“Lligands hemilàbils en la reacció de Pauson-Khand intermolecular i asimètrica”

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Apèndix I

Dades de difracció de raigs X

Table 1. Crystal data and structure refinement for **143a**.

Identification code	ISO_073_A	
Empirical formula	C34 H40 Co2 N O6 P S	
Formula weight	739.56	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 10.3233(6) Å	α= 90°.
	b = 11.2864(6) Å	β= 90°.
	c = 31.2034(18) Å	γ = 90°.
Volume	3635.6(4) Å^3	
Z	4	
Density (calculated)	1.351 Mg/m^3	
Absorption coefficient	1.055 mm^{-1}	
F(000) 1536		
Crystal size	0.19 x 0.16 x 0.14 mm^3	
Theta range for data collection	1.31 to 26.38°.	
Index ranges	-6<=h<=12, -13<=k<=14, -37<=l<=39	
Reflections collected	21097	
Independent reflections	7421 [R(int) = 0.0551]	
Completeness to theta = 26.38°	100.0 %	
Absorption correction	Semi-empirical	
Max. and min. transmission	0.8663 and 0.8247	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7421 / 0 / 407	
Goodness-of-fit on F^2	0.988	
Final R indices [I>2sigma(I)]	R1 = 0.0405, wR2 = 0.0765	
R indices (all data)	R1 = 0.0852, wR2 = 0.0999	
Absolute structure parameter	-0.005(16)	
Largest diff. peak and hole	0.307 and -0.311 e.Å^{-3}	

Table 2. Bond lengths [Å] and angles [°] for ISO_073_A.

Co(1)-C(13)	1.763(6)	O(2)-C(12)	1.157(5)	C(16)-C(17)	1.348(6)
Co(1)-C(12)	1.767(5)	O(3)-C(13)	1.140(6)	C(17)-C(18)	1.487(6)
Co(1)-C(16)	1.940(5)	O(4)-C(14)	1.147(6)	C(19)-C(20)	1.511(8)
Co(1)-C(17)	1.963(4)	O(5)-C(15)	1.153(5)	C(21)-C(22)	1.489(8)
Co(1)-S(1)	2.3039(12)	O(6)-C(18)	1.222(5)	C(23)-C(24)	1.381(5)
Co(1)-Co(2)	2.4904(8)	N(1)-C(18)	1.359(5)	C(23)-C(28)	1.389(6)
Co(2)-C(14)	1.761(6)	N(1)-C(19)	1.452(6)	C(24)-C(25)	1.387(6)
Co(2)-C(15)	1.780(5)	N(1)-C(21)	1.475(6)	C(25)-C(26)	1.367(7)
Co(2)-C(16)	1.922(5)	C(1)-C(2)	1.517(5)	C(26)-C(27)	1.361(6)
Co(2)-C(17)	1.974(4)	C(1)-C(6)	1.525(6)	C(27)-C(28)	1.384(6)
Co(2)-P(1)	2.2127(12)	C(2)-C(3)	1.515(6)	C(29)-C(34)	1.372(6)
S(1)-C(11)	1.824(4)	C(3)-C(4)	1.494(7)	C(29)-C(30)	1.373(6)
S(1)-C(7)	1.873(4)	C(3)-C(8)	1.539(6)	C(30)-C(31)	1.392(6)
P(1)-C(23)	1.835(4)	C(4)-C(5)	1.523(6)	C(31)-C(32)	1.354(7)
P(1)-C(29)	1.837(4)	C(5)-C(6)	1.532(6)	C(32)-C(33)	1.353(7)
P(1)-C(11)	1.844(4)	C(6)-C(7)	1.551(6)	C(33)-C(34)	1.375(7)
O(1)-C(11)	1.394(4)	C(7)-C(10)	1.528(5)		
O(1)-C(1)	1.443(5)	C(7)-C(9)	1.533(6)		

C(13)-Co(1)-C(12)	99.2(2)	C(15)-Co(2)-C(17)	138.5(2)
C(13)-Co(1)-C(16)	102.3(2)	C(16)-Co(2)-C(17)	40.45(17)
C(12)-Co(1)-C(16)	104.8(2)	C(14)-Co(2)-P(1)	98.73(18)
C(13)-Co(1)-C(17)	103.86(19)	C(15)-Co(2)-P(1)	109.71(17)
C(12)-Co(1)-C(17)	141.5(2)	C(16)-Co(2)-P(1)	138.71(14)
C(16)-Co(1)-C(17)	40.40(17)	C(17)-Co(2)-P(1)	105.49(12)
C(13)-Co(1)-S(1)	102.29(17)	C(14)-Co(2)-Co(1)	146.62(17)
C(12)-Co(1)-S(1)	99.41(15)	C(15)-Co(2)-Co(1)	106.34(16)
C(16)-Co(1)-S(1)	141.93(14)	C(16)-Co(2)-Co(1)	50.15(14)
C(17)-Co(1)-S(1)	105.13(12)	C(17)-Co(2)-Co(1)	50.56(12)
C(13)-Co(1)-Co(2)	150.74(16)	P(1)-Co(2)-Co(1)	91.99(4)
C(12)-Co(1)-Co(2)	96.46(16)	C(11)-S(1)-C(7)	97.56(18)
C(16)-Co(1)-Co(2)	49.52(13)	C(11)-S(1)-Co(1)	102.30(12)
C(17)-Co(1)-Co(2)	50.96(12)	C(7)-S(1)-Co(1)	118.51(14)
S(1)-Co(1)-Co(2)	99.34(3)	C(23)-P(1)-C(29)	104.74(19)
C(14)-Co(2)-C(15)	99.6(2)	C(23)-P(1)-C(11)	103.06(18)
C(14)-Co(2)-C(16)	106.2(2)	C(29)-P(1)-C(11)	98.57(17)
C(15)-Co(2)-C(16)	98.1(2)	C(23)-P(1)-Co(2)	120.80(14)
C(14)-Co(2)-C(17)	96.1(2)	C(29)-P(1)-Co(2)	118.64(15)

C(11)-P(1)-Co(2)	107.72(12)	C(17)-C(16)-Co(2)	71.9(3)
C(11)-O(1)-C(1)	112.5(3)	C(17)-C(16)-Co(1)	70.7(3)
C(18)-N(1)-C(19)	125.6(4)	Co(2)-C(16)-Co(1)	80.33(17)
C(18)-N(1)-C(21)	117.8(4)	C(16)-C(17)-C(18)	143.8(4)
C(19)-N(1)-C(21)	116.4(4)	C(16)-C(17)-Co(1)	68.9(3)
O(1)-C(1)-C(2)	105.6(3)	C(18)-C(17)-Co(1)	135.3(3)
O(1)-C(1)-C(6)	113.1(3)	C(16)-C(17)-Co(2)	67.7(3)
C(2)-C(1)-C(6)	112.5(4)	C(18)-C(17)-Co(2)	133.6(3)
C(3)-C(2)-C(1)	112.8(4)	Co(1)-C(17)-Co(2)	78.47(16)
C(4)-C(3)-C(2)	109.9(4)	O(6)-C(18)-N(1)	121.6(4)
C(4)-C(3)-C(8)	112.0(5)	O(6)-C(18)-C(17)	121.9(4)
C(2)-C(3)-C(8)	111.4(5)	N(1)-C(18)-C(17)	116.4(4)
C(3)-C(4)-C(5)	113.0(4)	N(1)-C(19)-C(20)	113.0(5)
C(4)-C(5)-C(6)	111.9(4)	N(1)-C(21)-C(22)	113.1(5)
C(1)-C(6)-C(5)	107.9(4)	C(24)-C(23)-C(28)	118.1(4)
C(1)-C(6)-C(7)	115.6(3)	C(24)-C(23)-P(1)	119.8(3)
C(5)-C(6)-C(7)	112.4(4)	C(28)-C(23)-P(1)	122.0(3)
C(10)-C(7)-C(9)	110.6(4)	C(23)-C(24)-C(25)	121.0(5)
C(10)-C(7)-C(6)	113.4(3)	C(26)-C(25)-C(24)	119.7(5)
C(9)-C(7)-C(6)	111.3(3)	C(27)-C(26)-C(25)	120.3(5)
C(10)-C(7)-S(1)	111.2(3)	C(26)-C(27)-C(28)	120.3(5)
C(9)-C(7)-S(1)	103.3(3)	C(27)-C(28)-C(23)	120.4(4)
C(6)-C(7)-S(1)	106.5(3)	C(34)-C(29)-C(30)	118.1(4)
O(1)-C(11)-S(1)	110.3(2)	C(34)-C(29)-P(1)	117.9(3)
O(1)-C(11)-P(1)	114.0(3)	C(30)-C(29)-P(1)	124.0(3)
S(1)-C(11)-P(1)	107.25(19)	C(29)-C(30)-C(31)	121.1(4)
O(2)-C(12)-Co(1)	175.7(4)	C(32)-C(31)-C(30)	119.4(5)
O(3)-C(13)-Co(1)	177.4(5)	C(33)-C(32)-C(31)	119.8(5)
O(4)-C(14)-Co(2)	178.8(6)	C(32)-C(33)-C(34)	121.2(5)
O(5)-C(15)-Co(2)	174.0(5)	C(29)-C(34)-C(33)	120.3(5)

Table 3. Crystal data and structure refinement for **149a**.

Identification code	JSO-285-A	
Empirical formula	C70 H106 Co4 N2 O13 P2 S3	
Formula weight	1577.41	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 12.4866(15) Å	α= 90°.
	b = 22.402(3) Å	β= 91.152(2)°.
	c = 13.3852(16) Å	γ= 90°.
Volume	3743.3(8) Å^3	
Z	2	
Density (calculated)	1.399 Mg/m^3	
Absorption coefficient	1.057 mm^{-1}	
F(000)	1660	
Crystal size	0.26 x 0.14 x 0.06 mm^3	
Theta range for data collection	1.52 to 29.21°.	
Index ranges	-17<=h<=16, -30<=k<=30, -17<=l<=17	
Reflections collected	47784	
Independent reflections	18439 [R(int) = 0.0773]	
Completeness to theta = 29.21°	94.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9432 and 0.7721	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	18439 / 1 / 847	
Goodness-of-fit on F^2	0.989	
Final R indices [I>2sigma(I)]	R1 = 0.0526, wR2 = 0.0731	
R indices (all data)	R1 = 0.0924, wR2 = 0.0845	
Absolute structure parameter	-0.024(9)	
Largest diff. peak and hole	0.438 and -0.514 e.Å^{-3}	

Table 4. Bond lengths [Å] and angles [°] for JSO-285-A.

Co(1)-C(11)	1.767(5)	O(6)-C(19)	1.451(4)	C(15)-H(15B)	0.9700
Co(1)-C(10)	1.789(5)	O(7)-C(37)	1.242(5)	C(16)-C(17)	1.522(5)
Co(1)-C(3)	1.945(4)	O(8)-C(42)	1.144(5)	C(16)-H(16A)	0.9700
Co(1)-C(2)	1.946(4)	O(9)-C(43)	1.149(5)	C(16)-H(16B)	0.9700
Co(1)-S(1)	2.2572(11)	O(10)-C(44)	1.152(5)	C(17)-C(18)	1.537(5)
Co(1)-Co(2)	2.4601(8)	O(11)-C(45)	1.153(5)	C(17)-C(20)	1.544(5)
Co(2)-C(8)	1.767(4)	O(12)-C(46)	1.404(4)	C(17)-H(17A)	0.9800
Co(2)-C(9)	1.785(5)	O(12)-C(53)	1.452(4)	C(18)-C(19)	1.529(5)
Co(2)-C(3)	1.942(4)	N(1)-C(1)	1.355(5)	C(18)-H(18A)	0.9700
Co(2)-C(2)	1.974(4)	N(1)-C(4)	1.473(5)	C(18)-H(18B)	0.9700
Co(2)-P(1)	2.2226(12)	N(1)-C(6)	1.473(5)	C(19)-H(19A)	0.9800
Co(3)-C(42)	1.771(4)	N(2)-C(37)	1.343(5)	C(20)-C(21)	1.540(5)
Co(3)-C(43)	1.778(4)	N(2)-C(40)	1.455(5)	C(20)-C(22)	1.544(5)
Co(3)-C(36)	1.937(4)	N(2)-C(38)	1.464(5)	C(21)-H(21A)	0.9600
Co(3)-C(35)	1.940(4)	C(1)-C(2)	1.470(6)	C(21)-H(21B)	0.9600
Co(3)-S(2)	2.2679(11)	C(2)-C(3)	1.352(5)	C(21)-H(21C)	0.9600
Co(3)-Co(4)	2.4762(8)	C(3)-H(3A)	0.9800	C(22)-H(22A)	0.9600
Co(4)-C(45)	1.764(5)	C(4)-C(5)	1.501(6)	C(22)-H(22B)	0.9600
Co(4)-C(44)	1.778(4)	C(4)-H(4A)	0.9700	C(22)-H(22C)	0.9600
Co(4)-C(35)	1.937(4)	C(4)-H(4B)	0.9700	C(23)-C(24)	1.530(5)
Co(4)-C(36)	1.976(4)	C(5)-H(5A)	0.9600	C(23)-C(28)	1.536(5)
Co(4)-P(2)	2.2244(12)	C(5)-H(5B)	0.9600	C(23)-H(23A)	0.9800
P(1)-C(12)	1.842(4)	C(5)-H(5C)	0.9600	C(24)-C(25)	1.530(5)
P(1)-C(23)	1.845(4)	C(6)-C(7)	1.514(5)	C(24)-H(24A)	0.9700
P(1)-C(29)	1.847(4)	C(6)-H(6A)	0.9700	C(24)-H(24B)	0.9700
P(2)-C(46)	1.830(4)	C(6)-H(6B)	0.9700	C(25)-C(26)	1.523(5)
P(2)-C(57)	1.842(4)	C(7)-H(7A)	0.9600	C(25)-H(25A)	0.9700
P(2)-C(63)	1.844(4)	C(7)-H(7B)	0.9600	C(25)-H(25B)	0.9700
S(1)-C(13)	1.821(4)	C(7)-H(7C)	0.9600	C(26)-C(27)	1.539(5)
S(1)-C(12)	1.826(4)	C(12)-H(12A)	0.9800	C(26)-H(26A)	0.9700
S(2)-C(47)	1.818(4)	C(13)-C(14)	1.511(5)	C(26)-H(26B)	0.9700
S(2)-C(46)	1.837(4)	C(13)-H(13A)	0.9700	C(27)-C(28)	1.531(5)
O(1)-C(1)	1.243(5)	C(13)-H(13B)	0.9700	C(27)-H(27A)	0.9700
O(2)-C(8)	1.148(5)	C(14)-C(20)	1.555(5)	C(27)-H(27B)	0.9700
O(3)-C(9)	1.145(5)	C(14)-C(19)	1.556(5)	C(28)-H(28A)	0.9700
O(4)-C(10)	1.144(5)	C(14)-C(15)	1.558(5)	C(28)-H(28B)	0.9700
O(5)-C(11)	1.145(5)	C(15)-C(16)	1.558(5)	C(29)-C(34)	1.528(5)
O(6)-C(12)	1.413(4)	C(15)-H(15A)	0.9700	C(29)-C(30)	1.532(5)

C(29)-H(29A)	0.9800	C(48)-C(53)	1.538(5)	C(60)-H(60A)	0.9700
C(30)-C(31)	1.524(5)	C(48)-C(49)	1.556(5)	C(60)-H(60B)	0.9700
C(30)-H(30A)	0.9700	C(48)-C(54)	1.575(5)	C(61)-C(62)	1.534(5)
C(30)-H(30B)	0.9700	C(49)-C(50)	1.544(5)	C(61)-H(61A)	0.9700
C(31)-C(32)	1.522(6)	C(49)-H(49A)	0.9700	C(61)-H(61B)	0.9700
C(31)-H(31A)	0.9700	C(49)-H(49B)	0.9700	C(62)-H(62A)	0.9700
C(31)-H(31B)	0.9700	C(50)-C(51)	1.544(5)	C(62)-H(62B)	0.9700
C(32)-C(33)	1.519(5)	C(50)-H(50A)	0.9700	C(63)-C(64)	1.532(5)
C(32)-H(32A)	0.9700	C(50)-H(50B)	0.9700	C(63)-C(68)	1.538(5)
C(32)-H(32B)	0.9700	C(51)-C(52)	1.535(5)	C(63)-H(63A)	0.9800
C(33)-C(34)	1.535(5)	C(51)-C(54)	1.544(5)	C(64)-C(65)	1.521(5)
C(33)-H(33A)	0.9700	C(51)-H(51A)	0.9800	C(64)-H(64A)	0.9700
C(33)-H(33B)	0.9700	C(52)-C(53)	1.545(5)	C(64)-H(64B)	0.9700
C(34)-H(34A)	0.9700	C(52)-H(52A)	0.9700	C(65)-C(66)	1.528(6)
C(34)-H(34B)	0.9700	C(52)-H(52B)	0.9700	C(65)-H(65A)	0.9700
C(35)-C(36)	1.343(5)	C(53)-H(53A)	0.9800	C(65)-H(65B)	0.9700
C(35)-H(35A)	0.9800	C(54)-C(56)	1.531(5)	C(66)-C(67)	1.508(6)
C(36)-C(37)	1.483(5)	C(54)-C(55)	1.532(6)	C(66)-H(66A)	0.9700
C(38)-C(39)	1.522(6)	C(55)-H(55A)	0.9600	C(66)-H(66B)	0.9700
C(38)-H(38A)	0.9700	C(55)-H(55B)	0.9600	C(67)-C(68)	1.529(5)
C(38)-H(38B)	0.9700	C(55)-H(55C)	0.9600	C(67)-H(67A)	0.9700
C(39)-H(39A)	0.9600	C(56)-H(56A)	0.9600	C(67)-H(67B)	0.9700
C(39)-H(39B)	0.9600	C(56)-H(56B)	0.9600	C(68)-H(68A)	0.9700
C(39)-H(39C)	0.9600	C(56)-H(56C)	0.9600	C(68)-H(68B)	0.9700
C(40)-C(41)	1.514(6)	C(57)-C(62)	1.528(5)	S(1S)-O(1S)	1.491(3)
C(40)-H(40A)	0.9700	C(57)-C(58)	1.549(5)	S(1S)-C(2S)	1.773(4)
C(40)-H(40B)	0.9700	C(57)-H(57A)	0.9800	S(1S)-C(1S)	1.778(4)
C(41)-H(41A)	0.9600	C(58)-C(59)	1.528(5)	C(1S)-H(1SB)	0.9600
C(41)-H(41B)	0.9600	C(58)-H(58A)	0.9700	C(1S)-H(1SC)	0.9600
C(41)-H(41C)	0.9600	C(58)-H(58B)	0.9700	C(1S)-H(1SD)	0.9600
C(46)-H(46A)	0.9800	C(59)-C(60)	1.535(6)	C(2S)-H(2SA)	0.9600
C(47)-C(48)	1.520(5)	C(59)-H(59A)	0.9700	C(2S)-H(2SB)	0.9600
C(47)-H(47A)	0.9700	C(59)-H(59B)	0.9700	C(2S)-H(2SC)	0.9600
C(47)-H(47B)	0.9700	C(60)-C(61)	1.516(5)		

C(11)-Co(1)-C(10)	104.8(2)	C(3)-Co(1)-C(2)	40.65(16)
C(11)-Co(1)-C(3)	101.39(18)	C(11)-Co(1)-S(1)	99.52(14)
C(10)-Co(1)-C(3)	107.69(19)	C(10)-Co(1)-S(1)	97.07(15)
C(11)-Co(1)-C(2)	97.25(18)	C(3)-Co(1)-S(1)	141.99(13)
C(10)-Co(1)-C(2)	145.30(18)	C(2)-Co(1)-S(1)	105.43(12)

C(11)-Co(1)-Co(2)	147.72(14)	C(35)-Co(4)-C(36)	40.12(15)
C(10)-Co(1)-Co(2)	99.99(13)	C(45)-Co(4)-P(2)	96.63(13)
C(3)-Co(1)-Co(2)	50.69(12)	C(44)-Co(4)-P(2)	104.42(14)
C(2)-Co(1)-Co(2)	51.64(12)	C(35)-Co(4)-P(2)	139.68(12)
S(1)-Co(1)-Co(2)	97.59(3)	C(36)-Co(4)-P(2)	103.95(12)
C(8)-Co(2)-C(9)	97.67(19)	C(45)-Co(4)-Co(3)	151.44(13)
C(8)-Co(2)-C(3)	107.66(18)	C(44)-Co(4)-Co(3)	101.23(14)
C(9)-Co(2)-C(3)	101.14(18)	C(35)-Co(4)-Co(3)	50.35(12)
C(8)-Co(2)-C(2)	107.37(18)	C(36)-Co(4)-Co(3)	50.06(11)
C(9)-Co(2)-C(2)	138.68(18)	P(2)-Co(4)-Co(3)	95.09(4)
C(3)-Co(2)-C(2)	40.36(15)	C(12)-P(1)-C(23)	106.62(18)
C(8)-Co(2)-P(1)	96.85(13)	C(12)-P(1)-C(29)	102.64(17)
C(9)-Co(2)-P(1)	108.72(14)	C(23)-P(1)-C(29)	102.87(17)
C(3)-Co(2)-P(1)	138.16(13)	C(12)-P(1)-Co(2)	108.39(12)
C(2)-Co(2)-P(1)	100.46(12)	C(23)-P(1)-Co(2)	119.91(14)
C(8)-Co(2)-Co(1)	156.25(14)	C(29)-P(1)-Co(2)	114.81(13)
C(9)-Co(2)-Co(1)	96.70(13)	C(46)-P(2)-C(57)	105.95(18)
C(3)-Co(2)-Co(1)	50.78(12)	C(46)-P(2)-C(63)	102.77(17)
C(2)-Co(2)-Co(1)	50.62(11)	C(57)-P(2)-C(63)	104.71(18)
P(1)-Co(2)-Co(1)	96.31(4)	C(46)-P(2)-Co(4)	107.81(13)
C(42)-Co(3)-C(43)	98.23(18)	C(57)-P(2)-Co(4)	119.03(14)
C(42)-Co(3)-C(36)	102.56(17)	C(63)-P(2)-Co(4)	115.06(13)
C(43)-Co(3)-C(36)	143.92(18)	C(13)-S(1)-C(12)	94.02(18)
C(42)-Co(3)-C(35)	100.37(18)	C(13)-S(1)-Co(1)	112.30(13)
C(43)-Co(3)-C(35)	106.92(18)	C(12)-S(1)-Co(1)	104.62(12)
C(36)-Co(3)-C(35)	40.52(15)	C(47)-S(2)-C(46)	93.75(17)
C(42)-Co(3)-S(2)	103.61(14)	C(47)-S(2)-Co(3)	115.42(13)
C(43)-Co(3)-S(2)	99.21(13)	C(46)-S(2)-Co(3)	104.60(12)
C(36)-Co(3)-S(2)	104.06(12)	C(12)-O(6)-C(19)	111.4(3)
C(35)-Co(3)-S(2)	141.30(12)	C(46)-O(12)-C(53)	110.7(3)
C(42)-Co(3)-Co(4)	149.62(14)	C(1)-N(1)-C(4)	118.3(4)
C(43)-Co(3)-Co(4)	98.28(13)	C(1)-N(1)-C(6)	124.7(4)
C(36)-Co(3)-Co(4)	51.44(11)	C(4)-N(1)-C(6)	116.7(3)
C(35)-Co(3)-Co(4)	50.25(11)	C(37)-N(2)-C(40)	125.0(3)
S(2)-Co(3)-Co(4)	98.69(3)	C(37)-N(2)-C(38)	117.8(3)
C(45)-Co(4)-C(44)	100.91(19)	C(40)-N(2)-C(38)	117.0(3)
C(45)-Co(4)-C(35)	106.94(17)	O(1)-C(1)-N(1)	119.8(4)
C(44)-Co(4)-C(35)	102.65(18)	O(1)-C(1)-C(2)	120.6(4)
C(45)-Co(4)-C(36)	101.71(17)	N(1)-C(1)-C(2)	119.6(4)
C(44)-Co(4)-C(36)	141.06(17)	C(3)-C(2)-C(1)	140.4(4)

C(3)-C(2)-Co(1)	69.6(2)	O(6)-C(12)-P(1)	115.4(3)
C(1)-C(2)-Co(1)	130.4(3)	S(1)-C(12)-P(1)	110.3(2)
C(3)-C(2)-Co(2)	68.6(2)	O(6)-C(12)-H(12A)	107.1
C(1)-C(2)-Co(2)	140.7(3)	S(1)-C(12)-H(12A)	107.1
Co(1)-C(2)-Co(2)	77.74(15)	P(1)-C(12)-H(12A)	107.1
C(2)-C(3)-Co(2)	71.1(2)	C(14)-C(13)-S(1)	112.8(3)
C(2)-C(3)-Co(1)	69.7(2)	C(14)-C(13)-H(13A)	109.0
Co(2)-C(3)-Co(1)	78.53(16)	S(1)-C(13)-H(13A)	109.0
C(2)-C(3)-H(3A)	136.4	C(14)-C(13)-H(13B)	109.0
Co(2)-C(3)-H(3A)	136.4	S(1)-C(13)-H(13B)	109.0
Co(1)-C(3)-H(3A)	136.4	H(13A)-C(13)-H(13B)	107.8
N(1)-C(4)-C(5)	113.6(4)	C(13)-C(14)-C(20)	120.8(3)
N(1)-C(4)-H(4A)	108.8	C(13)-C(14)-C(19)	115.0(3)
C(5)-C(4)-H(4A)	108.8	C(20)-C(14)-C(19)	103.0(3)
N(1)-C(4)-H(4B)	108.8	C(13)-C(14)-C(15)	111.5(3)
C(5)-C(4)-H(4B)	108.8	C(20)-C(14)-C(15)	101.6(3)
H(4A)-C(4)-H(4B)	107.7	C(19)-C(14)-C(15)	102.9(3)
C(4)-C(5)-H(5A)	109.5	C(14)-C(15)-C(16)	103.3(3)
C(4)-C(5)-H(5B)	109.5	C(14)-C(15)-H(15A)	111.1
H(5A)-C(5)-H(5B)	109.5	C(16)-C(15)-H(15A)	111.1
C(4)-C(5)-H(5C)	109.5	C(14)-C(15)-H(15B)	111.1
H(5A)-C(5)-H(5C)	109.5	C(16)-C(15)-H(15B)	111.1
H(5B)-C(5)-H(5C)	109.5	H(15A)-C(15)-H(15B)	109.1
N(1)-C(6)-C(7)	113.3(3)	C(17)-C(16)-C(15)	103.0(3)
N(1)-C(6)-H(6A)	108.9	C(17)-C(16)-H(16A)	111.2
C(7)-C(6)-H(6A)	108.9	C(15)-C(16)-H(16A)	111.2
N(1)-C(6)-H(6B)	108.9	C(17)-C(16)-H(16B)	111.2
C(7)-C(6)-H(6B)	108.9	C(15)-C(16)-H(16B)	111.2
H(6A)-C(6)-H(6B)	107.7	H(16A)-C(16)-H(16B)	109.1
C(6)-C(7)-H(7A)	109.5	C(16)-C(17)-C(18)	107.3(3)
C(6)-C(7)-H(7B)	109.5	C(16)-C(17)-C(20)	102.9(3)
H(7A)-C(7)-H(7B)	109.5	C(18)-C(17)-C(20)	102.4(3)
C(6)-C(7)-H(7C)	109.5	C(16)-C(17)-H(17A)	114.3
H(7A)-C(7)-H(7C)	109.5	C(18)-C(17)-H(17A)	114.3
H(7B)-C(7)-H(7C)	109.5	C(20)-C(17)-H(17A)	114.3
O(2)-C(8)-Co(2)	177.7(4)	C(19)-C(18)-C(17)	103.6(3)
O(3)-C(9)-Co(2)	177.3(4)	C(19)-C(18)-H(18A)	111.0
O(4)-C(10)-Co(1)	178.0(4)	C(17)-C(18)-H(18A)	111.0
O(5)-C(11)-Co(1)	176.3(4)	C(19)-C(18)-H(18B)	111.0
O(6)-C(12)-S(1)	109.4(2)	C(17)-C(18)-H(18B)	111.0

H(18A)-C(18)-H(18B)	109.0	C(26)-C(25)-H(25B)	108.9
O(6)-C(19)-C(18)	108.6(3)	C(24)-C(25)-H(25B)	108.9
O(6)-C(19)-C(14)	115.8(3)	H(25A)-C(25)-H(25B)	107.8
C(18)-C(19)-C(14)	103.6(3)	C(25)-C(26)-C(27)	109.6(3)
O(6)-C(19)-H(19A)	109.5	C(25)-C(26)-H(26A)	109.7
C(18)-C(19)-H(19A)	109.5	C(27)-C(26)-H(26A)	109.7
C(14)-C(19)-H(19A)	109.5	C(25)-C(26)-H(26B)	109.7
C(21)-C(20)-C(22)	106.4(3)	C(27)-C(26)-H(26B)	109.7
C(21)-C(20)-C(17)	113.0(3)	H(26A)-C(26)-H(26B)	108.2
C(22)-C(20)-C(17)	114.1(3)	C(28)-C(27)-C(26)	111.0(3)
C(21)-C(20)-C(14)	113.7(3)	C(28)-C(27)-H(27A)	109.4
C(22)-C(20)-C(14)	115.9(3)	C(26)-C(27)-H(27A)	109.4
C(17)-C(20)-C(14)	93.6(3)	C(28)-C(27)-H(27B)	109.4
C(20)-C(21)-H(21A)	109.5	C(26)-C(27)-H(27B)	109.4
C(20)-C(21)-H(21B)	109.5	H(27A)-C(27)-H(27B)	108.0
H(21A)-C(21)-H(21B)	109.5	C(27)-C(28)-C(23)	112.0(3)
C(20)-C(21)-H(21C)	109.5	C(27)-C(28)-H(28A)	109.2
H(21A)-C(21)-H(21C)	109.5	C(23)-C(28)-H(28A)	109.2
H(21B)-C(21)-H(21C)	109.5	C(27)-C(28)-H(28B)	109.2
C(20)-C(22)-H(22A)	109.5	C(23)-C(28)-H(28B)	109.2
C(20)-C(22)-H(22B)	109.5	H(28A)-C(28)-H(28B)	107.9
H(22A)-C(22)-H(22B)	109.5	C(34)-C(29)-C(30)	109.9(3)
C(20)-C(22)-H(22C)	109.5	C(34)-C(29)-P(1)	112.2(3)
H(22A)-C(22)-H(22C)	109.5	C(30)-C(29)-P(1)	117.2(3)
H(22B)-C(22)-H(22C)	109.5	C(34)-C(29)-H(29A)	105.5
C(24)-C(23)-C(28)	110.6(3)	C(30)-C(29)-H(29A)	105.5
C(24)-C(23)-P(1)	113.9(3)	P(1)-C(29)-H(29A)	105.5
C(28)-C(23)-P(1)	108.2(3)	C(31)-C(30)-C(29)	110.9(3)
C(24)-C(23)-H(23A)	108.0	C(31)-C(30)-H(30A)	109.5
C(28)-C(23)-H(23A)	108.0	C(29)-C(30)-H(30A)	109.5
P(1)-C(23)-H(23A)	108.0	C(31)-C(30)-H(30B)	109.5
C(23)-C(24)-C(25)	110.9(3)	C(29)-C(30)-H(30B)	109.5
C(23)-C(24)-H(24A)	109.5	H(30A)-C(30)-H(30B)	108.0
C(25)-C(24)-H(24A)	109.5	C(32)-C(31)-C(30)	111.6(3)
C(23)-C(24)-H(24B)	109.5	C(32)-C(31)-H(31A)	109.3
C(25)-C(24)-H(24B)	109.5	C(30)-C(31)-H(31A)	109.3
H(24A)-C(24)-H(24B)	108.1	C(32)-C(31)-H(31B)	109.3
C(26)-C(25)-C(24)	113.2(3)	C(30)-C(31)-H(31B)	109.3
C(26)-C(25)-H(25A)	108.9	H(31A)-C(31)-H(31B)	108.0
C(24)-C(25)-H(25A)	108.9	C(33)-C(32)-C(31)	110.7(3)

C(33)-C(32)-H(32A)	109.5	H(39A)-C(39)-H(39B)	109.5
C(31)-C(32)-H(32A)	109.5	C(38)-C(39)-H(39C)	109.5
C(33)-C(32)-H(32B)	109.5	H(39A)-C(39)-H(39C)	109.5
C(31)-C(32)-H(32B)	109.5	H(39B)-C(39)-H(39C)	109.5
H(32A)-C(32)-H(32B)	108.1	N(2)-C(40)-C(41)	112.4(4)
C(32)-C(33)-C(34)	111.4(3)	N(2)-C(40)-H(40A)	109.1
C(32)-C(33)-H(33A)	109.4	C(41)-C(40)-H(40A)	109.1
C(34)-C(33)-H(33A)	109.4	N(2)-C(40)-H(40B)	109.1
C(32)-C(33)-H(33B)	109.4	C(41)-C(40)-H(40B)	109.1
C(34)-C(33)-H(33B)	109.4	H(40A)-C(40)-H(40B)	107.9
H(33A)-C(33)-H(33B)	108.0	C(40)-C(41)-H(41A)	109.5
C(29)-C(34)-C(33)	111.6(3)	C(40)-C(41)-H(41B)	109.5
C(29)-C(34)-H(34A)	109.3	H(41A)-C(41)-H(41B)	109.5
C(33)-C(34)-H(34A)	109.3	C(40)-C(41)-H(41C)	109.5
C(29)-C(34)-H(34B)	109.3	H(41A)-C(41)-H(41C)	109.5
C(33)-C(34)-H(34B)	109.3	H(41B)-C(41)-H(41C)	109.5
H(34A)-C(34)-H(34B)	108.0	O(8)-C(42)-Co(3)	175.3(4)
C(36)-C(35)-Co(4)	71.5(2)	O(9)-C(43)-Co(3)	176.9(4)
C(36)-C(35)-Co(3)	69.6(2)	O(10)-C(44)-Co(4)	178.1(4)
Co(4)-C(35)-Co(3)	79.40(15)	O(11)-C(45)-Co(4)	178.3(4)
C(36)-C(35)-H(35A)	136.1	O(12)-C(46)-P(2)	114.3(2)
Co(4)-C(35)-H(35A)	136.1	O(12)-C(46)-S(2)	110.1(2)
Co(3)-C(35)-H(35A)	136.1	P(2)-C(46)-S(2)	110.78(19)
C(35)-C(36)-C(37)	143.0(4)	O(12)-C(46)-H(46A)	107.1
C(35)-C(36)-Co(3)	69.8(2)	P(2)-C(46)-H(46A)	107.1
C(37)-C(36)-Co(3)	133.9(3)	S(2)-C(46)-H(46A)	107.1
C(35)-C(36)-Co(4)	68.4(2)	C(48)-C(47)-S(2)	111.8(3)
C(37)-C(36)-Co(4)	134.7(3)	C(48)-C(47)-H(47A)	109.2
Co(3)-C(36)-Co(4)	78.50(14)	S(2)-C(47)-H(47A)	109.2
O(7)-C(37)-N(2)	120.9(4)	C(48)-C(47)-H(47B)	109.2
O(7)-C(37)-C(36)	120.2(4)	S(2)-C(47)-H(47B)	109.2
N(2)-C(37)-C(36)	118.9(4)	H(47A)-C(47)-H(47B)	107.9
N(2)-C(38)-C(39)	111.9(4)	C(47)-C(48)-C(53)	116.3(3)
N(2)-C(38)-H(38A)	109.2	C(47)-C(48)-C(49)	111.3(3)
C(39)-C(38)-H(38A)	109.2	C(53)-C(48)-C(49)	103.0(3)
N(2)-C(38)-H(38B)	109.2	C(47)-C(48)-C(54)	119.8(3)
C(39)-C(38)-H(38B)	109.2	C(53)-C(48)-C(54)	103.2(3)
H(38A)-C(38)-H(38B)	107.9	C(49)-C(48)-C(54)	101.0(3)
C(38)-C(39)-H(39A)	109.5	C(50)-C(49)-C(48)	104.6(3)
C(38)-C(39)-H(39B)	109.5	C(50)-C(49)-H(49A)	110.8

C(48)-C(49)-H(49A)	110.8	C(54)-C(56)-H(56A)	109.5
C(50)-C(49)-H(49B)	110.8	C(54)-C(56)-H(56B)	109.5
C(48)-C(49)-H(49B)	110.8	H(56A)-C(56)-H(56B)	109.5
H(49A)-C(49)-H(49B)	108.9	C(54)-C(56)-H(56C)	109.5
C(49)-C(50)-C(51)	102.4(3)	H(56A)-C(56)-H(56C)	109.5
C(49)-C(50)-H(50A)	111.3	H(56B)-C(56)-H(56C)	109.5
C(51)-C(50)-H(50A)	111.3	C(62)-C(57)-C(58)	111.7(3)
C(49)-C(50)-H(50B)	111.3	C(62)-C(57)-P(2)	112.8(3)
C(51)-C(50)-H(50B)	111.3	C(58)-C(57)-P(2)	107.8(3)
H(50A)-C(50)-H(50B)	109.2	C(62)-C(57)-H(57A)	108.2
C(52)-C(51)-C(50)	106.2(3)	C(58)-C(57)-H(57A)	108.2
C(52)-C(51)-C(54)	102.8(3)	P(2)-C(57)-H(57A)	108.2
C(50)-C(51)-C(54)	103.0(3)	C(59)-C(58)-C(57)	111.7(3)
C(52)-C(51)-H(51A)	114.5	C(59)-C(58)-H(58A)	109.3
C(50)-C(51)-H(51A)	114.5	C(57)-C(58)-H(58A)	109.3
C(54)-C(51)-H(51A)	114.5	C(59)-C(58)-H(58B)	109.3
C(51)-C(52)-C(53)	103.5(3)	C(57)-C(58)-H(58B)	109.3
C(51)-C(52)-H(52A)	111.1	H(58A)-C(58)-H(58B)	107.9
C(53)-C(52)-H(52A)	111.1	C(58)-C(59)-C(60)	109.5(3)
C(51)-C(52)-H(52B)	111.1	C(58)-C(59)-H(59A)	109.8
C(53)-C(52)-H(52B)	111.1	C(60)-C(59)-H(59A)	109.8
H(52A)-C(52)-H(52B)	109.0	C(58)-C(59)-H(59B)	109.8
O(12)-C(53)-C(48)	115.2(3)	C(60)-C(59)-H(59B)	109.8
O(12)-C(53)-C(52)	108.3(3)	H(59A)-C(59)-H(59B)	108.2
C(48)-C(53)-C(52)	103.6(3)	C(61)-C(60)-C(59)	110.3(4)
O(12)-C(53)-H(53A)	109.8	C(61)-C(60)-H(60A)	109.6
C(48)-C(53)-H(53A)	109.8	C(59)-C(60)-H(60A)	109.6
C(52)-C(53)-H(53A)	109.8	C(61)-C(60)-H(60B)	109.6
C(56)-C(54)-C(55)	106.7(3)	C(59)-C(60)-H(60B)	109.6
C(56)-C(54)-C(51)	112.7(3)	H(60A)-C(60)-H(60B)	108.1
C(55)-C(54)-C(51)	114.6(3)	C(60)-C(61)-C(62)	111.2(3)
C(56)-C(54)-C(48)	116.4(3)	C(60)-C(61)-H(61A)	109.4
C(55)-C(54)-C(48)	113.1(3)	C(62)-C(61)-H(61A)	109.4
C(51)-C(54)-C(48)	93.3(3)	C(60)-C(61)-H(61B)	109.4
C(54)-C(55)-H(55A)	109.5	C(62)-C(61)-H(61B)	109.4
C(54)-C(55)-H(55B)	109.5	H(61A)-C(61)-H(61B)	108.0
H(55A)-C(55)-H(55B)	109.5	C(57)-C(62)-C(61)	112.3(3)
C(54)-C(55)-H(55C)	109.5	C(57)-C(62)-H(62A)	109.1
H(55A)-C(55)-H(55C)	109.5	C(61)-C(62)-H(62A)	109.1
H(55B)-C(55)-H(55C)	109.5	C(57)-C(62)-H(62B)	109.1

C(61)-C(62)-H(62B)	109.1	C(66)-C(67)-H(67A)	109.3
H(62A)-C(62)-H(62B)	107.9	C(68)-C(67)-H(67A)	109.3
C(64)-C(63)-C(68)	109.0(3)	C(66)-C(67)-H(67B)	109.3
C(64)-C(63)-P(2)	112.2(3)	C(68)-C(67)-H(67B)	109.3
C(68)-C(63)-P(2)	117.2(3)	H(67A)-C(67)-H(67B)	107.9
C(64)-C(63)-H(63A)	105.9	C(67)-C(68)-C(63)	110.2(3)
C(68)-C(63)-H(63A)	105.9	C(67)-C(68)-H(68A)	109.6
P(2)-C(63)-H(63A)	105.9	C(63)-C(68)-H(68A)	109.6
C(65)-C(64)-C(63)	111.6(3)	C(67)-C(68)-H(68B)	109.6
C(65)-C(64)-H(64A)	109.3	C(63)-C(68)-H(68B)	109.6
C(63)-C(64)-H(64A)	109.3	H(68A)-C(68)-H(68B)	108.1
C(65)-C(64)-H(64B)	109.3	O(1S)-S(1S)-C(2S)	107.7(2)
C(63)-C(64)-H(64B)	109.3	O(1S)-S(1S)-C(1S)	107.3(2)
H(64A)-C(64)-H(64B)	108.0	C(2S)-S(1S)-C(1S)	97.2(2)
C(64)-C(65)-C(66)	110.5(3)	S(1S)-C(1S)-H(1SB)	109.5
C(64)-C(65)-H(65A)	109.6	S(1S)-C(1S)-H(1SC)	109.5
C(66)-C(65)-H(65A)	109.6	H(1SB)-C(1S)-H(1SC)	109.5
C(64)-C(65)-H(65B)	109.6	S(1S)-C(1S)-H(1SD)	109.5
C(66)-C(65)-H(65B)	109.6	H(1SB)-C(1S)-H(1SD)	109.5
H(65A)-C(65)-H(65B)	108.1	H(1SC)-C(1S)-H(1SD)	109.5
C(67)-C(66)-C(65)	111.6(4)	S(1S)-C(2S)-H(2SA)	109.5
C(67)-C(66)-H(66A)	109.3	S(1S)-C(2S)-H(2SB)	109.5
C(65)-C(66)-H(66A)	109.3	H(2SA)-C(2S)-H(2SB)	109.5
C(67)-C(66)-H(66B)	109.3	S(1S)-C(2S)-H(2SC)	109.5
C(65)-C(66)-H(66B)	109.3	H(2SA)-C(2S)-H(2SC)	109.5
H(66A)-C(66)-H(66B)	108.0	H(2SB)-C(2S)-H(2SC)	109.5
C(66)-C(67)-C(68)	111.7(3)		

Table 5. Crystal data and structure refinement for **149b**.

Identification code	jso285b.	
Empirical formula	C34 H50 Co2 N O6 P S	
Formula weight	749.64	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 14.3472(16) Å	α= 90°.
	b = 14.5361(17) Å	β= 90°.
	c = 17.177(2) Å	γ= 90°.
Volume	3582.3(7) $Å^3$	
Z	4	
Density (calculated)	1.390 Mg/m^3	
Absorption coefficient	1.072 mm^{-1}	
F(000)	1576	
Crystal size	0.20 x 0.12 x 0.07 mm^3	
Theta range for data collection	1.84 to 28.33°.	
Index ranges	-19<=h<=18, -19<=k<=19, -22<=l<=22	
Reflections collected	48797	
Independent reflections	8898 [R(int) = 0.1566]	
Completeness to theta = 28.33°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9287 and 0.8142	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8898 / 0 / 407	
Goodness-of-fit on F^2	0.983	
Final R indices [I>2sigma(I)]	R1 = 0.0563, wR2 = 0.0749	
R indices (all data)	R1 = 0.1043, wR2 = 0.0854	
Absolute structure parameter	-0.009(14)	
Extinction coefficient	0.00070(13)	
Largest diff. peak and hole	0.481 and -0.416 $e.Å^{-3}$	

Table 6. Bond lengths [Å] and angles [°] for JSO-285B.

Co(1)-C(8)	1.754(4)	C(25)-C(26)	1.527(5)
Co(1)-C(9)	1.795(4)	C(26)-C(27)	1.517(5)
Co(1)-C(2)	1.943(4)	C(27)-C(28)	1.524(5)
Co(1)-C(3)	1.956(4)	C(29)-C(30)	1.534(5)
Co(1)-P(1)	2.2182(12)	C(29)-C(34)	1.537(5)
Co(1)-Co(2)	2.4683(7)	C(30)-C(31)	1.531(5)
Co(2)-C(11)	1.762(5)	C(31)-C(32)	1.524(6)
Co(2)-C(10)	1.789(4)	C(32)-C(33)	1.521(5)
Co(2)-C(3)	1.939(4)	C(33)-C(34)	1.532(5)
Co(2)-C(2)	1.948(4)		
Co(2)-S(1)	2.2570(11)	C(8)-Co(1)-C(9)	97.19(18)
P(1)-C(23)	1.837(4)	C(8)-Co(1)-C(2)	105.95(17)
P(1)-C(12)	1.838(4)	C(9)-Co(1)-C(2)	104.27(17)
P(1)-C(29)	1.853(4)	C(8)-Co(1)-C(3)	104.41(17)
S(1)-C(12)	1.819(4)	C(9)-Co(1)-C(3)	142.23(17)
S(1)-C(13)	1.831(3)	C(2)-Co(1)-C(3)	40.15(15)
O(1)-C(1)	1.238(4)	C(8)-Co(1)-P(1)	96.10(13)
O(2)-C(8)	1.154(4)	C(9)-Co(1)-P(1)	109.97(14)
O(3)-C(9)	1.145(4)	C(2)-Co(1)-P(1)	136.22(12)
O(4)-C(10)	1.157(4)	C(3)-Co(1)-P(1)	98.24(12)
O(5)-C(11)	1.151(5)	C(8)-Co(1)-Co(2)	153.49(13)
O(6)-C(12)	1.414(4)	C(9)-Co(1)-Co(2)	100.82(12)
O(6)-C(19)	1.457(4)	C(2)-Co(1)-Co(2)	50.70(11)
N(1)-C(1)	1.365(5)	C(3)-Co(1)-Co(2)	50.36(11)
N(1)-C(4)	1.464(5)	P(1)-Co(1)-Co(2)	95.84(4)
N(1)-C(6)	1.466(5)	C(11)-Co(2)-C(10)	105.48(19)
C(1)-C(2)	1.476(5)	C(11)-Co(2)-C(3)	99.75(18)
C(2)-C(3)	1.339(5)	C(10)-Co(2)-C(3)	141.84(17)
C(4)-C(5)	1.514(6)	C(11)-Co(2)-C(2)	98.13(17)
C(6)-C(7)	1.505(6)	C(10)-Co(2)-C(2)	107.06(16)
C(13)-C(14)	1.517(5)	C(3)-Co(2)-C(2)	40.30(15)
C(14)-C(15)	1.549(5)	C(11)-Co(2)-S(1)	104.66(14)
C(14)-C(19)	1.560(5)	C(10)-Co(2)-S(1)	95.71(12)
C(14)-C(20)	1.570(5)	C(3)-Co(2)-S(1)	105.13(12)
C(15)-C(16)	1.564(5)	C(2)-Co(2)-S(1)	142.03(11)
C(16)-C(17)	1.548(5)	C(11)-Co(2)-Co(1)	147.07(14)
C(17)-C(18)	1.532(5)	C(10)-Co(2)-Co(1)	95.04(13)
C(17)-C(20)	1.547(5)	C(3)-Co(2)-Co(1)	51.00(12)
C(18)-C(19)	1.538(5)	C(2)-Co(2)-Co(1)	50.55(10)
C(20)-C(22)	1.532(5)	S(1)-Co(2)-Co(1)	98.46(3)
C(20)-C(21)	1.543(5)	C(23)-P(1)-C(12)	104.24(17)
C(23)-C(24)	1.536(5)	C(23)-P(1)-C(29)	104.96(17)
C(23)-C(28)	1.545(5)	C(12)-P(1)-C(29)	101.87(17)
C(24)-C(25)	1.529(5)	C(23)-P(1)-Co(1)	118.32(13)

C(12)-P(1)-Co(1)	110.85(13)	C(15)-C(14)-C(20)	102.0(3)
C(29)-P(1)-Co(1)	114.85(13)	C(19)-C(14)-C(20)	103.3(3)
C(12)-S(1)-C(13)	94.09(17)	C(14)-C(15)-C(16)	104.0(3)
C(12)-S(1)-Co(2)	105.76(12)	C(17)-C(16)-C(15)	102.3(3)
C(13)-S(1)-Co(2)	117.25(12)	C(18)-C(17)-C(20)	102.9(3)
C(12)-O(6)-C(19)	110.8(3)	C(18)-C(17)-C(16)	105.9(3)
C(1)-N(1)-C(4)	123.3(3)	C(20)-C(17)-C(16)	103.1(3)
C(1)-N(1)-C(6)	120.2(3)	C(17)-C(18)-C(19)	103.9(3)
C(4)-N(1)-C(6)	116.3(3)	O(6)-C(19)-C(18)	108.1(3)
O(1)-C(1)-N(1)	121.5(4)	O(6)-C(19)-C(14)	114.9(3)
O(1)-C(1)-C(2)	121.3(4)	C(18)-C(19)-C(14)	103.3(3)
N(1)-C(1)-C(2)	117.2(3)	C(22)-C(20)-C(21)	107.3(3)
C(3)-C(2)-C(1)	149.1(4)	C(22)-C(20)-C(17)	113.2(3)
C(3)-C(2)-Co(1)	70.4(2)	C(21)-C(20)-C(17)	113.6(3)
C(1)-C(2)-Co(1)	134.6(3)	C(22)-C(20)-C(14)	116.6(3)
C(3)-C(2)-Co(2)	69.5(2)	C(21)-C(20)-C(14)	112.5(3)
C(1)-C(2)-Co(2)	125.7(3)	C(17)-C(20)-C(14)	93.4(3)
Co(1)-C(2)-Co(2)	78.74(14)	C(24)-C(23)-C(28)	111.8(3)
C(2)-C(3)-Co(2)	70.2(2)	C(24)-C(23)-P(1)	111.4(2)
C(2)-C(3)-Co(1)	69.4(2)	C(28)-C(23)-P(1)	109.3(3)
Co(2)-C(3)-Co(1)	78.64(15)	C(25)-C(24)-C(23)	112.2(3)
N(1)-C(4)-C(5)	112.9(4)	C(26)-C(25)-C(24)	111.3(3)
N(1)-C(6)-C(7)	112.9(4)	C(27)-C(26)-C(25)	110.4(3)
O(2)-C(8)-Co(1)	177.9(4)	C(26)-C(27)-C(28)	111.3(3)
O(3)-C(9)-Co(1)	176.5(4)	C(27)-C(28)-C(23)	111.8(3)
O(4)-C(10)-Co(2)	175.4(4)	C(30)-C(29)-C(34)	109.9(3)
O(5)-C(11)-Co(2)	175.8(4)	C(30)-C(29)-P(1)	116.4(3)
O(6)-C(12)-S(1)	109.0(2)	C(34)-C(29)-P(1)	111.3(3)
O(6)-C(12)-P(1)	114.5(3)	C(31)-C(30)-C(29)	110.8(3)
S(1)-C(12)-P(1)	112.30(19)	C(32)-C(31)-C(30)	111.6(4)
C(14)-C(13)-S(1)	112.1(3)	C(33)-C(32)-C(31)	111.0(3)
C(13)-C(14)-C(15)	111.5(3)	C(32)-C(33)-C(34)	110.8(3)
C(13)-C(14)-C(19)	115.4(3)	C(33)-C(34)-C(29)	111.5(3)
C(15)-C(14)-C(19)	102.0(3)		
C(13)-C(14)-C(20)	120.4(3)		

Table 7. Crystal data and structure refinement for **153a**.

Identification code	xv323a	
Empirical formula	C36 H37 Co2 O7 P S2	
Formula weight	794.61	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 10.58900(10) Å	α= 90°.
	b = 16.9708(2) Å	β= 90°.
	c = 20.9719(2) Å	γ = 90°.
Volume	3768.73(7) $Å^3$	
Z	4	
Density (calculated)	1.400 Mg/m^3	
Absorption coefficient	1.078 mm^{-1}	
F(000)	1640	
Crystal size	0.40 x 0.20 x 0.20 mm^3	
Theta range for data collection	1.54 to 28.28°.	
Index ranges	-14<=h<=13, -20<=k<=22, -27<=l<=18	
Reflections collected	25918	
Independent reflections	9231 [R(int) = 0.0497]	
Completeness to theta = 28.28°	99.5 %	
Absorption correction	Empirical	
Max. and min. transmission	0.8132 and 0.6723	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9231 / 0 / 437	
Goodness-of-fit on F^2	1.088	
Final R indices [I>2sigma(I)]	R1 = 0.0494, wR2 = 0.0734	
R indices (all data)	R1 = 0.0950, wR2 = 0.0876	
Absolute structure parameter	0.009(13)	
Largest diff. peak and hole	0.268 and -0.330 $e.Å^{-3}$	

Table 8. Bond lengths [Å] and angles [°] for xv323a.

Co(1)-C(2)	1.762(5)	P(1)-C(12)	1.857(3)	C(17)-C(18)	1.376(5)
Co(1)-C(1)	1.797(5)	O(1)-C(1)	1.140(5)	C(18)-C(19)	1.366(6)
Co(1)-C(29)	1.913(4)	O(2)-C(2)	1.148(5)	C(19)-C(20)	1.351(6)
Co(1)-C(28)	1.930(4)	O(3)-C(3)	1.143(4)	C(20)-C(21)	1.384(5)
Co(1)-S(1)	2.2775(10)	O(4)-C(4)	1.139(4)	C(22)-C(27)	1.384(5)
Co(1)-Co(2)	2.4802(7)	O(5)-C(12)	1.394(4)	C(22)-C(23)	1.384(5)
Co(2)-C(4)	1.772(4)	O(5)-C(11)	1.438(4)	C(23)-C(24)	1.371(5)
Co(2)-C(3)	1.778(4)	C(5)-C(13)	1.527(5)	C(24)-C(25)	1.365(6)
Co(2)-C(28)	1.930(4)	C(5)-C(14)	1.530(5)	C(25)-C(26)	1.376(5)
Co(2)-C(29)	1.939(4)	C(5)-C(6)	1.548(5)	C(26)-C(27)	1.381(5)
Co(2)-P(1)	2.2338(10)	C(6)-C(11)	1.531(5)	C(28)-C(29)	1.341(5)
S(1)-C(12)	1.822(3)	C(6)-C(7)	1.545(5)	C(30)-C(35)	1.383(5)
S(1)-C(5)	1.869(4)	C(7)-C(8)	1.522(7)	C(30)-C(31)	1.400(5)
S(2)-O(7)	1.438(3)	C(8)-C(9)	1.514(6)	C(31)-C(32)	1.376(5)
S(2)-O(6)	1.443(3)	C(9)-C(15)	1.525(6)	C(32)-C(33)	1.371(6)
S(2)-C(28)	1.739(4)	C(9)-C(10)	1.526(5)	C(33)-C(34)	1.379(6)
S(2)-C(30)	1.760(4)	C(10)-C(11)	1.508(5)	C(33)-C(36)	1.515(5)
P(1)-C(16)	1.822(3)	C(16)-C(17)	1.383(5)	C(34)-C(35)	1.374(5)
P(1)-C(22)	1.828(3)	C(16)-C(21)	1.389(5)		

C(2)-Co(1)-C(1)	98.3(2)	C(3)-Co(2)-C(28)	142.29(17)
C(2)-Co(1)-C(29)	100.78(19)	C(4)-Co(2)-C(29)	100.32(18)
C(1)-Co(1)-C(29)	103.49(18)	C(3)-Co(2)-C(29)	105.44(17)
C(2)-Co(1)-C(28)	101.50(19)	C(28)-Co(2)-C(29)	40.56(14)
C(1)-Co(1)-C(28)	141.83(17)	C(4)-Co(2)-P(1)	104.46(14)
C(29)-Co(1)-C(28)	40.85(14)	C(3)-Co(2)-P(1)	104.41(13)
C(2)-Co(1)-S(1)	106.73(16)	C(28)-Co(2)-P(1)	99.95(11)
C(1)-Co(1)-S(1)	100.18(15)	C(29)-Co(2)-P(1)	137.90(12)
C(29)-Co(1)-S(1)	140.37(11)	C(4)-Co(2)-Co(1)	148.88(15)
C(28)-Co(1)-S(1)	104.81(11)	C(3)-Co(2)-Co(1)	98.10(13)
C(2)-Co(1)-Co(2)	148.80(15)	C(28)-Co(2)-Co(1)	50.01(10)
C(1)-Co(1)-Co(2)	100.09(14)	C(29)-Co(2)-Co(1)	49.45(11)
C(29)-Co(1)-Co(2)	50.37(11)	P(1)-Co(2)-Co(1)	97.47(3)
C(28)-Co(1)-Co(2)	50.01(11)	C(12)-S(1)-C(5)	97.62(16)
S(1)-Co(1)-Co(2)	94.56(3)	C(12)-S(1)-Co(1)	106.94(11)
C(4)-Co(2)-C(3)	97.51(18)	C(5)-S(1)-Co(1)	118.44(13)
C(4)-Co(2)-C(28)	103.79(17)	O(7)-S(2)-O(6)	118.28(18)

O(7)-S(2)-C(28)	107.69(17)	S(1)-C(12)-P(1)	107.77(17)
O(6)-S(2)-C(28)	109.82(17)	C(17)-C(16)-C(21)	117.9(3)
O(7)-S(2)-C(30)	108.29(17)	C(17)-C(16)-P(1)	122.8(3)
O(6)-S(2)-C(30)	107.88(17)	C(21)-C(16)-P(1)	119.3(3)
C(28)-S(2)-C(30)	103.93(17)	C(18)-C(17)-C(16)	120.6(4)
C(16)-P(1)-C(22)	103.97(16)	C(19)-C(18)-C(17)	120.6(4)
C(16)-P(1)-C(12)	101.43(15)	C(20)-C(19)-C(18)	119.8(4)
C(22)-P(1)-C(12)	103.75(15)	C(19)-C(20)-C(21)	120.5(4)
C(16)-P(1)-Co(2)	118.99(11)	C(20)-C(21)-C(16)	120.6(4)
C(22)-P(1)-Co(2)	117.53(11)	C(27)-C(22)-C(23)	117.4(3)
C(12)-P(1)-Co(2)	109.05(11)	C(27)-C(22)-P(1)	124.9(3)
C(12)-O(5)-C(11)	114.0(2)	C(23)-C(22)-P(1)	117.7(3)
O(1)-C(1)-Co(1)	173.7(5)	C(24)-C(23)-C(22)	121.9(4)
O(2)-C(2)-Co(1)	176.3(5)	C(25)-C(24)-C(23)	119.8(4)
O(3)-C(3)-Co(2)	178.2(4)	C(24)-C(25)-C(26)	119.8(4)
O(4)-C(4)-Co(2)	175.3(4)	C(25)-C(26)-C(27)	120.0(4)
C(13)-C(5)-C(14)	111.0(3)	C(26)-C(27)-C(22)	120.9(3)
C(13)-C(5)-C(6)	111.8(3)	C(29)-C(28)-S(2)	132.9(3)
C(14)-C(5)-C(6)	113.7(3)	C(29)-C(28)-Co(2)	70.1(2)
C(13)-C(5)-S(1)	103.2(3)	S(2)-C(28)-Co(2)	142.3(2)
C(14)-C(5)-S(1)	111.2(2)	C(29)-C(28)-Co(1)	68.9(2)
C(6)-C(5)-S(1)	105.3(2)	S(2)-C(28)-Co(1)	132.5(2)
C(11)-C(6)-C(7)	108.1(3)	Co(2)-C(28)-Co(1)	79.98(14)
C(11)-C(6)-C(5)	115.1(3)	C(28)-C(29)-Co(1)	70.3(2)
C(7)-C(6)-C(5)	112.5(3)	C(28)-C(29)-Co(2)	69.4(2)
C(8)-C(7)-C(6)	111.5(4)	Co(1)-C(29)-Co(2)	80.18(15)
C(9)-C(8)-C(7)	112.5(4)	C(35)-C(30)-C(31)	120.2(3)
C(8)-C(9)-C(15)	111.9(3)	C(35)-C(30)-S(2)	120.7(3)
C(8)-C(9)-C(10)	108.8(4)	C(31)-C(30)-S(2)	119.1(3)
C(15)-C(9)-C(10)	111.3(4)	C(32)-C(31)-C(30)	118.0(4)
C(11)-C(10)-C(9)	114.4(3)	C(33)-C(32)-C(31)	122.6(4)
O(5)-C(11)-C(10)	105.7(3)	C(32)-C(33)-C(34)	118.2(4)
O(5)-C(11)-C(6)	112.5(3)	C(32)-C(33)-C(36)	121.5(5)
C(10)-C(11)-C(6)	111.8(3)	C(34)-C(33)-C(36)	120.2(5)
O(5)-C(12)-S(1)	110.2(2)	C(35)-C(34)-C(33)	121.4(4)
O(5)-C(12)-P(1)	112.1(2)	C(34)-C(35)-C(30)	119.5(4)

Table 9. Crystal data and structure refinement for **172**.

Identification code	jso247g
Empirical formula	C23 H30 B O2 P S
Formula weight	412.31
Temperature	273(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 7.1021(2) Å α= 90°. b = 16.3353(5) Å β= 90°. c = 18.7391(5) Å γ= 90°.
Volume	2174.02(11) $Å^3$
Z	4
Density (calculated)	1.260 Mg/m^3
Absorption coefficient	2.132 mm^{-1}
F(000)	880
Crystal size	0.5 x 0.1 x 0.05 mm^3
Theta range for data collection	3.59 to 72.09°.
Index ranges	$-7 \le h \le 8$, $-19 \le k \le 20$, $-22 \le l \le 22$
Reflections collected	16848
Independent reflections	4091 [R(int) = 0.0649]
Completeness to theta = 72.09°	97.7 %
Absorption correction	SADABS (Bruker-AXS)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4091 / 0 / 374
Goodness-of-fit on F^2	1.088
Final R indices [I>2sigma(I)]	R1 = 0.0610, wR2 = 0.1743
R indices (all data)	R1 = 0.0614, wR2 = 0.1752
Absolute structure parameter	0.01(2)
Extinction coefficient	0.0070(9)
Largest diff. peak and hole	0.644 and -0.548 $e.Å^{-3}$

Table 10. Bond lengths [Å] and angles [°] for jso247g.

S(1)-O(2)	1.494(2)	C(2)-C(3)	1.513(5)	C(13)-C(14)	1.387(5)
S(1)-C(11)	1.820(4)	C(3)-C(4)	1.534(6)	C(14)-C(15)	1.387(6)
S(1)-C(10)	1.840(3)	C(3)-C(7)	1.541(5)	C(15)-C(16)	1.379(6)
O(1)-C(10)	1.403(4)	C(4)-C(5)	1.560(5)	C(16)-C(17)	1.389(5)
O(1)-C(1)	1.441(4)	C(5)-C(6)	1.543(5)	C(18)-C(23)	1.393(5)
C(1)-C(6)	1.534(5)	C(6)-C(11)	1.516(5)	C(18)-C(19)	1.395(5)
C(1)-C(2)	1.538(4)	C(6)-C(7)	1.552(5)	C(19)-C(20)	1.370(5)
P(1)-C(12)	1.801(3)	C(7)-C(8)	1.524(5)	C(20)-C(21)	1.379(5)
P(1)-C(18)	1.807(3)	C(7)-C(9)	1.530(5)	C(21)-C(22)	1.384(5)
P(1)-C(10)	1.838(3)	C(12)-C(17)	1.390(5)	C(22)-C(23)	1.380(5)
P(1)-B(1)	1.915(4)	C(12)-C(13)	1.394(5)		

O(2)-S(1)-C(11)	104.67(16)	C(8)-C(7)-C(3)	114.3(3)
O(2)-S(1)-C(10)	108.96(14)	C(9)-C(7)-C(3)	113.9(3)
C(11)-S(1)-C(10)	91.89(15)	C(8)-C(7)-C(6)	115.8(3)
C(10)-O(1)-C(1)	111.6(2)	C(9)-C(7)-C(6)	113.7(3)
O(1)-C(1)-C(6)	114.3(3)	C(3)-C(7)-C(6)	92.6(3)
O(1)-C(1)-C(2)	109.4(3)	O(1)-C(10)-P(1)	109.2(2)
C(6)-C(1)-C(2)	103.1(3)	O(1)-C(10)-S(1)	105.9(2)
C(12)-P(1)-C(18)	106.34(14)	P(1)-C(10)-S(1)	112.50(17)
C(12)-P(1)-C(10)	103.48(15)	C(6)-C(11)-S(1)	115.7(2)
C(18)-P(1)-C(10)	102.58(14)	C(17)-C(12)-C(13)	119.7(3)
C(12)-P(1)-B(1)	114.60(17)	C(17)-C(12)-P(1)	119.1(3)
C(18)-P(1)-B(1)	114.68(16)	C(13)-C(12)-P(1)	121.1(3)
C(10)-P(1)-B(1)	113.83(16)	C(14)-C(13)-C(12)	120.4(3)
C(3)-C(2)-C(1)	103.2(3)	C(13)-C(14)-C(15)	119.4(4)
C(2)-C(3)-C(4)	107.9(3)	C(16)-C(15)-C(14)	120.5(3)
C(2)-C(3)-C(7)	102.6(3)	C(15)-C(16)-C(17)	120.3(3)
C(4)-C(3)-C(7)	103.2(3)	C(16)-C(17)-C(12)	119.6(3)
C(3)-C(4)-C(5)	102.3(3)	C(23)-C(18)-C(19)	118.9(3)
C(6)-C(5)-C(4)	103.1(3)	C(23)-C(18)-P(1)	119.1(3)
C(11)-C(6)-C(1)	114.4(3)	C(19)-C(18)-P(1)	122.0(2)
C(11)-C(6)-C(5)	112.1(3)	C(20)-C(19)-C(18)	120.7(3)
C(1)-C(6)-C(5)	104.0(3)	C(19)-C(20)-C(21)	120.0(4)
C(11)-C(6)-C(7)	118.9(3)	C(20)-C(21)-C(22)	120.1(3)
C(1)-C(6)-C(7)	103.9(3)	C(23)-C(22)-C(21)	120.2(3)
C(5)-C(6)-C(7)	101.9(3)	C(22)-C(23)-C(18)	120.0(3)
C(8)-C(7)-C(9)	106.5(3)		

Table 11. Crystal data and structure refinement **176b**.

Identification code	jso299a_0m
Empirical formula	C79 H102 Co4 O20 P2 S6
Formula weight	1861.63
Temperature	273(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 15.1494(11) Å α= 90°. b = 10.6925(8) Å β= 102.233(2)°. c = 26.314(2) Å γ = 90°.
Volume	4165.7(5) Å^3
Z	2
Density (calculated)	1.484 Mg/m^3
Absorption coefficient	1.041 mm^{-1}
F(000)	1940
Crystal size	0.50 x 0.20 x 0.10 mm^3
Theta range for data collection	2.57 to 39.42°.
Index ranges	$-26 \le h \le 24$, $-13 \le k \le 18$, $-28 \le l \le 47$
Reflections collected	82318
Independent reflections	40305 [R(int) = 0.0316]
Completeness to theta = 39.42°	97.9 %
Absorption correction	SADABS (Bruker-AXS)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	40305 / 1 / 1000
Goodness-of-fit on F^2	0.999
Final R indices [I>2sigma(I)]	R1 = 0.0311, wR2 = 0.0746
R indices (all data)	R1 = 0.0368, wR2 = 0.0761
Absolute structure parameter	0.007(3)
Largest diff. peak and hole	1.283 and -0.594 e.Å^{-3}

Table 12. Bond lengths [Å] and angles [°] for JSO299A_0m.

Co(1A)-C(24A)	1.7996(13)	C(7A)-C(8A)	1.5303(16)
Co(1A)-C(25A)	1.8090(13)	C(7A)-C(9A)	1.5610(17)
Co(1A)-C(29A)	1.9215(11)	C(9A)-C(11A)	1.527(2)
Co(1A)-C(28A)	1.9665(11)	C(9A)-C(10A)	1.545(2)
Co(1A)-P(1A)	2.2269(4)	C(12A)-C(13A)	1.3900(18)
Co(1A)-Co(2A)	2.4492(2)	C(12A)-C(17A)	1.3968(19)
P(1A)-C(18A)	1.8225(12)	C(13A)-C(14A)	1.3948(19)
P(1A)-C(12A)	1.8270(12)	C(14A)-C(15A)	1.375(3)
P(1A)-C(1A)	1.8645(12)	C(15A)-C(16A)	1.381(3)
O(1A)-C(1A)	1.3967(14)	C(16A)-C(17A)	1.392(2)
O(1A)-C(2A)	1.4479(15)	C(18A)-C(23A)	1.3976(16)
C(1A)-S(1A)	1.8662(11)	C(18A)-C(19A)	1.4021(17)
Co(2A)-C(26A)	1.8052(13)	C(19A)-C(20A)	1.3904(18)
Co(2A)-C(27A)	1.8103(13)	C(20A)-C(21A)	1.3858(18)
Co(2A)-C(28A)	1.9330(11)	C(21A)-C(22A)	1.3888(18)
Co(2A)-C(29A)	1.9584(11)	C(22A)-C(23A)	1.3919(18)
Co(2A)-S(1A)	2.2001(3)	C(28A)-C(29A)	1.3721(15)
S(2A)-O(8A)	1.4431(11)	C(30A)-C(33A)	1.518(2)
S(2A)-O(7A)	1.4452(11)	C(30A)-C(32A)	1.525(2)
S(2A)-C(29A)	1.7488(11)	C(30A)-C(31A)	1.5326(18)
S(2A)-C(30A)	1.8279(13)	C(34A)-C(36A)	1.5182(18)
C(2A)-C(3A)	1.5423(16)	C(34A)-C(35A)	1.5264(18)
C(2A)-C(7A)	1.5528(16)	C(34A)-C(37A)	1.5269(19)
O(2A)-S(1A)	1.4767(9)	S(1B)-O(2B)	1.4813(9)
S(3A)-O(10A)	1.4438(10)	S(1B)-C(8B)	1.7965(13)
S(3A)-O(9A)	1.4466(9)	S(1B)-C(1B)	1.8745(12)
S(3A)-C(28A)	1.7581(12)	S(1B)-Co(4)	2.2018(3)
S(3A)-C(34A)	1.8245(13)	P(1B)-C(18B)	1.8292(13)
O(3A)-C(24A)	1.1366(16)	P(1B)-C(12B)	1.8346(12)
C(3A)-C(4A)	1.541(2)	P(1B)-C(1B)	1.8619(12)
O(4A)-C(25A)	1.1353(16)	P(1B)-Co(3)	2.2292(4)
C(4A)-C(5A)	1.541(2)	O(1B)-C(1B)	1.3993(14)
C(4A)-C(9A)	1.5475(18)	O(1B)-C(2B)	1.4437(15)
S(1A)-C(8A)	1.7956(12)	S(2B)-O(8B)	1.4438(13)
O(5A)-C(26A)	1.1405(16)	S(2B)-O(7B)	1.4453(11)
C(5A)-C(6A)	1.567(2)	S(2B)-C(28B)	1.7490(12)
O(6A)-C(27A)	1.1364(16)	S(2B)-C(30B)	1.8272(17)
C(6A)-C(7A)	1.5440(18)	C(2B)-C(3B)	1.5387(17)

C(2B)-C(7B)	1.5545(16)	C(9B)-C(11B)	1.540(2)
Co(3)-C(24B)	1.7993(13)	C(12B)-C(17B)	1.3997(18)
Co(3)-C(25B)	1.8048(13)	C(12B)-C(13B)	1.4002(18)
Co(3)-C(28B)	1.9142(13)	C(13B)-C(14B)	1.3958(19)
Co(3)-C(29B)	1.9760(12)	C(14B)-C(15B)	1.382(2)
Co(3)-Co(4)	2.4466(3)	C(15B)-C(16B)	1.394(2)
S(3B)-O(9B)	1.4464(12)	C(16B)-C(17B)	1.3894(18)
S(3B)-O(10B)	1.4502(10)	C(18B)-C(23B)	1.3983(19)
S(3B)-C(29B)	1.7510(11)	C(18B)-C(19B)	1.4021(19)
S(3B)-C(34B)	1.8232(15)	C(19B)-C(20B)	1.395(2)
O(3B)-C(24B)	1.1405(17)	C(20B)-C(21B)	1.383(3)
C(3B)-C(4B)	1.5370(19)	C(21B)-C(22B)	1.385(3)
Co(4)-C(26B)	1.8089(13)	C(22B)-C(23B)	1.392(2)
Co(4)-C(27B)	1.8138(14)	C(28B)-C(29B)	1.3734(17)
Co(4)-C(29B)	1.9233(11)	C(30B)-C(31B)	1.522(2)
Co(4)-C(28B)	1.9643(12)	C(30B)-C(32B)	1.525(3)
O(4B)-C(25B)	1.1404(16)	C(30B)-C(33B)	1.538(2)
C(4B)-C(9B)	1.5433(19)	C(34B)-C(37B)	1.521(3)
C(4B)-C(5B)	1.559(2)	C(34B)-C(35B)	1.527(2)
O(5B)-C(26B)	1.1382(16)	C(34B)-C(36B)	1.535(2)
C(5B)-C(6B)	1.563(2)	C(1L)-C(2L)	1.26(2)
O(6B)-C(27B)	1.1375(18)	C(2L)-C(3L)	1.669(14)
C(6B)-C(7B)	1.5340(19)	C(2L)-C(5L)#1	2.23(4)
C(7B)-C(8B)	1.5255(17)	C(3L)-C(4L)	1.763(14)
C(7B)-C(9B)	1.5656(18)	C(4L)-C(5L)	1.22(3)
C(9B)-C(10B)	1.530(2)	C(5L)-C(2L)#2	2.23(4)

C(24A)-Co(1A)-C(25A)	98.76(6)	P(1A)-Co(1A)-Co(2A)	93.200(11)
C(24A)-Co(1A)-C(29A)	110.38(5)	C(18A)-P(1A)-C(12A)	103.88(6)
C(25A)-Co(1A)-C(29A)	99.61(5)	C(18A)-P(1A)-C(1A)	104.15(5)
C(24A)-Co(1A)-C(28A)	101.03(5)	C(12A)-P(1A)-C(1A)	103.06(5)
C(25A)-Co(1A)-C(28A)	140.52(5)	C(18A)-P(1A)-Co(1A)	117.50(4)
C(29A)-Co(1A)-C(28A)	41.31(5)	C(12A)-P(1A)-Co(1A)	113.72(4)
C(24A)-Co(1A)-P(1A)	94.82(4)	C(1A)-P(1A)-Co(1A)	113.00(4)
C(25A)-Co(1A)-P(1A)	104.37(4)	C(1A)-O(1A)-C(2A)	112.25(9)
C(29A)-Co(1A)-P(1A)	141.90(3)	O(1A)-C(1A)-P(1A)	110.10(8)
C(28A)-Co(1A)-P(1A)	107.57(3)	O(1A)-C(1A)-S(1A)	114.44(8)
C(24A)-Co(1A)-Co(2A)	151.46(4)	P(1A)-C(1A)-S(1A)	110.49(6)
C(25A)-Co(1A)-Co(2A)	105.68(4)	C(26A)-Co(2A)-C(27A)	99.71(6)
C(29A)-Co(1A)-Co(2A)	51.53(3)	C(26A)-Co(2A)-C(28A)	140.11(5)
C(28A)-Co(1A)-Co(2A)	50.48(3)	C(27A)-Co(2A)-C(28A)	105.64(5)

C(26A)-Co(2A)-C(29A)	102.66(5)	C(6A)-C(7A)-C(2A)	103.94(10)
C(27A)-Co(2A)-C(29A)	105.02(5)	C(8A)-C(7A)-C(9A)	114.60(10)
C(28A)-Co(2A)-C(29A)	41.29(5)	C(6A)-C(7A)-C(9A)	102.51(10)
C(26A)-Co(2A)-S(1A)	107.54(4)	C(2A)-C(7A)-C(9A)	103.58(10)
C(27A)-Co(2A)-S(1A)	95.10(4)	C(7A)-C(8A)-S(1A)	110.72(8)
C(28A)-Co(2A)-S(1A)	100.39(3)	C(11A)-C(9A)-C(10A)	106.94(12)
C(29A)-Co(2A)-S(1A)	140.06(3)	C(11A)-C(9A)-C(4A)	113.70(13)
C(26A)-Co(2A)-Co(1A)	94.51(4)	C(10A)-C(9A)-C(4A)	114.33(11)
C(27A)-Co(2A)-Co(1A)	153.95(4)	C(11A)-C(9A)-C(7A)	115.98(11)
C(28A)-Co(2A)-Co(1A)	51.70(3)	C(10A)-C(9A)-C(7A)	113.05(12)
C(29A)-Co(2A)-Co(1A)	50.19(3)	C(4A)-C(9A)-C(7A)	92.68(9)
S(1A)-Co(2A)-Co(1A)	101.297(10)	C(13A)-C(12A)-C(17A)	118.95(12)
O(8A)-S(2A)-O(7A)	117.41(7)	C(13A)-C(12A)-P(1A)	122.74(10)
O(8A)-S(2A)-C(29A)	106.52(6)	C(17A)-C(12A)-P(1A)	117.74(10)
O(7A)-S(2A)-C(29A)	108.24(6)	C(12A)-C(13A)-C(14A)	119.94(14)
O(8A)-S(2A)-C(30A)	107.71(6)	C(15A)-C(14A)-C(13A)	120.88(15)
O(7A)-S(2A)-C(30A)	108.15(6)	C(14A)-C(15A)-C(16A)	119.59(13)
C(29A)-S(2A)-C(30A)	108.54(6)	C(15A)-C(16A)-C(17A)	120.29(16)
O(1A)-C(2A)-C(3A)	111.04(10)	C(16A)-C(17A)-C(12A)	120.35(15)
O(1A)-C(2A)-C(7A)	111.26(9)	C(23A)-C(18A)-C(19A)	118.52(11)
C(3A)-C(2A)-C(7A)	103.78(9)	C(23A)-C(18A)-P(1A)	119.21(9)
O(10A)-S(3A)-O(9A)	117.21(6)	C(19A)-C(18A)-P(1A)	122.25(9)
O(10A)-S(3A)-C(28A)	107.24(6)	C(20A)-C(19A)-C(18A)	120.16(11)
O(9A)-S(3A)-C(28A)	107.08(5)	C(21A)-C(20A)-C(19A)	120.85(12)
O(10A)-S(3A)-C(34A)	107.83(6)	C(20A)-C(21A)-C(22A)	119.47(12)
O(9A)-S(3A)-C(34A)	107.76(6)	C(21A)-C(22A)-C(23A)	120.07(11)
C(28A)-S(3A)-C(34A)	109.59(5)	C(22A)-C(23A)-C(18A)	120.90(11)
C(4A)-C(3A)-C(2A)	102.31(10)	O(3A)-C(24A)-Co(1A)	177.33(13)
C(3A)-C(4A)-C(5A)	107.51(11)	O(4A)-C(25A)-Co(1A)	176.40(12)
C(3A)-C(4A)-C(9A)	102.35(10)	O(5A)-C(26A)-Co(2A)	176.10(12)
C(5A)-C(4A)-C(9A)	103.08(12)	O(6A)-C(27A)-Co(2A)	178.35(12)
O(2A)-S(1A)-C(8A)	106.70(6)	C(29A)-C(28A)-S(3A)	141.38(9)
O(2A)-S(1A)-C(1A)	107.05(5)	C(29A)-C(28A)-Co(2A)	70.35(6)
C(8A)-S(1A)-C(1A)	97.16(5)	S(3A)-C(28A)-Co(2A)	144.55(6)
O(2A)-S(1A)-Co(2A)	115.39(4)	C(29A)-C(28A)-Co(1A)	67.59(7)
C(8A)-S(1A)-Co(2A)	117.50(4)	S(3A)-C(28A)-Co(1A)	123.16(6)
C(1A)-S(1A)-Co(2A)	111.14(4)	Co(2A)-C(28A)-Co(1A)	77.81(4)
C(4A)-C(5A)-C(6A)	103.35(10)	C(28A)-C(29A)-S(2A)	148.55(10)
C(7A)-C(6A)-C(5A)	102.19(11)	C(28A)-C(29A)-Co(1A)	71.10(7)
C(8A)-C(7A)-C(6A)	117.98(11)	S(2A)-C(29A)-Co(1A)	137.85(7)
C(8A)-C(7A)-C(2A)	112.59(9)	C(28A)-C(29A)-Co(2A)	68.36(6)

S(2A)-C(29A)-Co(2A)	121.31(6)	C(25B)-Co(3)-C(28B)	95.26(6)
Co(1A)-C(29A)-Co(2A)	78.28(4)	C(24B)-Co(3)-C(29B)	100.84(6)
C(33A)-C(30A)-C(32A)	113.12(14)	C(25B)-Co(3)-C(29B)	135.52(5)
C(33A)-C(30A)-C(31A)	111.31(13)	C(28B)-Co(3)-C(29B)	41.31(5)
C(32A)-C(30A)-C(31A)	109.13(12)	C(24B)-Co(3)-P(1B)	93.60(5)
C(33A)-C(30A)-S(2A)	108.90(9)	C(25B)-Co(3)-P(1B)	105.64(5)
C(32A)-C(30A)-S(2A)	109.44(10)	C(28B)-Co(3)-P(1B)	144.08(4)
C(31A)-C(30A)-S(2A)	104.58(9)	C(29B)-Co(3)-P(1B)	108.87(4)
C(36A)-C(34A)-C(35A)	111.88(12)	C(24B)-Co(3)-Co(4)	150.99(5)
C(36A)-C(34A)-C(37A)	110.69(13)	C(25B)-Co(3)-Co(4)	99.93(4)
C(35A)-C(34A)-C(37A)	109.81(11)	C(28B)-Co(3)-Co(4)	51.81(4)
C(36A)-C(34A)-S(3A)	109.25(9)	C(29B)-Co(3)-Co(4)	50.18(3)
C(35A)-C(34A)-S(3A)	109.95(8)	P(1B)-Co(3)-Co(4)	95.278(11)
C(37A)-C(34A)-S(3A)	105.03(10)	O(9B)-S(3B)-O(10B)	117.60(6)
O(2B)-S(1B)-C(8B)	107.37(6)	O(9B)-S(3B)-C(29B)	105.97(6)
O(2B)-S(1B)-C(1B)	106.94(5)	O(10B)-S(3B)-C(29B)	107.59(6)
C(8B)-S(1B)-C(1B)	96.43(6)	O(9B)-S(3B)-C(34B)	107.43(7)
O(2B)-S(1B)-Co(4)	113.28(4)	O(10B)-S(3B)-C(34B)	106.73(7)
C(8B)-S(1B)-Co(4)	119.41(4)	C(29B)-S(3B)-C(34B)	111.60(6)
C(1B)-S(1B)-Co(4)	111.63(4)	C(4B)-C(3B)-C(2B)	102.07(10)
C(18B)-P(1B)-C(12B)	104.07(6)	C(26B)-Co(4)-C(27B)	97.69(6)
C(18B)-P(1B)-C(1B)	103.28(6)	C(26B)-Co(4)-C(29B)	142.58(6)
C(12B)-P(1B)-C(1B)	101.63(5)	C(27B)-Co(4)-C(29B)	105.60(6)
C(18B)-P(1B)-Co(3)	119.71(5)	C(26B)-Co(4)-C(28B)	104.75(6)
C(12B)-P(1B)-Co(3)	115.65(4)	C(27B)-Co(4)-C(28B)	104.69(6)
C(1B)-P(1B)-Co(3)	110.36(4)	C(29B)-Co(4)-C(28B)	41.36(5)
C(1B)-O(1B)-C(2B)	111.92(9)	C(26B)-Co(4)-S(1B)	107.39(4)
O(1B)-C(1B)-P(1B)	110.19(8)	C(27B)-Co(4)-S(1B)	97.38(5)
O(1B)-C(1B)-S(1B)	114.40(8)	C(29B)-Co(4)-S(1B)	98.31(4)
P(1B)-C(1B)-S(1B)	111.37(6)	C(28B)-Co(4)-S(1B)	137.79(3)
O(8B)-S(2B)-O(7B)	117.67(7)	C(26B)-Co(4)-Co(3)	96.26(4)
O(8B)-S(2B)-C(28B)	107.81(7)	C(27B)-Co(4)-Co(3)	153.73(5)
O(7B)-S(2B)-C(28B)	106.01(6)	C(29B)-Co(4)-Co(3)	52.11(4)
O(8B)-S(2B)-C(30B)	107.90(8)	C(28B)-Co(4)-Co(3)	49.99(4)
O(7B)-S(2B)-C(30B)	106.75(7)	S(1B)-Co(4)-Co(3)	99.529(11)
C(28B)-S(2B)-C(30B)	110.66(7)	C(3B)-C(4B)-C(9B)	102.75(11)
O(1B)-C(2B)-C(3B)	112.29(10)	C(3B)-C(4B)-C(5B)	107.17(12)
O(1B)-C(2B)-C(7B)	111.24(9)	C(9B)-C(4B)-C(5B)	102.08(11)
C(3B)-C(2B)-C(7B)	104.29(9)	C(4B)-C(5B)-C(6B)	103.53(11)
C(24B)-Co(3)-C(25B)	104.14(6)	C(7B)-C(6B)-C(5B)	102.29(11)
C(24B)-Co(3)-C(28B)	109.44(6)	C(8B)-C(7B)-C(6B)	117.21(11)

C(8B)-C(7B)-C(2B)	112.72(10)
C(6B)-C(7B)-C(2B)	103.72(10)
C(8B)-C(7B)-C(9B)	115.87(10)
C(6B)-C(7B)-C(9B)	101.90(10)
C(2B)-C(7B)-C(9B)	103.70(10)
C(7B)-C(8B)-S(1B)	109.93(8)
C(10B)-C(9B)-C(11B)	107.41(13)
C(10B)-C(9B)-C(4B)	113.76(13)
C(11B)-C(9B)-C(4B)	113.59(13)
C(10B)-C(9B)-C(7B)	115.02(11)
C(11B)-C(9B)-C(7B)	113.75(12)
C(4B)-C(9B)-C(7B)	93.06(10)
C(17B)-C(12B)-C(13B)	118.88(11)
C(17B)-C(12B)-P(1B)	118.89(9)
C(13B)-C(12B)-P(1B)	121.83(10)
C(14B)-C(13B)-C(12B)	119.93(13)
C(15B)-C(14B)-C(13B)	120.82(14)
C(14B)-C(15B)-C(16B)	119.57(12)
C(17B)-C(16B)-C(15B)	120.12(14)
C(16B)-C(17B)-C(12B)	120.64(13)
C(23B)-C(18B)-C(19B)	118.51(12)
C(23B)-C(18B)-P(1B)	120.46(10)
C(19B)-C(18B)-P(1B)	121.02(10)
C(20B)-C(19B)-C(18B)	120.00(14)
C(21B)-C(20B)-C(19B)	120.86(15)
C(20B)-C(21B)-C(22B)	119.57(14)
C(21B)-C(22B)-C(23B)	120.20(15)
C(22B)-C(23B)-C(18B)	120.84(14)
O(3B)-C(24B)-Co(3)	177.57(13)
O(4B)-C(25B)-Co(3)	173.83(12)
O(5B)-C(26B)-Co(4)	175.49(12)
O(6B)-C(27B)-Co(4)	178.59(14)
C(29B)-C(28B)-S(2B)	148.26(10)
C(29B)-C(28B)-Co(3)	71.76(7)
S(2B)-C(28B)-Co(3)	137.08(8)
C(29B)-C(28B)-Co(4)	67.72(7)
S(2B)-C(28B)-Co(4)	122.76(7)
Co(3)-C(28B)-Co(4)	78.21(4)
C(28B)-C(29B)-S(3B)	137.99(10)
C(28B)-C(29B)-Co(4)	70.92(7)
S(3B)-C(29B)-Co(4)	146.77(8)
C(28B)-C(29B)-Co(3)	66.93(7)
S(3B)-C(29B)-Co(3)	123.99(7)
Co(4)-C(29B)-Co(3)	77.71(4)
C(31B)-C(30B)-C(32B)	111.08(15)
C(31B)-C(30B)-C(33B)	111.18(14)
C(32B)-C(30B)-C(33B)	110.22(17)
C(31B)-C(30B)-S(2B)	109.57(13)
C(32B)-C(30B)-S(2B)	111.34(10)
C(33B)-C(30B)-S(2B)	103.20(13)
C(37B)-C(34B)-C(35B)	112.14(15)
C(37B)-C(34B)-C(36B)	110.65(13)
C(35B)-C(34B)-C(36B)	110.39(13)
C(37B)-C(34B)-S(3B)	109.75(10)
C(35B)-C(34B)-S(3B)	109.48(11)
C(36B)-C(34B)-S(3B)	104.12(11)
C(1L)-C(2L)-C(3L)	111.9(13)
C(1L)-C(2L)-C(5L)#1	78.2(16)
C(3L)-C(2L)-C(5L)#1	158.7(8)
C(2L)-C(3L)-C(4L)	140.5(7)
C(5L)-C(4L)-C(3L)	118.4(15)
C(4L)-C(5L)-C(2L)#2	79(2)

Table 13. Crystal data and structure refinement for **191**.

Identification code	JSO 446	
Empirical formula	C23 H26 N O P S	
Formula weight	395.48	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2	
Unit cell dimensions	a = 22.5509(11) Å	α= 90°.
	b = 6.1310(3) Å	β= 119.507(2)°.
	c = 17.2557(9) Å	γ = 90°.
Volume	2076.32(18) $Å^3$	
Z	4	
Density (calculated)	1.265 Mg/m^3	
Absorption coefficient	0.246 mm^{-1}	
F(000)	840	
Crystal size	0.50 x 0.21 x 0.13 mm^3	
Theta range for data collection	1.36 to 26.37°.	
Index ranges	-28<=h<=28, -7<=k<=7, -20<=l<=21	
Reflections collected	13715	
Independent reflections	3920 [R(int) = 0.0275]	
Completeness to theta = 26.37°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9688 and 0.8871	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3920 / 1 / 244	
Goodness-of-fit on F^2	1.166	
Final R indices [I>2sigma(I)]	R1 = 0.0249, wR2 = 0.0689	
R indices (all data)	R1 = 0.0271, wR2 = 0.0823	
Absolute structure parameter	0.04(6)	
Largest diff. peak and hole	0.230 and -0.297 $e.Å^{-3}$	

Table 14. Bond lengths [Å] and angles [°] for JSO 446.

S(1)-O(1)	1.4891(14)	C(8)-C(9)	1.398(3)
S(1)-N(1)	1.6794(17)	C(9)-C(10)	1.391(3)
S(1)-C(20)	1.8605(19)	C(10)-C(11)	1.381(3)
P(1)-N(1)	1.7283(16)	C(11)-C(12)	1.386(3)
P(1)-C(14)	1.8321(19)	C(12)-C(13)	1.397(3)
P(1)-C(8)	1.8408(18)	C(14)-C(15)	1.385(3)
N(1)-C(1)	1.498(2)	C(14)-C(19)	1.402(3)
C(1)-C(2)	1.512(2)	C(15)-C(16)	1.397(3)
C(2)-C(3)	1.386(3)	C(16)-C(17)	1.381(3)
C(2)-C(7)	1.392(3)	C(17)-C(18)	1.383(3)
C(3)-C(4)	1.391(3)	C(18)-C(19)	1.383(3)
C(4)-C(5)	1.385(3)	C(20)-C(21)	1.518(3)
C(5)-C(6)	1.374(3)	C(20)-C(23)	1.519(3)
C(6)-C(7)	1.394(3)	C(20)-C(22)	1.532(3)
C(8)-C(13)	1.394(3)		
		C(8)-C(13)-C(12)	120.60(19)
O(1)-S(1)-N(1)	107.75(8)	C(15)-C(14)-C(19)	118.68(18)
O(1)-S(1)-C(20)	104.24(8)	C(15)-C(14)-P(1)	125.58(14)
N(1)-S(1)-C(20)	104.19(8)	C(19)-C(14)-P(1)	115.74(15)
N(1)-P(1)-C(14)	106.34(8)	C(14)-C(15)-C(16)	120.66(19)
N(1)-P(1)-C(8)	102.83(8)	C(17)-C(16)-C(15)	119.8(2)
C(14)-P(1)-C(8)	99.31(8)	C(16)-C(17)-C(18)	120.2(2)
C(1)-N(1)-S(1)	118.49(12)	C(17)-C(18)-C(19)	120.1(2)
C(1)-N(1)-P(1)	115.44(12)	C(18)-C(19)-C(14)	120.60(19)
S(1)-N(1)-P(1)	124.30(9)	C(21)-C(20)-C(23)	111.69(17)
N(1)-C(1)-C(2)	112.75(14)	C(21)-C(20)-C(22)	110.95(18)
C(3)-C(2)-C(7)	118.97(17)	C(23)-C(20)-C(22)	110.81(18)
C(3)-C(2)-C(1)	120.27(18)	C(21)-C(20)-S(1)	107.43(13)
C(7)-C(2)-C(1)	120.75(19)	C(23)-C(20)-S(1)	112.43(13)
C(2)-C(3)-C(4)	120.6(2)	C(22)-C(20)-S(1)	103.20(14)
C(5)-C(4)-C(3)	120.0(2)		
C(6)-C(5)-C(4)	119.79(18)		
C(5)-C(6)-C(7)	120.4(2)		
C(2)-C(7)-C(6)	120.1(2)		
C(13)-C(8)-C(9)	119.01(17)		
C(13)-C(8)-P(1)	123.98(14)		
C(9)-C(8)-P(1)	116.96(15)		
C(10)-C(9)-C(8)	120.3(2)		
C(11)-C(10)-C(9)	120.05(19)		
C(10)-C(11)-C(12)	120.61(18)		
C(11)-C(12)-C(13)	119.4(2)		

Table 15. Crystal data and structure refinement for **202**.

Identification code	jso-459_0m	
Empirical formula	C36 H42 Co2 N O8 P S	
Formula weight	797.60	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 12.0566(13) Å	a= 90°.
	b = 10.6639(13) Å	b= 109.093(5)°.
	c = 15.1828(18) Å	g = 90°.
Volume	1844.7(4) $Å^3$	
Z	2	
Density (calculated)	1.436 Mg/m^3	
Absorption coefficient	1.050 mm^{-1}	
F(000)	828	
Crystal size	0.30 x 0.20 x 0.10 mm^3	
Theta range for data collection	2.84 to 39.64°.	
Index ranges	-21<=h<=9, -17<=k<=16, -26<=l<=26	
Reflections collected	31722	
Independent reflections	16994 [R(int) = 0.0240]	
Completeness to theta = 39.64°	86.6 %	
Absorption correction	SADABS (Bruker-Nonius)	
Max. and min. transmission	0.9023 and 0.7436	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16994 / 1 / 476	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R1 = 0.0248, wR2 = 0.0680	
R indices (all data)	R1 = 0.0259, wR2 = 0.0684	
Absolute structure parameter	0.016(4)	
Largest diff. peak and hole	0.812 and -0.365 $e.Å^{-3}$	

Table 16. Bond lengths [Å] and angles [°] for JSO-459_0m.

Co(1)-C(9)	1.7760(14)	O(2)-C(6)	1.1458(14)
Co(1)-C(8)	1.7920(10)	C(2)-C(3)	1.5128(15)
Co(1)-C(1)	1.9469(9)	O(3)-C(7)	1.1455(14)
Co(1)-C(2)	1.9614(9)	C(3)-C(5)	1.516(2)
Co(1)-P(1)	2.1986(4)	C(3)-C(4)	1.5217(16)
Co(1)-Co(2)	2.4273(3)	O(4)-C(8)	1.1421(13)
S(1)-O(6)	1.4799(8)	O(5)-C(9)	1.1404(18)
S(1)-N(1)	1.7010(9)	C(10)-C(11)	1.5223(15)
S(1)-C(10)	1.8596(14)	C(10)-C(12)	1.5319(17)
S(1)-Co(2)	2.1883(3)	C(10)-C(13)	1.5328(17)
N(1)-C(14)	1.4876(13)	C(14)-C(15)	1.5144(17)
N(1)-P(1)	1.7226(10)	C(15)-C(20)	1.3952(15)
P(1)-C(27)	1.8268(10)	C(15)-C(16)	1.3977(16)
P(1)-C(21)	1.8294(11)	C(16)-C(17)	1.3868(18)
O(1)-C(3)	1.4359(13)	C(17)-C(18)	1.3945(19)
C(1)-C(2)	1.3503(13)	C(18)-C(19)	1.390(2)
C(1)-Co(2)	1.9577(13)	C(19)-C(20)	1.389(2)
Co(2)-C(7)	1.7817(11)	C(21)-C(22)	1.3975(16)
Co(2)-C(6)	1.7991(11)	C(21)-C(26)	1.4016(15)
Co(2)-C(2)	1.9585(12)		

C(22)-C(23)	1.3880(17)	C(1S')-C(2S')	1.461(14)
C(23)-C(24)	1.3989(17)	C(2S')-O(2S')	1.369(10)
C(24)-C(25)	1.388(2)	O(2S')-C(3S')	1.407(12)
C(25)-C(26)	1.3924(19)	C(3S')-C(4S')	1.538(14)
C(27)-C(32)	1.3916(18)		
C(27)-C(28)	1.4022(16)		
C(28)-C(29)	1.3927(17)		
C(29)-C(30)	1.385(3)		
C(30)-C(31)	1.394(2)		
C(31)-C(32)	1.3900(16)		
O(1S)-C(2S)	1.202(3)		
C(1S)-C(2S)	1.516(4)		
C(2S)-O(2S)	1.338(3)		
O(2S)-C(3S)	1.456(3)		
C(3S)-C(4S)	1.494(4)		
O(1S')-C(2S')	1.208(9)		

C(9)-Co(1)-C(8)	100.91(5)	C(6)-Co(2)-S(1)	111.12(4)
C(9)-Co(1)-C(1)	103.35(5)	C(1)-Co(2)-S(1)	100.37(3)
C(8)-Co(1)-C(1)	143.26(5)	C(2)-Co(2)-S(1)	138.90(3)
C(9)-Co(1)-C(2)	104.53(5)	C(7)-Co(2)-Co(1)	147.26(5)
C(8)-Co(1)-C(2)	106.58(4)	C(6)-Co(2)-Co(1)	102.19(4)
C(1)-Co(1)-C(2)	40.42(4)	C(1)-Co(2)-Co(1)	51.36(3)
C(9)-Co(1)-P(1)	97.42(3)	C(2)-Co(2)-Co(1)	51.79(3)
C(8)-Co(1)-P(1)	105.68(4)	S(1)-Co(2)-Co(1)	97.891(12)
C(1)-Co(1)-P(1)	98.11(3)	C(1)-C(2)-C(3)	138.98(10)
C(2)-Co(1)-P(1)	136.29(3)	C(1)-C(2)-Co(2)	69.80(7)
C(9)-Co(1)-Co(2)	153.53(4)	C(3)-C(2)-Co(2)	133.13(8)
C(8)-Co(1)-Co(2)	97.77(4)	C(1)-C(2)-Co(1)	69.21(6)
C(1)-Co(1)-Co(2)	51.76(4)	C(3)-C(2)-Co(1)	139.75(8)
C(2)-Co(1)-Co(2)	51.69(4)	Co(2)-C(2)-Co(1)	76.52(4)
P(1)-Co(1)-Co(2)	95.386(12)	O(1)-C(3)-C(2)	108.48(9)
O(6)-S(1)-N(1)	105.43(5)	O(1)-C(3)-C(5)	109.84(10)
O(6)-S(1)-C(10)	103.90(6)	C(2)-C(3)-C(5)	109.14(10)
N(1)-S(1)-C(10)	104.99(5)	O(1)-C(3)-C(4)	105.24(10)
O(6)-S(1)-Co(2)	114.64(4)	C(2)-C(3)-C(4)	112.16(10)
N(1)-S(1)-Co(2)	111.60(4)	C(5)-C(3)-C(4)	111.86(11)
C(10)-S(1)-Co(2)	115.28(3)	O(2)-C(6)-Co(2)	176.06(12)
C(14)-N(1)-S(1)	117.15(7)	O(3)-C(7)-Co(2)	177.50(12)
C(14)-N(1)-P(1)	123.99(8)	O(4)-C(8)-Co(1)	179.00(12)
S(1)-N(1)-P(1)	117.99(5)	O(5)-C(9)-Co(1)	178.06(10)
N(1)-P(1)-C(27)	105.36(5)	C(11)-C(10)-C(12)	111.31(9)
N(1)-P(1)-C(21)	102.89(5)	C(11)-C(10)-C(13)	110.62(9)
C(27)-P(1)-C(21)	99.66(5)	C(12)-C(10)-C(13)	109.78(11)
N(1)-P(1)-Co(1)	112.99(3)	C(11)-C(10)-S(1)	110.23(9)
C(27)-P(1)-Co(1)	117.48(3)	C(12)-C(10)-S(1)	110.33(8)
C(21)-P(1)-Co(1)	116.54(4)	C(13)-C(10)-S(1)	104.36(8)
C(2)-C(1)-Co(1)	70.37(5)	N(1)-C(14)-C(15)	116.07(10)
C(2)-C(1)-Co(2)	69.86(7)	C(20)-C(15)-C(16)	118.90(11)
Co(1)-C(1)-Co(2)	76.87(4)	C(20)-C(15)-C(14)	118.46(11)
C(7)-Co(2)-C(6)	100.50(5)	C(16)-C(15)-C(14)	122.58(9)
C(7)-Co(2)-C(1)	96.89(5)	C(17)-C(16)-C(15)	120.18(11)
C(6)-Co(2)-C(1)	142.02(5)	C(16)-C(17)-C(18)	120.76(13)
C(7)-Co(2)-C(2)	100.11(5)	C(19)-C(18)-C(17)	119.12(13)
C(6)-Co(2)-C(2)	103.02(5)	C(20)-C(19)-C(18)	120.27(11)
C(1)-Co(2)-C(2)	40.34(4)	C(19)-C(20)-C(15)	120.71(12)
C(7)-Co(2)-S(1)	95.59(4)	C(22)-C(21)-C(26)	118.83(11)

C(22)-C(21)-P(1)	118.51(7)	C(32)-C(27)-P(1)	123.41(8)
C(26)-C(21)-P(1)	122.62(9)	C(28)-C(27)-P(1)	117.65(9)
C(23)-C(22)-C(21)	120.66(10)	C(29)-C(28)-C(27)	120.18(13)
C(22)-C(23)-C(24)	120.12(12)	C(30)-C(29)-C(28)	120.45(13)
C(25)-C(24)-C(23)	119.63(12)	C(29)-C(30)-C(31)	119.70(11)
C(24)-C(25)-C(26)	120.28(11)	C(32)-C(31)-C(30)	119.94(14)
C(25)-C(26)-C(21)	120.47(12)	C(31)-C(32)-C(27)	120.87(12)
C(32)-C(27)-C(28)	118.85(10)		

Table 17. Crystal data and structure refinement for **242b**.

Identification code	ISO123B	
Empirical formula	C20 H21 N O2	
Formula weight	307.38	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 19.8555(18) Å	α= 90°.
	b = 12.3548(11) Å	β= 112.805(2)°.
	c = 14.8624(13) Å	γ = 90°.
Volume	3360.9(5) $Å^3$	
Z	8	
Density (calculated)	1.215 Mg/m^3	
Absorption coefficient	0.078 mm^{-1}	
F(000)	1312	
Crystal size	0.44 x 0.17 x 0.16 mm^3	
Theta range for data collection	1.99 to 26.37°.	
Index ranges	-24<=h<=24, -15<=k<=12, -18<=l<=14	
Reflections collected	9559	
Independent reflections	3434 [R(int) = 0.0189]	
Completeness to theta = 26.37°	99.7 %	
Absorption correction	Semi-empirical	
Max. and min. transmission	0.9876 and 0.9665	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3434 / 0 / 208	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2sigma(I)]	R1 = 0.0605, wR2 = 0.1808	
R indices (all data)	R1 = 0.0822, wR2 = 0.2005	
Largest diff. peak and hole	0.340 and -0.261 $e.Å^{-3}$	

Table 18. Bond lengths [Å] and angles [°] for ISO123B.

O(1)-C(8)	1.216(3)		
O(2)-C(11)	1.224(3)	C(8)-C(9)	1.475(3)
N(1)-C(11)	1.352(3)	C(9)-C(10)	1.330(3)
N(1)-C(12)	1.431(3)	C(9)-C(11)	1.498(3)
C(1)-C(2)	1.496(4)	C(12)-C(17)	1.396(3)
C(1)-C(5)	1.521(4)	C(12)-C(13)	1.401(3)
C(1)-C(6)	1.552(4)	C(13)-C(14)	1.392(3)
C(2)-C(3)	1.315(5)	C(13)-C(18)	1.498(4)
C(3)-C(4)	1.494(4)	C(14)-C(15)	1.381(4)
C(4)-C(5)	1.535(3)	C(15)-C(16)	1.379(4)
C(4)-C(7)	1.550(3)	C(15)-C(19)	1.513(3)
C(6)-C(10)	1.490(4)	C(16)-C(17)	1.393(3)
C(6)-C(7)	1.518(4)	C(17)-C(20)	1.497(4)
C(7)-C(8)	1.513(3)		

C(11)-N(1)-C(12)	125.79(19)	C(8)-C(9)-C(11)	126.8(2)
C(2)-C(1)-C(5)	100.3(2)	C(9)-C(10)-C(6)	114.7(2)
C(2)-C(1)-C(6)	106.8(2)	O(2)-C(11)-N(1)	124.2(2)
C(5)-C(1)-C(6)	99.4(2)	O(2)-C(11)-C(9)	121.8(2)
C(3)-C(2)-C(1)	108.2(3)	N(1)-C(11)-C(9)	114.0(2)
C(2)-C(3)-C(4)	107.2(3)	C(17)-C(12)-C(13)	121.3(2)
C(3)-C(4)-C(5)	100.5(2)	C(17)-C(12)-N(1)	117.8(2)
C(3)-C(4)-C(7)	107.4(2)	C(13)-C(12)-N(1)	120.8(2)
C(5)-C(4)-C(7)	98.9(2)	C(14)-C(13)-C(12)	117.4(2)
C(1)-C(5)-C(4)	93.34(18)	C(14)-C(13)-C(18)	119.8(2)
C(10)-C(6)-C(7)	103.62(19)	C(12)-C(13)-C(18)	122.8(2)
C(10)-C(6)-C(1)	117.6(3)	C(15)-C(14)-C(13)	123.0(2)
C(7)-C(6)-C(1)	103.0(2)	C(16)-C(15)-C(14)	117.8(2)
C(8)-C(7)-C(6)	105.54(19)	C(16)-C(15)-C(19)	120.7(3)
C(8)-C(7)-C(4)	117.1(2)	C(14)-C(15)-C(19)	121.5(3)
C(6)-C(7)-C(4)	103.30(19)	C(15)-C(16)-C(17)	122.3(2)
O(1)-C(8)-C(9)	126.2(2)	C(16)-C(17)-C(12)	118.2(2)
O(1)-C(8)-C(7)	125.9(2)	C(16)-C(17)-C(20)	120.1(2)
C(9)-C(8)-C(7)	107.97(19)	C(12)-C(17)-C(20)	121.6(2)
C(10)-C(9)-C(8)	108.2(2)		
C(10)-C(9)-C(11)	125.1(2)		