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Synthesis and Characterization of Compounds 1-4

General Procedures. All operations with compounds **2-4** were performed in a nitrogen-filled glovebox (Vacuum Atmospheres with an MO-40 purifier). (tmeda)$PdMe_2$ was prepared as previously reported.[14a] All solvents were reagent grade or better. Pentane, diethyl ether, and THF were distilled over sodium/benzophenone ketyl. All solvents were degassed and stored under high-purity nitrogen after distillation. All deuterated solvents (Aldrich) were stored under high-purity nitrogen on molecular sieves (3 Å).

^1H, ^{31}P, and ^{13}C NMR spectra were recorded using a Bruker DPX250 spectrometer. ^1H and ^{13}C chemical shifts are reported in ppm downfield from TMS and referenced to the residual solvent h_1 (7.24 ppm chloroform-*d*, 2.04 ppm acetone-d_6, 7.15 ppm benzene-d_6) and all-*d* solvent peaks (77.00 ppm chloroform, 29.8 ppm acetone, 128.00 ppm benzene), respectively. ^{31}P chemical shifts are reported in ppm downfield from H_3PO_4 and referenced to an external 85% phosphoric acid sample. All measurements were performed at 21°C.

Synthesis of 1. A DMF (35 mL) solution of 2,6-di-t-butyl-4-methylphenol (5.2 g, 0.023 mol) and 1,1,1,3,3,3-hexamethyldisilazane (15 mL, 0.071 mol) was refluxed under argon atmosphere for 20 hours. The solution turned blue as reflux started. Upon concentration by distillation under reduced pressure, a white precipitate was formed, which was collected on a sinter, washed with DMF and dried under vacuum, giving pure phenyl silyl ether (3.2 g, 47%), as identified by ^1H-NMR.

^1H NMR ($CDCl_3$) : δ = 0.38 (s, 9H, $SiMe_3$), 1.38 (s, 18H, *t*-Bu), 2.24 (s, 3H, CH_3), 7.02 (s, 2H, Ar-H).

To a CCl_4 solution (30 mL) of the phenyl silyl ether (500 mg, 1.7 mmol), N-bromosuccinimide (400 mg, 2.2 mmol) and azobisisobutyronitrile (10 mg) were added.

The mixture was irradiated at close range with a 100-W lamp, which initiated reflux. After 20-30 min. the mixture was cooled and the floating imine was filtered out. The solvent was removed on a rotary evaporator and the residue was extracted with hexane. When the dilute hexane solution (10 mL) was cooled at 4°C for 6 hours, by-products precipitated. From the concentrated supernatant (ca. 4 mL) **1** crystallized (310 mg, 49%).

^{1}H NMR ($CDCl_3$) : δ = 0.41 (s, 9H, $SiMe_3$), 1.40 (s, 18H, *t*-Bu), 4.49 (s, 2H, CH_2Br), 7.26 (s, 2H, Ar-H). ^{13}C {^{1}H} NMR ($CDCl_3$) : δ = 3.97 ($SiMe_3$), 31.12 (*t*-Bu), 35.13 (*t*-Bu), 35.27 (CH_2Br), 126.81 (Ar-H), 129.09 (Ar-C), 141.15 (Ar-C), 153.41 (Ar-O). The assignment was confirmed by a DEPT experiment.

Synthesis of 2. A cold acetone solution of **1** (57 mg, 0.154 mmol) was added to a cold acetone solution of (tmeda)$PdMe_2$ (36 mg, 0.143 mmol). After standing for 15 min. at -30°C, the solvent was evaporated *in vacuo*, the residue was washed with pentane and **2** was extracted by diethyl ether. Evaporation of the solvent gave pure **2** (67 mg, 79%).

^{1}H NMR (d_6-acetone) : δ = 0.37 (s, 9H, $SiMe_3$), 1.39 (s, 18H, *t*-Bu), 2.43 (s, 6H, NMe_2), 2.49 (s, 6H, NMe_2), 2.79 (t, 2H, J_{HH}=5.5Hz, NCH_2CH_2N), 2.84 (s, 2H, CH_2Pd), 7.55 (s, 2H, Ar-H). A second triplet (δ = 2.50) is obscured by the methyl signal. The ^{1}H NMR of this complex in $CDCl_3$ is similar to the reported spectrum of bromo($PhCH_2$)(tmeda)palladium.[14b] ^{13}C{^{1}H} NMR (d_6-acetone) : δ = 3.70 ($SiMe_3$), 14.84 (CH_2Pd), 32.00 (*t*-Bu), 35.49 (*t*-Bu), 48.65 (NMe_2), 49.66 (NMe_2), 57.82 (NCH_2CH_2N), 63.79 (NCH_2CH_2N), 127.87 (Ar-H), 140.11 (Ar-C), 140.32 (Ar-C), 149.72 (Ar-O). The assignment was confirmed by a DEPT experiment.

Synthesis of 3. A THF solution of dppe (35 mg, 0.088 mmol) was added to a THF solution of **2** (52 mg, 0.088 mmol) at -30°C. After 30 min. the solvent was removed *in*

vacuo, the residue was washed with pentane and **3** was extracted by diethyl ether. Evaporation of the solvent gave pure **3** (70 mg, 91%).

$^{31}P\{^1H\}$ NMR (C_6D_6) : δ = 30.12 (d, J_{PP}=40.6Hz), 52.90 (d, J_{PP}=40.6Hz). ^1H NMR (C_6D_6) : δ = 0.40 (s, 9H, $SiMe_3$), 1.45 (s, 18H, *t*-Bu), 1.50 (m overlapping with signal of *t*-Bu, 2H, PCH_2CH_2P), 1.91 (dtd, J_{PH}=27.0Hz, J_{HH}=8.4Hz, J_{PH}=5.2Hz, 2H, PCH_2CH_2P), 3.94 (dd, J_{PH}=10.5Hz and 5.4Hz, 2H, CH_2Pd), 6.97-7.10 (m, 12H, dppe), 7.31-7.40 (m, 4H, dppe), 7.75 (d, J_{PH}=1.9Hz, 2H, Ar-H), 7.91-7.99 (m, 4H, dppe)

Synthesis of 4. To a THF solution of **3** (70 mg, 0.080 mmol), 1 equiv. of tetra-n-butylammonium fluoride trihydrate (25 mg, 0.080 mmol) was added. After staying at room temperature for 15 min., the solvent was removed *in vacuo*, the residue was washed with pentane and **4** was extracted by diethyl ether. Evaporation of the solvent gave pure **4** (53 mg, 91%)

$^{31}P\{^1H\}$ NMR (C_6D_6) : δ = 29.07 (d, J_{PP}=14.2Hz), 37.49 (d, J_{PP}=14.2Hz). ^1H NMR (C_6D_6) : δ = 1.61 (s, 18H, *t*-Bu), 1.83 (m, 2H, PCH_2CH_2P), 1.91 (m, 2H, PCH_2CH_2P), 3.40 (dd, J_{PH}=7.1Hz and 3.8Hz, 2H, exo CH_2), 6.93-7.55 (22H, Ar-H and QM-ring C-H). $^{13}C\{^1H\}$ NMR (C_6D_6) : δ = 25.53 (dd, J_{PC}=26.1Hz and 16.3Hz, PCH_2CH_2P), 26.60 (dd, J_{PC}=26.5Hz and 16.8Hz, PCH_2CH_2P), 51.34 (d, 30.7Hz, exo CH_2), 82.28 (dd, J_{PC}=12.5Hz and 4.8Hz, $C{=}CH_2$), 125-142 (Ar and QM ring), 183.96 (br d, J_{PC}=3.7Hz, C=O). The assignment was confirmed by a DEPT and a C-H correlation experiment.

Elemental analysis: Found (Calc.) C 68.55 (68.10); H 7.05 (6.41)

Displacement and Trapping of BHT-QM. A C_6D_6 solution of dibenzylidene acetone (3 mg, 0.013 mmol) was added to a C_6D_6 solution of **4** (7 mg, 0.010 mmol) at room temperature. Based on $^{31}P\{^1H\}$ NMR integration, ca. 90% conversion of **4** to the known[18d] (dppe)Pd(DBA) was observed within 10 min. Concomitant formation of free BHT-QM was detected by ^1H NMR spectroscopy. Excess of MeOH was added and the volatiles were removed *in vacuo*. Extraction by pentane gave **5**, which was identified by GC-MS analysis and ^1H NMR spectroscopy. Yields are quantitative based on ^1H NMR integration.

BHT-QM: ^1H NMR (C_6D_6) : δ = 1.37 (s, 18H, *t*-Bu), 5.20 (s, 2H, CH_2), 6.77 (s, 2H, C-H).[8b]

5: ^1H NMR (C_6D_6) : δ = 1.37 (s, 18H, *t*-Bu), 3.21 (s, 3H, OMe), 4.33 (s, 2H, CH_2O), 4.94 (s, 1H, OH), 7.31 (s, 2H, Ar-H).

GC-MS (EI): M^+= 250, (M^+ - CH_3)= 235, (M^+ - OCH_3)= 219.[20]

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X-ray crystal structure analysis 22001119
$C_{41}H_{46}OP_2Pd$

CRYSTAL DATA: $C_{41}H_{46}OP_2Pd$, orange, prisma, 0.3 x 0.3 x 0.3mm^3, Monoclinic, P2(1)/n (No. 14), a=9.553(2), b=28.122(6), c=13.774(3)Å, β=107.52(3)°, from 25 reflections, T=110K, V=3528.7(13)Å^3, Z=4, Fw=723.12, Dc=1.4361Mg/m^3, μ =0.648mm^{-1}.

Data collection and treatment: Rigaku AFC5R four-circle diffractometer, MoKα, graphite monochromator (λ=0.71073Å), 14156 reflections collected, 1.45°≤Θ≤27.50°, -12≤h≤7, 0≤k≤36, -17≤l≤17, ω scan method, scan width=1.4°, scan speed 12°/min, typical half-height peak width=0.25°, 3 standards collected 72 times each, with an 4% change in intensity, 8109 independent reflections (R-int=0.0560).

Solution and refinement: Structure solved by direct methods (SHELXS-96). Full-matrix least-squares refinement based on F^2 (SHELXL-93). Idealized hydrogens were placed and refined in a riding mode 412 parameters with 0 restraints, final R_1=0.0290(based on F^2) for data with I>2sigmaI and , R_1=0.0336 for all data based on all 8104 reflections, goodness-of-fit on F^2=1.061, largest electron density=0.972 e/Å^{-3}

Table 1. Crystal data and structure refinement for 4

Identification code	4 ; m120
Empirical formula	C41 H46 O P2 Pd
Formula weight	723.12
Temperature	110 K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	P2(1)/n
Unit cell dimensions	a = 9.553(2) A alpha = 90 deg. b = 28.122(6) A beta = 107.52(3) deg. c = 13.774(3) A gamma = 90 deg.
Volume	3528.7(13) A^3
Z	4
Density (calculated)	1.361 Mg/m^3
Absorption coefficient	0.648 mm^-1
F(000)	1504
Crystal size	0.3 x 0.3 x 0.3 mm
Theta range for data collection	1.45 to 27.50 deg.
Index ranges	-12<=h<=7, -4<=k<=36, -17<=l<=17
Reflections collected	14156
Independent reflections	8109 [R(int) = 0.0560]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8104 / 0 / 412
Goodness-of-fit on F^2	1.061
Final R indices [I>2sigma(I)]	R1 = 0.0290, wR2 = 0.0723
R indices (all data)	R1 = 0.0336, wR2 = 0.0768
Largest diff. peak and hole	0.972 and -0.698 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for m120. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pd(1)	8816(1)	1131(1)	458(1)	14(1)
P(2)	6874(1)	1291(1)	-960(1)	17(1)
P(3)	9277(1)	1939(1)	543(1)	17(1)
O(5)	13648(2)	1079(1)	3856(1)	28(1)
C(16)	6796(2)	1947(1)	-1140(2)	23(1)
C(17)	8308(2)	2178(1)	-729(1)	22(1)
C(211)	4964(2)	1172(1)	-1031(1)	17(1)
C(212)	4081(2)	848(1)	-1713(1)	21(1)
C(213)	2620(2)	782(1)	-1746(2)	28(1)
C(214)	2030(2)	1034(1)	-1106(2)	30(1)
C(215)	2906(3)	1350(1)	-405(2)	29(1)
C(216)	4363(2)	1413(1)	-364(2)	24(1)
C(217)	7062(2)	1048(1)	-2139(1)	18(1)
C(218)	8078(2)	685(1)	-2087(1)	20(1)
C(219)	8217(2)	476(1)	-2971(2)	24(1)
C(220)	7332(2)	628(1)	-3912(2)	26(1)
C(221)	6313(2)	988(1)	-3979(2)	28(1)
C(222)	6186(2)	1199(1)	-3099(2)	26(1)
C(311)	11056(2)	2233(1)	864(1)	20(1)
C(312)	12167(2)	2051(1)	1683(2)	25(1)
C(313)	13550(2)	2261(1)	1977(2)	31(1)
C(314)	13832(2)	2653(1)	1453(2)	37(1)
C(315)	12737(3)	2837(1)	643(2)	38(1)
C(316)	11351(2)	2629(1)	346(2)	30(1)
C(317)	8458(2)	2226(1)	1432(1)	19(1)
C(318)	7970(2)	1942(1)	2091(2)	25(1)
C(319)	7486(2)	2145(1)	2854(2)	28(1)
C(320)	7479(2)	2634(1)	2958(2)	27(1)
C(321)	7925(2)	2921(1)	2287(2)	25(1)
C(322)	8421(2)	2721(1)	1531(2)	22(1)
C(1)	8862(2)	405(1)	786(1)	19(1)
C(2)	10098(2)	602(1)	1554(1)	16(1)
C(3)	11572(2)	570(1)	1485(1)	16(1)
C(4)	12787(2)	681(1)	2269(1)	17(1)
C(5)	12589(2)	896(1)	3195(1)	19(1)
C(6)	11111(2)	885(1)	3321(1)	19(1)
C(7)	9948(2)	749(1)	2521(1)	18(1)
C(8)	14354(2)	583(1)	2229(1)	20(1)
C(9)	15228(2)	1049(1)	2291(2)	26(1)
C(10)	14342(2)	323(1)	1248(2)	23(1)
C(11)	15159(2)	263(1)	3135(2)	25(1)
C(12)	10916(2)	1040(1)	4338(2)	27(1)
C(13)	9339(3)	969(1)	4361(2)	33(1)
C(14)	11921(3)	741(1)	5212(2)	45(1)
C(15)	11287(3)	1571(1)	4514(2)	41(1)

Table 3. Bond lengths [A] and angles [deg] for m120.

Pd(1)-C(1)	2.088(2)
Pd(1)-C(2)	2.208(2)
Pd(1)-P(2)	2.2976(10)
Pd(1)-P(3)	2.3120(7)
P(2)-C(217)	1.819(2)
P(2)-C(211)	1.829(2)
P(2)-C(16)	1.861(2)
P(3)-C(311)	1.821(2)
P(3)-C(317)	1.828(2)
P(3)-C(17)	1.844(2)
O(5)-C(5)	1.251(2)
C(16)-C(17)	1.528(3)
C(211)-C(212)	1.395(3)
C(211)-C(216)	1.397(3)
C(212)-C(213)	1.395(3)
C(213)-C(214)	1.377(3)
C(214)-C(215)	1.392(3)
C(215)-C(216)	1.388(3)
C(217)-C(218)	1.396(3)
C(217)-C(222)	1.401(3)
C(218)-C(219)	1.393(3)
C(219)-C(220)	1.385(3)
C(220)-C(221)	1.390(3)
C(221)-C(222)	1.386(3)
C(311)-C(312)	1.394(3)
C(311)-C(316)	1.396(3)
C(312)-C(313)	1.393(3)
C(313)-C(314)	1.387(4)
C(314)-C(315)	1.380(4)
C(315)-C(316)	1.391(3)
C(317)-C(318)	1.390(3)
C(317)-C(322)	1.399(3)
C(318)-C(319)	1.391(3)
C(319)-C(320)	1.385(3)
C(320)-C(321)	1.387(3)
C(321)-C(322)	1.388(3)
C(1)-C(2)	1.437(2)
C(2)-C(7)	1.441(2)
C(2)-C(3)	1.443(3)
C(3)-C(4)	1.362(2)
C(4)-C(5)	1.474(3)
C(4)-C(8)	1.539(3)
C(5)-C(6)	1.474(3)
C(6)-C(7)	1.364(3)
C(6)-C(12)	1.530(3)
C(8)-C(10)	1.533(3)
C(8)-C(9)	1.541(3)
C(8)-C(11)	1.543(3)
C(12)-C(13)	1.530(3)
C(12)-C(15)	1.536(3)
C(12)-C(14)	1.544(3)

C(1)-Pd(1)-C(2)	38.97(6)
C(1)-Pd(1)-P(2)	109.57(5)
C(2)-Pd(1)-P(2)	148.53(5)
C(1)-Pd(1)-P(3)	163.52(5)
C(2)-Pd(1)-P(3)	124.72(5)
P(2)-Pd(1)-P(3)	86.73(2)
C(217)-P(2)-C(211)	104.38(9)
C(217)-P(2)-C(16)	105.37(9)
C(211)-P(2)-C(16)	100.07(9)
C(217)-P(2)-Pd(1)	114.48(6)
C(211)-P(2)-Pd(1)	123.11(6)
C(16)-P(2)-Pd(1)	107.30(6)
C(311)-P(3)-C(317)	101.13(8)
C(311)-P(3)-C(17)	103.32(9)
C(317)-P(3)-C(17)	106.36(9)
C(311)-P(3)-Pd(1)	127.52(6)
C(317)-P(3)-Pd(1)	110.75(6)
C(17)-P(3)-Pd(1)	106.06(6)
C(17)-C(16)-P(2)	112.06(13)
C(16)-C(17)-P(3)	110.25(13)
C(212)-C(211)-C(216)	118.4(2)
C(212)-C(211)-P(2)	123.14(15)
C(216)-C(211)-P(2)	118.46(14)
C(213)-C(212)-C(211)	120.3(2)
C(214)-C(213)-C(212)	120.6(2)
C(213)-C(214)-C(215)	119.8(2)
C(216)-C(215)-C(214)	119.8(2)
C(215)-C(216)-C(211)	121.1(2)
C(218)-C(217)-C(222)	118.5(2)
C(218)-C(217)-P(2)	118.89(14)
C(222)-C(217)-P(2)	122.5(2)
C(219)-C(218)-C(217)	120.8(2)
C(220)-C(219)-C(218)	119.8(2)
C(219)-C(220)-C(221)	120.3(2)
C(222)-C(221)-C(220)	119.9(2)
C(221)-C(222)-C(217)	120.8(2)
C(312)-C(311)-C(316)	119.1(2)
C(312)-C(311)-P(3)	117.17(15)
C(316)-C(311)-P(3)	123.74(15)
C(313)-C(312)-C(311)	120.2(2)
C(314)-C(313)-C(312)	120.2(2)
C(315)-C(314)-C(313)	120.0(2)
C(314)-C(315)-C(316)	120.2(2)
C(315)-C(316)-C(311)	120.4(2)
C(318)-C(317)-C(322)	118.9(2)
C(318)-C(317)-P(3)	118.64(14)
C(322)-C(317)-P(3)	122.2(2)
C(319)-C(318)-C(317)	120.8(2)

C(320)-C(319)-C(318)	119.8(2)
C(319)-C(320)-C(321)	119.9(2)
C(322)-C(321)-C(320)	120.4(2)
C(321)-C(322)-C(317)	120.1(2)
C(2)-C(1)-Pd(1)	75.06(10)
C(1)-C(2)-C(7)	120.1(2)
C(1)-C(2)-C(3)	122.0(2)
C(7)-C(2)-C(3)	116.7(2)
C(1)-C(2)-Pd(1)	65.97(10)
C(7)-C(2)-Pd(1)	104.45(12)
C(3)-C(2)-Pd(1)	110.38(12)
C(4)-C(3)-C(2)	123.3(2)
C(3)-C(4)-C(5)	118.6(2)
C(3)-C(4)-C(8)	122.5(2)
C(5)-C(4)-C(8)	118.9(2)
O(5)-C(5)-C(6)	121.0(2)
O(5)-C(5)-C(4)	120.9(2)
C(6)-C(5)-C(4)	118.1(2)
C(7)-C(6)-C(5)	119.1(2)
C(7)-C(6)-C(12)	121.8(2)
C(5)-C(6)-C(12)	119.1(2)
C(6)-C(7)-C(2)	123.0(2)
C(10)-C(8)-C(4)	111.5(2)
C(10)-C(8)-C(9)	108.3(2)
C(4)-C(8)-C(9)	111.3(2)
C(10)-C(8)-C(11)	107.8(2)
C(4)-C(8)-C(11)	109.1(2)
C(9)-C(8)-C(11)	108.7(2)
C(13)-C(12)-C(6)	111.9(2)
C(13)-C(12)-C(15)	107.8(2)
C(6)-C(12)-C(15)	109.6(2)
C(13)-C(12)-C(14)	107.3(2)
C(6)-C(12)-C(14)	109.9(2)
C(15)-C(12)-C(14)	110.3(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for m120. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Pd(1)	16(1)	13(1)	12(1)	0(1)	0(1)	0(1)
P(2)	17(1)	15(1)	14(1)	1(1)	-1(1)	1(1)
P(3)	19(1)	14(1)	16(1)	0(1)	1(1)	-1(1)
O(5)	21(1)	40(1)	19(1)	-7(1)	-1(1)	-5(1)
C(16)	24(1)	15(1)	24(1)	3(1)	-2(1)	1(1)
C(17)	25(1)	17(1)	20(1)	2(1)	1(1)	-1(1)
C(211)	16(1)	18(1)	15(1)	5(1)	2(1)	1(1)
C(212)	23(1)	18(1)	20(1)	2(1)	2(1)	1(1)
C(213)	25(1)	29(1)	25(1)	6(1)	0(1)	-6(1)
C(214)	22(1)	37(1)	31(1)	11(1)	7(1)	1(1)
C(215)	35(1)	31(1)	26(1)	7(1)	14(1)	8(1)
C(216)	30(1)	21(1)	19(1)	1(1)	5(1)	3(1)
C(217)	18(1)	20(1)	15(1)	1(1)	2(1)	-2(1)
C(218)	18(1)	21(1)	18(1)	3(1)	2(1)	-2(1)
C(219)	25(1)	25(1)	24(1)	-1(1)	10(1)	-2(1)
C(220)	29(1)	33(1)	18(1)	-4(1)	9(1)	-8(1)
C(221)	28(1)	39(1)	15(1)	4(1)	2(1)	-3(1)
C(222)	23(1)	32(1)	18(1)	4(1)	1(1)	4(1)
C(311)	21(1)	18(1)	21(1)	-5(1)	7(1)	-3(1)
C(312)	25(1)	22(1)	26(1)	-4(1)	6(1)	0(1)
C(313)	23(1)	35(1)	31(1)	-7(1)	1(1)	0(1)
C(314)	23(1)	43(1)	43(1)	-8(1)	8(1)	-11(1)
C(315)	35(1)	40(1)	39(1)	6(1)	10(1)	-14(1)
C(316)	27(1)	30(1)	29(1)	4(1)	5(1)	-5(1)
C(317)	16(1)	17(1)	20(1)	-2(1)	1(1)	-1(1)
C(318)	28(1)	18(1)	32(1)	-2(1)	11(1)	-1(1)
C(319)	29(1)	26(1)	33(1)	0(1)	14(1)	-3(1)
C(320)	23(1)	28(1)	29(1)	-10(1)	7(1)	-1(1)
C(321)	21(1)	18(1)	32(1)	-7(1)	3(1)	-2(1)
C(322)	21(1)	18(1)	24(1)	-2(1)	1(1)	-2(1)
C(1)	19(1)	15(1)	18(1)	1(1)	0(1)	0(1)
C(2)	20(1)	13(1)	13(1)	2(1)	0(1)	1(1)
C(3)	20(1)	14(1)	14(1)	1(1)	2(1)	2(1)
C(4)	18(1)	16(1)	15(1)	2(1)	3(1)	1(1)
C(5)	19(1)	21(1)	15(1)	2(1)	1(1)	-1(1)
C(6)	22(1)	19(1)	13(1)	1(1)	3(1)	0(1)
C(7)	19(1)	17(1)	17(1)	3(1)	4(1)	2(1)
C(8)	19(1)	20(1)	20(1)	1(1)	4(1)	1(1)
C(9)	22(1)	24(1)	30(1)	2(1)	7(1)	-4(1)
C(10)	21(1)	24(1)	25(1)	1(1)	7(1)	3(1)
C(11)	19(1)	27(1)	24(1)	6(1)	1(1)	3(1)
C(12)	27(1)	38(1)	15(1)	-5(1)	5(1)	-3(1)
C(13)	33(1)	48(1)	22(1)	-8(1)	14(1)	-4(1)
C(14)	39(1)	78(2)	15(1)	6(1)	5(1)	6(1)
C(15)	41(1)	46(1)	39(1)	-26(1)	15(1)	-12(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for m120.

	x	y	z	U(eq)
H(16A)	6396(2)	2019(1)	-1860(2)	28
H(16B)	6142(2)	2082(1)	-794(2)	28
H(17A)	8199(2)	2519(1)	-686(1)	26
H(17B)	8879(2)	2115(1)	-1190(1)	26
H(212)	4469(2)	675(1)	-2147(1)	26
H(213)	2040(2)	566(1)	-2204(2)	34
H(214)	1049(2)	993(1)	-1143(2)	36
H(215)	2517(3)	1518(1)	35(2)	35
H(216)	4949(2)	1620(1)	114(2)	28
H(218)	8668(2)	581(1)	-1456(1)	24
H(219)	8902(2)	236(1)	-2928(2)	29
H(220)	7420(2)	487(1)	-4503(2)	31
H(221)	5718(2)	1088(1)	-4613(2)	34
H(222)	5511(2)	1443(1)	-3147(2)	31
H(312)	11983(2)	1787(1)	2035(2)	30
H(313)	14287(2)	2139(1)	2526(2)	37
H(314)	14758(2)	2792(1)	1649(2)	44
H(315)	12926(3)	3101(1)	294(2)	45
H(316)	10617(2)	2755(1)	-200(2)	35
H(318)	7967(2)	1613(1)	2021(2)	30
H(319)	7169(2)	1951(1)	3294(2)	34
H(320)	7175(2)	2770(1)	3476(2)	33
H(321)	7891(2)	3250(1)	2345(2)	30
H(322)	8730(2)	2916(1)	1089(2)	26
H(1A)	8066(2)	287(1)	1022(1)	22
H(10B)	9093(2)	195(1)	296(1)	22
H(3)	11700(2)	469(1)	875(1)	20
H(7)	9016(2)	751(1)	2602(1)	21
H(9C)	15381(17)	1191(3)	2948(5)	38
H(9D)	14688(9)	1264(3)	1772(9)	38
H(9E)	16160(8)	981(1)	2191(13)	38
H(10F)	15332(2)	260(5)	1254(6)	35
H(10G)	13866(16)	518(3)	671(2)	35
H(10H)	13819(16)	29(3)	1204(6)	35
H(11A)	15206(17)	422(3)	3761(2)	37
H(11B)	16136(7)	200(5)	3112(8)	37
H(11C)	14636(11)	-31(3)	3096(8)	37
H(13D)	9269(5)	1058(6)	5017(5)	50
H(13E)	9070(7)	641(2)	4233(14)	50
H(13F)	8688(3)	1163(5)	3846(9)	50
H(14G)	11808(20)	844(6)	5848(2)	67
H(14H)	12925(4)	781(7)	5225(11)	67
H(14I)	11657(17)	411(2)	5105(10)	67
H(15J)	11152(23)	1668(2)	5148(8)	61
H(15K)	10650(16)	1753(1)	3968(9)	61
H(15L)	12289(8)	1623(2)	4536(16)	61