Synthesis and luminescence behaviour of novel heterodecanuclear silver(I)-rhenium(I) alkynyl complexes. X-Ray crystal structures of $[Ag_6(\mu\text{-dppm})_4\{\mu_3\text{-}C{\equiv}CC{\equiv}C\text{-}Re(Me_2bpy)(CO)_3\}_4](PF_6)_2$ and $[Ag_6(\mu\text{-dppm})_4\{\mu_3\text{-}C{\equiv}CC{\equiv}C\text{-}Re(Br_2phen)(CO)_3\}_4](PF_6)_2$

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Supplementary Information

Characterizations

[Ag_6(μ-dppm)$_4${μ_3-C≡CC≡C-Re(^{t}Bu$_2$bpy)(CO)$_3$}$_4$](PF$_6$)$_2$ (1):

^{1}H NMR (300 MHz, acetone-d_6, 298K)/ ppm: 1.2-1.4 (m, 72H, ^{t}Bu), 3.4-3.8 (m, 8H, -CH_2), 6.5-8.6 (m, 104H, pyridyl Hs and -Ph). IR (nujol mull, KBr), ν/cm^{-1}: 2005s, 1896m [(C≡O)], 2085w [ν(C≡C)]. Positive FAB-MS: m/z: 2265 {M–2PF_6}$^{2+}$. Anal. Calc. for $Ag_6Re_4C_{200}H_{184}N_8O_{12}P_{10}F_{12}$: C, 49.82; H, 3.85; N, 2.33. Found: C, 49.73; H, 3.82; N, 2.43.

[Ag_6(μ-dppm)$_4${μ_3-C≡CC≡C-Re(Me$_2$bpy)(CO)$_3$}$_4$](PF$_6$)$_2$ (2):

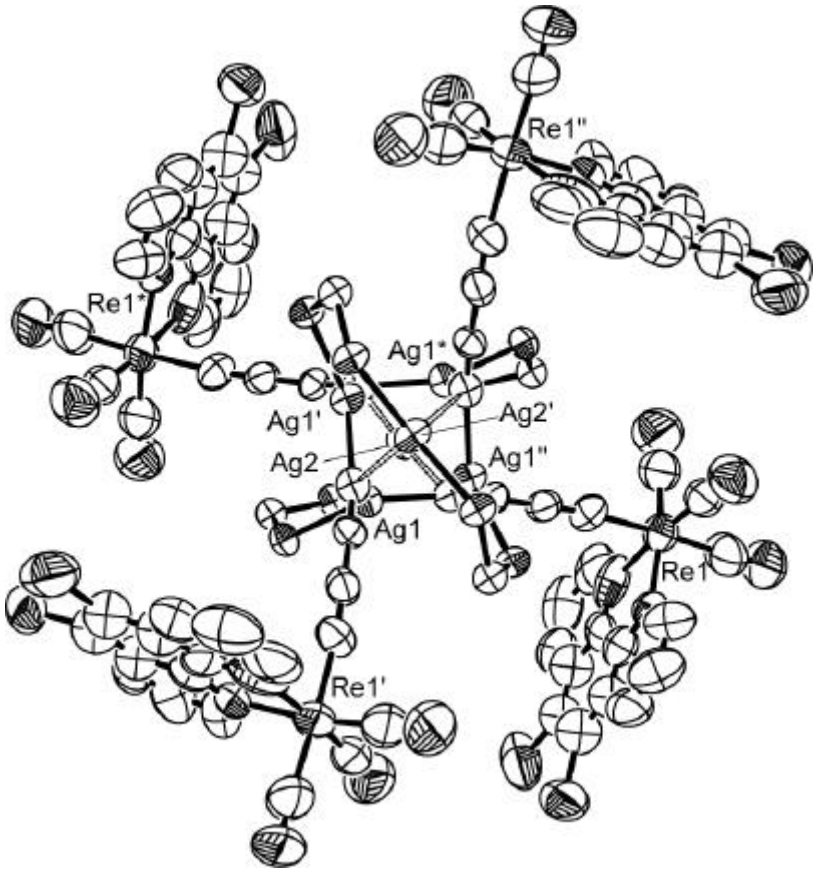
^{1}H NMR (300 MHz, acetone-d_6, 298K)/ppm: 2.1-2.2 (m, 24H, -Me), 3.4-3.5 (m, 8H, -CH_2), 6.4-8.7 (m, 104H, pyridyl Hs and -Ph). IR (nujol mull, KBr), ν/cm^{-1}: 2004s, 1891m [(C≡O)], 2087w [ν(C≡C)]. Positive FAB-MS: m/z: 2097{M–2PF_6}$^{2+}$. Anal. Calc. for $Ag_6Re_4C_{176}H_{136}N_8O_{12}P_{10}F_{12}$: C, 47.13; H, 3.06; N, 2.50. Found: C, 47.36; H, 3.25; N, 2.47.

[Ag_6(μ-dppm)$_4${μ_3-C≡CC≡C-Re(phen)(CO)$_3$}$_4$](PF$_6$)$_2$ (3):

^{1}H NMR (300 MHz, acetone-d_6, 298K)/ppm: 3.5-3.6 (m, 8H, -CH_2), 6.0-9.3 (m, 112H, pyridyl Hs and -Ph). IR (nujol mull, KBr), ν/cm^{-1}: 2007s, 1900m [(C≡O)], 2084w [ν(C≡C)]. Positive FAB-MS: m/z: 2089 {M–2PF_6}$^{2+}$. Anal. Calc. for $Ag_6Re_4C_{176}H_{120}N_8O_{12}P_{10}F_{12}$: C, 47.30; H, 2.71; N, 2.51. Found: C, 47.22; H, 2.90; N, 2.57.

[Ag_6(μ-dppm)$_4${μ_3-C≡CC≡C-Re(Br$_2$phen)(CO)$_3$}$_4$](PF$_6$)$_2$ (4):

^{1}H NMR (300 MHz, acetone-d_6, 298K)/ppm: 3.4-3.7 (m, 8H, -CH_2), 5.9-9.4 (m, 104H, pyridyl Hs and -Ph). IR (nujol mull, KBr), ν/cm^{-1}: 2009s, 1900m [(C≡O)], 2086w [ν(C≡C)]. Positive FAB-MS: m/z: 2405 {M–2PF_6}$^{2+}$. Anal. Calc. for $Ag_6Re_4C_{176}H_{112}N_8O_{12}Br_8P_{10}F_{12}$: C, 41.45; H, 2.21; N, 2.20. Found: C, 41.45; H, 2.41; N, 2.20.



Perspective drawing of the complex cation of **4** with atomic numbering scheme. Hydrogen atoms and phenyl rings have been omitted for clarity. Thermal ellipsoids are shown at the 30% probability level.

Crystal data: $[C_{176}\ H_{136}\ Ag_6\ F_{12}\ N_8\ O_{12}\ P_{10}\ Re_4]$ (**2**) ; formula weight = 4484.65, Orthorhombic, P $2_1\ 2_1\ 2_1$, a = 20.082(4) Å, b = 29.961(6) Å, c = 35.827(7) Å, V = 21556(7) $Å^3$, Z = 4, D_c = 1.382 g cm^{-3}, μ(Mo-Kα) = 2.901 mm^{-1}, F(000) = 8736, T = 293 K.

Data collection: A crystal of dimensions 0.3 x 0.1 x 0.05 mm mounted in a glass capillary with mother liquor was used for data collection at 20°C on a MAR diffractometer with a 300 mm image plate detector using graphite monochromatized Mo-K_α radiation (λ = 0.71073 Å). Data collection was made with 1.5° oscillation step of φ, 600 seconds exposure time and scanner distance at 140 mm. 120 images were collected.

Data reduction: The images were interpreted and intensities integrated using program DENZO [1].

Structure solution: The structure was solved by direct methods employing SIR-97 program[2] on PC. Ag, Re and P atoms were located according to the direct methods and the successive least-square Fourier cycles. Positions of other non-hydrogen atoms were found after successful refinement by full-matrix least-squares using program SHELXL-97 [3] on PC. Two PF_6^- anions were located; and for convergence of refinement, the geometry of the anions was assumed to be normal octahedral with the same P-F and adjacent F…F distances; and thermal parameters of each six F atoms were assumed to be the same. Since some Re atoms have high thermal parameters, restrains had to be applied for the coordinated organic ligands. Pyridine rings of bpy ligand were assumed to be normal hexagon rings with bond lengths of 1.39 Å. For each $Re(CO)_3$(bpy)-fragment, Re-CO bond lengths and distances of Re…O were assumed to be similar; three Re(4)-CO bond lengths were extraordinarily assumed to be around 1.90(2) Å; C atoms of each three carbonyls were assumed to be similarly separated; for Re(3) and Re(4), four groups of planarity were assumed for two CO's, Re and bound C of C_4; planarity of bpy and Re(4) was also assumed; for the four bpy$(Me)_2$-ligands, all the C-Me bond lengths and N…N distances were assumed to be similar; and the C-C bonds connecting two py rings were also assumed to be similar; thermal parameters of C and O atoms of the three CO's bound to Re(4) were assumed to be the same respectively. The absolute structure was assisted by the Flack parameter of 0.005(9).

Structure refinement: According to the SHELXL-97 program [3], all 18181 independent reflections (R_{int} [4] equal to 0.0553, 11341 reflections larger than $4\sigma(F_o)$) from a total 41373 reflections were participated in the full-matrix least-square refinement against F^2. These reflections were in the range -21<=h<= 20, -29<=k<= 28, -37=l<= 26 with $2\theta_{max}$ equal to 45.44°.

One crystallographic asymmetric unit consists of one formula unit. In the final stage of least-squares refinement, only Ag, Re, P atoms were refined anisotropically, other non-hydrogen atoms isotropically. H atoms were generated by program SHELXL-97. The positions of H atoms were calculated based on riding mode with thermal parameters equal to 1.2 times that of the associated C atoms, and participated in the calculation of final R-indices[5].

Convergence ($(\Delta/\sigma)_{max}$ = 0.06, av. 0.006) for 711 variable parameters by full-matrix least-squares refinement on F^2 reaches to R_1 = 0.0683 and wR_2 = 0.1819 with a goodness-of-fit of 0.996, the parameters a and b for weighting scheme are 0.1164 and 0. The final difference Fourier map shows maximum rest peaks and holes of 1.214 and -1.261 $eÅ^{-3}$ respectively.

Drawing: The ORTEP [6] drawing of the molecule was made with thermal ellipsoids at the 30 % probability level. Screen drawing is provided for reference. Drawing with high quality can be provided upon request.

Tables: Table (1) of Crystallographic and refinement data, table (2) of atomic coordinates, table (3) of full bond lengths and bond angles and this report [7] are provided. The other supplementary materials, such as table of

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[1] Otwinowski, Z. and Minor, W., "Processing of X-ray Diffraction Data Collected in Oscillation Mode", Methods in Enzymology, Volume 276: Macromolecular Crystallography, part A, p. 307-326, 1997. Carter C. W., Sweet Jr. & R. M., Eds., Academic Press.

[2] A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A.G.G. Moliterni, G. Polidori, R. Spagna. ***Sir97****: a new tool for crystal structure determination and refinement. J. Appl. Cryst.*, **1998**, *32*, 115-119.

[3] SHELXL97, Sheldrick, G. M. (1997). SHELX97. Programs for Crystal Structure Analysis (Release 97-2). University of Goetingen, Germany.

[4] $R_{int} = \Sigma\ |\ F_o^2 - F_o^2(mean)\ |\ /\ \Sigma\ [\ F_o^2]$

[5] Since the structure refinements are against F^2, R-indices based on F^2 are larger than (more than double) those based on F. For comparison with older refinements based on F and an OMIT threshold, a conventional index R_1 based on observed F values larger than $4\sigma(F_o)$ is also given (corresponding to Intensity≥2σ(I)). $wR_2 = \{\ \Sigma\ [\ w(\ F_o^2 - F_c^2)^2]\ /\ \Sigma\ [\ w(F_o^2)^2]\ \}^{1/2}$, $R_1 = \Sigma\ ||F_o| - |F_c||\ /\ \Sigma\ |F_o|$, The Goodness of Fit is always based on F^2: $GooF = S = \{\ \Sigma\ [\ w(\ F_o^2 - F_c^2)^2]\ /\ (\ n - p)\ \}^{1/2}$, where n is the number of reflections and p is the total number of parameters refined. The weighting scheme is: $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP\ ]$, where P is $[\ 2\ F_c^2 + Max(\ F_o^2, 0)\ ]/3$.

[6] ORTEP3 for Windows - Farrugia, L. J. (1997) J. Appl. Cryst. 30, 565.

anisotropic displacement parameters, table of hydrogen coordinates and/or other tables and/or CIF, RES-files, can be provided under request by notifying the identification code.

[7] Crystallographic data summarized in this report are abstracted from tables of crystallographic data and data collection record.

Table 1. Crystal data and structure refinement for mar499.

Identification code	mar499	
Empirical formula	C_{176} H_{136} Ag_6 F_{12} N_8 O_{12} P_{10} Re_4	
Formula weight	4484.65	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 2_1 2_1 2_1	
Unit cell dimensions	a = 20.082(4) Å	α= 90°.
	b = 29.961(6) Å	β= 90°.
	c = 35.827(7) Å	γ = 90°.
Volume	21556(7) $Å^3$	
Z	4	
Density (calculated)	1.382 Mg/m^3	
Absorption coefficient	2.901 mm^{-1}	
F(000)	8736	
Crystal size	0.3 x 0.1 x 0.05 mm^3	
Theta range for data collection	0.89 to 22.72°.	
Index ranges	-21<=h<=20, -29<=k<=28, -37<=l<=26	
Reflections collected	41373	
Independent reflections	18181 [R(int) = 0.0553]	
Completeness to theta = 22.72°	69.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	18181 / 295 / 711	
Goodness-of-fit on F^2	0.996	
Final R indices [I>2sigma(I)]	R1 = 0.0683, wR2 = 0.1819	
R indices (all data)	R1 = 0.1131, wR2 = 0.2123	
Absolute structure parameter	0.005(9)	
Largest diff. peak and hole	1.214 and -1.261 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mar499. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ag(1)	875(1)	4137(1)	1664(1)	81(1)
Ag(2)	1107(1)	3583(1)	2329(1)	76(1)
Ag(3)	1516(1)	3303(1)	1415(1)	83(1)
Ag(4)	865(1)	2698(1)	1976(1)	83(1)
Ag(5)	2392(1)	3199(1)	2086(1)	79(1)
Ag(6)	2099(1)	2254(1)	2246(1)	90(1)
Re(2)	-2383(1)	3155(1)	1354(1)	105(1)
Re(1)	3694(1)	5429(1)	2002(1)	148(1)
Re(3)	3441(1)	1578(1)	554(1)	159(1)
Re(4)	1180(1)	2555(1)	4133(1)	186(1)
P(1)	639(3)	4737(2)	2116(2)	78(2)
P(2)	1311(3)	4218(2)	2743(2)	78(2)
P(3)	552(3)	4215(2)	1012(2)	87(2)
P(4)	859(3)	3244(2)	839(2)	86(2)
P(5)	3527(3)	3056(2)	1867(2)	89(2)
P(6)	3322(3)	2141(2)	2224(3)	102(2)
P(7)	113(3)	2271(2)	2377(2)	87(2)
P(8)	1325(3)	1657(2)	2435(2)	90(2)
O(1)	4565(13)	6257(8)	2049(10)	211(11)
O(2)	2631(13)	6004(9)	2362(10)	225(12)
O(3)	4316(17)	5116(12)	2726(9)	280(17)
O(4)	-3863(8)	3006(7)	1195(7)	153(7)
O(5)	-2193(11)	3673(8)	626(6)	171(8)
O(6)	-2105(9)	2267(6)	962(7)	147(7)
O(7)	4176(10)	1058(7)	-52(6)	181(9)
O(8)	4575(15)	1337(12)	1061(11)	283(17)
O(9)	4330(20)	2343(13)	367(18)	390(30)
O(10)	930(20)	2441(14)	4960(7)	312(11)
O(11)	669(19)	1629(9)	3956(15)	312(11)
O(12)	-188(14)	2960(12)	4045(16)	312(11)
C(1)	627(7)	5305(4)	1926(5)	72(6)

C(2)	1223(6)	5515(6)	1836(6)	148(11)
C(3)	1216(7)	5935(6)	1671(7)	152(12)
C(4)	614(10)	6144(5)	1595(6)	143(11)
C(5)	18(7)	5934(5)	1686(6)	109(8)
C(6)	25(6)	5514(5)	1851(5)	98(8)
C(7)	-185(6)	4686(5)	2339(5)	79(6)
C(8)	-620(7)	4374(5)	2188(4)	101(8)
C(9)	-1229(7)	4292(5)	2359(5)	98(7)
C(10)	-1403(6)	4522(6)	2682(5)	126(9)
C(11)	-968(8)	4835(5)	2833(4)	120(9)
C(12)	-359(7)	4916(4)	2662(5)	90(7)
C(13)	2111(7)	4231(6)	2981(6)	86(7)
C(14)	2281(9)	3855(5)	3188(6)	135(10)
C(15)	2883(11)	3841(6)	3379(6)	150(12)
C(16)	3315(8)	4203(8)	3363(7)	149(12)
C(17)	3145(9)	4579(6)	3156(7)	181(15)
C(18)	2543(10)	4593(5)	2965(6)	156(12)
C(19)	750(8)	4280(6)	3131(5)	92(7)
C(20)	240(9)	3969(5)	3173(6)	122(9)
C(21)	-197(8)	4003(7)	3472(7)	179(14)
C(22)	-126(10)	4347(8)	3729(6)	178(15)
C(23)	383(11)	4657(6)	3687(5)	160(12)
C(24)	821(8)	4624(5)	3388(6)	108(8)
C(25)	1227(9)	4764(6)	2466(7)	74(6)
C(26)	1197(9)	4408(6)	689(7)	115(9)
C(27)	1838(11)	4488(6)	820(6)	129(10)
C(28)	2345(8)	4593(7)	571(8)	191(15)
C(29)	2211(11)	4617(7)	191(7)	157(12)
C(30)	1571(13)	4537(7)	60(6)	171(14)
C(31)	1064(9)	4433(6)	309(7)	142(11)
C(32)	-164(9)	4611(6)	944(7)	100(8)
C(33)	-19(8)	5057(7)	874(8)	143(11)
C(34)	-531(11)	5368(5)	849(8)	138(10)
C(35)	-1188(9)	5233(7)	896(8)	145(11)
C(36)	-1333(8)	4787(8)	967(9)	189(15)
C(37)	-821(11)	4476(5)	991(8)	172(14)

C(38)	1310(9)	3285(6)	384(5)	103(8)
C(39)	963(7)	3260(6)	48(7)	139(11)
C(40)	1305(11)	3283(7)	-288(5)	182(15)
C(41)	1993(11)	3332(6)	-290(5)	136(11)
C(42)	2340(7)	3358(6)	45(7)	146(11)
C(43)	1998(9)	3334(6)	382(5)	131(10)
C(44)	375(9)	2722(5)	763(7)	107(8)
C(45)	-291(9)	2734(5)	659(7)	132(10)
C(46)	-631(7)	2338(7)	590(8)	166(13)
C(47)	-305(10)	1931(6)	626(8)	140(11)
C(48)	361(10)	1920(5)	730(7)	146(11)
C(49)	702(7)	2315(7)	799(7)	122(9)
C(50)	236(10)	3703(7)	808(8)	94(7)
C(51)	4198(7)	3318(6)	2126(5)	88(7)
C(52)	4864(9)	3239(6)	2042(5)	126(9)
C(53)	5361(6)	3415(7)	2268(7)	134(10)
C(54)	5193(10)	3670(7)	2578(6)	181(15)
C(55)	4528(12)	3749(7)	2663(5)	184(15)
C(56)	4030(8)	3573(6)	2437(6)	128(10)
C(57)	3687(8)	3262(6)	1401(6)	82(6)
C(58)	3837(12)	2984(5)	1102(8)	260(20)
C(59)	3947(15)	3165(10)	750(7)	420(50)
C(60)	3907(13)	3624(11)	697(6)	222(19)
C(61)	3756(10)	3902(6)	996(8)	153(12)
C(62)	3646(8)	3721(6)	1348(7)	126(9)
C(63)	3710(13)	2310(6)	2659(7)	127(10)
C(64)	4398(12)	2358(8)	2682(7)	164(13)
C(65)	4689(10)	2511(9)	3009(9)	290(30)
C(66)	4293(16)	2618(8)	3315(7)	198(17)
C(67)	3605(15)	2570(7)	3293(7)	182(15)
C(68)	3314(9)	2417(8)	2965(9)	191(15)
C(69)	3522(13)	1546(7)	2125(8)	119(9)
C(70)	4124(11)	1385(9)	1990(9)	176(14)
C(71)	4220(15)	928(11)	1951(11)	260(20)
C(72)	3710(20)	633(6)	2046(12)	260(20)
C(73)	3112(18)	794(10)	2181(12)	310(30)

C(74)	3016(12)	1251(11)	2221(10)	300(30)
C(75)	3743(10)	2450(6)	1841(7)	83(7)
C(76)	-402(8)	2562(6)	2728(6)	105(8)
C(77)	-516(10)	2386(5)	3081(7)	176(14)
C(78)	-942(11)	2603(7)	3327(5)	164(13)
C(79)	-1254(8)	2997(7)	3220(6)	130(10)
C(80)	-1140(8)	3173(5)	2867(6)	124(9)
C(81)	-714(9)	2956(6)	2621(5)	111(9)
C(82)	-503(7)	1915(5)	2121(6)	88(7)
C(83)	-895(9)	1599(6)	2301(5)	143(11)
C(84)	-1341(8)	1341(5)	2097(7)	131(10)
C(85)	-1396(8)	1400(6)	1713(7)	156(12)
C(86)	-1005(10)	1716(7)	1533(5)	143(11)
C(87)	-558(8)	1974(5)	1737(6)	108(8)
C(88)	1624(8)	1256(6)	2783(5)	99(8)
C(89)	1844(9)	1423(5)	3123(6)	126(10)
C(90)	2065(9)	1132(8)	3399(5)	163(13)
C(91)	2066(9)	674(7)	3334(6)	158(12)
C(92)	1846(8)	508(4)	2994(6)	117(9)
C(93)	1626(8)	799(6)	2718(5)	105(8)
C(94)	1045(8)	1322(5)	2048(5)	88(7)
C(95)	472(8)	1062(6)	2053(5)	121(9)
C(96)	271(8)	840(5)	1731(7)	133(10)
C(97)	643(11)	878(6)	1406(5)	150(12)
C(98)	1216(10)	1138(7)	1401(5)	167(13)
C(99)	1417(7)	1360(5)	1723(6)	137(10)
C(100)	534(10)	1870(8)	2673(8)	100(7)
C(101)	2032(9)	3848(7)	1734(7)	72(6)
C(102)	2309(9)	4169(7)	1791(7)	69(6)
C(103)	2711(13)	4549(9)	1876(10)	118(9)
C(104)	3089(12)	4893(8)	1961(9)	105(8)
C(105)	4240(15)	5931(9)	2069(13)	198(17)
C(106)	3065(15)	5760(9)	2270(10)	167(14)
C(107)	4004(14)	5272(11)	2480(9)	171(14)
N(1)	3512(8)	5550(5)	1443(5)	111(6)
C(108)	3010(8)	5832(5)	1318(6)	149(12)

C(109)	2922(9)	5903(6)	938(7)	176(14)
C(110)	3337(12)	5692(8)	682(5)	177(14)
C(111)	3839(10)	5409(7)	807(6)	158(12)
C(112)	3926(7)	5338(5)	1187(7)	121(9)
N(2)	4404(7)	5008(5)	1692(6)	136(8)
C(113)	4373(7)	5033(5)	1305(6)	99(8)
C(114)	4771(9)	4755(6)	1089(5)	118(9)
C(115)	5198(8)	4452(5)	1259(6)	149(12)
C(116)	5229(7)	4428(5)	1646(7)	123(9)
C(117)	4831(9)	4705(6)	1863(5)	142(11)
C(118)	3220(20)	5828(15)	262(8)	250(20)
C(119)	5538(17)	4112(11)	985(11)	197(16)
C(120)	387(10)	3449(6)	1904(7)	78(6)
C(121)	-172(9)	3372(6)	1747(7)	70(6)
C(122)	-815(11)	3323(7)	1622(8)	90(7)
C(123)	-1438(12)	3256(8)	1516(8)	102(8)
C(124)	-3285(10)	3069(7)	1246(8)	105(8)
C(125)	-2257(12)	3463(8)	907(7)	138(11)
C(126)	-2190(11)	2615(7)	1103(8)	126(10)
N(3)	-2470(7)	2883(5)	1905(4)	101(6)
C(127)	-2337(7)	2441(4)	1996(5)	122(9)
C(128)	-2446(9)	2289(4)	2357(6)	142(11)
C(129)	-2688(9)	2580(7)	2628(4)	155(12)
C(130)	-2821(8)	3022(6)	2537(5)	112(9)
C(131)	-2712(7)	3174(4)	2175(5)	89(7)
N(4)	-2623(6)	3705(4)	1713(4)	91(5)
C(132)	-2752(7)	3605(4)	2085(5)	87(7)
C(133)	-2976(7)	3937(6)	2326(4)	100(8)
C(134)	-3071(7)	4368(5)	2194(5)	114(9)
C(135)	-2942(8)	4469(3)	1823(5)	122(9)
C(136)	-2718(7)	4137(5)	1582(4)	102(8)
C(137)	-2840(20)	2369(14)	3015(9)	224(19)
C(138)	-3295(15)	4757(9)	2454(10)	158(12)
C(139)	1698(10)	2555(7)	1615(8)	83(7)
C(140)	2089(11)	2368(7)	1408(8)	88(7)
C(141)	2523(12)	2139(8)	1161(8)	98(8)

C(142)	2924(14)	1888(10)	948(11)	126(10)
C(143)	3901(8)	1256(5)	177(5)	213(18)
C(144)	4257(16)	1527(12)	838(12)	250(20)
C(145)	3860(20)	2102(11)	346(9)	450(50)
N(5)	2537(6)	1657(6)	229(5)	117(7)
C(146)	2411(8)	2042(5)	24(6)	151(12)
C(147)	1789(10)	2109(6)	-136(6)	154(12)
C(148)	1292(7)	1790(7)	-92(6)	136(10)
C(149)	1417(8)	1405(6)	113(6)	140(11)
C(150)	2040(9)	1339(5)	273(6)	118(9)
N(6)	2811(7)	1032(5)	695(5)	120(7)
C(151)	2219(8)	992(5)	498(5)	99(8)
C(152)	1809(7)	624(6)	555(6)	125(10)
C(153)	1992(10)	297(5)	811(7)	150(12)
C(154)	2585(11)	337(6)	1008(6)	173(14)
C(155)	2995(8)	705(6)	950(5)	157(12)
C(156)	606(14)	1797(13)	-295(12)	199(16)
C(157)	1537(19)	-112(11)	881(16)	230(20)
C(158)	1782(10)	2979(7)	2556(9)	83(7)
C(159)	1666(10)	2858(7)	2859(9)	83(7)
C(160)	1543(13)	2746(9)	3208(11)	109(8)
C(161)	1402(14)	2673(10)	3529(12)	140(11)
C(162)	994(13)	2453(9)	4648(4)	350(20)
C(163)	950(30)	1948(6)	4024(14)	350(20)
C(164)	261(12)	2723(17)	4059(15)	350(20)
N(7)	1596(11)	3201(5)	4206(7)	184(12)
C(165)	1249(8)	3602(7)	4191(10)	184(15)
C(166)	1589(12)	4004(5)	4224(8)	191(16)
C(167)	2276(12)	4005(6)	4270(8)	169(14)
C(168)	2623(8)	3604(8)	4284(8)	156(12)
C(169)	2283(11)	3202(6)	4252(5)	156(12)
N(8)	2145(8)	2434(8)	4222(8)	189(13)
C(170)	2545(14)	2793(6)	4322(9)	188(15)
C(171)	3222(13)	2730(9)	4382(11)	260(20)
C(172)	3499(9)	2308(11)	4342(11)	270(30)
C(173)	3100(13)	1949(8)	4242(11)	210(18)

C(174)	2422(13)	2012(7)	4182(10)	310(30)
C(175)	2590(20)	4476(11)	4353(18)	290(30)
C(176)	4234(18)	2140(20)	4410(30)	450(50)
P(9)	-2938(7)	3976(5)	3499(4)	270(9)
F(1)	-3523(12)	3974(9)	3241(7)	318(7)
F(2)	-3099(13)	3515(7)	3615(8)	318(7)
F(3)	-2350(12)	3973(9)	3750(7)	318(7)
F(4)	-2777(13)	4441(7)	3375(8)	318(7)
F(5)	-3355(13)	4156(9)	3801(7)	318(7)
F(6)	-2510(13)	3801(9)	3191(7)	318(7)
P(10)	4541(7)	4582(5)	-220(4)	239(8)
F(7)	4039(17)	4934(11)	-396(12)	450(14)
F(8)	5062(17)	4960(11)	-139(12)	450(14)
F(9)	5018(17)	4215(11)	-41(12)	450(14)
F(10)	3993(16)	4194(11)	-301(12)	450(14)
F(11)	4850(20)	4490(14)	-620(8)	450(14)
F(12)	4210(20)	4651(14)	179(8)	450(14)

Table 3. Bond lengths [Å] and angles [°] for mar499.

Ag(1)-P(3)	2.438(8)	Re(1)-C(106)	1.87(3)
Ag(1)-C(120)	2.44(2)	Re(1)-C(105)	1.88(3)
Ag(1)-P(1)	2.466(7)	Re(1)-C(107)	1.88(3)
Ag(1)-C(101)	2.492(18)	Re(1)-C(104)	2.02(3)
Ag(1)-Ag(2)	2.940(3)	Re(1)-N(1)	2.070(18)
Ag(1)-Ag(3)	2.949(2)	Re(1)-N(2)	2.202(13)
Ag(2)-C(120)	2.14(2)	Re(3)-C(143)	1.901(18)
Ag(2)-C(158)	2.40(2)	Re(3)-C(145)	1.929(19)
Ag(2)-P(2)	2.447(6)	Re(3)-C(144)	1.935(18)
Ag(2)-Ag(5)	2.957(2)	Re(3)-C(142)	1.98(3)
Ag(2)-Ag(4)	2.978(2)	Re(3)-N(6)	2.128(12)
Ag(3)-C(101)	2.25(2)	Re(3)-N(5)	2.171(13)
Ag(3)-C(139)	2.38(2)	Re(4)-C(162)	1.907(14)
Ag(3)-P(4)	2.456(7)	Re(4)-C(163)	1.915(14)
Ag(3)-Ag(5)	2.996(3)	Re(4)-C(164)	1.931(14)
Ag(3)-Ag(4)	3.007(3)	Re(4)-N(8)	1.996(15)
Ag(4)-C(139)	2.16(2)	Re(4)-N(7)	2.125(14)
Ag(4)-P(7)	2.444(7)	Re(4)-C(161)	2.24(4)
Ag(4)-C(120)	2.459(19)	P(1)-C(25)	1.72(2)
Ag(4)-Ag(6)	2.974(2)	P(1)-C(1)	1.831(14)
Ag(5)-C(158)	2.19(3)	P(1)-C(7)	1.843(13)
Ag(5)-C(101)	2.43(2)	P(2)-C(19)	1.800(17)
Ag(5)-P(5)	2.449(6)	P(2)-C(13)	1.819(15)
Ag(5)-Ag(6)	2.948(2)	P(2)-C(25)	1.92(2)
Ag(6)-P(8)	2.464(6)	P(3)-C(50)	1.81(2)
Ag(6)-P(6)	2.480(6)	P(3)-C(26)	1.829(18)
Ag(6)-C(158)	2.52(2)	P(3)-C(32)	1.879(16)
Ag(6)-C(139)	2.56(3)	P(4)-C(44)	1.859(15)
Re(2)-C(125)	1.87(2)	P(4)-C(50)	1.86(2)
Re(2)-C(124)	1.87(2)	P(4)-C(38)	1.870(18)
Re(2)-C(126)	1.89(2)	P(5)-C(57)	1.81(2)
Re(2)-C(123)	2.01(2)	P(5)-C(51)	1.815(16)
Re(2)-N(3)	2.141(14)	P(5)-C(75)	1.87(2)
Re(2)-N(4)	2.145(11)	P(6)-C(63)	1.82(2)

P(6)-C(75)	1.86(2)	C(16)-C(17)	1.3900
P(6)-C(69)	1.86(2)	C(17)-C(18)	1.3900
P(7)-C(100)	1.81(3)	C(19)-C(20)	1.3900
P(7)-C(76)	1.847(17)	C(19)-C(24)	1.3900
P(7)-C(82)	1.874(15)	C(20)-C(21)	1.3900
P(8)-C(94)	1.801(17)	C(21)-C(22)	1.3900
P(8)-C(88)	1.831(16)	C(22)-C(23)	1.3900
P(8)-C(100)	1.91(2)	C(23)-C(24)	1.3900
O(1)-C(105)	1.18(3)	C(26)-C(27)	1.3900
O(2)-C(106)	1.18(3)	C(26)-C(31)	1.3900
O(3)-C(107)	1.18(3)	C(27)-C(28)	1.3900
O(4)-C(124)	1.191(19)	C(28)-C(29)	1.3900
O(5)-C(125)	1.19(2)	C(29)-C(30)	1.3900
O(6)-C(126)	1.17(2)	C(30)-C(31)	1.3900
O(7)-C(143)	1.15(2)	C(32)-C(33)	1.3900
O(8)-C(144)	1.17(3)	C(32)-C(37)	1.3900
O(9)-C(145)	1.19(3)	C(33)-C(34)	1.3900
O(10)-C(162)	1.13(2)	C(34)-C(35)	1.3900
O(11)-C(163)	1.14(3)	C(35)-C(36)	1.3900
O(12)-C(164)	1.15(3)	C(36)-C(37)	1.3900
C(1)-C(2)	1.3900	C(38)-C(39)	1.3900
C(1)-C(6)	1.3900	C(38)-C(43)	1.3900
C(2)-C(3)	1.3900	C(39)-C(40)	1.3900
C(3)-C(4)	1.3900	C(40)-C(41)	1.3900
C(4)-C(5)	1.3900	C(41)-C(42)	1.3900
C(5)-C(6)	1.3900	C(42)-C(43)	1.3900
C(7)-C(8)	1.3900	C(44)-C(45)	1.3900
C(7)-C(12)	1.3900	C(44)-C(49)	1.3900
C(8)-C(9)	1.3900	C(45)-C(46)	1.3900
C(9)-C(10)	1.3900	C(46)-C(47)	1.3900
C(10)-C(11)	1.3900	C(47)-C(48)	1.3900
C(11)-C(12)	1.3900	C(48)-C(49)	1.3900
C(13)-C(14)	1.3900	C(51)-C(52)	1.3900
C(13)-C(18)	1.3900	C(51)-C(56)	1.3900
C(14)-C(15)	1.3900	C(52)-C(53)	1.3900
C(15)-C(16)	1.3900	C(53)-C(54)	1.3900

C(54)-C(55)	1.3900	C(91)-C(92)	1.3900
C(55)-C(56)	1.3900	C(92)-C(93)	1.3900
C(57)-C(58)	1.3900	C(94)-C(95)	1.3900
C(57)-C(62)	1.3900	C(94)-C(99)	1.3900
C(58)-C(59)	1.3900	C(95)-C(96)	1.3900
C(59)-C(60)	1.3900	C(96)-C(97)	1.3900
C(60)-C(61)	1.3900	C(97)-C(98)	1.3900
C(61)-C(62)	1.3900	C(98)-C(99)	1.3900
C(63)-C(64)	1.3900	C(101)-C(102)	1.13(2)
C(63)-C(68)	1.3900	C(102)-C(103)	1.43(3)
C(64)-C(65)	1.3900	C(103)-C(104)	1.32(3)
C(65)-C(66)	1.3900	N(1)-C(108)	1.3900
C(66)-C(67)	1.3900	N(1)-C(112)	1.3900
C(67)-C(68)	1.3900	C(108)-C(109)	1.3900
C(69)-C(70)	1.3900	C(109)-C(110)	1.3900
C(69)-C(74)	1.3900	C(110)-C(111)	1.3900
C(70)-C(71)	1.3900	C(110)-C(118)	1.58(2)
C(71)-C(72)	1.3900	C(111)-C(112)	1.3900
C(72)-C(73)	1.3900	C(112)-C(113)	1.350(14)
C(73)-C(74)	1.3900	N(2)-C(113)	1.3900
C(76)-C(77)	1.3900	N(2)-C(117)	1.3900
C(76)-C(81)	1.3900	C(113)-C(114)	1.3900
C(77)-C(78)	1.3900	C(114)-C(115)	1.3900
C(78)-C(79)	1.3900	C(115)-C(116)	1.3900
C(79)-C(80)	1.3900	C(115)-C(119)	1.57(2)
C(80)-C(81)	1.3900	C(116)-C(117)	1.3900
C(82)-C(83)	1.3900	C(120)-C(121)	1.28(3)
C(82)-C(87)	1.3900	C(121)-C(122)	1.37(3)
C(83)-C(84)	1.3900	C(122)-C(123)	1.32(3)
C(84)-C(85)	1.3900	N(3)-C(127)	1.3900
C(85)-C(86)	1.3900	N(3)-C(131)	1.3900
C(86)-C(87)	1.3900	C(127)-C(128)	1.3900
C(88)-C(89)	1.3900	C(128)-C(129)	1.3900
C(88)-C(93)	1.3900	C(129)-C(130)	1.3900
C(89)-C(90)	1.3900	C(129)-C(137)	1.55(2)
C(90)-C(91)	1.3900	C(130)-C(131)	1.3900

C(131)-C(132)	1.334(12)	C(169)-C(170)	1.356(15)
N(4)-C(132)	1.3900	N(8)-C(170)	1.3900
N(4)-C(136)	1.3900	N(8)-C(174)	1.3900
C(132)-C(133)	1.3900	C(170)-C(171)	1.3900
C(133)-C(134)	1.3900	C(171)-C(172)	1.3900
C(134)-C(135)	1.3900	C(172)-C(173)	1.3900
C(134)-C(138)	1.556(19)	C(172)-C(176)	1.57(2)
C(135)-C(136)	1.3900	C(173)-C(174)	1.3900
C(139)-C(140)	1.22(3)	P(9)-F(5)	1.468(17)
C(140)-C(141)	1.42(3)	P(9)-F(2)	1.479(17)
C(141)-C(142)	1.34(4)	P(9)-F(3)	1.484(17)
N(5)-C(146)	1.3900	P(9)-F(6)	1.494(17)
N(5)-C(150)	1.3900	P(9)-F(1)	1.496(17)
C(146)-C(147)	1.3900	P(9)-F(4)	1.496(17)
C(147)-C(148)	1.3900	P(10)-F(8)	1.57(2)
C(148)-C(149)	1.3900	P(10)-F(11)	1.59(2)
C(148)-C(156)	1.56(2)	P(10)-F(7)	1.59(2)
C(149)-C(150)	1.3900	P(10)-F(9)	1.59(2)
C(150)-C(151)	1.363(14)	P(10)-F(12)	1.59(2)
N(6)-C(151)	1.3900	P(10)-F(10)	1.63(2)
N(6)-C(155)	1.3900		
C(151)-C(152)	1.3900	P(3)-Ag(1)-C(120)	108.2(6)
C(152)-C(153)	1.3900	P(3)-Ag(1)-P(1)	120.5(2)
C(153)-C(154)	1.3900	C(120)-Ag(1)-P(1)	108.0(6)
C(153)-C(157)	1.55(2)	P(3)-Ag(1)-C(101)	112.2(6)
C(154)-C(155)	1.3900	C(120)-Ag(1)-C(101)	92.6(7)
C(158)-C(159)	1.17(3)	P(1)-Ag(1)-C(101)	111.5(6)
C(159)-C(160)	1.32(4)	P(3)-Ag(1)-Ag(2)	150.89(17)
C(160)-C(161)	1.20(4)	C(120)-Ag(1)-Ag(2)	45.7(6)
N(7)-C(165)	1.3900	P(1)-Ag(1)-Ag(2)	84.88(17)
N(7)-C(169)	1.3900	C(101)-Ag(1)-Ag(2)	64.8(5)
C(165)-C(166)	1.3900	P(3)-Ag(1)-Ag(3)	84.68(16)
C(166)-C(167)	1.3900	C(120)-Ag(1)-Ag(3)	64.2(5)
C(167)-C(168)	1.3900	P(1)-Ag(1)-Ag(3)	154.27(17)
C(167)-C(175)	1.57(2)	C(101)-Ag(1)-Ag(3)	47.9(5)
C(168)-C(169)	1.3900	Ag(2)-Ag(1)-Ag(3)	72.41(7)

C(120)-Ag(2)-C(158)	118.8(8)	C(139)-Ag(4)-Ag(2)	107.7(6)
C(120)-Ag(2)-P(2)	133.7(5)	P(7)-Ag(4)-Ag(2)	108.54(19)
C(158)-Ag(2)-P(2)	106.6(6)	C(120)-Ag(4)-Ag(2)	45.1(5)
C(120)-Ag(2)-Ag(1)	54.7(6)	Ag(6)-Ag(4)-Ag(2)	97.13(7)
C(158)-Ag(2)-Ag(1)	142.1(7)	C(139)-Ag(4)-Ag(3)	51.8(6)
P(2)-Ag(2)-Ag(1)	94.47(17)	P(7)-Ag(4)-Ag(3)	167.62(18)
C(120)-Ag(2)-Ag(5)	107.9(6)	C(120)-Ag(4)-Ag(3)	63.1(5)
C(158)-Ag(2)-Ag(5)	46.7(7)	Ag(6)-Ag(4)-Ag(3)	97.14(7)
P(2)-Ag(2)-Ag(5)	109.55(14)	Ag(2)-Ag(4)-Ag(3)	71.07(6)
Ag(1)-Ag(2)-Ag(5)	96.88(8)	C(158)-Ag(5)-C(101)	118.3(7)
C(120)-Ag(2)-Ag(4)	54.5(5)	C(158)-Ag(5)-P(5)	135.8(6)
C(158)-Ag(2)-Ag(4)	64.2(6)	C(101)-Ag(5)-P(5)	104.6(5)
P(2)-Ag(2)-Ag(4)	167.73(19)	C(158)-Ag(5)-Ag(6)	56.5(6)
Ag(1)-Ag(2)-Ag(4)	97.67(8)	C(101)-Ag(5)-Ag(6)	144.1(5)
Ag(5)-Ag(2)-Ag(4)	70.82(6)	P(5)-Ag(5)-Ag(6)	94.55(16)
C(101)-Ag(3)-C(139)	117.4(8)	C(158)-Ag(5)-Ag(2)	53.2(6)
C(101)-Ag(3)-P(4)	136.7(6)	C(101)-Ag(5)-Ag(2)	65.2(5)
C(139)-Ag(3)-P(4)	105.5(6)	P(5)-Ag(5)-Ag(2)	167.23(16)
C(101)-Ag(3)-Ag(1)	55.4(5)	Ag(6)-Ag(5)-Ag(2)	98.17(6)
C(139)-Ag(3)-Ag(1)	140.7(6)	C(158)-Ag(5)-Ag(3)	108.7(6)
P(4)-Ag(3)-Ag(1)	94.65(16)	C(101)-Ag(5)-Ag(3)	47.5(6)
C(101)-Ag(3)-Ag(5)	52.8(6)	P(5)-Ag(5)-Ag(3)	107.9(2)
C(139)-Ag(3)-Ag(5)	64.6(6)	Ag(6)-Ag(5)-Ag(3)	97.93(7)
P(4)-Ag(3)-Ag(5)	169.30(17)	Ag(2)-Ag(5)-Ag(3)	71.50(6)
Ag(1)-Ag(3)-Ag(5)	95.80(8)	P(8)-Ag(6)-P(6)	122.3(2)
C(101)-Ag(3)-Ag(4)	107.4(6)	P(8)-Ag(6)-C(158)	110.1(6)
C(139)-Ag(3)-Ag(4)	45.4(6)	P(6)-Ag(6)-C(158)	112.5(5)
P(4)-Ag(3)-Ag(4)	106.57(17)	P(8)-Ag(6)-C(139)	107.4(5)
Ag(1)-Ag(3)-Ag(4)	96.82(8)	P(6)-Ag(6)-C(139)	109.3(5)
Ag(5)-Ag(3)-Ag(4)	69.89(7)	C(158)-Ag(6)-C(139)	90.4(8)
C(139)-Ag(4)-P(7)	136.6(6)	P(8)-Ag(6)-Ag(5)	151.19(16)
C(139)-Ag(4)-C(120)	114.9(8)	P(6)-Ag(6)-Ag(5)	85.83(17)
P(7)-Ag(4)-C(120)	107.4(5)	C(158)-Ag(6)-Ag(5)	46.3(6)
C(139)-Ag(4)-Ag(6)	57.3(7)	C(139)-Ag(6)-Ag(5)	63.5(5)
P(7)-Ag(4)-Ag(6)	95.19(17)	P(8)-Ag(6)-Ag(4)	83.55(16)
C(120)-Ag(4)-Ag(6)	140.2(5)	P(6)-Ag(6)-Ag(4)	151.2(2)

C(158)-Ag(6)-Ag(4)	63.1(5)	C(143)-Re(3)-C(142)	176.9(9)
C(139)-Ag(6)-Ag(4)	45.1(5)	C(145)-Re(3)-C(142)	96.9(17)
Ag(5)-Ag(6)-Ag(4)	70.99(6)	C(144)-Re(3)-C(142)	96.2(17)
C(125)-Re(2)-C(124)	91.3(10)	C(143)-Re(3)-N(6)	93.9(6)
C(125)-Re(2)-C(126)	89.2(10)	C(145)-Re(3)-N(6)	167.1(14)
C(124)-Re(2)-C(126)	89.0(9)	C(144)-Re(3)-N(6)	108.6(13)
C(125)-Re(2)-C(123)	92.5(11)	C(142)-Re(3)-N(6)	83.1(9)
C(124)-Re(2)-C(123)	175.1(12)	C(143)-Re(3)-N(5)	94.6(7)
C(126)-Re(2)-C(123)	94.1(10)	C(145)-Re(3)-N(5)	93.8(14)
C(125)-Re(2)-N(3)	171.9(10)	C(144)-Re(3)-N(5)	178.0(13)
C(124)-Re(2)-N(3)	93.4(9)	C(142)-Re(3)-N(5)	83.8(10)
C(126)-Re(2)-N(3)	97.4(10)	N(6)-Re(3)-N(5)	73.4(5)
C(123)-Re(2)-N(3)	82.5(9)	C(162)-Re(4)-C(163)	89.9(15)
C(125)-Re(2)-N(4)	99.5(10)	C(162)-Re(4)-C(164)	89.2(16)
C(124)-Re(2)-N(4)	90.7(8)	C(163)-Re(4)-C(164)	89.3(15)
C(126)-Re(2)-N(4)	171.2(10)	C(162)-Re(4)-N(8)	90.4(12)
C(123)-Re(2)-N(4)	85.6(8)	C(163)-Re(4)-N(8)	95.5(18)
N(3)-Re(2)-N(4)	73.8(5)	C(164)-Re(4)-N(8)	175.1(17)
C(106)-Re(1)-C(105)	84.5(12)	C(162)-Re(4)-N(7)	95.9(10)
C(106)-Re(1)-C(107)	83.8(12)	C(163)-Re(4)-N(7)	170(2)
C(105)-Re(1)-C(107)	83.8(13)	C(164)-Re(4)-N(7)	98.9(17)
C(106)-Re(1)-C(104)	93.0(12)	N(8)-Re(4)-N(7)	76.3(7)
C(105)-Re(1)-C(104)	176.8(17)	C(162)-Re(4)-C(161)	179.8(4)
C(107)-Re(1)-C(104)	93.8(13)	C(163)-Re(4)-C(161)	90.1(16)
C(106)-Re(1)-N(1)	106.4(12)	C(164)-Re(4)-C(161)	91.0(16)
C(105)-Re(1)-N(1)	94.9(14)	N(8)-Re(4)-C(161)	89.4(11)
C(107)-Re(1)-N(1)	169.6(11)	N(7)-Re(4)-C(161)	84.0(10)
C(104)-Re(1)-N(1)	87.8(10)	C(25)-P(1)-C(1)	103.6(9)
C(106)-Re(1)-N(2)	177.1(10)	C(25)-P(1)-C(7)	107.7(10)
C(105)-Re(1)-N(2)	98.4(12)	C(1)-P(1)-C(7)	103.2(7)
C(107)-Re(1)-N(2)	95.8(11)	C(25)-P(1)-Ag(1)	112.3(7)
C(104)-Re(1)-N(2)	84.1(8)	C(1)-P(1)-Ag(1)	115.8(7)
N(1)-Re(1)-N(2)	74.2(6)	C(7)-P(1)-Ag(1)	113.4(6)
C(143)-Re(3)-C(145)	85.9(14)	C(19)-P(2)-C(13)	100.8(9)
C(143)-Re(3)-C(144)	85.5(14)	C(19)-P(2)-C(25)	104.9(9)
C(145)-Re(3)-C(144)	84.3(13)	C(13)-P(2)-C(25)	107.6(9)

C(19)-P(2)-Ag(2)	116.3(7)	C(94)-P(8)-Ag(6)	112.9(7)
C(13)-P(2)-Ag(2)	116.6(6)	C(88)-P(8)-Ag(6)	117.1(6)
C(25)-P(2)-Ag(2)	109.6(8)	C(100)-P(8)-Ag(6)	113.9(8)
C(50)-P(3)-C(26)	105.1(12)	C(2)-C(1)-C(6)	120.0
C(50)-P(3)-C(32)	102.4(10)	C(2)-C(1)-P(1)	119.7(9)
C(26)-P(3)-C(32)	105.2(10)	C(6)-C(1)-P(1)	120.2(9)
C(50)-P(3)-Ag(1)	113.3(10)	C(3)-C(2)-C(1)	120.0
C(26)-P(3)-Ag(1)	116.6(8)	C(2)-C(3)-C(4)	120.0
C(32)-P(3)-Ag(1)	112.8(9)	C(5)-C(4)-C(3)	120.0
C(44)-P(4)-C(50)	105.2(9)	C(6)-C(5)-C(4)	120.0
C(44)-P(4)-C(38)	100.5(10)	C(5)-C(6)-C(1)	120.0
C(50)-P(4)-C(38)	103.0(11)	C(8)-C(7)-C(12)	120.0
C(44)-P(4)-Ag(3)	117.6(8)	C(8)-C(7)-P(1)	116.8(9)
C(50)-P(4)-Ag(3)	110.9(9)	C(12)-C(7)-P(1)	123.0(10)
C(38)-P(4)-Ag(3)	117.9(7)	C(9)-C(8)-C(7)	120.0
C(57)-P(5)-C(51)	101.1(9)	C(8)-C(9)-C(10)	120.0
C(57)-P(5)-C(75)	104.1(11)	C(9)-C(10)-C(11)	120.0
C(51)-P(5)-C(75)	105.9(9)	C(12)-C(11)-C(10)	120.0
C(57)-P(5)-Ag(5)	113.6(6)	C(11)-C(12)-C(7)	120.0
C(51)-P(5)-Ag(5)	116.8(7)	C(14)-C(13)-C(18)	120.0
C(75)-P(5)-Ag(5)	113.7(7)	C(14)-C(13)-P(2)	116.8(12)
C(63)-P(6)-C(75)	107.5(11)	C(18)-C(13)-P(2)	123.2(12)
C(63)-P(6)-C(69)	109.7(11)	C(15)-C(14)-C(13)	120.0
C(75)-P(6)-C(69)	103.8(12)	C(16)-C(15)-C(14)	120.0
C(63)-P(6)-Ag(6)	111.1(9)	C(15)-C(16)-C(17)	120.0
C(75)-P(6)-Ag(6)	114.0(7)	C(18)-C(17)-C(16)	120.0
C(69)-P(6)-Ag(6)	110.5(9)	C(17)-C(18)-C(13)	120.0
C(100)-P(7)-C(76)	100.1(12)	C(20)-C(19)-C(24)	120.0
C(100)-P(7)-C(82)	102.6(10)	C(20)-C(19)-P(2)	118.4(12)
C(76)-P(7)-C(82)	103.5(8)	C(24)-C(19)-P(2)	121.5(12)
C(100)-P(7)-Ag(4)	113.7(8)	C(19)-C(20)-C(21)	120.0
C(76)-P(7)-Ag(4)	119.9(7)	C(22)-C(21)-C(20)	120.0
C(82)-P(7)-Ag(4)	114.7(8)	C(23)-C(22)-C(21)	120.0
C(94)-P(8)-C(88)	105.1(9)	C(22)-C(23)-C(24)	120.0
C(94)-P(8)-C(100)	105.6(10)	C(23)-C(24)-C(19)	120.0
C(88)-P(8)-C(100)	100.8(11)	P(1)-C(25)-P(2)	113.3(10)

C(27)-C(26)-C(31)	120.0	C(53)-C(52)-C(51)	120.0
C(27)-C(26)-P(3)	119.8(14)	C(54)-C(53)-C(52)	120.0
C(31)-C(26)-P(3)	120.0(15)	C(53)-C(54)-C(55)	120.0
C(28)-C(27)-C(26)	120.0	C(56)-C(55)-C(54)	120.0
C(27)-C(28)-C(29)	120.0	C(55)-C(56)-C(51)	120.0
C(28)-C(29)-C(30)	120.0	C(58)-C(57)-C(62)	120.0
C(31)-C(30)-C(29)	120.0	C(58)-C(57)-P(5)	123.1(15)
C(30)-C(31)-C(26)	120.0	C(62)-C(57)-P(5)	116.9(15)
C(33)-C(32)-C(37)	120.0	C(57)-C(58)-C(59)	120.0
C(33)-C(32)-P(3)	118.0(12)	C(58)-C(59)-C(60)	120.0
C(37)-C(32)-P(3)	121.8(12)	C(61)-C(60)-C(59)	120.0
C(32)-C(33)-C(34)	120.0	C(62)-C(61)-C(60)	120.0
C(35)-C(34)-C(33)	120.0	C(61)-C(62)-C(57)	120.0
C(36)-C(35)-C(34)	120.0	C(64)-C(63)-C(68)	120.0
C(35)-C(36)-C(37)	120.0	C(64)-C(63)-P(6)	120.3(17)
C(36)-C(37)-C(32)	120.0	C(68)-C(63)-P(6)	119.6(17)
C(39)-C(38)-C(43)	120.0	C(65)-C(64)-C(63)	120.0
C(39)-C(38)-P(4)	120.5(13)	C(64)-C(65)-C(66)	120.0
C(43)-C(38)-P(4)	119.5(13)	C(67)-C(66)-C(65)	120.0
C(40)-C(39)-C(38)	120.0	C(68)-C(67)-C(66)	120.0
C(39)-C(40)-C(41)	120.0	C(67)-C(68)-C(63)	120.0
C(42)-C(41)-C(40)	120.0	C(70)-C(69)-C(74)	120.0
C(43)-C(42)-C(41)	120.0	C(70)-C(69)-P(6)	126.0(18)
C(42)-C(43)-C(38)	120.0	C(74)-C(69)-P(6)	113.9(18)
C(45)-C(44)-C(49)	120.0	C(69)-C(70)-C(71)	120.0
C(45)-C(44)-P(4)	121.4(11)	C(72)-C(71)-C(70)	120.0
C(49)-C(44)-P(4)	118.6(11)	C(71)-C(72)-C(73)	120.0
C(46)-C(45)-C(44)	120.0	C(74)-C(73)-C(72)	120.0
C(47)-C(46)-C(45)	120.0	C(73)-C(74)-C(69)	120.0
C(46)-C(47)-C(48)	120.0	P(6)-C(75)-P(5)	109.9(12)
C(49)-C(48)-C(47)	120.0	C(77)-C(76)-C(81)	120.0
C(48)-C(49)-C(44)	120.0	C(77)-C(76)-P(7)	122.1(13)
P(3)-C(50)-P(4)	111.5(12)	C(81)-C(76)-P(7)	117.7(13)
C(52)-C(51)-C(56)	120.0	C(76)-C(77)-C(78)	120.0
C(52)-C(51)-P(5)	121.9(12)	C(79)-C(78)-C(77)	120.0
C(56)-C(51)-P(5)	117.8(12)	C(78)-C(79)-C(80)	120.0

C(79)-C(80)-C(81)	120.0	O(1)-C(105)-Re(1)	169(4)
C(80)-C(81)-C(76)	120.0	O(2)-C(106)-Re(1)	165(3)
C(83)-C(82)-C(87)	120.0	O(3)-C(107)-Re(1)	163(4)
C(83)-C(82)-P(7)	122.3(13)	C(108)-N(1)-C(112)	120.0
C(87)-C(82)-P(7)	117.7(13)	C(108)-N(1)-Re(1)	123.2(11)
C(84)-C(83)-C(82)	120.0	C(112)-N(1)-Re(1)	116.8(11)
C(83)-C(84)-C(85)	120.0	C(109)-C(108)-N(1)	120.0
C(86)-C(85)-C(84)	120.0	C(108)-C(109)-C(110)	120.0
C(87)-C(86)-C(85)	120.0	C(111)-C(110)-C(109)	120.0
C(86)-C(87)-C(82)	120.0	C(111)-C(110)-C(118)	125(2)
C(89)-C(88)-C(93)	120.0	C(109)-C(110)-C(118)	115(2)
C(89)-C(88)-P(8)	117.7(13)	C(112)-C(111)-C(110)	120.0
C(93)-C(88)-P(8)	122.2(13)	C(113)-C(112)-C(111)	119.7(19)
C(88)-C(89)-C(90)	120.0	C(113)-C(112)-N(1)	120.1(19)
C(91)-C(90)-C(89)	120.0	C(111)-C(112)-N(1)	120.0
C(92)-C(91)-C(90)	120.0	C(113)-N(2)-C(117)	120.0
C(91)-C(92)-C(93)	120.0	C(113)-N(2)-Re(1)	116.4(11)
C(92)-C(93)-C(88)	120.0	C(117)-N(2)-Re(1)	123.5(11)
C(95)-C(94)-C(99)	120.0	C(112)-C(113)-C(114)	127.8(18)
C(95)-C(94)-P(8)	124.2(12)	C(112)-C(113)-N(2)	112.2(18)
C(99)-C(94)-P(8)	115.6(12)	C(114)-C(113)-N(2)	120.0
C(96)-C(95)-C(94)	120.0	C(113)-C(114)-C(115)	120.0
C(95)-C(96)-C(97)	120.0	C(116)-C(115)-C(114)	120.0
C(98)-C(97)-C(96)	120.0	C(116)-C(115)-C(119)	125(2)
C(99)-C(98)-C(97)	120.0	C(114)-C(115)-C(119)	115(2)
C(98)-C(99)-C(94)	120.0	C(117)-C(116)-C(115)	120.0
P(7)-C(100)-P(8)	110.3(15)	C(116)-C(117)-N(2)	120.0
C(102)-C(101)-Ag(3)	160(2)	C(121)-C(120)-Ag(2)	160(2)
C(102)-C(101)-Ag(5)	116.1(18)	C(121)-C(120)-Ag(1)	110.6(16)
Ag(3)-C(101)-Ag(5)	79.6(7)	Ag(2)-C(120)-Ag(1)	79.6(6)
C(102)-C(101)-Ag(1)	100.4(15)	C(121)-C(120)-Ag(4)	103.0(14)
Ag(3)-C(101)-Ag(1)	76.8(6)	Ag(2)-C(120)-Ag(4)	80.4(7)
Ag(5)-C(101)-Ag(1)	127.5(9)	Ag(1)-C(120)-Ag(4)	130.8(9)
C(101)-C(102)-C(103)	174(2)	C(120)-C(121)-C(122)	172(2)
C(104)-C(103)-C(102)	178(3)	C(123)-C(122)-C(121)	176(3)
C(103)-C(104)-Re(1)	171(3)	C(122)-C(123)-Re(2)	180(3)

O(4)-C(124)-Re(2)	177(3)	O(7)-C(143)-Re(3)	179.4(9)
O(5)-C(125)-Re(2)	177(3)	O(8)-C(144)-Re(3)	149(4)
O(6)-C(126)-Re(2)	175(2)	O(9)-C(145)-Re(3)	144(3)
C(127)-N(3)-C(131)	120.0	C(146)-N(5)-C(150)	120.0
C(127)-N(3)-Re(2)	124.3(9)	C(146)-N(5)-Re(3)	121.7(10)
C(131)-N(3)-Re(2)	115.6(9)	C(150)-N(5)-Re(3)	117.6(10)
N(3)-C(127)-C(128)	120.0	C(147)-C(146)-N(5)	120.0
C(129)-C(128)-C(127)	120.0	C(148)-C(147)-C(146)	120.0
C(128)-C(129)-C(130)	120.0	C(147)-C(148)-C(149)	120.0
C(128)-C(129)-C(137)	116(2)	C(147)-C(148)-C(156)	125(2)
C(130)-C(129)-C(137)	124(2)	C(149)-C(148)-C(156)	115(2)
C(131)-C(130)-C(129)	120.0	C(150)-C(149)-C(148)	120.0
C(132)-C(131)-C(130)	122.2(15)	C(151)-C(150)-C(149)	126.2(15)
C(132)-C(131)-N(3)	117.3(15)	C(151)-C(150)-N(5)	113.7(15)
C(130)-C(131)-N(3)	120.0	C(149)-C(150)-N(5)	120.0
C(132)-N(4)-C(136)	120.0	C(151)-N(6)-C(155)	120.0
C(132)-N(4)-Re(2)	116.8(8)	C(151)-N(6)-Re(3)	117.1(10)
C(136)-N(4)-Re(2)	122.9(8)	C(155)-N(6)-Re(3)	122.7(10)
C(131)-C(132)-C(133)	124.2(14)	C(150)-C(151)-C(152)	122.5(15)
C(131)-C(132)-N(4)	115.4(14)	C(150)-C(151)-N(6)	117.3(15)
C(133)-C(132)-N(4)	120.0	C(152)-C(151)-N(6)	120.0
C(132)-C(133)-C(134)	120.0	C(151)-C(152)-C(153)	120.0
C(135)-C(134)-C(133)	120.0	C(154)-C(153)-C(152)	120.0
C(135)-C(134)-C(138)	117.6(18)	C(154)-C(153)-C(157)	119(2)
C(133)-C(134)-C(138)	122.3(18)	C(152)-C(153)-C(157)	121(2)
C(136)-C(135)-C(134)	120.0	C(153)-C(154)-C(155)	120.0
C(135)-C(136)-N(4)	120.0	C(154)-C(155)-N(6)	120.0
C(140)-C(139)-Ag(4)	163.2(19)	C(159)-C(158)-Ag(5)	157(2)
C(140)-C(139)-Ag(3)	110(2)	C(159)-C(158)-Ag(2)	115.9(19)
Ag(4)-C(139)-Ag(3)	82.8(7)	Ag(5)-C(158)-Ag(2)	80.1(9)
C(140)-C(139)-Ag(6)	100.0(18)	C(159)-C(158)-Ag(6)	101.1(18)
Ag(4)-C(139)-Ag(6)	77.6(8)	Ag(5)-C(158)-Ag(6)	77.2(8)
Ag(3)-C(139)-Ag(6)	130.1(10)	Ag(2)-C(158)-Ag(6)	129.9(12)
C(139)-C(140)-C(141)	178(3)	C(158)-C(159)-C(160)	177(3)
C(142)-C(141)-C(140)	175(3)	C(161)-C(160)-C(159)	175(3)
C(141)-C(142)-Re(3)	169(3)	C(160)-C(161)-Re(4)	178(3)

O(10)-C(162)-Re(4)	171(3)	F(6)-P(9)-F(1)	89.6(8)
O(11)-C(163)-Re(4)	164(5)	F(5)-P(9)-F(4)	90.0(8)
O(12)-C(164)-Re(4)	157(4)	F(2)-P(9)-F(4)	179.0(10)
C(165)-N(7)-C(169)	120.0	F(3)-P(9)-F(4)	90.7(8)
C(165)-N(7)-Re(4)	125.9(13)	F(6)-P(9)-F(4)	89.0(8)
C(169)-N(7)-Re(4)	114.0(13)	F(1)-P(9)-F(4)	89.4(8)
C(166)-C(165)-N(7)	120.0	F(8)-P(10)-F(11)	91.7(8)
C(165)-C(166)-C(167)	120.0	F(8)-P(10)-F(7)	91.0(8)
C(166)-C(167)-C(168)	120.0	F(11)-P(10)-F(7)	90.4(8)
C(166)-C(167)-C(175)	115(3)	F(8)-P(10)-F(9)	91.3(8)
C(168)-C(167)-C(175)	124(3)	F(11)-P(10)-F(9)	90.4(8)
C(169)-C(168)-C(167)	120.0	F(7)-P(10)-F(9)	177.6(10)
C(170)-C(169)-C(168)	125(2)	F(8)-P(10)-F(12)	91.3(8)
C(170)-C(169)-N(7)	114(2)	F(11)-P(10)-F(12)	176.9(10)
C(168)-C(169)-N(7)	120.0	F(7)-P(10)-F(12)	90.2(8)
C(170)-N(8)-C(174)	120.0	F(9)-P(10)-F(12)	89.0(8)
C(170)-N(8)-Re(4)	117.5(16)	F(8)-P(10)-F(10)	179.3(11)
C(174)-N(8)-Re(4)	122.5(16)	F(11)-P(10)-F(10)	88.9(8)
C(169)-C(170)-C(171)	122(2)	F(7)-P(10)-F(10)	88.5(8)
C(169)-C(170)-N(8)	115(2)	F(9)-P(10)-F(10)	89.2(8)
C(171)-C(170)-N(8)	120.0	F(12)-P(10)-F(10)	88.1(8)
C(172)-C(171)-C(170)	120.0		
C(171)-C(172)-C(173)	120.0		
C(171)-C(172)-C(176)	130(4)		
C(173)-C(172)-C(176)	110(4)		
C(172)-C(173)-C(174)	120.0		
C(173)-C(174)-N(8)	120.0		
F(5)-P(9)-F(2)	90.8(8)		
F(5)-P(9)-F(3)	90.7(8)		
F(2)-P(9)-F(3)	89.9(8)		
F(5)-P(9)-F(6)	179.0(11)		
F(2)-P(9)-F(6)	90.2(8)		
F(3)-P(9)-F(6)	89.2(8)		
F(5)-P(9)-F(1)	90.5(8)		
F(2)-P(9)-F(1)	89.9(8)		
F(3)-P(9)-F(1)	178.8(11)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for mar499. 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}
Ag(1)	88(1)	82(1)	73(2)	-5(1)	-11(1)	0(1)
Ag(2)	71(1)	82(1)	75(2)	-6(1)	-7(1)	-1(1)
Ag(3)	88(1)	81(1)	78(2)	5(1)	-9(1)	-4(1)
Ag(4)	86(1)	79(1)	84(2)	6(1)	5(1)	-5(1)
Ag(5)	62(1)	93(1)	83(2)	9(1)	3(1)	2(1)
Ag(6)	86(1)	85(1)	100(2)	17(1)	11(1)	0(1)
Re(2)	76(1)	140(1)	100(1)	-19(1)	-20(1)	-17(1)
Re(1)	129(1)	171(1)	143(2)	-50(1)	31(1)	-77(1)
Re(3)	130(1)	215(2)	133(2)	-73(1)	67(1)	-50(1)
Re(4)	282(2)	208(2)	68(1)	-4(1)	12(1)	-116(2)
P(1)	79(4)	78(4)	76(6)	-6(4)	-6(3)	-2(3)
P(2)	74(3)	84(4)	77(6)	-6(4)	-14(3)	-2(3)
P(3)	102(4)	84(4)	75(6)	1(4)	-9(4)	3(3)
P(4)	95(4)	98(5)	65(5)	-5(4)	-4(4)	4(3)
P(5)	65(3)	92(5)	111(7)	7(4)	1(4)	9(3)
P(6)	93(4)	103(5)	109(8)	21(5)	6(4)	21(4)
P(7)	89(4)	91(4)	80(6)	12(4)	5(4)	-9(3)
P(8)	105(4)	76(4)	90(6)	12(4)	9(4)	2(3)
P(9)	248(14)	370(20)	190(20)	-121(17)	42(13)	-85(15)
P(10)	240(13)	292(17)	185(18)	43(13)	101(13)	72(13)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mar499.

	x	y	z	U(eq)
H(2)	1626	5375	1886	177
H(3)	1615	6075	1610	183
H(4)	609	6425	1485	172
H(5)	-385	6074	1635	131
H(6)	-374	5374	1911	118
H(8)	-504	4220	1972	122
H(9)	-1521	4084	2258	117
H(10)	-1811	4468	2796	152
H(11)	-1084	4989	3049	144
H(12)	-67	5125	2763	108
H(14)	1991	3613	3198	162
H(15)	2996	3590	3517	180
H(16)	3718	4194	3491	179
H(17)	3434	4821	3145	217
H(18)	2429	4844	2827	188
H(20)	193	3739	3001	147
H(21)	-538	3796	3500	215
H(22)	-419	4370	3930	213
H(23)	431	4888	3859	192
H(24)	1162	4831	3360	130
H(25A)	1108	5003	2637	88
H(25B)	1655	4838	2357	88
H(27)	1927	4471	1074	155
H(28)	2773	4646	659	229
H(29)	2550	4688	24	188
H(30)	1481	4554	-194	205
H(31)	635	4379	221	171
H(33)	421	5147	842	172
H(34)	-434	5666	802	165
H(35)	-1531	5441	880	174

H(36)	-1772	4697	998	226
H(37)	-918	4178	1038	206
H(39)	502	3227	50	167
H(40)	1073	3266	-513	219
H(41)	2221	3348	-516	164
H(42)	2800	3391	44	175
H(43)	2230	3351	606	157
H(45)	-509	3006	636	158
H(46)	-1077	2346	521	200
H(47)	-533	1667	580	167
H(48)	579	1648	754	175
H(49)	1147	2308	869	146
H(50A)	124	3755	549	113
H(50B)	-167	3615	938	113
H(52)	4976	3069	1834	151
H(53)	5806	3363	2211	161
H(54)	5526	3788	2729	217
H(55)	4416	3919	2870	221
H(56)	3585	3625	2493	153
H(58)	3864	2677	1137	317
H(59)	4048	2979	550	502
H(60)	3980	3745	462	267
H(61)	3729	4209	961	183
H(62)	3546	3906	1548	152
H(64)	4663	2287	2477	197
H(65)	5149	2543	3024	353
H(66)	4488	2720	3534	238
H(67)	3340	2642	3497	219
H(68)	2854	2385	2950	230
H(70)	4463	1582	1927	212
H(71)	4623	820	1860	306
H(72)	3778	327	2019	317
H(73)	2773	597	2245	377
H(74)	2613	1359	2311	355
H(75A)	3603	2330	1602	100
H(75B)	4221	2413	1861	100

H(77)	-307	2122	3153	211
H(78)	-1019	2485	3563	196
H(79)	-1540	3142	3384	156
H(80)	-1349	3437	2795	149
H(81)	-637	3074	2385	133
H(83)	-858	1560	2557	171
H(84)	-1603	1129	2217	157
H(85)	-1695	1227	1577	187
H(86)	-1042	1755	1277	171
H(87)	-296	2185	1616	130
H(89)	1843	1729	3167	151
H(90)	2211	1243	3627	196
H(91)	2214	480	3519	190
H(92)	1847	202	2950	140
H(93)	1479	688	2490	125
H(95)	223	1037	2271	145
H(96)	-112	666	1734	160
H(97)	509	729	1191	180
H(98)	1465	1163	1184	201
H(99)	1800	1534	1720	164
H(10A)	239	1621	2724	120
H(10B)	648	2009	2909	120
H(108)	2732	5974	1489	179
H(109)	2587	6092	854	211
H(111)	4116	5268	636	189
H(114)	4750	4771	830	142
H(116)	5515	4225	1760	147
H(117)	4851	4689	2122	170
H(11A)	2848	6031	247	372
H(11B)	3121	5565	117	372
H(11C)	3609	5969	165	372
H(11D)	5448	4198	732	296
H(11E)	5364	3819	1030	296
H(11F)	6010	4112	1027	296
H(127)	-2175	2247	1815	147
H(128)	-2357	1994	2418	170

H(130)	-2983	3216	2718	134
H(133)	-3062	3869	2575	120
H(135)	-3006	4758	1735	147
H(136)	-2632	4204	1333	123
H(13A)	-3007	2595	3181	337
H(13B)	-2443	2242	3116	337
H(13C)	-3173	2140	2986	337
H(13D)	-3334	5027	2310	237
H(13E)	-2971	4799	2647	237
H(13F)	-3718	4686	2563	237
H(146)	2744	2256	-6	181
H(147)	1705	2367	-273	185
H(149)	1085	1192	142	168
H(152)	1412	597	423	150
H(154)	2708	119	1179	208
H(155)	3391	732	1082	188
H(15A)	348	1543	-220	298
H(15B)	675	1787	-560	298
H(15C)	371	2066	-232	298
H(15D)	1147	-90	727	344
H(15E)	1407	-119	1139	344
H(15F)	1774	-381	821	344
H(165)	789	3601	4160	221
H(166)	1357	4272	4214	230
H(168)	3083	3605	4316	187
H(171)	3489	2971	4449	318
H(173)	3285	1666	4215	252
H(174)	2155	1771	4115	375
H(17A)	3065	4445	4383	433
H(17B)	2404	4596	4578	433
H(17C)	2501	4674	4149	433
H(17D)	4506	2389	4483	671
H(17E)	4406	2020	4179	671
H(17F)	4238	1917	4597	671

Crystal data: [C_{176} H_{112} Ag_6 Br_8 F_{12} N_8 O_{12} P_{10} Re_4] (**4**); formula weight = 5099.74, Tetragonal, P $4_2/n$, a = 27.379(4) Å, c = 16.984(3) Å, V = 12731(4) $Å^3$, Z = 2, D_c = 1.330 g cm^{-3}, μ(Mo-Kα) = 3.712 mm^{-1}, F(000) = 4880, T = 253 K.

Data collection: A crystal of dimensions 0.4 x 0.2 x 0.1 mm mounted in a glass capilliary was used for data collection at -20^{o}C on a MAR diffractometer with a 300 mm image plate detector using graphite monochromatized Mo-K_α radiation (λ = 0.71073 Å). Data collection was made with 1^o oscillation step of φ, 10 minutes exposure time and scanner distance at 120 mm. 180 images were collected.

Data reduction: The images were interpreted and intensities integrated using program DENZO [i].

Structure solution: The structure was solved by direct methods employing SHELXS-97 program[ii] on PC. Re, Ag, Br and many non-H atoms were located according to the direct methods. The positions of the other non-hydrogen atoms were found after successful refinement by full-matrix least-squares using program SHELXL-97 [iii] on PC. Due to high thermal displacements, two Br atoms were restrained to have similar Br-C bond lengths and 1,3-Br…C distances, respectively; meanwhile, four C atoms of C(11), C(14) C(18) and C(19) were refined isotropically.

Structure refinement: According to the SHELXL-97 program [3], all 9110 independent reflections (R_{int} [iv] equal to 0.0518, 5662 reflections larger than $4\sigma(F_o)$) from a total 53215 reflections were participated in the full-matrix least-square refinement against F^2. These reflections were in the range -31<=h<= 31, -30<=k<= 31, -19<=l<= 19 with $2\theta_{max}$ equal to 50.94^o.

One crystallographic asymmetric unit consists of one fourth of formula unit, including half of PF_6^- anion. In the final stage of least-squares refinement, four C atoms were refined isotropically, the other non-H atoms were refined anisotropically. H atoms were generated by program SHELXL-97. The positions of H atoms were calculated based on riding mode with thermal parameters equal to 1.2 times that of the associated C atoms, and participated in the calculation of final R-indices[v].

Convergence (($\Delta/\sigma)_{max}$ = 0.001, av. 0.001) for 502 variable parameters by full-matrix least-squares refinement on F^2 reaches to R_1 = 0.0665 and wR_2 = 0.2207 with a goodness-of-fit of 1.019, the parameters a and b for weighting scheme are 0.1643 and 0.0. The final difference Fourier map shows maximum rest peaks and holes of 1.300 and -1.625 e$Å^{-3}$ respectively.

Drawing: The ORTEP [vi] drawing of the molecule was made with thermal ellipsoids at the 30 % probability level. Screen drawing is provided for reference. The drawing with high quality can be provided upon request.

Tables: Table (1) of Crystallographic and refinement data, table (3) of full bond lengths and bond angles and this report [vii] are provided. The other supplementary materials, such as table of atomic coordinates with thermal parameters, table of anisotropic displacement parameters, table of hydrogen coordinates and/or other tables and/or CIF, RES-files, can be provided under request by notifying the identification code.

Table 1. Crystal data and structure refinement for mar867.

Identification code	mar867	
Empirical formula	C_{176} H_{112} Ag_6 Br_8 F_{12} N_8 O_{12} P_{10} Re_4	
Formula weight	5099.74	
Temperature	253(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	P 4_2/n	
Unit cell dimensions	a = 27.379(4) Å	α= 90°.
	b = 27.379(4) Å	β= 90°.
	c = 16.984(3) Å	γ = 90°.
Volume	12731(4) $Å^3$	
Z	2	
Density (calculated)	1.330 Mg/m^3	
Absorption coefficient	3.712 mm^{-1}	
F(000)	4880	
Crystal size	0.4 x 0.2 x 0.1 mm^3	
Theta range for data collection	1.41 to 25.47°.	
Index ranges	-31<=h<=31, -30<=k<=31, -19<=l<=19	
Reflections collected	53215	
Independent reflections	9110 [R(int) = 0.0518]	
Completeness to theta = 25.47°	77.1 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9110 / 2 / 502	
Goodness-of-fit on F^2	1.019	
Final R indices [I>2sigma(I)]	R1 = 0.0665, wR2 = 0.2207	
R indices (all data)	R1 = 0.1023, wR2 = 0.2395	
Largest diff. peak and hole	1.300 and -1.625 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mar867. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	8077(1)	9971(1)	413(1)	107(1)
Ag(1)	8066(1)	7213(1)	1984(1)	59(1)
Ag(2)	7500	7500	514(1)	60(1)
Br(1)	10599(1)	9301(1)	885(2)	194(1)
Br(2)	10353(1)	8963(1)	-929(2)	218(1)
P(1)	8495(1)	6516(1)	1439(1)	57(1)
P(2)	8093(1)	6925(1)	-122(1)	57(1)
O(1)	8270(5)	11015(5)	-214(9)	186(6)
O(2)	7539(5)	10473(5)	1802(8)	163(5)
O(3)	7131(6)	9912(6)	-499(9)	187(6)
N(1)	8781(4)	9900(4)	1021(9)	107(4)
N(2)	8579(7)	9623(4)	-431(7)	127(5)
C(1)	7944(3)	7962(4)	1602(4)	57(2)
C(2)	7930(4)	8366(4)	1348(5)	59(2)
C(3)	7946(4)	8837(5)	1041(6)	78(3)
C(4)	7965(5)	9265(5)	820(7)	93(4)
C(5)	8213(7)	10625(7)	54(12)	142(6)
C(6)	7726(6)	10272(6)	1224(13)	138(6)
C(7)	7493(7)	9941(6)	-148(10)	128(5)
C(8)	8869(6)	10033(6)	1809(10)	125(5)
C(9)	9311(8)	9936(8)	2105(10)	149(7)
C(10)	9677(7)	9758(6)	1711(12)	143(7)
C(11)	9620(4)	9614(4)	937(4)	113(4)
C(12)	9156(4)	9690(3)	630(6)	106(4)
C(13)	9051(3)	9549(4)	-138(7)	107(4)
C(14)	9410(4)	9332(4)	-598(5)	131(5)
C(19)	9874(3)	9256(4)	-291(4)	121(5)
C(18)	9979(3)	9397(4)	477(5)	138(6)
C(15)	9290(9)	9217(7)	-1347(15)	163(9)
C(16)	8862(12)	9251(8)	-1648(12)	173(10)
C(17)	8476(8)	9486(7)	-1135(16)	161(8)

C(20)	8275(4)	6373(3)	443(4)	55(2)
C(21)	8466(4)	5919(4)	1934(5)	67(3)
C(22)	8484(5)	5484(4)	1516(7)	100(4)
C(23)	8479(6)	5044(5)	1951(9)	117(5)
C(24)	8452(5)	5035(5)	2728(9)	98(4)
C(25)	8424(5)	5451(5)	3099(6)	93(4)
C(26)	8432(4)	5902(4)	2728(5)	76(3)
C(27)	9151(4)	6609(4)	1324(5)	64(3)
C(28)	9457(5)	6263(4)	989(6)	84(3)
C(29)	9958(5)	6351(6)	920(8)	107(4)
C(30)	10150(5)	6775(6)	1202(9)	107(4)
C(31)	9852(6)	7118(5)	1544(11)	122(5)
C(32)	9357(4)	7045(4)	1602(7)	85(3)
C(33)	7892(4)	6643(4)	-1056(5)	68(3)
C(34)	8160(4)	6258(4)	-1398(5)	78(3)
C(35)	7990(6)	6052(5)	-2098(6)	105(4)
C(36)	7562(6)	6235(6)	-2432(7)	111(5)
C(37)	7307(5)	6611(5)	-2085(7)	99(4)
C(38)	7480(4)	6815(4)	-1412(5)	77(3)
C(39)	8662(4)	7225(4)	-321(5)	58(2)
C(40)	9081(5)	7011(5)	-557(6)	81(3)
C(41)	9506(5)	7238(6)	-697(8)	101(4)
C(42)	9537(6)	7722(8)	-608(8)	116(5)
C(43)	9128(7)	7965(6)	-356(8)	115(5)
C(44)	8686(5)	7717(5)	-205(6)	85(3)
P(3)	9592(4)	9540(5)	-3830(6)	162(5)
F(1)	9705(12)	9122(12)	-3183(18)	241(12)
F(2)	9560(12)	9925(12)	-3065(18)	242(13)
F(3)	9130(10)	9398(9)	-3633(14)	190(9)
F(4)	9538(9)	9101(9)	-4429(12)	167(7)
F(5)	10060(20)	9620(20)	-3970(30)	390(30)
F(6)	9447(14)	9954(14)	-4430(20)	270(15)

Table 3. Bond lengths [Å] and angles [°] for mar867.

Re(1)-C(7)	1.86(2)	C(2)-C(3)	1.390(16)
Re(1)-C(6)	1.87(2)	C(3)-C(4)	1.232(16)
Re(1)-C(5)	1.930(18)	C(8)-C(9)	1.34(2)
Re(1)-C(4)	2.074(14)	C(9)-C(10)	1.30(2)
Re(1)-N(1)	2.196(12)	C(10)-C(11)	1.38(2)
Re(1)-N(2)	2.203(15)	C(11)-C(12)	1.3900
Ag(1)-C(1)	2.178(11)	C(11)-C(18)	1.3900
Ag(1)-P(1)	2.423(3)	C(12)-C(13)	1.3900
Ag(1)-C(1)#1	2.456(7)	C(13)-C(14)	1.3900
Ag(1)-Ag(1)#1	3.0206(11)	C(14)-C(15)	1.35(3)
Ag(1)-Ag(1)#2	3.0206(11)	C(14)-C(19)	1.3900
Ag(1)-Ag(2)	3.0415(10)	C(19)-C(18)	1.3900
Ag(2)-P(2)#3	2.506(2)	C(15)-C(16)	1.28(3)
Ag(2)-P(2)	2.506(2)	C(16)-C(17)	1.51(3)
Ag(2)-C(1)	2.549(8)	C(21)-C(26)	1.352(13)
Ag(2)-C(1)#3	2.549(8)	C(21)-C(22)	1.387(15)
Ag(2)-Ag(1)#3	3.0415(10)	C(22)-C(23)	1.414(16)
Br(1)-C(18)	1.852(8)	C(23)-C(24)	1.323(17)
Br(2)-C(19)	1.880(8)	C(24)-C(25)	1.304(17)
P(1)-C(27)	1.825(11)	C(25)-C(26)	1.386(16)
P(1)-C(20)	1.837(7)	C(27)-C(28)	1.387(14)
P(1)-C(21)	1.840(10)	C(27)-C(32)	1.402(14)
P(2)-C(39)	1.794(11)	C(28)-C(29)	1.396(17)
P(2)-C(33)	1.848(9)	C(29)-C(30)	1.360(18)
P(2)-C(20)	1.858(9)	C(30)-C(31)	1.37(2)
O(1)-C(5)	1.171(17)	C(31)-C(32)	1.372(17)
O(2)-C(6)	1.24(2)	C(33)-C(38)	1.365(14)
O(3)-C(7)	1.160(19)	C(33)-C(34)	1.412(14)
N(1)-C(12)	1.350(13)	C(34)-C(35)	1.396(14)
N(1)-C(8)	1.407(18)	C(35)-C(36)	1.395(19)
N(2)-C(17)	1.28(2)	C(36)-C(37)	1.377(18)
N(2)-C(13)	1.398(18)	C(37)-C(38)	1.358(15)
C(1)-C(2)	1.188(13)	C(39)-C(40)	1.350(15)
C(1)-Ag(1)#2	2.456(7)	C(39)-C(44)	1.363(15)

C(40)-C(41)	1.341(17)	C(1)-Ag(1)-Ag(2)	55.5(2)
C(41)-C(42)	1.34(2)	P(1)-Ag(1)-Ag(2)	97.91(6)
C(42)-C(43)	1.37(2)	C(1)#1-Ag(1)-Ag(2)	142.0(3)
C(43)-C(44)	1.410(19)	Ag(1)#1-Ag(1)-Ag(2)	98.47(3)
P(3)-F(5)	1.31(6)	Ag(1)#2-Ag(1)-Ag(2)	98.47(3)
P(3)-F(3)	1.37(3)	P(2)#3-Ag(2)-P(2)	128.92(10)
P(3)-F(6)	1.58(4)	P(2)#3-Ag(2)-C(1)	108.1(2)
P(3)-F(4)	1.58(2)	P(2)-Ag(2)-C(1)	108.4(2)
P(3)-F(1)	1.62(3)	P(2)#3-Ag(2)-C(1)#3	108.4(2)
P(3)-F(2)	1.68(3)	P(2)-Ag(2)-C(1)#3	108.1(2)
		C(1)-Ag(2)-C(1)#3	87.1(4)
C(7)-Re(1)-C(6)	87.5(8)	P(2)#3-Ag(2)-Ag(1)#3	82.01(5)
C(7)-Re(1)-C(5)	92.6(7)	P(2)-Ag(2)-Ag(1)#3	147.83(6)
C(6)-Re(1)-C(5)	85.6(7)	C(1)-Ag(2)-Ag(1)#3	61.3(2)
C(7)-Re(1)-C(4)	90.2(6)	C(1)#3-Ag(2)-Ag(1)#3	44.8(2)
C(6)-Re(1)-C(4)	95.2(6)	P(2)#3-Ag(2)-Ag(1)	147.83(6)
C(5)-Re(1)-C(4)	177.1(7)	P(2)-Ag(2)-Ag(1)	82.01(5)
C(7)-Re(1)-N(1)	172.0(6)	C(1)-Ag(2)-Ag(1)	44.8(2)
C(6)-Re(1)-N(1)	98.2(7)	C(1)#3-Ag(2)-Ag(1)	61.3(2)
C(5)-Re(1)-N(1)	93.5(6)	Ag(1)#3-Ag(2)-Ag(1)	69.74(3)
C(4)-Re(1)-N(1)	83.7(4)	C(27)-P(1)-C(20)	104.7(4)
C(7)-Re(1)-N(2)	100.6(7)	C(27)-P(1)-C(21)	102.4(5)
C(6)-Re(1)-N(2)	171.9(8)	C(20)-P(1)-C(21)	102.6(4)
C(5)-Re(1)-N(2)	94.2(6)	C(27)-P(1)-Ag(1)	114.1(3)
C(4)-Re(1)-N(2)	84.7(4)	C(20)-P(1)-Ag(1)	111.1(3)
N(1)-Re(1)-N(2)	73.7(6)	C(21)-P(1)-Ag(1)	120.3(3)
C(1)-Ag(1)-P(1)	134.6(2)	C(39)-P(2)-C(33)	106.7(4)
C(1)-Ag(1)-C(1)#1	116.0(3)	C(39)-P(2)-C(20)	103.7(4)
P(1)-Ag(1)-C(1)#1	106.9(2)	C(33)-P(2)-C(20)	100.6(4)
C(1)-Ag(1)-Ag(1)#1	107.0(2)	C(39)-P(2)-Ag(2)	110.9(3)
P(1)-Ag(1)-Ag(1)#1	113.41(7)	C(33)-P(2)-Ag(2)	116.1(4)
C(1)#1-Ag(1)-Ag(1)#1	45.4(3)	C(20)-P(2)-Ag(2)	117.5(3)
C(1)-Ag(1)-Ag(1)#2	53.46(19)	C(12)-N(1)-C(8)	116.6(12)
P(1)-Ag(1)-Ag(1)#2	162.42(7)	C(12)-N(1)-Re(1)	118.2(10)
C(1)#1-Ag(1)-Ag(1)#2	62.5(2)	C(8)-N(1)-Re(1)	125.1(11)
Ag(1)#1-Ag(1)-Ag(1)#2	70.29(2)	C(17)-N(2)-C(13)	119.5(17)

C(17)-N(2)-Re(1)	126.4(18)	C(15)-C(16)-C(17)	116(2)
C(13)-N(2)-Re(1)	114.1(9)	N(2)-C(17)-C(16)	120(2)
C(2)-C(1)-Ag(1)	172.1(8)	P(1)-C(20)-P(2)	113.0(5)
C(2)-C(1)-Ag(1)#2	104.0(7)	C(26)-C(21)-C(22)	119.0(10)
Ag(1)-C(1)-Ag(1)#2	81.1(3)	C(26)-C(21)-P(1)	119.3(8)
C(2)-C(1)-Ag(2)	100.5(6)	C(22)-C(21)-P(1)	121.7(7)
Ag(1)-C(1)-Ag(2)	79.7(3)	C(21)-C(22)-C(23)	117.6(11)
Ag(1)#2-C(1)-Ag(2)	133.1(4)	C(24)-C(23)-C(22)	122.5(14)
C(1)-C(2)-C(3)	176.1(11)	C(25)-C(24)-C(23)	117.9(13)
C(4)-C(3)-C(2)	175.6(12)	C(24)-C(25)-C(26)	124.0(10)
C(3)-C(4)-Re(1)	173.7(11)	C(21)-C(26)-C(25)	118.9(11)
O(1)-C(5)-Re(1)	174.5(19)	C(28)-C(27)-C(32)	118.4(10)
O(2)-C(6)-Re(1)	173.5(17)	C(28)-C(27)-P(1)	122.9(9)
O(3)-C(7)-Re(1)	178.6(18)	C(32)-C(27)-P(1)	118.6(8)
C(9)-C(8)-N(1)	117.5(17)	C(27)-C(28)-C(29)	120.6(12)
C(10)-C(9)-C(8)	125.3(19)	C(30)-C(29)-C(28)	119.9(13)
C(9)-C(10)-C(11)	120.6(17)	C(29)-C(30)-C(31)	120.1(13)
C(10)-C(11)-C(12)	114.7(11)	C(32)-C(31)-C(30)	121.2(13)
C(10)-C(11)-C(18)	125.3(11)	C(31)-C(32)-C(27)	119.8(11)
C(12)-C(11)-C(18)	120.0	C(38)-C(33)-C(34)	120.4(9)
N(1)-C(12)-C(13)	115.0(10)	C(38)-C(33)-P(2)	118.8(8)
N(1)-C(12)-C(11)	125.0(10)	C(34)-C(33)-P(2)	120.8(8)
C(13)-C(12)-C(11)	120.0	C(35)-C(34)-C(33)	118.6(11)
C(12)-C(13)-C(14)	120.0	C(36)-C(35)-C(34)	118.8(12)
C(12)-C(13)-N(2)	119.0(9)	C(37)-C(36)-C(35)	121.5(11)
C(14)-C(13)-N(2)	121.0(9)	C(38)-C(37)-C(36)	119.4(12)
C(15)-C(14)-C(19)	122.8(13)	C(37)-C(38)-C(33)	121.3(11)
C(15)-C(14)-C(13)	117.2(13)	C(40)-C(39)-C(44)	115.6(11)
C(19)-C(14)-C(13)	120.0	C(40)-C(39)-P(2)	126.5(9)
C(14)-C(19)-C(18)	120.0	C(44)-C(39)-P(2)	117.8(8)
C(14)-C(19)-Br(2)	119.0(5)	C(41)-C(40)-C(39)	126.0(13)
C(18)-C(19)-Br(2)	121.0(5)	C(42)-C(41)-C(40)	119.7(14)
C(19)-C(18)-C(11)	120.0	C(41)-C(42)-C(43)	117.7(14)
C(19)-C(18)-Br(1)	120.1(5)	C(42)-C(43)-C(44)	121.5(15)
C(11)-C(18)-Br(1)	119.9(5)	C(39)-C(44)-C(43)	119.4(13)
C(16)-C(15)-C(14)	126(2)	F(5)-P(3)-F(3)	172(3)

F(5)-P(3)-F(6)	90(3)
F(3)-P(3)-F(6)	97.3(19)
F(5)-P(3)-F(4)	96(3)
F(3)-P(3)-F(4)	81.7(14)
F(6)-P(3)-F(4)	96.2(15)
F(5)-P(3)-F(1)	94(3)
F(3)-P(3)-F(1)	79.0(16)
F(6)-P(3)-F(1)	176(2)
F(4)-P(3)-F(1)	85.3(15)
F(5)-P(3)-F(2)	95(3)
F(3)-P(3)-F(2)	86.6(17)
F(6)-P(3)-F(2)	91.9(19)
F(4)-P(3)-F(2)	166.5(16)
F(1)-P(3)-F(2)	85.9(15)

Symmetry transformations used to generate equivalent atoms:

#1 y,-x+3/2,-z+1/2 #2 -y+3/2,x,-z+1/2 #3 -x+3/2,-y+3/2,z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for mar867. 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}
Re(1)	101(1)	73(1)	148(1)	38(1)	12(1)	-4(1)
Ag(1)	69(1)	60(1)	48(1)	1(1)	2(1)	8(1)
Ag(2)	70(1)	65(1)	47(1)	0	0	16(1)
Br(1)	99(1)	141(2)	343(3)	109(2)	39(2)	-3(1)
Br(2)	207(2)	113(2)	333(3)	44(2)	161(2)	23(2)
P(1)	67(2)	58(2)	47(1)	2(1)	-4(1)	10(1)
P(2)	68(2)	59(2)	43(1)	-2(1)	-2(1)	12(1)
O(1)	160(12)	104(9)	293(16)	94(10)	33(11)	0(8)
O(2)	150(11)	152(11)	188(11)	11(9)	48(9)	18(9)
O(3)	148(12)	167(13)	245(16)	62(11)	-57(11)	6(10)
N(1)	78(8)	71(7)	173(12)	34(7)	12(8)	-14(6)
N(2)	208(16)	76(8)	97(8)	26(6)	8(9)	-40(9)
C(1)	66(6)	73(7)	33(4)	-7(4)	5(4)	-4(5)
C(2)	66(7)	58(7)	54(5)	5(5)	-4(4)	-7(5)
C(3)	66(7)	82(9)	86(7)	1(6)	4(5)	-10(6)
C(4)	92(9)	86(9)	100(8)	9(7)	5(7)	-19(7)
C(5)	123(14)	115(14)	189(15)	51(13)	23(12)	15(11)
C(6)	94(11)	85(11)	230(20)	46(12)	43(12)	-2(9)
C(7)	118(14)	109(12)	157(13)	47(10)	6(11)	3(11)
C(8)	98(12)	160(16)	116(11)	22(10)	-6(9)	-20(11)
C(9)	136(17)	190(20)	124(12)	12(12)	2(13)	-46(15)
C(10)	94(12)	124(14)	211(18)	63(13)	18(12)	-17(10)
C(12)	111(12)	72(9)	134(11)	36(8)	16(10)	-18(8)
C(13)	108(12)	63(8)	150(13)	35(8)	21(11)	6(8)
C(15)	149(18)	101(13)	240(30)	58(15)	12(17)	-21(14)
C(16)	270(30)	116(16)	130(14)	7(12)	70(20)	-20(20)
C(17)	190(20)	92(13)	200(20)	64(14)	-32(18)	-27(13)
C(20)	64(6)	62(6)	40(4)	-3(4)	-3(4)	4(5)
C(21)	71(7)	60(7)	71(6)	3(5)	-12(5)	12(5)
C(22)	156(13)	61(8)	84(7)	10(6)	-21(7)	17(8)
C(23)	150(14)	67(9)	133(12)	15(8)	-19(10)	-17(9)

C(24)	101(10)	75(9)	119(10)	26(8)	-9(8)	6(7)
C(25)	110(10)	108(11)	61(6)	20(7)	11(6)	16(8)
C(26)	104(9)	71(7)	52(5)	20(5)	0(5)	12(6)
C(27)	70(7)	63(7)	60(5)	8(5)	-1(5)	16(6)
C(28)	78(9)	82(8)	92(7)	-13(6)	4(6)	13(7)
C(29)	87(11)	114(12)	121(10)	-11(9)	8(8)	34(9)
C(30)	73(9)	115(12)	132(11)	23(9)	-5(8)	-15(9)
C(31)	89(11)	81(10)	197(15)	-12(10)	9(10)	-11(8)
C(32)	63(8)	65(8)	126(9)	-17(7)	1(6)	6(6)
C(33)	83(8)	72(7)	51(5)	-6(5)	0(5)	1(6)
C(34)	109(9)	78(7)	47(5)	-17(5)	-3(5)	6(7)
C(35)	159(14)	100(10)	56(6)	-12(6)	-5(7)	10(9)
C(36)	137(13)	128(12)	69(7)	-12(8)	-18(8)	-16(10)
C(37)	101(10)	115(11)	80(8)	-12(7)	-24(7)	14(8)
C(38)	92(9)	83(8)	57(6)	-10(5)	-10(6)	20(7)
C(39)	75(7)	48(6)	51(5)	4(4)	9(4)	13(5)
C(40)	93(10)	83(8)	68(6)	13(5)	-3(6)	6(8)
C(41)	66(9)	108(12)	127(10)	31(9)	22(7)	13(8)
C(42)	76(10)	163(18)	109(10)	31(10)	8(8)	-18(11)
C(43)	143(15)	89(10)	113(10)	15(8)	-16(10)	-27(11)
C(44)	90(9)	99(10)	66(6)	4(6)	-5(6)	-11(8)
P(3)	119(8)	222(12)	144(7)	18(8)	-33(6)	-82(8)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mar867.

	x	y	z	U(eq)
H(8)	8629	10183	2111	150
H(9)	9360	10001	2636	179
H(10)	9980	9728	1953	171
H(15)	9539	9104	-1671	196
H(16)	8793	9137	-2152	208
H(17)	8162	9532	-1330	193
H(20A)	7997	6155	482	66
H(20B)	8531	6204	158	66
H(22)	8499	5483	969	120
H(23)	8497	4749	1680	140
H(24)	8452	4741	3002	118
H(25)	8397	5445	3644	112
H(26)	8413	6189	3021	91
H(28)	9328	5970	808	101
H(29)	10159	6121	682	129
H(30)	10484	6832	1164	128
H(31)	9987	7405	1738	147
H(32)	9159	7284	1825	102
H(34)	8445	6143	-1162	94
H(35)	8158	5797	-2337	126
H(36)	7447	6101	-2899	134
H(37)	7018	6724	-2309	119
H(38)	7314	7078	-1189	93
H(40)	9074	6674	-629	97
H(41)	9778	7060	-855	121
H(42)	9826	7888	-713	140
H(43)	9142	8302	-284	138
H(44)	8414	7888	-28	102

[i] Otwinowski, Z. and Minor, W., "Processing of X-ray Diffraction Data Collected in Oscillation Mode", Methods in Enzymology, Volume 276: Macromolecular Crystallography, part A, p. 307-326, 1997. Carter C. W., Sweet Jr. & R. M., Eds., Academic Press.

[ii] SHELXS97, Sheldrick, G. M. (1997). SHELX97. Programs for Crystal Structure Analysis (Release 97-2). University of Goetingen, Germany.

[iii] SHELXL97, Sheldrick, G. M. (1997). SHELX97. Programs for Crystal Structure Analysis (Release 97-2). University of Goetingen, Germany.

[iv] $R_{int} = \Sigma \mid F_o^2 - F_o^2(mean) \mid / \Sigma [F_o^2]$

[v] Since the structure refinements are against F^2, R-indices based on F^2 are larger than (more than double) those based on F. For comparison with older refinements based on F and an OMIT threshold, a conventional index R_1 based on observed F values larger than $4\sigma(F_o)$ is also given (corresponding to Intensity$\geq 2\sigma(I)$). $wR_2 = \{ \Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2] \}^{1/2}$, $R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$, The Goodness of Fit is always based on F^2: $GooF = S = \{ \Sigma [w(F_o^2 - F_c^2)^2] / (n - p) \}^{1/2}$, where n is the number of reflections and p is the total number of parameters refined. The weighting scheme is: $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, where P is $[2 F_c^2 + Max(F_o^2, 0)]/3$.

[vi] ORTEP3 for Windows - Farrugia, L. J. (1997) J. Appl. Cryst. 30, 565.

[vii] The crystallographic data summarized in this reported are abstracted from the previous tables and the experiment record.