 15817 reflections]	R1 = 0.0301, *w*R2 = 0.0673
R indices (all data)	R1 = 0.0409, *w*R2 = 0.0701
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.003
Average shift/error	0.000
Largest diff. peak and hole	1.677 and -0.800 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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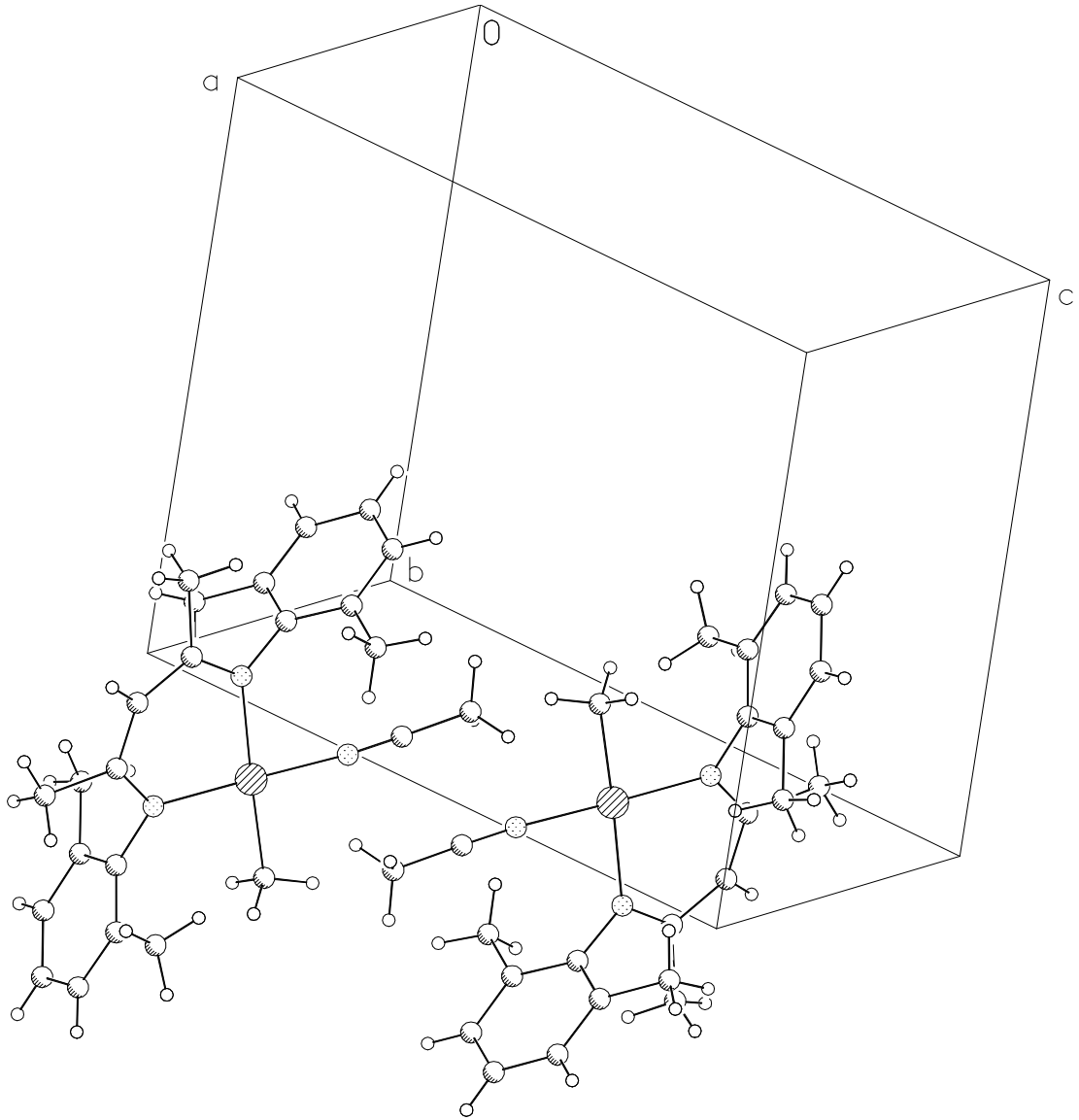
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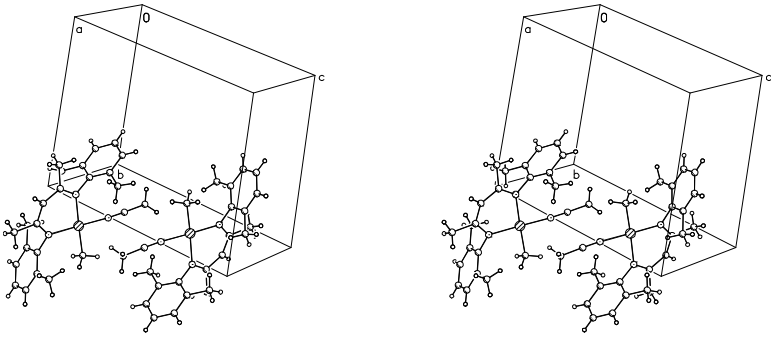
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c
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Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 6 (CCDC 296075). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Pd(1)	7947(1)	9405(1)	7206(1)	13(1)
N(1)	6030(1)	8793(1)	8008(1)	13(1)
N(2)	6434(1)	11458(1)	7054(1)	13(1)
N(3)	9910(1)	9956(1)	6432(1)	18(1)
C(1)	4376(1)	9624(1)	8077(1)	14(1)
C(2)	3739(1)	11044(1)	7666(1)	15(1)
C(3)	4741(1)	11900(1)	7274(1)	14(1)
C(4)	3049(1)	9034(1)	8681(1)	20(1)
C(5)	3791(1)	13397(1)	7162(1)	19(1)
C(6)	6490(1)	7410(1)	8641(1)	14(1)
C(7)	6108(1)	6446(1)	8323(1)	17(1)
C(8)	6558(1)	5119(1)	8974(1)	22(1)
C(9)	7396(1)	4750(1)	9905(1)	23(1)
C(10)	7783(1)	5714(1)	10204(1)	21(1)
C(11)	7333(1)	7052(1)	9581(1)	16(1)
C(12)	5223(2)	6815(1)	7312(1)	26(1)
C(13)	7763(2)	8094(1)	9907(1)	24(1)
C(14)	7329(1)	12424(1)	6802(1)	14(1)
C(15)	7391(1)	13164(1)	5797(1)	18(1)
C(16)	8221(1)	14141(1)	5584(1)	23(1)
C(17)	8975(1)	14370(1)	6341(1)	23(1)
C(18)	8953(1)	13597(1)	7331(1)	19(1)
C(19)	8143(1)	12615(1)	7569(1)	14(1)
C(20)	6544(2)	12936(1)	4977(1)	26(1)
C(21)	8091(1)	11787(1)	8638(1)	17(1)
C(22)	10984(1)	10341(1)	6001(1)	19(1)
C(23)	12303(2)	10874(1)	5444(1)	28(1)
C(24)	9516(1)	7434(1)	7334(1)	22(1)

Table S8. Selected bond lengths [Å] and angles [°] for 6 (CCDC 296075).

Pd(1)-N(3)	2.0135(9)	N(3)-Pd(1)-N(1)	178.19(3)
Pd(1)-N(1)	2.0262(8)	N(3)-Pd(1)-C(24)	87.01(4)
Pd(1)-C(24)	2.0526(9)	N(1)-Pd(1)-C(24)	91.41(4)
Pd(1)-N(2)	2.1113(7)	N(3)-Pd(1)-N(2)	90.54(3)
		N(1)-Pd(1)-N(2)	91.03(3)
		C(24)-Pd(1)-N(2)	177.45(4)

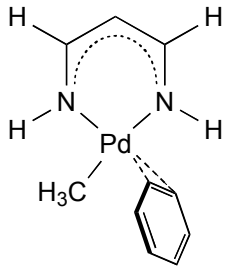
Table S9. Bond lengths [Å] and angles [°] for 6 (CCDC 296075).

Pd(1)-N(3)	2.0135(9)	C(7)-C(6)-C(11)	121.00(8)
Pd(1)-N(1)	2.0262(8)	C(7)-C(6)-N(1)	120.62(8)
Pd(1)-C(24)	2.0526(9)	C(11)-C(6)-N(1)	118.38(8)
Pd(1)-N(2)	2.1113(7)	C(8)-C(7)-C(6)	118.28(9)
N(1)-C(1)	1.3372(11)	C(8)-C(7)-C(12)	120.28(9)
N(1)-C(6)	1.4381(11)	C(6)-C(7)-C(12)	121.44(8)
N(2)-C(3)	1.3203(11)	C(9)-C(8)-C(7)	121.31(10)
N(2)-C(14)	1.4278(12)	C(10)-C(9)-C(8)	119.66(9)
N(3)-C(22)	1.1457(13)	C(9)-C(10)-C(11)	120.74(9)
C(1)-C(2)	1.4031(12)	C(10)-C(11)-C(6)	118.99(9)
C(1)-C(4)	1.5154(13)	C(10)-C(11)-C(13)	120.58(9)
C(2)-C(3)	1.4100(13)	C(6)-C(11)-C(13)	120.43(8)
C(3)-C(5)	1.5186(12)	C(19)-C(14)-C(15)	120.93(8)
C(6)-C(7)	1.4023(13)	C(19)-C(14)-N(2)	118.97(7)
C(6)-C(11)	1.4051(12)	C(15)-C(14)-N(2)	120.11(8)
C(7)-C(8)	1.3993(14)	C(16)-C(15)-C(14)	118.32(9)
C(7)-C(12)	1.5057(14)	C(16)-C(15)-C(20)	121.01(9)
C(8)-C(9)	1.3901(16)	C(14)-C(15)-C(20)	120.65(9)
C(9)-C(10)	1.3877(16)	C(17)-C(16)-C(15)	121.08(9)
C(10)-C(11)	1.3961(12)	C(16)-C(17)-C(18)	119.88(9)
C(11)-C(13)	1.5075(14)	C(19)-C(18)-C(17)	120.53(10)
C(14)-C(19)	1.4021(13)	C(18)-C(19)-C(14)	119.18(8)
C(14)-C(15)	1.4069(11)	C(18)-C(19)-C(21)	120.96(8)
C(15)-C(16)	1.4021(15)	C(14)-C(19)-C(21)	119.84(8)
C(15)-C(20)	1.5030(15)	N(3)-C(22)-C(23)	178.08(11)
C(16)-C(17)	1.3868(18)		
C(17)-C(18)	1.3944(14)		
C(18)-C(19)	1.3937(13)		
C(19)-C(21)	1.5078(12)		
C(22)-C(23)	1.4533(15)		
N(3)-Pd(1)-N(1)	178.19(3)		
N(3)-Pd(1)-C(24)	87.01(4)		
N(1)-Pd(1)-C(24)	91.41(4)		
N(3)-Pd(1)-N(2)	90.54(3)		
N(1)-Pd(1)-N(2)	91.03(3)		
C(24)-Pd(1)-N(2)	177.45(4)		
C(1)-N(1)-C(6)	116.01(7)		
C(1)-N(1)-Pd(1)	124.39(6)		
C(6)-N(1)-Pd(1)	119.23(5)		
C(3)-N(2)-C(14)	116.66(7)		
C(3)-N(2)-Pd(1)	124.45(6)		
C(14)-N(2)-Pd(1)	118.53(5)		
C(22)-N(3)-Pd(1)	176.10(8)		
N(1)-C(1)-C(2)	125.72(8)		
N(1)-C(1)-C(4)	119.28(7)		
C(2)-C(1)-C(4)	114.95(7)		
C(1)-C(2)-C(3)	127.84(8)		
N(2)-C(3)-C(2)	123.68(8)		
N(2)-C(3)-C(5)	120.14(8)		
C(2)-C(3)-C(5)	116.10(8)		

Table S10. Anisotropic displacement parameters ($Å^2 x 10^4$) for 6 (CCDC 296075). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	117(1)	137(1)	106(1)	-38(1)	7(1)	-21(1)
N(1)	125(2)	128(2)	131(3)	-35(2)	3(2)	-32(2)
N(2)	116(2)	140(2)	124(2)	-33(2)	1(2)	-30(2)
N(3)	151(3)	185(3)	165(3)	-57(2)	30(2)	-30(2)
C(1)	125(3)	158(3)	136(3)	-47(2)	4(2)	-44(2)
C(2)	110(3)	159(3)	171(3)	-47(2)	1(2)	-30(2)
C(3)	117(3)	140(3)	134(3)	-36(2)	-13(2)	-25(2)
C(4)	165(3)	198(4)	236(4)	-55(3)	51(3)	-70(3)
C(5)	125(3)	146(3)	252(4)	-39(3)	2(3)	-18(2)
C(6)	132(3)	135(3)	144(3)	-39(2)	2(2)	-38(2)
C(7)	148(3)	172(3)	213(4)	-84(3)	3(3)	-45(2)
C(8)	197(4)	165(3)	299(5)	-84(3)	48(3)	-71(3)
C(9)	214(4)	156(3)	262(4)	-13(3)	54(3)	-51(3)
C(10)	198(4)	196(4)	170(4)	4(3)	6(3)	-45(3)
C(11)	166(3)	172(3)	138(3)	-30(2)	-3(2)	-49(2)
C(12)	251(5)	260(4)	285(5)	-141(4)	-61(4)	-60(4)
C(13)	309(5)	244(4)	175(4)	-63(3)	-54(3)	-105(4)
C(14)	116(3)	140(3)	126(3)	-19(2)	16(2)	-26(2)
C(15)	160(3)	191(3)	126(3)	-2(2)	21(2)	-20(3)
C(16)	184(4)	223(4)	192(4)	24(3)	59(3)	-54(3)
C(17)	159(3)	208(4)	281(5)	1(3)	57(3)	-81(3)
C(18)	126(3)	196(3)	233(4)	-36(3)	22(3)	-69(3)
C(19)	114(3)	146(3)	144(3)	-21(2)	14(2)	-39(2)
C(20)	289(5)	292(5)	129(4)	-31(3)	-14(3)	-56(4)
C(21)	188(3)	194(3)	131(3)	-22(2)	-8(2)	-77(3)
C(22)	179(4)	236(4)	161(3)	-75(3)	40(3)	-66(3)
C(23)	279(5)	419(6)	212(4)	-121(4)	96(4)	-207(5)
C(24)	193(4)	176(4)	258(4)	-66(3)	66(3)	-22(3)

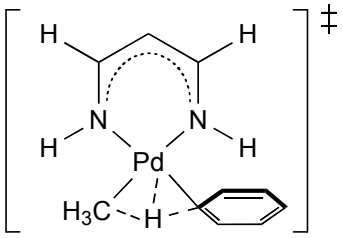
Part II



7

Total internal energy, Utot (SCFE + ZPE + U): -625.513570 hartrees
Total enthalpy, Htot (Utot + pV): -625.512626 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -625.569917 hartrees

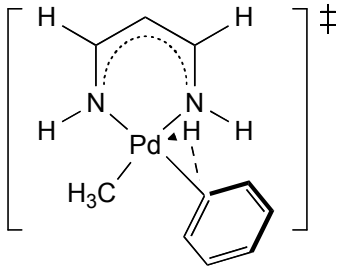
Pd	0.5110670752	-1.0297235332	-0.4375121409
N	1.2398121850	-1.5455930247	1.3702149999
C	2.5141166615	-1.6117385304	1.7148123980
C	3.6329046911	-1.3469610543	0.9227009374
C	3.5993558526	-0.9504594030	-0.4246367458
N	2.5197100071	-0.7653645078	-1.1548587445
C	-1.3384659059	-1.3258715180	0.4062913973
H	-1.4018840182	-2.3589263368	0.7653915134
H	-1.4563587942	-0.6348622714	1.2481679465
H	-2.1220156441	-1.1444509241	-0.3314069528
H	2.7424779226	-0.4787653596	-2.1041931694
H	4.5736186216	-0.7842041998	-0.8966502503
H	4.6060697726	-1.4570455466	1.3868928504
H	2.7138430859	-1.9111976507	2.7480127386
H	0.5857873874	-1.7804515364	2.1060105538
C	-0.2057582150	0.2783890416	-2.4132623064
C	-1.4480051468	0.9351457470	-2.2744014951
H	0.7091399558	0.8564787407	-2.3433075429
H	-1.4689558552	1.9781524897	-1.9731295808
C	-0.1741252278	-1.0720192405	-2.8209229693
C	-1.3848693877	-1.7485100294	-3.0854399789
C	-2.5947205394	-1.0869015415	-2.9549657282
C	-2.6264354624	0.2605732293	-2.5473676582
H	0.7659234802	-1.5529085784	-3.0682801410
H	-1.3570709481	-2.7837472653	-3.4120005183
H	-3.5239478714	-1.6062568052	-3.1716580483
H	-3.5799452791	0.7722261820	-2.4519442767
X	-0.1916365000	-0.3955365000	-2.6159500000



TS_{σ}

Total internal energy, Utot (SCFE + ZPE + U): -625.481457 hartrees
Total enthalpy, Htot (Utot + pV): -625.480513 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -625.536980 hartrees

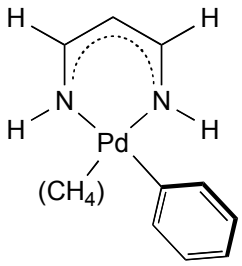
C	-0.0041279313	-0.6761349349	0.0225222100
C	-0.0078737432	0.3134878644	1.0080206558
C	1.1995228772	0.8111601688	1.5251434779
C	2.4087416159	0.2702337755	1.0583345692
C	2.4132788305	-0.7190111397	0.0727259622
C	1.2064071785	-1.1895789563	-0.4488653298
Pd	1.2102220835	2.7388497195	2.4531323077
C	1.2315030064	1.5771230320	4.3483724062
N	1.2252712395	4.5530083642	3.4168661275
C	1.2169217012	5.7473287868	2.8554918059
C	1.1983187987	6.0217268450	1.4837407143
C	1.1859998025	5.0426070372	0.4824181373
N	1.1890400687	3.7375298194	0.6636031738
H	2.1433365998	1.9883370626	4.7836951905
H	1.2395472558	0.4944448790	4.5130743748
H	0.3322089238	1.9817305126	4.8144002288
H	1.2382423442	4.5718171302	4.4305427769
H	1.2255704268	6.6115713925	3.5261994615
H	1.1935390076	7.0603531348	1.1756025002
H	1.1726129722	5.3999303955	-0.5516016093
H	1.1784175600	3.1901365384	-0.1886636811
H	3.3509670530	0.6285129418	1.4647649135
H	3.3562054361	-1.1225820083	-0.2872794087
H	1.2089171934	-1.9614195139	-1.2140000450
H	-0.9441888206	-1.0475825317	-0.3772166617
H	-0.9531966980	0.7043723236	1.3744493909
H	1.1993634860	1.1126208055	2.9367614880



TS$_{oxad}$

Total internal energy, Utot (SCFE + ZPE + U): -625.466570 hartrees
Total enthalpy, Htot (Utot + pV): -625.465626 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -625.521719 hartrees

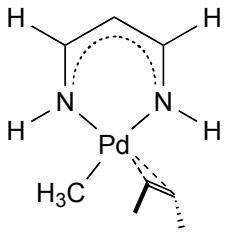
Pd	0.0066270874	0.1742617817	-0.0378580966
N	0.0021209495	-0.1013543323	2.0323486801
C	1.0520027752	-0.2848419952	2.8204323105
C	2.3943483712	-0.3154611920	2.4391551296
C	2.8670899929	-0.1676274579	1.1245744048
N	2.1321516164	-0.0049020831	0.0453709827
C	-2.0524441641	0.3303126502	0.0325346869
H	-2.3099316795	0.9499398751	0.8956318793
H	-2.4884536650	0.7520556324	-0.8716465812
H	-2.4203984056	-0.6911260452	0.1725482727
H	-0.8804197163	-0.0968647162	2.5317007819
H	0.8524182511	-0.4245954778	3.8871160611
H	3.1313762220	-0.4649362684	3.2194782772
H	3.9538784034	-0.1997636848	0.9979644211
H	2.6729987749	0.0970899633	-0.8073953175
C	-0.0553037845	-0.1730011837	-2.0634012811
C	-0.8483048098	0.4719140681	-3.0225371177
C	-0.8639128197	0.0259941137	-4.3469120949
C	-0.0901449633	-1.0682886757	-4.7329773240
C	0.7070018642	-1.7113020213	-3.7860597324
C	0.7368311804	-1.2621254935	-2.4623549931
H	-1.4631850420	1.3226984718	-2.7477999260
H	-1.4841355144	0.5398842691	-5.0769904809
H	-0.1058815194	-1.4156494075	-5.7623533431
H	1.3105919168	-2.5692141518	-4.0719202186
H	1.3642847524	-1.7770304170	-1.7423706074
H	0.0314186852	1.4193456702	-0.8932984967



8

Total internal energy, Utot (SCFE + ZPE + U): -625.512504 hartrees
Total enthalpy, Htot (Utot + pV): -625.511560 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -625.569443 hartrees

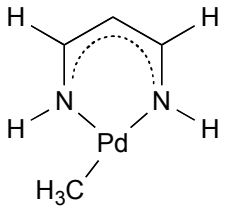
C	0.0045918692	-0.1251704108	-0.2095360052
C	-0.1179602466	-0.1098886098	1.1883906940
C	1.0549301907	-0.1284773843	1.9600450832
C	2.3142448774	-0.1398441947	1.3505674567
C	2.4226130258	-0.1406745718	-0.0417278680
C	1.2640869629	-0.1336723118	-0.8199835586
Pd	-1.9266885076	-0.0197383858	2.0830509826
C	-1.3091286207	2.2778477432	3.1764816042
N	-3.8334756975	0.0298241224	2.9960331142
C	-4.7522587113	-0.8984923038	2.8396994706
C	-4.6210944563	-2.0676625993	2.0694463645
C	-3.4914539829	-2.4212825695	1.3326989053
N	-2.3582611569	-1.7519423834	1.2047179512
H	-2.0006091854	2.9018086069	3.7451981658
H	-0.3182639526	2.7273477161	3.1100838964
H	-1.6992896337	2.1822492771	2.1491358674
H	-4.1382555185	0.7961131478	3.5878838607
H	-5.7114922279	-0.7630712411	3.3498027570
H	-5.4646498755	-2.7473530735	2.0426596278
H	-3.5410546213	-3.3659451457	0.7841957358
H	-1.6461908873	-2.1795034388	0.6280961671
H	0.9971431108	-0.1400854700	3.0465678541
H	3.2109868147	-0.1555438793	1.9661520583
H	3.4010215685	-0.1514154957	-0.5147595999
H	1.3377087802	-0.1342842275	-1.9052617202
H	-0.8867460769	-0.1217717724	-0.8329621444
H	-1.2048886838	1.3163825363	3.7063509603



9

Total internal energy, Utot (SCFE + ZPE + U): -550.502069 hartrees
Total enthalpy, Htot (Utot + pV): -550.501125 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -550.557870 hartrees

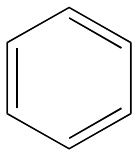
C	0.0198828305	-0.0064335461	0.0303068984
Pd	-0.0184890581	0.0051688930	2.0967879566
C	2.2508251428	-0.0053986698	2.1309774634
C	1.8224345621	-1.3218958538	2.1287324448
N	-1.9495818771	0.6318156303	1.9122043952
C	-2.8029483470	0.9102849029	2.8836616249
C	-2.5734555395	0.8382396254	4.2579726953
C	-1.3620857613	0.4457490050	4.8506680533
N	-0.2636388310	0.0872939521	4.2204188447
X	2.0107585000	-0.6557270000	2.1107505000
H	-0.7549479125	-0.6959092454	-0.3221107405
H	-0.2036501832	1.0068639494	-0.3206934829
H	0.9835918133	-0.3180401075	-0.3859480394
H	0.4846211377	-0.1546556724	4.8603666090
H	-1.3455226855	0.4426737158	5.9457732538
H	-3.3913378024	1.1052870485	4.9169022679
H	-3.8015540565	1.2342479830	2.5753625521
H	-2.3261269088	0.7530028678	0.9797631605
C	1.8732377927	-2.2886803320	3.2842759047
C	2.8599164546	0.7424967396	3.2895024693
H	1.6947144506	-1.7947669014	1.1581331655
H	2.4268024144	0.4552932907	1.1620433907
H	3.9529025315	0.7594651732	3.1764655803
H	2.5183266165	1.7812496223	3.3093469347
H	2.6382325870	0.2938545376	4.2595454122
H	2.7477459357	-2.9444432394	3.1711370525
H	1.9551795692	-1.7983757034	4.2560294993
H	0.9863330006	-2.9282943691	3.3001139061



10

Total internal energy, Utot (SCFE + ZPE + U): -393.349654 hartrees
Total enthalpy, Htot (Utot + pV): -393.348710 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -393.392660 hartrees

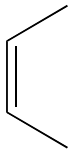
C	0.3264673997	-0.7728700545	-0.3564467263
Pd	1.1386183380	-1.6319484721	1.3020277712
N	1.9343345364	-2.5362415623	3.0451833342
C	3.2230594134	-2.6371169032	3.2797807862
C	4.2539446878	-2.1756526493	2.4367924360
C	4.0768583605	-1.5349210306	1.2140336472
N	2.9443360969	-1.2297945813	0.5982100277
H	0.6153132149	-1.2958844962	-1.2735398342
H	-0.7611337439	-0.8739837968	-0.2099209894
H	0.5812881478	0.2887001136	-0.4350828944
H	3.0257445585	-0.7598758678	-0.2925627790
H	4.9846500253	-1.2389524163	0.6809682171
H	5.2740727395	-2.3320231716	2.7668712493
H	3.5446834672	-3.1201782522	4.2079517438
H	1.3641749256	-2.9353652413	3.7845931361



Total internal energy, Utot (SCFE + ZPE + U): -232.148098 hartrees
Total enthalpy, Htot (Utot + pV): -232.147154 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -232.177603 hartrees

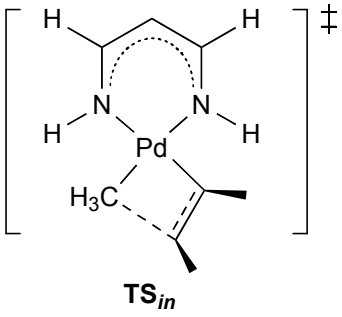
H	-0.0000021880	-0.0000003872	0.0061696424
C	-0.0000020980	-0.0000007121	1.0926771102
C	1.2092448642	0.0000007663	1.7908399241
C	1.2092504050	-0.0000003048	3.1871635923
C	0.0000005060	0.0000001360	3.8853259998
C	-1.2092442684	0.0000014152	3.1871587461
C	-1.2092483672	-0.0000010567	1.7908362062
H	2.1501801707	0.0000020950	1.2475751584

H	2.1501949683	-0.0000028304	3.7304117679
H	-0.0000140915	-0.0000011033	4.9718337304
H	-2.1501845428	0.0000019674	3.7304147450
H	-2.1501867200	-0.0000026445	1.2475761590



Total internal energy, Utot (SCFE + ZPE + U): -157.119376 hartrees
Total enthalpy, Htot (Utot + pV): -157.118432 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -157.152537 hartrees

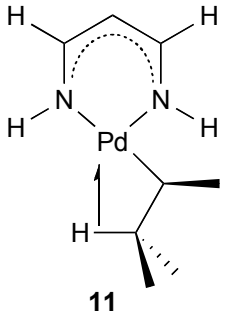
C	-0.2444048889	0.0000055380	-0.2856971209
C	0.0287074582	0.0000093468	1.1922588611
C	1.2168881117	0.0000046551	1.8074930424
H	-0.8605049799	0.0000086348	1.8228553689
H	1.2147120102	0.0000073002	2.8977506048
C	2.5817278615	-0.0000152965	1.1779587071
H	2.5469085077	-0.0000290818	0.0860117856
H	3.1577228782	0.8792363705	1.4943383934
H	3.1576994904	-0.8792746979	1.4943588862
H	0.6678792783	0.0000700551	-0.8867841939
H	-0.8349244346	-0.8793488545	-0.5736520561
H	-0.8350426091	0.8792797478	-0.5736428401



TS*in*

Total internal energy, Utot (SCFE + ZPE + U): -550.462113 hartrees
Total enthalpy, Htot (Utot + pV): -550.461169 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -550.515560 hartrees

C	-0.0730584401	0.0122840692	0.0090698590
Pd	-0.0560528196	0.0015420447	2.2794220641
C	1.8570561778	0.0604112173	0.7729113487
C	2.0177854047	0.0579778326	2.2112770502
N	-2.1584702494	-0.0002450203	2.2259127188
C	-2.9586723797	-0.0038312157	3.2714580180
C	-2.5613540623	-0.0281461754	4.6174768224
C	-1.2362602528	-0.0456334238	5.0624563653
N	-0.1414259652	-0.0387248486	4.3222755357
H	-1.0921588008	-0.0667589247	6.1472552021
H	-3.3406858832	-0.0323500681	5.3706783613
H	-4.0380594649	0.0131585915	3.0875319772
H	-2.6512788048	0.0242072129	1.3371863337
H	2.0611983404	-0.9031088466	0.3112429563
C	2.3678184694	1.2429360808	-0.0300567054
C	2.6204852722	1.2510985791	2.9339956749
H	2.3401456266	-0.9049433776	2.6147696991
H	0.7156089297	-0.0596998901	4.8610309157
H	-0.7458634266	-0.8451698016	0.0951648748
H	-0.6096100979	0.9625568158	-0.0369625899
H	0.4735607001	-0.1130761762	-0.9201604022
H	3.4513168889	1.3324211266	0.1191945297
H	2.1859410932	1.1253883102	-1.1014201839
H	1.9140153911	2.1839786073	0.2900579217
H	3.7039396178	1.3260373014	2.7553522257
H	2.1682259878	2.1985209754	2.6276052940
H	2.4810282326	1.1637857070	4.0159876615



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Total internal energy, Utot (SCFE + ZPE + U): -550.503979 hartrees
Total enthalpy, Htot (Utot + pV): -550.503034 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -550.557890 hartrees

C	1.3322031638	1.2361725031	-0.7802080427
C	1.0880964849	-0.0589196077	0.0107070052
C	1.9077216300	-0.1715529026	1.2674708994
Pd	0.0740722241	0.0446553638	2.1806403950
N	-1.9404146197	0.2631144961	2.7822164565
C	-2.3449816126	0.3090939323	4.0341260473
C	-1.5299840950	0.2315568735	5.1764223145
C	-0.1417271495	0.0862072107	5.1715738930
N	0.6562422852	-0.0019907972	4.1200339653
H	-0.0528991425	0.0536743865	0.3478581256
H	0.3433843593	0.0394977645	6.1516314805
H	-2.0192274805	0.2861833989	6.1420792860
H	-3.4190544506	0.4180492975	4.2199676498
H	-2.7042617279	0.3334970483	2.1193854924
C	1.0401506575	-1.2932041094	-0.9017893949
H	2.5076795440	0.7232781206	1.4572050656
C	2.6728928508	-1.4431323806	1.5835096710
H	1.6365447361	-0.1046743091	4.3485261373
H	2.3038559105	1.1815601249	-1.2844496456
H	0.5638839707	1.3929743837	-1.5448282033
H	1.3390831625	2.1058941168	-0.1176539889
H	0.3175905031	-1.1499458184	-1.7118359838
H	2.0243177452	-1.4593965844	-1.3546145082
H	0.7606629715	-2.1962313676	-0.3549984368
H	3.5147165462	-1.5976132604	0.8904045601
H	3.0974899323	-1.3903524939	2.5915147831
H	2.0438602399	-2.3368556601	1.5426037190
X	1.5033035000	-0.0921970000	0.6343335000