

## Supporting Information

### Crystallographic Data of Complexes 2, 3 and 8

#### Complex 2

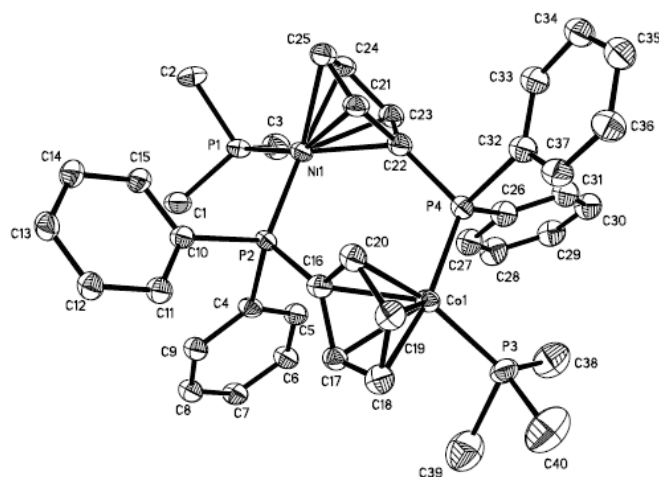


Table 1. Crystal data and structure refinement for complex 2.

Identification code	sun904a
Empirical formula	C <sub>40</sub> H <sub>46</sub> Co Ni P <sub>4</sub>
Formula weight	768.29
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 25.604(5) Å    alpha = 90 deg. b = 18.385(4) Å    beta = 98.91(3) deg. c = 17.539(4) Å    gamma = 90 deg.
Volume	8156(3) Å <sup>3</sup>
Z, Calculated density	8, 1.251 Mg/m <sup>3</sup>

Absorption coefficient	1.050 mm <sup>-1</sup>
F(000)	3208
Crystal size	0.31 x 0.30 x 0.27 mm
Theta range for data collection	1.37 to 25.66 deg.
Limiting indices	-30<=h<=15, -22<=k<=21, -20<=l<=21
Reflections collected / unique	23945 / 13110 [R(int) = 0.1434]
Completeness to theta = 25.66	84.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7646 and 0.7366
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	13110 / 1626 / 841
Goodness-of-fit on F <sup>2</sup>	0.946
Final R indices [I>2sigma(I)]	R1 = 0.1016, wR2 = 0.1963
R indices (all data)	R1 = 0.2057, wR2 = 0.2367
Largest diff. peak and hole	0.654 and -0.578 e. Å <sup>-3</sup>

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for complex 2.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ni (1)	-8 (1)	6891 (1)	4305 (1)	34 (1)
Ni (2)	5258 (1)	6872 (1)	4805 (1)	37 (1)
Co (1)	1337 (1)	8110 (1)	5459 (1)	35 (1)
Co (2)	6481 (1)	8381 (1)	5786 (1)	34 (1)
P (1)	-820 (1)	6707 (1)	4368 (2)	36 (1)
P (2)	31 (1)	8036 (1)	4471 (1)	28 (1)
P (3)	1756 (2)	8207 (2)	6609 (2)	53 (1)
P (4)	1323 (1)	6965 (1)	5298 (2)	33 (1)
P (5)	5154 (1)	8002 (1)	4936 (1)	30 (1)
P (6)	4748 (2)	6687 (1)	3739 (2)	47 (1)
P (7)	6585 (1)	7242 (1)	5646 (2)	35 (1)
P (8)	7211 (2)	8803 (2)	5534 (2)	48 (1)
C (1)	-1289 (6)	7411 (6)	4502 (7)	54 (3)
C (2)	-1193 (7)	6285 (6)	3503 (7)	59 (3)
C (3)	-949 (8)	6056 (7)	5082 (8)	65 (3)
C (4)	-302 (5)	8396 (5)	5250 (6)	36 (2)
C (5)	-240 (6)	7996 (5)	5943 (6)	41 (2)
C (6)	-488 (6)	8225 (5)	6541 (6)	45 (2)
C (7)	-806 (6)	8823 (5)	6478 (6)	42 (2)
C (8)	-866 (6)	9220 (5)	5812 (6)	41 (2)
C (9)	-626 (6)	9019 (5)	5208 (6)	39 (2)
C (10)	-251 (5)	8626 (5)	3642 (6)	35 (2)
C (11)	-126 (6)	9356 (5)	3602 (6)	41 (2)
C (12)	-338 (6)	9770 (5)	2965 (6)	41 (2)
C (13)	-682 (6)	9447 (6)	2387 (6)	45 (2)
C (14)	-804 (6)	8738 (6)	2400 (6)	45 (2)
C (15)	-593 (6)	8319 (5)	3035 (6)	41 (2)
C (16)	675 (5)	8474 (5)	4717 (6)	37 (2)
C (17)	820 (5)	8991 (5)	5304 (6)	39 (2)
C (18)	1339 (6)	9222 (6)	5293 (7)	48 (2)
C (19)	1526 (6)	8874 (5)	4642 (7)	45 (2)
C (20)	1117 (5)	8403 (5)	4311 (6)	41 (2)
C (21)	666 (6)	6710 (5)	3822 (6)	42 (2)

C (22)	768 (6)	6561 (5)	4648 (6)	42 (2)
C (23)	434 (6)	5987 (5)	4772 (7)	45 (2)
C (24)	100 (6)	5816 (5)	4062 (6)	45 (2)
C (25)	269 (6)	6225 (6)	3466 (7)	48 (2)
C (26)	1304 (6)	6380 (6)	6141 (7)	48 (2)
C (27)	880 (7)	6481 (6)	6535 (7)	53 (2)
C (28)	827 (7)	6110 (7)	7203 (7)	60 (2)
C (29)	1208 (7)	5622 (6)	7477 (7)	54 (2)
C (30)	1631 (7)	5509 (6)	7113 (7)	54 (2)
C (31)	1681 (6)	5880 (6)	6415 (7)	50 (2)
C (32)	1876 (6)	6556 (6)	4857 (6)	46 (2)
C (33)	1843 (6)	5845 (6)	4557 (7)	49 (2)
C (34)	2238 (7)	5566 (7)	4197 (7)	54 (2)
C (35)	2685 (7)	5965 (6)	4173 (7)	56 (2)
C (36)	2730 (7)	6684 (6)	4448 (7)	56 (2)
C (37)	2307 (6)	6955 (7)	4801 (7)	52 (2)
C (38)	1804 (10)	7552 (9)	7364 (10)	94 (4)
C (39)	1441 (10)	8899 (10)	7205 (11)	103 (5)
C (40)	2295 (11)	8812 (12)	6742 (12)	119 (5)
C (41)	4221 (7)	6010 (6)	3783 (8)	61 (3)
C (42)	4344 (8)	7398 (7)	3170 (9)	68 (3)
C (43)	5076 (7)	6326 (7)	2997 (7)	66 (3)
C (44)	7614 (7)	9249 (7)	6345 (9)	64 (4)
C (45)	7147 (8)	9536 (7)	4831 (8)	67 (4)
C (46)	7716 (8)	8271 (7)	5211 (9)	70 (4)
C (47)	5162 (6)	8572 (5)	4060 (6)	43 (2)
C (48)	5502 (6)	8411 (6)	3610 (6)	45 (2)
C (49)	5562 (6)	8813 (6)	2952 (6)	46 (2)
C (50)	5216 (6)	9363 (6)	2759 (7)	47 (2)
C (51)	4843 (6)	9529 (6)	3173 (6)	45 (2)
C (52)	4799 (6)	9143 (5)	3852 (6)	41 (2)
C (53)	4571 (6)	8316 (5)	5331 (6)	40 (2)
C (54)	4161 (6)	7815 (6)	5378 (7)	47 (2)
C (55)	3721 (6)	8004 (6)	5703 (7)	53 (2)
C (56)	3681 (6)	8697 (6)	6001 (7)	51 (2)
C (57)	4079 (6)	9175 (6)	5978 (7)	48 (2)
C (58)	4530 (6)	8991 (6)	5647 (6)	43 (2)
C (59)	5894 (6)	6139 (6)	4876 (7)	45 (2)
C (60)	6010 (6)	6675 (5)	5470 (6)	42 (2)
C (61)	5576 (6)	6600 (6)	5914 (7)	45 (2)
C (62)	5231 (6)	6050 (6)	5611 (7)	49 (2)
C (63)	5422 (6)	5778 (6)	4968 (7)	46 (2)
C (64)	5649 (5)	8501 (5)	5582 (6)	40 (2)
C (65)	5855 (5)	8366 (5)	6381 (6)	40 (2)

C (66)	6181 (6)	8926 (5)	6688 (6)	40 (2)
C (67)	6247 (5)	9397 (5)	6087 (6)	41 (2)
C (68)	5908 (5)	9164 (5)	5401 (6)	38 (2)
C (69)	6919 (6)	6894 (6)	4843 (7)	49 (2)
C (70)	6785 (6)	7270 (6)	4142 (7)	49 (2)
C (71)	6941 (6)	7007 (7)	3499 (7)	56 (2)
C (72)	7270 (6)	6373 (7)	3534 (7)	54 (2)
C (73)	7410 (6)	6042 (7)	4228 (7)	55 (2)
C (74)	7243 (6)	6297 (6)	4882 (7)	51 (2)
C (75)	6959 (6)	6743 (6)	6477 (7)	53 (2)
C (76)	6841 (7)	6045 (7)	6681 (7)	56 (2)
C (77)	7160 (7)	5695 (8)	7310 (8)	65 (2)
C (78)	7559 (8)	6045 (8)	7700 (9)	68 (2)
C (79)	7701 (7)	6712 (8)	7510 (8)	68 (2)
C (80)	7412 (7)	7103 (7)	6895 (8)	60 (2)

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Table 3. Bond lengths [Å] and angles [deg] for complex 2.

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Ni (1)–C (24)	2.050(10)
Ni (1)–C (21)	2.063(15)
Ni (1)–C (22)	2.074(13)
Ni (1)–C (23)	2.103(11)
Ni (1)–C (25)	2.120(13)
Ni (1)–P (2)	2.125(3)
Ni (1)–P (1)	2.127(4)
Ni (2)–C (61)	2.052(11)
Ni (2)–C (63)	2.066(11)
Ni (2)–C (62)	2.078(12)
Ni (2)–C (59)	2.103(13)
Ni (2)–P (5)	2.112(3)
Ni (2)–C (60)	2.123(12)
Ni (2)–P (6)	2.135(3)
Co (1)–C (18)	2.065(11)
Co (1)–C (20)	2.076(10)
Co (1)–C (16)	2.081(11)
Co (1)–C (17)	2.084(11)
Co (1)–C (19)	2.116(12)
Co (1)–P (4)	2.124(3)
Co (1)–P (3)	2.140(3)
Co (2)–C (65)	2.043(15)
Co (2)–C (67)	2.057(10)
Co (2)–C (68)	2.092(11)
Co (2)–C (66)	2.117(12)
Co (2)–C (64)	2.117(14)
Co (2)–P (7)	2.128(3)
Co (2)–P (8)	2.132(5)
P (1)–C (3)	1.799(15)
P (1)–C (1)	1.804(14)
P (1)–C (2)	1.833(11)
P (2)–C (16)	1.826(13)
P (2)–C (4)	1.842(12)
P (2)–C (10)	1.867(9)
P (3)–C (40)	1.76(2)
P (3)–C (38)	1.779(17)
P (3)–C (39)	1.90(2)
P (4)–C (26)	1.834(12)
P (4)–C (22)	1.836(12)
P (4)–C (32)	1.872(16)

P(5)–C(64)	1.811(11)
P(5)–C(53)	1.836(15)
P(5)–C(47)	1.862(12)
P(6)–C(43)	1.783(16)
P(6)–C(41)	1.846(16)
P(6)–C(42)	1.858(12)
P(7)–C(60)	1.792(14)
P(7)–C(75)	1.858(11)
P(7)–C(69)	1.870(14)
P(8)–C(46)	1.783(19)
P(8)–C(45)	1.818(14)
P(8)–C(44)	1.820(12)
C(4)–C(5)	1.408(14)
C(4)–C(9)	1.410(16)
C(5)–C(6)	1.374(18)
C(6)–C(7)	1.363(17)
C(7)–C(8)	1.365(14)
C(8)–C(9)	1.354(18)
C(10)–C(11)	1.386(14)
C(10)–C(15)	1.387(14)
C(11)–C(12)	1.390(13)
C(12)–C(13)	1.371(15)
C(13)–C(14)	1.343(15)
C(14)–C(15)	1.393(13)
C(16)–C(17)	1.409(13)
C(16)–C(20)	1.432(19)
C(17)–C(18)	1.40(2)
C(18)–C(19)	1.45(2)
C(19)–C(20)	1.414(17)
C(21)–C(25)	1.420(17)
C(21)–C(22)	1.458(14)
C(22)–C(23)	1.396(19)
C(23)–C(24)	1.433(15)
C(24)–C(25)	1.409(19)
C(26)–C(31)	1.365(17)
C(26)–C(27)	1.39(2)
C(27)–C(28)	1.380(18)
C(28)–C(29)	1.36(2)
C(29)–C(30)	1.35(2)
C(30)–C(31)	1.425(17)
C(32)–C(37)	1.34(2)
C(32)–C(33)	1.406(15)
C(33)–C(34)	1.37(2)
C(34)–C(35)	1.37(2)

C (35)–C (36)	1. 406 (16)
C (36)–C (37)	1. 42 (2)
C (47)–C (48)	1. 29 (2)
C (47)–C (52)	1. 413 (17)
C (48)–C (49)	1. 399 (16)
C (49)–C (50)	1. 352 (18)
C (50)–C (51)	1. 32 (2)
C (51)–C (52)	1. 407 (16)
C (53)–C (58)	1. 369 (14)
C (53)–C (54)	1. 409 (18)
C (54)–C (55)	1. 38 (2)
C (55)–C (56)	1. 388 (16)
C (56)–C (57)	1. 35 (2)
C (57)–C (58)	1. 41 (2)
C (59)–C (63)	1. 41 (2)
C (59)–C (60)	1. 433 (14)
C (60)–C (61)	1. 46 (2)
C (61)–C (62)	1. 392 (17)
C (62)–C (63)	1. 39 (2)
C (64)–C (65)	1. 441 (14)
C (64)–C (68)	1. 448 (16)
C (65)–C (66)	1. 382 (15)
C (66)–C (67)	1. 394 (16)
C (67)–C (68)	1. 435 (14)
C (69)–C (74)	1. 372 (18)
C (69)–C (70)	1. 406 (16)
C (70)–C (71)	1. 343 (19)
C (71)–C (72)	1. 434 (19)
C (72)–C (73)	1. 358 (17)
C (73)–C (74)	1. 37 (2)
C (75)–C (76)	1. 379 (18)
C (75)–C (80)	1. 43 (2)
C (76)–C (77)	1. 421 (16)
C (77)–C (78)	1. 31 (2)
C (78)–C (79)	1. 34 (2)
C (79)–C (80)	1. 406 (17)
C (24)–Ni (1)–C (21)	67. 1 (5)
C (24)–Ni (1)–C (22)	68. 0 (5)
C (21)–Ni (1)–C (22)	41. 3 (4)
C (24)–Ni (1)–C (23)	40. 3 (4)
C (21)–Ni (1)–C (23)	66. 4 (5)
C (22)–Ni (1)–C (23)	39. 0 (5)
C (24)–Ni (1)–C (25)	39. 5 (5)



C(21)–Ni(1)–C(25)	39.7(5)
C(22)–Ni(1)–C(25)	67.9(5)
C(23)–Ni(1)–C(25)	66.2(5)
C(24)–Ni(1)–P(2)	168.1(5)
C(21)–Ni(1)–P(2)	101.0(3)
C(22)–Ni(1)–P(2)	103.2(3)
C(23)–Ni(1)–P(2)	135.9(3)
C(25)–Ni(1)–P(2)	130.8(4)
C(24)–Ni(1)–P(1)	91.2(4)
C(21)–Ni(1)–P(1)	151.8(3)
C(22)–Ni(1)–P(1)	147.0(3)
C(23)–Ni(1)–P(1)	109.0(4)
C(25)–Ni(1)–P(1)	112.3(4)
P(2)–Ni(1)–P(1)	100.14(13)
C(61)–Ni(2)–C(63)	65.7(4)
C(61)–Ni(2)–C(62)	39.4(5)
C(63)–Ni(2)–C(62)	39.2(5)
C(61)–Ni(2)–C(59)	66.3(5)
C(63)–Ni(2)–C(59)	39.5(6)
C(62)–Ni(2)–C(59)	66.4(6)
C(61)–Ni(2)–P(5)	100.0(3)
C(63)–Ni(2)–P(5)	165.8(3)
C(62)–Ni(2)–P(5)	128.6(4)
C(59)–Ni(2)–P(5)	137.2(4)
C(61)–Ni(2)–C(60)	40.9(5)
C(63)–Ni(2)–C(60)	67.1(5)
C(62)–Ni(2)–C(60)	68.0(5)
C(59)–Ni(2)–C(60)	39.6(4)
P(5)–Ni(2)–C(60)	103.1(3)
C(61)–Ni(2)–P(6)	153.0(4)
C(63)–Ni(2)–P(6)	92.9(3)
C(62)–Ni(2)–P(6)	113.6(4)
C(59)–Ni(2)–P(6)	108.2(3)
P(5)–Ni(2)–P(6)	100.47(11)
C(60)–Ni(2)–P(6)	146.5(3)
C(18)–Co(1)–C(20)	67.2(4)
C(18)–Co(1)–C(16)	67.2(5)
C(20)–Co(1)–C(16)	40.3(5)
C(18)–Co(1)–C(17)	39.4(5)
C(20)–Co(1)–C(17)	66.4(5)
C(16)–Co(1)–C(17)	39.6(4)
C(18)–Co(1)–C(19)	40.6(5)
C(20)–Co(1)–C(19)	39.4(5)
C(16)–Co(1)–C(19)	67.2(5)

C (17)–Co (1)–C (19)	66.6 (5)
C (18)–Co (1)–P (4)	164.3 (4)
C (20)–Co (1)–P (4)	97.6 (3)
C (16)–Co (1)–P (4)	103.9 (3)
C (17)–Co (1)–P (4)	139.2 (3)
C (19)–Co (1)–P (4)	124.7 (4)
C (18)–Co (1)–P (3)	92.2 (3)
C (20)–Co (1)–P (3)	156.0 (3)
C (16)–Co (1)–P (3)	143.5 (3)
C (17)–Co (1)–P (3)	105.9 (3)
C (19)–Co (1)–P (3)	116.6 (3)
P (4)–Co (1)–P (3)	101.75 (11)
C (65)–Co (2)–C (67)	66.3 (5)
C (65)–Co (2)–C (68)	66.9 (5)
C (67)–Co (2)–C (68)	40.5 (4)
C (65)–Co (2)–C (66)	38.8 (4)
C (67)–Co (2)–C (66)	39.0 (4)
C (68)–Co (2)–C (66)	66.3 (4)
C (65)–Co (2)–C (64)	40.5 (4)
C (67)–Co (2)–C (64)	67.8 (5)
C (68)–Co (2)–C (64)	40.2 (4)
C (66)–Co (2)–C (64)	66.7 (4)
C (65)–Co (2)–P (7)	99.7 (3)
C (67)–Co (2)–P (7)	165.9 (4)
C (68)–Co (2)–P (7)	137.2 (3)
C (66)–Co (2)–P (7)	128.2 (3)
C (64)–Co (2)–P (7)	103.0 (3)
C (65)–Co (2)–P (8)	153.2 (3)
C (67)–Co (2)–P (8)	91.3 (4)
C (68)–Co (2)–P (8)	106.0 (4)
C (66)–Co (2)–P (8)	114.4 (4)
C (64)–Co (2)–P (8)	144.9 (3)
P (7)–Co (2)–P (8)	101.78 (15)
C (3)–P (1)–C (1)	100.9 (8)
C (3)–P (1)–C (2)	99.6 (7)
C (1)–P (1)–C (2)	98.0 (7)
C (3)–P (1)–Ni (1)	115.3 (6)
C (1)–P (1)–Ni (1)	124.6 (5)
C (2)–P (1)–Ni (1)	114.4 (6)
C (16)–P (2)–C (4)	99.8 (5)
C (16)–P (2)–C (10)	98.9 (5)
C (4)–P (2)–C (10)	101.6 (5)
C (16)–P (2)–Ni (1)	119.4 (4)
C (4)–P (2)–Ni (1)	116.1 (3)

C(10)-P(2)-Ni(1)	117.7(3)
C(40)-P(3)-C(38)	111.5(9)
C(40)-P(3)-C(39)	83.9(12)
C(38)-P(3)-C(39)	91.7(10)
C(40)-P(3)-Co(1)	116.5(7)
C(38)-P(3)-Co(1)	127.7(6)
C(39)-P(3)-Co(1)	112.4(6)
C(26)-P(4)-C(22)	98.6(5)
C(26)-P(4)-C(32)	102.4(6)
C(22)-P(4)-C(32)	98.2(6)
C(26)-P(4)-Co(1)	118.4(4)
C(22)-P(4)-Co(1)	118.6(3)
C(32)-P(4)-Co(1)	117.1(4)
C(64)-P(5)-C(53)	97.8(5)
C(64)-P(5)-C(47)	97.8(5)
C(53)-P(5)-C(47)	104.4(6)
C(64)-P(5)-Ni(2)	118.6(4)
C(53)-P(5)-Ni(2)	118.3(4)
C(47)-P(5)-Ni(2)	116.5(4)
C(43)-P(6)-C(41)	102.1(7)
C(43)-P(6)-C(42)	99.0(8)
C(41)-P(6)-C(42)	98.5(8)
C(43)-P(6)-Ni(2)	113.9(5)
C(41)-P(6)-Ni(2)	115.0(4)
C(42)-P(6)-Ni(2)	124.9(4)
C(60)-P(7)-C(75)	99.0(6)
C(60)-P(7)-C(69)	97.5(6)
C(75)-P(7)-C(69)	100.5(6)
C(60)-P(7)-Co(2)	118.5(4)
C(75)-P(7)-Co(2)	117.0(4)
C(69)-P(7)-Co(2)	120.2(4)
C(46)-P(8)-C(45)	100.6(9)
C(46)-P(8)-C(44)	98.3(8)
C(45)-P(8)-C(44)	100.1(7)
C(46)-P(8)-Co(2)	124.7(5)
C(45)-P(8)-Co(2)	114.9(6)
C(44)-P(8)-Co(2)	114.3(7)
C(5)-C(4)-C(9)	117.2(11)
C(5)-C(4)-P(2)	116.7(8)
C(9)-C(4)-P(2)	126.1(8)
C(6)-C(5)-C(4)	119.6(10)
C(7)-C(6)-C(5)	121.8(10)
C(6)-C(7)-C(8)	119.2(13)
C(9)-C(8)-C(7)	121.2(11)

C(8)–C(9)–C(4)	121.0(10)
C(11)–C(10)–C(15)	118.7(9)
C(11)–C(10)–P(2)	122.5(8)
C(15)–C(10)–P(2)	118.9(7)
C(10)–C(11)–C(12)	120.4(10)
C(13)–C(12)–C(11)	119.0(10)
C(14)–C(13)–C(12)	122.1(10)
C(13)–C(14)–C(15)	119.3(10)
C(10)–C(15)–C(14)	120.6(9)
C(17)–C(16)–C(20)	106.6(11)
C(17)–C(16)–P(2)	126.6(11)
C(20)–C(16)–P(2)	126.6(8)
C(17)–C(16)–Co(1)	70.3(6)
C(20)–C(16)–Co(1)	69.7(7)
P(2)–C(16)–Co(1)	128.7(5)
C(18)–C(17)–C(16)	109.7(12)
C(18)–C(17)–Co(1)	69.6(7)
C(16)–C(17)–Co(1)	70.1(6)
C(17)–C(18)–C(19)	108.0(11)
C(17)–C(18)–Co(1)	71.0(6)
C(19)–C(18)–Co(1)	71.6(6)
C(20)–C(19)–C(18)	106.1(14)
C(20)–C(19)–Co(1)	68.8(6)
C(18)–C(19)–Co(1)	67.8(7)
C(19)–C(20)–C(16)	109.5(11)
C(19)–C(20)–Co(1)	71.8(6)
C(16)–C(20)–Co(1)	70.0(6)
C(25)–C(21)–C(22)	109.0(11)
C(25)–C(21)–Ni(1)	72.3(9)
C(22)–C(21)–Ni(1)	69.8(8)
C(23)–C(22)–C(21)	106.1(10)
C(23)–C(22)–P(4)	130.0(8)
C(21)–C(22)–P(4)	122.9(10)
C(23)–C(22)–Ni(1)	71.6(8)
C(21)–C(22)–Ni(1)	69.0(7)
P(4)–C(22)–Ni(1)	132.6(6)
C(22)–C(23)–C(24)	109.2(10)
C(22)–C(23)–Ni(1)	69.4(6)
C(24)–C(23)–Ni(1)	67.8(6)
C(25)–C(24)–C(23)	108.5(12)
C(25)–C(24)–Ni(1)	72.9(6)
C(23)–C(24)–Ni(1)	71.8(6)
C(24)–C(25)–C(21)	106.9(10)
C(24)–C(25)–Ni(1)	67.6(7)

C (21)–C (25)–Ni (1)	68.0 (7)
C (31)–C (26)–C (27)	118.6 (12)
C (31)–C (26)–P (4)	125.0 (13)
C (27)–C (26)–P (4)	116.4 (9)
C (28)–C (27)–C (26)	123.0 (13)
C (29)–C (28)–C (27)	117.9 (17)
C (30)–C (29)–C (28)	121.2 (13)
C (29)–C (30)–C (31)	121.1 (13)
C (26)–C (31)–C (30)	118.2 (15)
C (37)–C (32)–C (33)	118.9 (14)
C (37)–C (32)–P (4)	119.6 (9)
C (33)–C (32)–P (4)	121.5 (11)
C (34)–C (33)–C (32)	120.9 (14)
C (35)–C (34)–C (33)	119.6 (13)
C (34)–C (35)–C (36)	121.3 (15)
C (35)–C (36)–C (37)	116.8 (14)
C (32)–C (37)–C (36)	122.2 (12)
C (48)–C (47)–C (52)	119.3 (11)
C (48)–C (47)–P (5)	118.0 (9)
C (52)–C (47)–P (5)	122.6 (11)
C (47)–C (48)–C (49)	123.6 (12)
C (50)–C (49)–C (48)	116.7 (15)
C (51)–C (50)–C (49)	122.4 (12)
C (50)–C (51)–C (52)	120.6 (12)
C (51)–C (52)–C (47)	117.2 (14)
C (58)–C (53)–C (54)	117.7 (13)
C (58)–C (53)–P (5)	123.8 (10)
C (54)–C (53)–P (5)	118.3 (9)
C (55)–C (54)–C (53)	121.4 (12)
C (54)–C (55)–C (56)	119.8 (13)
C (57)–C (56)–C (55)	119.2 (15)
C (56)–C (57)–C (58)	121.6 (12)
C (53)–C (58)–C (57)	120.2 (12)
C (63)–C (59)–C (60)	109.0 (13)
C (63)–C (59)–Ni (2)	68.8 (8)
C (60)–C (59)–Ni (2)	70.9 (7)
C (59)–C (60)–C (61)	103.5 (11)
C (59)–C (60)–P (7)	126.7 (11)
C (61)–C (60)–P (7)	129.6 (8)
C (59)–C (60)–Ni (2)	69.4 (7)
C (61)–C (60)–Ni (2)	66.9 (7)
P (7)–C (60)–Ni (2)	130.3 (5)
C (62)–C (61)–C (60)	110.8 (11)
C (62)–C (61)–Ni (2)	71.3 (6)

C (60)–C (61)–Ni (2)	72.2 (7)
C (63)–C (62)–C (61)	106.8 (14)
C (63)–C (62)–Ni (2)	69.9 (7)
C (61)–C (62)–Ni (2)	69.3 (7)
C (62)–C (63)–C (59)	109.8 (11)
C (62)–C (63)–Ni (2)	70.9 (6)
C (59)–C (63)–Ni (2)	71.7 (7)
C (65)–C (64)–C (68)	104.3 (9)
C (65)–C (64)–P (5)	129.6 (9)
C (68)–C (64)–P (5)	126.1 (8)
C (65)–C (64)–Co (2)	67.0 (7)
C (68)–C (64)–Co (2)	69.0 (8)
P (5)–C (64)–Co (2)	129.9 (6)
C (66)–C (65)–C (64)	111.1 (10)
C (66)–C (65)–Co (2)	73.5 (9)
C (64)–C (65)–Co (2)	72.5 (8)
C (65)–C (66)–C (67)	107.7 (9)
C (65)–C (66)–Co (2)	67.7 (7)
C (67)–C (66)–Co (2)	68.2 (7)
C (66)–C (67)–C (68)	108.8 (10)
C (66)–C (67)–Co (2)	72.8 (6)
C (68)–C (67)–Co (2)	71.1 (6)
C (67)–C (68)–C (64)	107.8 (9)
C (67)–C (68)–Co (2)	68.4 (6)
C (64)–C (68)–Co (2)	70.8 (6)
C (74)–C (69)–C (70)	120.1 (13)
C (74)–C (69)–P (7)	125.4 (10)
C (70)–C (69)–P (7)	114.4 (9)
C (71)–C (70)–C (69)	119.6 (12)
C (70)–C (71)–C (72)	120.4 (12)
C (73)–C (72)–C (71)	118.3 (13)
C (72)–C (73)–C (74)	121.6 (13)
C (73)–C (74)–C (69)	119.9 (12)
C (76)–C (75)–C (80)	119.3 (11)
C (76)–C (75)–P (7)	123.8 (10)
C (80)–C (75)–P (7)	116.7 (10)
C (75)–C (76)–C (77)	120.0 (14)
C (78)–C (77)–C (76)	119.5 (15)
C (77)–C (78)–C (79)	122.8 (13)
C (78)–C (79)–C (80)	122.0 (15)
C (79)–C (80)–C (75)	116.3 (14)

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Symmetry transformations used to generate equivalent atoms:



Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for complex 2.  
 The anisotropic displacement factor exponent takes the form:  
 $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$

	U11	U22	U33	U23	U13	U12
Ni (1)	46(1)	27(1)	30(1)	-1(1)	9(1)	5(1)
Ni (2)	47(1)	28(1)	37(1)	-1(1)	12(1)	-1(1)
Co(1)	44(1)	27(1)	33(1)	3(1)	6(1)	1(1)
Co(2)	37(1)	35(1)	32(1)	-8(1)	6(1)	5(1)
P(1)	42(2)	30(1)	38(1)	-7(1)	11(1)	-2(1)
P(2)	36(2)	24(1)	26(1)	2(1)	10(1)	5(1)
P(3)	67(3)	37(2)	48(2)	1(1)	-11(2)	-7(1)
P(4)	39(2)	32(1)	29(1)	6(1)	9(1)	4(1)
P(5)	40(2)	23(1)	28(1)	-2(1)	4(1)	-1(1)
P(6)	62(3)	36(1)	41(2)	-10(1)	2(2)	-1(1)
P(7)	39(2)	38(1)	30(1)	-1(1)	7(1)	10(1)
P(8)	36(2)	50(2)	57(2)	-21(1)	11(2)	-1(1)
C(1)	57(7)	47(5)	56(5)	-15(5)	7(5)	-2(5)
C(2)	72(8)	51(5)	51(6)	-23(5)	0(6)	-5(5)
C(3)	78(8)	55(6)	61(6)	1(5)	12(7)	1(6)
C(4)	52(4)	31(3)	27(3)	-1(3)	11(3)	3(3)
C(5)	57(4)	35(3)	32(3)	2(3)	6(3)	2(3)
C(6)	61(5)	39(4)	35(4)	3(3)	13(4)	6(4)
C(7)	60(5)	42(4)	28(3)	0(3)	17(4)	2(4)
C(8)	55(5)	36(3)	33(4)	4(3)	14(4)	3(3)
C(9)	54(4)	32(3)	30(3)	7(3)	10(3)	2(3)
C(10)	49(4)	32(3)	27(3)	3(3)	8(3)	1(3)
C(11)	54(4)	36(3)	33(3)	6(3)	8(3)	2(3)
C(12)	53(5)	37(3)	34(4)	9(3)	9(4)	3(3)
C(13)	56(5)	42(4)	36(4)	9(3)	6(4)	9(4)
C(14)	53(5)	46(4)	35(4)	6(3)	2(4)	2(4)
C(15)	49(4)	39(3)	33(3)	2(3)	2(4)	2(3)
C(16)	53(3)	30(3)	30(3)	4(2)	9(3)	1(3)
C(17)	51(4)	32(3)	33(3)	1(3)	5(3)	4(3)
C(18)	57(5)	44(4)	41(4)	8(3)	7(4)	-3(4)
C(19)	52(5)	42(4)	43(4)	9(4)	10(4)	-8(4)
C(20)	51(4)	36(3)	35(3)	8(3)	10(3)	2(3)
C(21)	55(4)	39(3)	32(3)	-4(3)	9(3)	7(3)
C(22)	57(3)	36(3)	33(3)	2(3)	6(3)	8(3)



C(23)	59(4)	37(3)	39(3)	3(3)	9(3)	8(3)
C(24)	62(5)	34(4)	40(4)	-5(3)	8(4)	6(4)
C(25)	59(5)	41(4)	41(4)	-5(3)	6(4)	8(4)
C(26)	63(4)	45(3)	36(3)	7(3)	8(3)	2(3)
C(27)	67(4)	55(4)	37(3)	8(3)	5(3)	4(3)
C(28)	73(5)	66(4)	41(4)	12(4)	10(4)	-1(4)
C(29)	73(5)	56(4)	35(4)	10(4)	11(4)	-5(4)
C(30)	69(5)	49(4)	40(4)	9(4)	3(4)	2(4)
C(31)	66(4)	46(3)	37(3)	9(3)	6(3)	5(3)
C(32)	60(4)	42(3)	36(3)	4(3)	8(3)	4(3)
C(33)	60(4)	45(3)	43(3)	3(3)	11(3)	5(3)
C(34)	62(5)	51(4)	49(4)	0(4)	14(4)	9(4)
C(35)	62(5)	57(4)	51(4)	5(4)	13(4)	9(4)
C(36)	64(5)	52(4)	56(4)	1(4)	18(4)	1(4)
C(37)	60(5)	49(4)	48(4)	-4(4)	14(4)	2(4)
C(38)	103(8)	107(7)	70(6)	-4(6)	2(7)	-10(7)
C(39)	99(10)	132(9)	78(8)	-3(8)	8(8)	-4(8)
C(40)	111(11)	159(10)	81(9)	-5(9)	1(9)	-29(9)
C(41)	77(8)	55(6)	52(6)	-18(5)	11(6)	-12(6)
C(42)	77(8)	57(6)	60(6)	-7(5)	-15(6)	2(6)
C(43)	87(9)	66(6)	45(6)	-25(5)	10(6)	-1(6)
C(44)	49(8)	66(7)	78(7)	-13(6)	16(7)	-18(6)
C(45)	64(8)	70(6)	69(7)	-9(6)	20(7)	-19(6)
C(46)	65(8)	71(7)	78(7)	-20(6)	23(7)	-10(6)
C(47)	51(4)	40(3)	39(3)	-3(3)	10(3)	-2(3)
C(48)	53(4)	44(3)	39(3)	-1(3)	8(3)	-1(3)
C(49)	55(5)	48(4)	36(4)	4(3)	12(4)	-3(4)
C(50)	57(5)	44(4)	41(4)	4(3)	11(4)	-4(4)
C(51)	54(5)	41(4)	40(4)	0(3)	10(4)	-2(4)
C(52)	50(4)	39(3)	36(3)	3(3)	8(3)	-1(3)
C(53)	46(4)	38(3)	38(3)	2(3)	11(3)	2(3)
C(54)	48(5)	47(4)	49(4)	-4(4)	20(4)	-8(4)
C(55)	53(5)	53(4)	56(4)	-4(4)	16(4)	-1(4)
C(56)	51(5)	53(4)	51(4)	-2(4)	17(4)	0(4)
C(57)	52(5)	48(4)	46(4)	-3(4)	16(4)	-1(4)
C(58)	49(4)	41(3)	41(3)	-2(3)	11(3)	0(3)
C(59)	52(4)	46(3)	39(3)	0(3)	10(3)	9(3)
C(60)	50(3)	41(3)	37(3)	-3(3)	10(3)	10(3)
C(61)	53(4)	40(3)	42(3)	3(3)	9(3)	9(3)
C(62)	54(5)	45(4)	49(4)	6(4)	14(4)	5(4)
C(63)	51(5)	41(4)	46(4)	3(3)	11(4)	5(4)
C(64)	47(3)	37(3)	35(3)	-2(3)	9(3)	4(3)
C(65)	47(4)	38(3)	34(3)	-3(3)	9(3)	3(3)
C(66)	46(5)	40(4)	34(4)	-8(3)	9(4)	-1(4)

C(67)	45(5)	35(4)	43(4)	-10(3)	8(4)	-1(3)
C(68)	44(4)	34(3)	36(3)	-1(3)	9(3)	0(3)
C(69)	53(4)	51(3)	42(3)	-5(3)	10(3)	9(3)
C(70)	54(4)	56(4)	40(3)	-10(3)	13(3)	4(3)
C(71)	57(5)	66(4)	46(4)	-9(4)	15(4)	4(4)
C(72)	51(5)	66(4)	47(4)	-14(4)	14(4)	-1(4)
C(73)	55(5)	61(4)	49(4)	-15(4)	13(4)	8(4)
C(74)	54(4)	57(3)	43(3)	-6(3)	10(3)	10(3)
C(75)	57(4)	58(3)	45(3)	-2(3)	7(3)	16(3)
C(76)	58(4)	59(3)	49(3)	3(3)	6(3)	18(3)
C(77)	66(5)	72(4)	57(4)	7(4)	5(4)	26(4)
C(78)	67(5)	78(4)	58(4)	2(4)	4(4)	23(4)
C(79)	65(5)	79(4)	59(4)	-6(4)	2(4)	22(4)
C(80)	58(4)	69(4)	50(4)	-4(3)	2(4)	19(4)

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Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for complex 2.

	x	y	z	U(eq)
H(1A)	-1641	7219	4392	80
H(1B)	-1252	7808	4159	80
H(1C)	-1222	7580	5026	80
H(2A)	-1026	5837	3397	89
H(2B)	-1200	6609	3072	89
H(2C)	-1548	6189	3589	89
H(3A)	-794	6222	5585	97
H(3B)	-799	5595	4978	97
H(3C)	-1324	6003	5063	97
H(5)	-32	7579	5996	50
H(6)	-437	7965	7002	53
H(7)	-981	8959	6883	50
H(8)	-1075	9636	5772	49
H(9)	-677	9296	4759	46
H(11)	102	9571	4004	49
H(12)	-248	10258	2933	49
H(13)	-835	9729	1971	54
H(14)	-1028	8528	1991	54
H(15)	-681	7829	3053	49
H(17)	595	9153	5676	47
H(18)	1534	9579	5642	57
H(19)	1871	8944	4474	55
H(20)	1130	8084	3867	49
H(21)	849	7074	3553	50
H(23)	412	5763	5273	54
H(24)	-176	5442	3993	54
H(25)	125	6201	2915	57
H(27)	620	6814	6341	64
H(28)	539	6191	7457	72
H(29)	1179	5361	7923	65
H(30)	1892	5183	7322	64
H(31)	1962	5784	6153	60
H(33)	1549	5560	4603	59
H(34)	2201	5107	3971	65
H(35)	2965	5757	3970	67

H(36)	3024	6969	4401	68
H(37)	2329	7424	5000	62
H(38A)	2117	7643	7729	142
H(38B)	1822	7073	7151	142
H(38C)	1499	7587	7618	142
H(39A)	1101	8725	7290	155
H(39B)	1399	9354	6933	155
H(39C)	1664	8968	7692	155
H(40A)	2223	9215	6393	178
H(40B)	2607	8564	6643	178
H(40C)	2348	8988	7264	178
H(41A)	4065	5876	3269	92
H(41B)	3955	6216	4049	92
H(41C)	4369	5586	4055	92
H(42A)	4573	7767	3018	102
H(42B)	4107	7612	3479	102
H(42C)	4145	7181	2718	102
H(43A)	5305	5936	3203	99
H(43B)	5282	6702	2805	99
H(43C)	4819	6145	2584	99
H(44A)	7760	8891	6716	96
H(44B)	7400	9583	6583	96
H(44C)	7896	9510	6166	96
H(45A)	7485	9765	4836	100
H(45B)	6898	9888	4959	100
H(45C)	7026	9343	4326	100
H(46A)	7590	8084	4705	105
H(46B)	7809	7874	5561	105
H(46C)	8022	8570	5192	105
H(48)	5717	8007	3731	54
H(49)	5827	8707	2661	55
H(50)	5242	9635	2319	56
H(51)	4607	9904	3013	54
H(52)	4541	9259	4153	49
H(54)	4187	7347	5186	56
H(55)	3452	7667	5721	64
H(56)	3385	8831	6214	61
H(57)	4055	9637	6186	57
H(58)	4799	9329	5643	52
H(59)	6105	6044	4466	55
H(61)	5536	6890	6371	54
H(62)	4918	5881	5817	58
H(63)	5258	5386	4636	55
H(65)	5758	7948	6676	47

H(66)	6355	8966	7225	48
H(67)	6467	9835	6135	49
H(68)	5861	9410	4899	46
H(70)	6589	7697	4123	59
H(71)	6834	7236	3028	67
H(72)	7386	6194	3093	65
H(73)	7624	5632	4259	65
H(74)	7348	6065	5352	62
H(76)	6552	5803	6407	67
H(77)	7086	5220	7443	79
H(78)	7753	5820	8128	82
H(79)	8000	6925	7792	82
H(80)	7510	7569	6767	72

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Table 6. Torsion angles [deg] for complex 2.

Complex 3

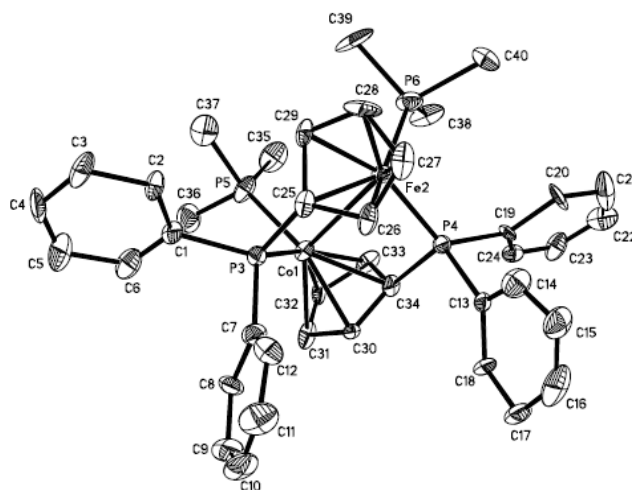


Table 1. Crystal data and structure refinement for Complex 3

Identification code	test
Empirical formula	C <sub>40</sub> H <sub>46</sub> Co Fe P <sub>4</sub>
Formula weight	765.43
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, Cc
Unit cell dimensions	a = 13.2681(19) Å    alpha = 90 deg. b = 15.846(2) Å    beta = 93.362(2) deg. c = 17.926(3) Å    gamma = 90 deg.

Volume	3762.4(10) Å <sup>3</sup>
Z, Calculated density	4, 1.351 Mg/m <sup>3</sup>
Absorption coefficient	1.024 mm <sup>-1</sup>
F(000)	1596
Crystal size	0.18 x 0.15 x 0.12 mm
Theta range for data collection	2.00 to 27.52 deg.
Limiting indices	-16<=h<=17, -18<=k<=20, -23<=l<=17
Reflections collected / unique	10802 / 6063 [R(int) = 0.0253]
Completeness to theta = 27.52	97.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8870 and 0.8372
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	6063 / 2 / 421
Goodness-of-fit on F <sup>2</sup>	1.022
Final R indices [I>2sigma(I)]	R1 = 0.0450, wR2 = 0.1161
R indices (all data)	R1 = 0.0581, wR2 = 0.1243
Absolute structure parameter	0.20(4)
Largest diff. peak and hole	0.726 and -0.362 e.Å <sup>-3</sup>

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for Complex 3

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Co(1)	8002(1)	2906(1)	3430(1)	33(1)
Fe(2)	5950(1)	2903(1)	3953(1)	30(1)
P(3)	7101(2)	2280(2)	2550(2)	29(1)
P(4)	6853(2)	2269(2)	4816(2)	27(1)
P(5)	8145(3)	4124(2)	2874(2)	45(1)
P(6)	5810(3)	4111(2)	4513(2)	48(1)
C(1)	6949(9)	2591(7)	1557(6)	36(3)
C(2)	5975(10)	2730(8)	1217(7)	39(3)
C(3)	5917(13)	2948(8)	416(8)	60(4)
C(4)	6831(14)	2983(9)	40(7)	67(5)
C(5)	7705(11)	2769(9)	373(8)	69(4)
C(6)	7738(10)	2577(9)	1159(7)	58(4)
C(7)	7317(10)	1153(8)	2389(7)	43(3)
C(8)	8373(10)	932(8)	2283(8)	42(3)
C(9)	8597(12)	72(10)	2159(8)	71(5)
C(10)	7797(14)	-536(7)	2074(9)	70(4)
C(11)	6963(14)	-269(9)	2153(10)	77(5)
C(12)	6642(10)	534(9)	2324(9)	55(3)
C(13)	6579(8)	1135(7)	4994(6)	28(2)
C(14)	5638(11)	881(9)	5067(9)	58(4)
C(15)	5358(11)	101(9)	5273(9)	62(4)
C(16)	6012(13)	-475(9)	5309(10)	81(5)
C(17)	7143(13)	-313(8)	5248(9)	70(4)
C(18)	7367(10)	539(7)	5110(8)	50(3)
C(19)	7043(8)	2574(6)	5816(6)	34(3)
C(20)	6159(10)	2629(9)	6242(7)	52(3)
C(21)	6289(15)	2821(10)	6982(9)	87(6)
C(22)	7262(13)	2955(9)	7326(8)	67(5)
C(23)	8045(12)	2933(8)	6913(8)	53(4)
C(24)	7940(10)	2755(7)	6212(7)	41(3)
C(25)	5870(7)	2351(6)	2885(6)	31(2)
C(26)	5417(10)	1801(8)	3427(6)	45(3)



C (27)	4631 (9)	2207 (7)	3719 (7)	51 (3)
C (28)	4568 (8)	3029 (8)	3399 (8)	54 (4)
C (29)	5300 (9)	3148 (7)	2895 (5)	38 (3)
C (30)	8522 (7)	1802 (5)	3966 (6)	26 (2)
C (31)	9375 (7)	2232 (7)	3650 (6)	42 (3)
C (32)	9469 (8)	3022 (8)	3966 (5)	38 (3)
C (33)	8684 (8)	3106 (6)	4478 (7)	37 (3)
C (34)	8132 (7)	2343 (6)	4498 (6)	29 (2)
C (35)	8538 (12)	5013 (9)	3477 (9)	75 (4)
C (36)	9159 (12)	4257 (9)	2332 (8)	69 (3)
C (37)	7235 (12)	4586 (8)	2251 (8)	66 (4)
C (38)	6831 (12)	4621 (6)	5129 (7)	62 (4)
C (39)	5528 (13)	5045 (8)	3910 (8)	80 (5)
C (40)	4717 (12)	4083 (9)	5202 (9)	73 (4)

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Table 3. Bond lengths [Å] and angles [deg] for Complex 3

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Co(1)–C(33)	2.061(11)
Co(1)–C(30)	2.092(9)
Co(1)–C(34)	2.109(10)
Co(1)–C(31)	2.128(10)
Co(1)–C(32)	2.127(11)
Co(1)–P(3)	2.164(3)
Co(1)–P(5)	2.186(3)
Co(1)–Fe(2)	2.9319(9)
Fe(2)–C(28)	2.043(10)
Fe(2)–C(29)	2.073(10)
Fe(2)–C(26)	2.087(12)
Fe(2)–C(27)	2.090(10)
Fe(2)–C(25)	2.102(10)
Fe(2)–P(4)	2.149(3)
Fe(2)–P(6)	2.175(4)
P(3)–C(25)	1.776(11)
P(3)–C(7)	1.834(13)
P(3)–C(1)	1.846(11)
P(4)–C(34)	1.825(10)
P(4)–C(19)	1.861(11)
P(4)–C(13)	1.864(11)
P(5)–C(36)	1.717(14)
P(5)–C(37)	1.756(14)
P(5)–C(35)	1.833(15)
P(6)–C(39)	1.858(12)
P(6)–C(38)	1.879(11)
P(6)–C(40)	1.960(14)
C(1)–C(6)	1.301(16)
C(1)–C(2)	1.414(15)
C(2)–C(3)	1.475(18)
C(2)–H(2)	0.9300
C(3)–C(4)	1.42(2)
C(3)–H(3)	0.9300
C(4)–C(5)	1.32(2)
C(4)–H(4)	0.9300
C(5)–C(6)	1.440(19)
C(5)–H(5)	0.9300
C(6)–H(6)	0.9300
C(7)–C(12)	1.328(18)

C (7)–C (8)	1. 467 (18)
C (8)–C (9)	1. 416 (18)
C (8)–H (8)	0. 9300
C (9)–C (10)	1. 43 (2)
C (9)–H (9)	0. 9300
C (10)–C (11)	1. 20 (2)
C (10)–H (10)	0. 9300
C (11)–C (12)	1. 382 (19)
C (11)–H (11)	0. 9300
C (12)–H (12)	0. 9300
C (13)–C (14)	1. 325 (18)
C (13)–C (18)	1. 415 (15)
C (14)–C (15)	1. 348 (19)
C (14)–H (14)	0. 9300
C (15)–C (16)	1. 26 (2)
C (15)–H (15)	0. 9300
C (16)–C (17)	1. 53 (2)
C (16)–H (16)	0. 9300
C (17)–C (18)	1. 407 (15)
C (17)–H (17)	0. 9300
C (18)–H (18)	0. 9300
C (19)–C (24)	1. 378 (16)
C (19)–C (20)	1. 440 (13)
C (20)–C (21)	1. 36 (2)
C (20)–H (20)	0. 9300
C (21)–C (22)	1. 41 (2)
C (21)–H (21)	0. 9300
C (22)–C (23)	1. 31 (2)
C (22)–H (22)	0. 9300
C (23)–C (24)	1. 287 (18)
C (23)–H (23)	0. 9300
C (24)–H (24)	0. 9300
C (25)–C (29)	1. 472 (14)
C (25)–C (26)	1. 461 (15)
C (26)–C (27)	1. 356 (17)
C (26)–H (26)	0. 9800
C (27)–C (28)	1. 424 (17)
C (27)–H (27)	0. 9800
C (28)–C (29)	1. 377 (18)
C (28)–H (28)	0. 9799
C (29)–H (29)	0. 9800
C (30)–C (34)	1. 403 (14)
C (30)–C (31)	1. 463 (11)
C (30)–H (30)	0. 9800

C (31)–C (32)	1. 377 (16)
C (31)–H (31)	0. 9799
C (32)–C (33)	1. 434 (16)
C (32)–H (32)	0. 9800
C (33)–C (34)	1. 416 (11)
C (33)–H (33)	0. 9800
C (35)–H (35A)	0. 9600
C (35)–H (35B)	0. 9600
C (35)–H (35C)	0. 9600
C (36)–H (36A)	0. 9600
C (36)–H (36B)	0. 9600
C (36)–H (36C)	0. 9600
C (37)–H (37A)	0. 9600
C (37)–H (37B)	0. 9600
C (37)–H (37C)	0. 9600
C (38)–H (38A)	0. 9600
C (38)–H (38B)	0. 9600
C (38)–H (38C)	0. 9600
C (39)–H (39A)	0. 9600
C (39)–H (39B)	0. 9600
C (39)–H (39C)	0. 9600
C (40)–H (40A)	0. 9600
C (40)–H (40B)	0. 9600
C (40)–H (40C)	0. 9600
C (33)–Co (1)–C (30)	66. 2 (4)
C (33)–Co (1)–C (34)	39. 7 (3)
C (30)–Co (1)–C (34)	39. 0 (4)
C (33)–Co (1)–C (31)	65. 4 (5)
C (30)–Co (1)–C (31)	40. 6 (3)
C (34)–Co (1)–C (31)	66. 2 (4)
C (33)–Co (1)–C (32)	40. 0 (4)
C (30)–Co (1)–C (32)	66. 3 (4)
C (34)–Co (1)–C (32)	66. 6 (4)
C (31)–Co (1)–C (32)	37. 8 (4)
C (33)–Co (1)–P (3)	158. 4 (3)
C (30)–Co (1)–P (3)	96. 0 (3)
C (34)–Co (1)–P (3)	118. 7 (3)
C (31)–Co (1)–P (3)	109. 6 (4)
C (32)–Co (1)–P (3)	145. 2 (3)
C (33)–Co (1)–P (5)	103. 5 (3)
C (30)–Co (1)–P (5)	155. 9 (3)
C (34)–Co (1)–P (5)	141. 5 (3)
C (31)–Co (1)–P (5)	115. 6 (3)

C (32)–Co (1)–P (5)	91.6 (3)
P (3)–Co (1)–P (5)	97.52 (13)
C (33)–Co (1)–Fe (2)	94.3 (3)
C (30)–Co (1)–Fe (2)	98.0 (2)
C (34)–Co (1)–Fe (2)	74.8 (3)
C (31)–Co (1)–Fe (2)	137.8 (3)
C (32)–Co (1)–Fe (2)	134.3 (3)
P (3)–Co (1)–Fe (2)	75.42 (9)
P (5)–Co (1)–Fe (2)	104.71 (12)
C (28)–Fe (2)–C (29)	39.1 (5)
C (28)–Fe (2)–C (26)	65.9 (5)
C (29)–Fe (2)–C (26)	68.4 (4)
C (28)–Fe (2)–C (27)	40.3 (5)
C (29)–Fe (2)–C (27)	67.5 (5)
C (26)–Fe (2)–C (27)	37.9 (5)
C (28)–Fe (2)–C (25)	66.5 (4)
C (29)–Fe (2)–C (25)	41.3 (4)
C (26)–Fe (2)–C (25)	40.8 (4)
C (27)–Fe (2)–C (25)	66.5 (4)
C (28)–Fe (2)–P (4)	147.4 (4)
C (29)–Fe (2)–P (4)	158.4 (3)
C (26)–Fe (2)–P (4)	95.4 (3)
C (27)–Fe (2)–P (4)	108.8 (4)
C (25)–Fe (2)–P (4)	117.2 (3)
C (28)–Fe (2)–P (6)	92.3 (4)
C (29)–Fe (2)–P (6)	102.4 (4)
C (26)–Fe (2)–P (6)	155.4 (4)
C (27)–Fe (2)–P (6)	117.7 (4)
C (25)–Fe (2)–P (6)	141.8 (3)
P (4)–Fe (2)–P (6)	97.97 (13)
C (28)–Fe (2)–Co (1)	131.9 (4)
C (29)–Fe (2)–Co (1)	92.9 (3)
C (26)–Fe (2)–Co (1)	98.8 (4)
C (27)–Fe (2)–Co (1)	136.0 (4)
C (25)–Fe (2)–Co (1)	73.0 (3)
P (4)–Fe (2)–Co (1)	75.00 (9)
P (6)–Fe (2)–Co (1)	104.59 (13)
C (25)–P (3)–C (7)	105.7 (6)
C (25)–P (3)–C (1)	105.0 (5)
C (7)–P (3)–C (1)	96.8 (6)
C (25)–P (3)–Co (1)	101.8 (3)
C (7)–P (3)–Co (1)	118.4 (4)
C (1)–P (3)–Co (1)	127.2 (4)
C (34)–P (4)–C (19)	102.0 (5)

C(34)-P(4)-C(13)	108.1(5)
C(19)-P(4)-C(13)	95.8(5)
C(34)-P(4)-Fe(2)	103.6(3)
C(19)-P(4)-Fe(2)	127.6(3)
C(13)-P(4)-Fe(2)	117.9(4)
C(36)-P(5)-C(37)	96.9(8)
C(36)-P(5)-C(35)	91.9(7)
C(37)-P(5)-C(35)	102.5(7)
C(36)-P(5)-Co(1)	117.3(5)
C(37)-P(5)-Co(1)	125.7(5)
C(35)-P(5)-Co(1)	116.1(5)
C(39)-P(6)-C(38)	96.5(6)
C(39)-P(6)-C(40)	104.7(7)
C(38)-P(6)-C(40)	100.0(8)
C(39)-P(6)-Fe(2)	116.9(5)
C(38)-P(6)-Fe(2)	124.9(4)
C(40)-P(6)-Fe(2)	110.9(5)
C(6)-C(1)-C(2)	120.7(11)
C(6)-C(1)-P(3)	118.6(8)
C(2)-C(1)-P(3)	120.2(9)
C(1)-C(2)-C(3)	116.8(13)
C(1)-C(2)-H(2)	121.6
C(3)-C(2)-H(2)	121.6
C(4)-C(3)-C(2)	118.2(14)
C(4)-C(3)-H(3)	120.9
C(2)-C(3)-H(3)	120.9
C(5)-C(4)-C(3)	121.9(12)
C(5)-C(4)-H(4)	119.0
C(3)-C(4)-H(4)	119.1
C(4)-C(5)-C(6)	118.2(12)
C(4)-C(5)-H(5)	120.9
C(6)-C(5)-H(5)	120.9
C(1)-C(6)-C(5)	123.7(12)
C(1)-C(6)-H(6)	118.2
C(5)-C(6)-H(6)	118.2
C(12)-C(7)-C(8)	117.2(12)
C(12)-C(7)-P(3)	128.4(11)
C(8)-C(7)-P(3)	114.3(10)
C(9)-C(8)-C(7)	117.4(13)
C(9)-C(8)-H(8)	121.3
C(7)-C(8)-H(8)	121.3
C(10)-C(9)-C(8)	120.1(14)
C(10)-C(9)-H(9)	119.9
C(8)-C(9)-H(9)	119.9

C(11)-C(10)-C(9)	115.6(13)
C(11)-C(10)-H(10)	122.2
C(9)-C(10)-H(10)	122.2
C(10)-C(11)-C(12)	130.5(16)
C(10)-C(11)-H(11)	114.8
C(12)-C(11)-H(11)	114.7
C(7)-C(12)-C(11)	118.9(14)
C(7)-C(12)-H(12)	120.5
C(11)-C(12)-H(12)	120.5
C(14)-C(13)-C(18)	118.3(12)
C(14)-C(13)-P(4)	120.3(10)
C(18)-C(13)-P(4)	121.2(9)
C(13)-C(14)-C(15)	125.6(14)
C(13)-C(14)-H(14)	117.2
C(15)-C(14)-H(14)	117.2
C(16)-C(15)-C(14)	118.6(14)
C(16)-C(15)-H(15)	120.7
C(14)-C(15)-H(15)	120.7
C(15)-C(16)-C(17)	123.3(12)
C(15)-C(16)-H(16)	118.3
C(17)-C(16)-H(16)	118.4
C(18)-C(17)-C(16)	113.0(12)
C(18)-C(17)-H(17)	123.5
C(16)-C(17)-H(17)	123.5
C(17)-C(18)-C(13)	120.3(13)
C(17)-C(18)-H(18)	119.8
C(13)-C(18)-H(18)	119.9
C(24)-C(19)-C(20)	114.8(11)
C(24)-C(19)-P(4)	127.9(8)
C(20)-C(19)-P(4)	117.3(9)
C(21)-C(20)-C(19)	118.0(14)
C(21)-C(20)-H(20)	121.0
C(19)-C(20)-H(20)	121.0
C(20)-C(21)-C(22)	121.2(14)
C(20)-C(21)-H(21)	119.4
C(22)-C(21)-H(21)	119.4
C(23)-C(22)-C(21)	118.9(13)
C(23)-C(22)-H(22)	120.5
C(21)-C(22)-H(22)	120.5
C(24)-C(23)-C(22)	120.9(14)
C(24)-C(23)-H(23)	119.6
C(22)-C(23)-H(23)	119.6
C(23)-C(24)-C(19)	126.0(14)
C(23)-C(24)-H(24)	117.0

C (19)–C (24)–H (24)	117.0
C (29)–C (25)–C (26)	105.8 (10)
C (29)–C (25)–P (3)	122.8 (8)
C (26)–C (25)–P (3)	127.5 (9)
C (29)–C (25)–Fe (2)	68.3 (5)
C (26)–C (25)–Fe (2)	69.0 (6)
P (3)–C (25)–Fe (2)	109.7 (4)
C (27)–C (26)–C (25)	109.2 (11)
C (27)–C (26)–Fe (2)	71.2 (7)
C (25)–C (26)–Fe (2)	70.1 (6)
C (27)–C (26)–H (26)	125.4
C (25)–C (26)–H (26)	125.4
Fe (2)–C (26)–H (26)	125.4
C (26)–C (27)–C (28)	107.8 (11)
C (26)–C (27)–Fe (2)	70.9 (7)
C (28)–C (27)–Fe (2)	68.1 (6)
C (26)–C (27)–H (27)	126.2
C (28)–C (27)–H (27)	126.0
Fe (2)–C (27)–H (27)	126.1
C (29)–C (28)–C (27)	111.3 (11)
C (29)–C (28)–Fe (2)	71.6 (6)
C (27)–C (28)–Fe (2)	71.7 (7)
C (29)–C (28)–H (28)	124.4
C (27)–C (28)–H (28)	124.4
Fe (2)–C (28)–H (28)	124.3
C (28)–C (29)–C (25)	105.9 (10)
C (28)–C (29)–Fe (2)	69.3 (6)
C (25)–C (29)–Fe (2)	70.4 (5)
C (28)–C (29)–H (29)	127.0
C (25)–C (29)–H (29)	127.1
Fe (2)–C (29)–H (29)	127.1
C (34)–C (30)–C (31)	107.6 (8)
C (34)–C (30)–Co (1)	71.1 (5)
C (31)–C (30)–Co (1)	71.0 (5)
C (34)–C (30)–H (30)	126.2
C (31)–C (30)–H (30)	126.1
Co (1)–C (30)–H (30)	126.2
C (32)–C (31)–C (30)	108.5 (10)
C (32)–C (31)–Co (1)	71.1 (7)
C (30)–C (31)–Co (1)	68.4 (5)
C (32)–C (31)–H (31)	125.7
C (30)–C (31)–H (31)	125.7
Co (1)–C (31)–H (31)	125.7
C (31)–C (32)–C (33)	107.2 (10)



C (31)–C (32)–Co (1)	71.1 (6)
C (33)–C (32)–Co (1)	67.5 (6)
C (31)–C (32)–H (32)	126.4
C (33)–C (32)–H (32)	126.4
Co (1)–C (32)–H (32)	126.4
C (34)–C (33)–C (32)	109.5 (10)
C (34)–C (33)–Co (1)	72.0 (6)
C (32)–C (33)–Co (1)	72.5 (7)
C (34)–C (33)–H (33)	125.2
C (32)–C (33)–H (33)	125.3
Co (1)–C (33)–H (33)	125.1
C (30)–C (34)–C (33)	107.0 (9)
C (30)–C (34)–P (4)	124.0 (7)
C (33)–C (34)–P (4)	123.7 (8)
C (30)–C (34)–Co (1)	69.9 (6)
C (33)–C (34)–Co (1)	68.3 (6)
P (4)–C (34)–Co (1)	106.4 (5)
P (5)–C (35)–H (35A)	109.5
P (5)–C (35)–H (35B)	109.5
H (35A)–C (35)–H (35B)	109.5
P (5)–C (35)–H (35C)	109.5
H (35A)–C (35)–H (35C)	109.5
H (35B)–C (35)–H (35C)	109.5
P (5)–C (36)–H (36A)	109.5
P (5)–C (36)–H (36B)	109.5
H (36A)–C (36)–H (36B)	109.5
P (5)–C (36)–H (36C)	109.5
H (36A)–C (36)–H (36C)	109.5
H (36B)–C (36)–H (36C)	109.5
P (5)–C (37)–H (37A)	109.5
P (5)–C (37)–H (37B)	109.5
H (37A)–C (37)–H (37B)	109.5
P (5)–C (37)–H (37C)	109.5
H (37A)–C (37)–H (37C)	109.5
H (37B)–C (37)–H (37C)	109.5
P (6)–C (38)–H (38A)	109.5
P (6)–C (38)–H (38B)	109.5
H (38A)–C (38)–H (38B)	109.5
P (6)–C (38)–H (38C)	109.5
H (38A)–C (38)–H (38C)	109.5
H (38B)–C (38)–H (38C)	109.5
P (6)–C (39)–H (39A)	109.5
P (6)–C (39)–H (39B)	109.5
H (39A)–C (39)–H (39B)	109.5

P (6) -C (39) -H (39C)	109.5
H (39A) -C (39) -H (39C)	109.5
H (39B) -C (39) -H (39C)	109.5
P (6) -C (40) -H (40A)	109.5
P (6) -C (40) -H (40B)	109.5
H (40A) -C (40) -H (40B)	109.5
P (6) -C (40) -H (40C)	109.5
H (40A) -C (40) -H (40C)	109.5
H (40B) -C (40) -H (40C)	109.5

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{Å}^2 \times 10^3$ ) for Complex 3

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$$

	U11	U22	U33	U23	U13	U12
Co(1)	36(1)	31(1)	31(1)	6(1)	-2(1)	-3(1)
Fe(2)	26(1)	32(1)	30(1)	-3(1)	-6(1)	6(1)
P(3)	31(1)	28(1)	28(2)	1(1)	0(1)	-1(1)
P(4)	30(1)	26(1)	24(1)	-1(1)	0(1)	1(1)
P(5)	54(2)	37(2)	42(2)	15(1)	-12(2)	-21(2)
P(6)	61(2)	37(2)	46(2)	-9(1)	-10(2)	16(2)
C(1)	43(6)	41(6)	23(5)	-6(4)	-16(4)	3(5)
C(2)	44(6)	53(6)	19(4)	0(4)	-12(4)	-13(5)
C(3)	88(10)	48(7)	43(7)	24(5)	-12(7)	-24(6)
C(4)	117(12)	65(8)	25(6)	3(5)	32(7)	-4(7)
C(5)	65(8)	90(9)	53(9)	32(7)	17(6)	-29(7)
C(6)	59(7)	68(8)	44(7)	7(6)	-21(6)	-7(6)
C(7)	50(6)	40(6)	38(7)	-1(5)	-6(5)	11(5)
C(8)	40(6)	43(6)	45(7)	-9(5)	6(5)	16(5)
C(9)	91(10)	73(9)	45(7)	-15(6)	-35(7)	46(8)
C(10)	111(11)	23(5)	74(9)	2(5)	-7(8)	-5(6)
C(11)	85(9)	51(8)	92(11)	-5(7)	-14(8)	-12(7)
C(12)	48(7)	60(8)	57(8)	-9(6)	10(6)	4(6)
C(13)	37(5)	26(5)	21(5)	1(4)	4(4)	2(4)
C(14)	52(7)	61(8)	59(9)	8(6)	-7(6)	-2(6)
C(15)	60(8)	53(7)	75(9)	18(6)	9(6)	-15(6)
C(16)	103(11)	60(8)	80(11)	27(7)	6(8)	-48(8)
C(17)	83(8)	37(6)	95(10)	34(6)	38(7)	22(5)
C(18)	66(8)	27(5)	58(7)	20(5)	20(6)	19(5)
C(19)	47(6)	23(5)	34(5)	-4(4)	24(5)	12(4)
C(20)	52(6)	64(7)	46(6)	-13(5)	39(5)	2(5)
C(21)	116(14)	103(11)	47(9)	-2(7)	39(9)	-30(9)
C(22)	97(10)	61(8)	39(7)	-20(5)	-30(7)	23(7)
C(23)	68(8)	55(7)	33(6)	9(5)	-18(6)	-18(6)
C(24)	54(7)	28(5)	43(7)	1(4)	6(5)	9(4)
C(25)	26(4)	41(5)	24(5)	-1(4)	-11(4)	-20(4)
C(26)	57(7)	54(7)	21(5)	4(5)	-8(5)	-18(6)
C(27)	55(7)	63(7)	35(6)	1(5)	-4(5)	-40(5)

C(28)	21(5)	57(7)	82(9)	-27(6)	-23(5)	22(4)
C(29)	40(6)	57(6)	15(4)	6(4)	-10(4)	-7(5)
C(30)	18(4)	20(4)	40(5)	14(4)	15(4)	1(3)
C(31)	17(4)	71(7)	38(6)	23(5)	1(4)	-17(4)
C(32)	36(5)	63(7)	16(4)	7(4)	0(3)	0(4)
C(33)	33(5)	25(4)	53(7)	10(4)	-9(5)	-18(4)
C(34)	30(4)	24(4)	35(6)	3(4)	8(4)	-16(3)
C(35)	86(9)	51(8)	87(11)	19(7)	0(7)	-27(7)
C(36)	74(7)	70(7)	63(7)	10(6)	21(6)	-10(5)
C(37)	78(8)	56(7)	63(8)	-5(6)	-1(7)	-20(6)
C(38)	93(9)	24(5)	62(8)	-25(5)	-51(7)	8(5)
C(39)	126(12)	34(6)	70(9)	-5(5)	-67(8)	31(6)
C(40)	79(8)	71(7)	72(8)	-1(5)	35(6)	33(6)

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Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for Complex 3

	x	y	z	U(eq)
H(2)	5398	2685	1485	47
H(3)	5299	3060	163	72
H(4)	6811	3162	-455	81
H(5)	8286	2742	107	83
H(6)	8357	2435	1396	70
H(8)	8876	1342	2297	51
H(9)	9264	-100	2132	85
H(10)	7916	-1100	1965	84
H(11)	6450	-667	2089	92
H(12)	5964	639	2393	66
H(14)	5128	1274	4966	69
H(15)	4695	-8	5387	75
H(16)	5798	-1028	5376	97
H(17)	7631	-733	5297	84
H(18)	8035	711	5096	60
H(20)	5518	2536	6019	63
H(21)	5727	2866	7267	105
H(22)	7346	3057	7837	80
H(23)	8685	3047	7129	64
H(24)	8522	2749	5948	49
H(26)	5642	1228	3556	53
H(27)	4187	1978	4087	61
H(28)	4066	3454	3519	65
H(29)	5399	3650	2588	45
H(30)	8291	1227	3850	31
H(31)	9801	1999	3272	50
H(32)	9977	3448	3860	46
H(33)	8577	3601	4791	45
H(35A)	8627	5506	3175	112
H(35B)	9164	4878	3746	112
H(35C)	8030	5122	3824	112
H(36A)	9145	3832	1951	103
H(36B)	9773	4210	2639	103
H(36C)	9124	4805	2103	103

H(37A)	7520	5072	2022	99
H(37B)	6662	4754	2518	99
H(37C)	7026	4184	1872	99
H(38A)	7465	4574	4900	93
H(38B)	6878	4344	5606	93
H(38C)	6673	5206	5197	93
H(39A)	5251	5487	4202	119
H(39B)	5049	4891	3511	119
H(39C)	6139	5240	3705	119
H(40A)	4578	4646	5365	109
H(40B)	4916	3740	5627	109
H(40C)	4121	3849	4951	109

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Table 6. Torsion angles [deg] for Complex 3

Complex 8

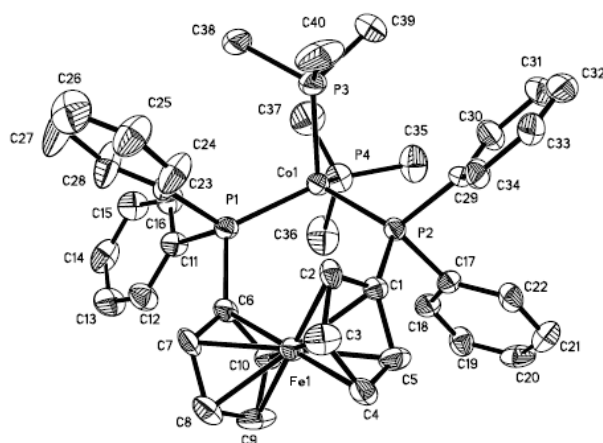


Table 1. Crystal data and structure refinement for Complex 8.

Identification code	test1	
Empirical formula	C40 H46 Co Fe P4	
Formula weight	765.43	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Triclinic, P-1	
Unit cell dimensions	a = 10.524(3) Å	alpha = 69.857(6) deg.
	b = 18.946(6) Å	beta = 87.349(6) deg.
	c = 20.071(6) Å	gamma = 87.141(6) deg.
Volume	3750.7(19) Å <sup>3</sup>	

Z, Calculated density	2, 1.355 Mg/m <sup>3</sup>
Absorption coefficient	1.027 mm <sup>-1</sup>
F(000)	1596.0
Crystal size	0.36 x 0.32 x 0.28 mm
Theta range for data collection	1.08 to 24.00 deg.
Limiting indices	-11<=h<=12, -20<=k<=21, -21<=l<=22
Reflections collected / unique	17348 / 11701 [R(int) = 0.0646]
Completeness to theta = 24.00	99.4 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	11701 / 0 / 841
Goodness-of-fit on F <sup>2</sup>	0.999
Final R indices [I>2sigma(I)]	R1 = 0.0692, wR2 = 0.1623
R indices (all data)	R1 = 0.1587, wR2 = 0.2498
Largest diff. peak and hole	0.567 and -0.589 e.Å <sup>-3</sup>



Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for Complex 8.

$U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	$U(\text{eq})$
C(1)	1699(9)	602(5)	3745(5)	38(2)
C(2)	2727(9)	113(5)	3675(5)	42(2)
C(3)	3586(11)	25(6)	4231(6)	59(3)
C(4)	3098(10)	454(6)	4637(5)	54(3)
C(5)	1943(11)	808(6)	4345(5)	54(3)
C(6)	3671(10)	1798(5)	2572(5)	44(3)
C(7)	4830(9)	1486(6)	2861(6)	51(3)
C(8)	5053(10)	1693(6)	3449(6)	60(3)
C(9)	4006(14)	2155(6)	3532(6)	71(4)
C(10)	3113(10)	2231(5)	2997(5)	47(3)
C(11)	3328(10)	2674(5)	1150(5)	49(3)
C(12)	4207(11)	3123(6)	1263(6)	66(3)
C(13)	4524(13)	3794(6)	740(7)	79(4)
C(14)	3994(14)	4003(7)	92(7)	76(4)
C(15)	3121(12)	3567(7)	-36(7)	72(4)
C(16)	2747(11)	2925(6)	497(6)	65(3)
C(17)	-532(9)	1492(5)	3591(5)	40(2)
C(18)	-556(10)	2271(6)	3312(6)	52(3)
C(19)	-1188(10)	2716(6)	3630(7)	60(3)
C(20)	-1834(12)	2401(7)	4230(7)	69(4)
C(21)	-1858(11)	1626(7)	4543(6)	66(3)
C(22)	-1207(9)	1176(6)	4209(6)	52(3)
C(23)	3970(9)	1131(6)	1512(5)	42(2)
C(24)	4141(13)	394(7)	1904(7)	83(4)
C(25)	4850(15)	-128(7)	1728(8)	90(5)
C(26)	5483(14)	91(8)	1095(10)	101(5)
C(27)	5351(18)	817(9)	667(9)	144(8)
C(28)	4593(13)	1327(7)	896(8)	98(5)
C(29)	-627(9)	108(5)	3414(5)	42(2)
C(30)	-1765(11)	170(7)	3135(6)	64(3)
C(31)	-2559(13)	-440(10)	3326(7)	95(5)
C(32)	-2127(17)	-1125(8)	3793(8)	85(5)
C(33)	-995(12)	-1199(7)	4058(6)	61(3)

C (34)	-221 (11)	-589 (5)	3861 (5)	52 (3)
C (35)	-2171 (10)	2355 (7)	1749 (7)	87 (4)
C (36)	-282 (13)	3391 (6)	1423 (8)	101 (5)
C (37)	-838 (14)	2656 (8)	500 (6)	98 (5)
C (38)	1272 (12)	808 (8)	596 (6)	87 (4)
C (39)	-1208 (12)	536 (8)	1266 (7)	96 (5)
C (40)	960 (17)	-327 (6)	1907 (7)	116 (6)
C (41)	4491 (8)	4899 (5)	2465 (5)	38 (2)
C (42)	5426 (10)	5235 (6)	1952 (5)	50 (3)
C (43)	6484 (11)	4690 (7)	2002 (6)	65 (3)
C (44)	6105 (11)	4020 (6)	2550 (6)	60 (3)
C (45)	4920 (9)	4129 (5)	2843 (6)	49 (3)
C (46)	6118 (9)	5776 (5)	3316 (5)	39 (2)
C (47)	7421 (9)	5635 (5)	3068 (6)	47 (3)
C (48)	7834 (11)	4889 (6)	3469 (6)	61 (3)
C (49)	6771 (11)	4560 (6)	3969 (6)	61 (3)
C (50)	5746 (10)	5104 (5)	3859 (5)	48 (3)
C (51)	5087 (9)	7044 (5)	3650 (5)	39 (2)
C (52)	5483 (10)	6670 (6)	4344 (5)	54 (3)
C (53)	5382 (11)	7013 (7)	4864 (6)	66 (3)
C (54)	4879 (10)	7735 (8)	4686 (7)	65 (4)
C (55)	4481 (10)	8109 (6)	4017 (6)	60 (3)
C (56)	4604 (9)	7767 (5)	3515 (6)	47 (3)
C (57)	6287 (9)	7252 (5)	2352 (5)	40 (2)
C (58)	7086 (10)	7704 (6)	2539 (6)	60 (3)
C (59)	7904 (10)	8208 (6)	2056 (6)	61 (3)
C (60)	7982 (11)	8240 (7)	1383 (7)	64 (3)
C (61)	7273 (13)	7784 (7)	1165 (6)	81 (4)
C (62)	6428 (11)	7298 (6)	1644 (6)	63 (3)
C (63)	2390 (9)	4662 (6)	3421 (5)	45 (3)
C (64)	2310 (9)	4779 (6)	4074 (6)	54 (3)
C (65)	1747 (13)	4240 (8)	4688 (6)	84 (4)
C (66)	1329 (13)	3578 (7)	4660 (8)	83 (4)
C (67)	1446 (12)	3452 (7)	4025 (8)	78 (4)
C (68)	1984 (10)	3982 (6)	3405 (7)	63 (3)
C (69)	1992 (9)	5320 (5)	1953 (5)	41 (2)
C (70)	679 (12)	5517 (7)	1998 (7)	77 (4)
C (71)	-164 (12)	5545 (7)	1466 (7)	76 (4)
C (72)	334 (15)	5359 (7)	903 (7)	84 (4)
C (73)	1612 (12)	5158 (8)	857 (7)	82 (4)
C (74)	2377 (11)	5145 (7)	1375 (6)	67 (3)
C (75)	137 (9)	6482 (7)	3350 (6)	62 (3)
C (76)	1958 (11)	6635 (6)	4283 (5)	66 (3)
C (77)	1307 (12)	7859 (6)	3103 (7)	76 (4)

C (78)	3389 (13)	8306 (5)	1347 (6)	78 (4)
C (79)	3518 (11)	7164 (7)	738 (5)	67 (3)
C (80)	1250 (12)	7554 (8)	1283 (7)	88 (4)
Co (1)	802 (1)	1494 (1)	1982 (1)	40 (1)
Co (2)	3195 (1)	6547 (1)	2621 (1)	38 (1)
Fe (1)	3378 (1)	1131 (1)	3603 (1)	41 (1)
Fe (2)	6155 (1)	4889 (1)	2945 (1)	42 (1)
P (1)	2811 (3)	1762 (2)	1804 (1)	42 (1)
P (2)	382 (2)	942 (1)	3115 (1)	37 (1)
P (3)	462 (3)	667 (2)	1470 (2)	59 (1)
P (4)	-526 (3)	2436 (2)	1452 (2)	60 (1)
P (5)	5102 (2)	6625 (1)	2959 (1)	35 (1)
P (6)	3043 (2)	5403 (1)	2638 (1)	40 (1)
P (7)	2856 (3)	7331 (2)	1543 (2)	51 (1)
P (8)	1754 (3)	6849 (2)	3325 (2)	47 (1)

---

Table 3. Bond lengths [Å] and angles [deg] for Complex 8.

---

C(1)–C(5)	1.424(13)
C(1)–C(2)	1.422(12)
C(1)–P(2)	1.857(10)
C(1)–Fe(1)	2.035(9)
C(2)–C(3)	1.428(14)
C(2)–Fe(1)	2.036(9)
C(3)–C(4)	1.401(14)
C(3)–Fe(1)	2.047(10)
C(4)–C(5)	1.408(14)
C(4)–Fe(1)	2.046(10)
C(5)–Fe(1)	2.032(11)
C(6)–C(7)	1.388(13)
C(6)–C(10)	1.462(13)
C(6)–P(1)	1.847(10)
C(6)–Fe(1)	2.037(9)
C(7)–C(8)	1.397(14)
C(7)–Fe(1)	2.051(10)
C(8)–C(9)	1.413(16)
C(8)–Fe(1)	2.060(10)
C(9)–C(10)	1.424(14)
C(9)–Fe(1)	2.036(10)
C(10)–Fe(1)	2.032(10)
C(11)–C(12)	1.365(13)
C(11)–C(16)	1.390(14)
C(11)–P(1)	1.863(10)
C(12)–C(13)	1.386(14)
C(13)–C(14)	1.360(17)
C(14)–C(15)	1.355(16)
C(15)–C(16)	1.376(14)
C(17)–C(22)	1.361(13)
C(17)–C(18)	1.386(13)
C(17)–P(2)	1.851(9)
C(18)–C(19)	1.356(13)
C(19)–C(20)	1.317(15)
C(20)–C(21)	1.386(15)
C(21)–C(22)	1.392(14)
C(23)–C(28)	1.314(14)
C(23)–C(24)	1.355(14)
C(23)–P(1)	1.878(10)
C(24)–C(25)	1.342(15)

C (25)–C (26)	1. 349 (17)
C (26)–C (27)	1. 352 (18)
C (27)–C (28)	1. 407 (17)
C (29)–C (30)	1. 328 (14)
C (29)–C (34)	1. 376 (13)
C (29)–P (2)	1. 855 (9)
C (30)–C (31)	1. 393 (15)
C (31)–C (32)	1. 384 (19)
C (32)–C (33)	1. 309 (18)
C (33)–C (34)	1. 380 (13)
C (35)–P (4)	1. 801 (11)
C (36)–P (4)	1. 822 (12)
C (37)–P (4)	1. 853 (13)
C (38)–P (3)	1. 853 (11)
C (39)–P (3)	1. 870 (12)
C (40)–P (3)	1. 843 (13)
C (41)–C (42)	1. 397 (12)
C (41)–C (45)	1. 452 (13)
C (41)–P (6)	1. 842 (9)
C (41)–Fe (2)	2. 034 (9)
C (42)–C (43)	1. 464 (14)
C (42)–Fe (2)	2. 045 (11)
C (43)–C (44)	1. 425 (15)
C (43)–Fe (2)	2. 066 (11)
C (44)–C (45)	1. 391 (14)
C (44)–Fe (2)	2. 061 (10)
C (45)–Fe (2)	2. 053 (9)
C (46)–C (50)	1. 420 (13)
C (46)–C (47)	1. 480 (13)
C (46)–P (5)	1. 830 (10)
C (46)–Fe (2)	2. 057 (9)
C (47)–C (48)	1. 422 (14)
C (47)–Fe (2)	2. 071 (9)
C (48)–C (49)	1. 478 (15)
C (48)–Fe (2)	2. 097 (11)
C (49)–C (50)	1. 424 (14)
C (49)–Fe (2)	2. 057 (11)
C (50)–Fe (2)	2. 034 (10)
C (51)–C (56)	1. 376 (13)
C (51)–C (52)	1. 400 (13)
C (51)–P (5)	1. 821 (9)
C (52)–C (53)	1. 405 (14)
C (53)–C (54)	1. 374 (15)
C (54)–C (55)	1. 359 (15)

C (55)–C (56)	1. 372 (13)
C (57)–C (58)	1. 378 (13)
C (57)–C (62)	1. 395 (13)
C (57)–P (5)	1. 861 (9)
C (58)–C (59)	1. 400 (13)
C (59)–C (60)	1. 329 (15)
C (60)–C (61)	1. 361 (16)
C (61)–C (62)	1. 398 (14)
C (63)–C (68)	1. 388 (13)
C (63)–C (64)	1. 401 (14)
C (63)–P (6)	1. 841 (10)
C (64)–C (65)	1. 427 (15)
C (65)–C (66)	1. 370 (17)
C (66)–C (67)	1. 374 (17)
C (67)–C (68)	1. 416 (15)
C (69)–C (74)	1. 351 (13)
C (69)–C (70)	1. 421 (14)
C (69)–P (6)	1. 856 (10)
C (70)–C (71)	1. 405 (15)
C (71)–C (72)	1. 370 (17)
C (72)–C (73)	1. 388 (17)
C (73)–C (74)	1. 337 (15)
C (75)–P (8)	1. 862 (10)
C (76)–P (8)	1. 845 (10)
C (77)–P (8)	1. 851 (10)
C (78)–P (7)	1. 863 (10)
C (79)–P (7)	1. 850 (10)
C (80)–P (7)	1. 779 (12)
Co (1)–P (2)	2. 184 (3)
Co (1)–P (1)	2. 184 (3)
Co (1)–P (3)	2. 199 (3)
Co (1)–P (4)	2. 203 (3)
Co (2)–P (6)	2. 170 (3)
Co (2)–P (5)	2. 176 (3)
Co (2)–P (7)	2. 197 (3)
Co (2)–P (8)	2. 211 (3)
C (5)–C (1)–C (2)	106. 8 (9)
C (5)–C (1)–P (2)	128. 4 (8)
C (2)–C (1)–P (2)	124. 7 (7)
C (5)–C (1)–Fe (1)	69. 4 (6)
C (2)–C (1)–Fe (1)	69. 6 (5)
P (2)–C (1)–Fe (1)	122. 7 (4)
C (1)–C (2)–C (3)	108. 0 (9)

C(1)–C(2)–Fe(1)	69.5(5)
C(3)–C(2)–Fe(1)	69.9(6)
C(4)–C(3)–C(2)	108.1(10)
C(4)–C(3)–Fe(1)	70.0(6)
C(2)–C(3)–Fe(1)	69.1(5)
C(3)–C(4)–C(5)	108.2(9)
C(3)–C(4)–Fe(1)	70.0(6)
C(5)–C(4)–Fe(1)	69.2(6)
C(4)–C(5)–C(1)	108.8(10)
C(4)–C(5)–Fe(1)	70.3(6)
C(1)–C(5)–Fe(1)	69.6(6)
C(7)–C(6)–C(10)	107.7(9)
C(7)–C(6)–P(1)	132.9(8)
C(10)–C(6)–P(1)	119.4(8)
C(7)–C(6)–Fe(1)	70.7(6)
C(10)–C(6)–Fe(1)	68.8(5)
P(1)–C(6)–Fe(1)	126.0(5)
C(6)–C(7)–C(8)	110.1(10)
C(6)–C(7)–Fe(1)	69.6(5)
C(8)–C(7)–Fe(1)	70.5(6)
C(7)–C(8)–C(9)	107.4(10)
C(7)–C(8)–Fe(1)	69.8(6)
C(9)–C(8)–Fe(1)	68.9(6)
C(8)–C(9)–C(10)	109.3(10)
C(8)–C(9)–Fe(1)	70.7(6)
C(10)–C(9)–Fe(1)	69.3(6)
C(9)–C(10)–C(6)	105.5(10)
C(9)–C(10)–Fe(1)	69.7(6)
C(6)–C(10)–Fe(1)	69.1(5)
C(12)–C(11)–C(16)	117.3(10)
C(12)–C(11)–P(1)	125.6(8)
C(16)–C(11)–P(1)	117.1(8)
C(11)–C(12)–C(13)	121.1(12)
C(14)–C(13)–C(12)	120.2(12)
C(15)–C(14)–C(13)	120.0(11)
C(14)–C(15)–C(16)	119.8(12)
C(15)–C(16)–C(11)	121.3(12)
C(22)–C(17)–C(18)	116.8(9)
C(22)–C(17)–P(2)	123.7(7)
C(18)–C(17)–P(2)	119.5(7)
C(19)–C(18)–C(17)	123.3(10)
C(20)–C(19)–C(18)	119.1(11)
C(19)–C(20)–C(21)	121.1(11)
C(20)–C(21)–C(22)	119.1(11)

C (17)–C (22)–C (21)	120.6 (10)
C (28)–C (23)–C (24)	113.4 (10)
C (28)–C (23)–P (1)	124.8 (9)
C (24)–C (23)–P (1)	121.5 (8)
C (25)–C (24)–C (23)	127.3 (12)
C (24)–C (25)–C (26)	117.9 (13)
C (25)–C (26)–C (27)	118.5 (14)
C (26)–C (27)–C (28)	119.8 (14)
C (23)–C (28)–C (27)	123.1 (13)
C (30)–C (29)–C (34)	118.0 (10)
C (30)–C (29)–P (2)	118.1 (9)
C (34)–C (29)–P (2)	123.6 (8)
C (29)–C (30)–C (31)	121.0 (12)
C (32)–C (31)–C (30)	119.1 (13)
C (33)–C (32)–C (31)	120.5 (13)
C (32)–C (33)–C (34)	119.5 (13)
C (29)–C (34)–C (33)	121.7 (11)
C (42)–C (41)–C (45)	108.0 (9)
C (42)–C (41)–P (6)	123.6 (8)
C (45)–C (41)–P (6)	128.2 (7)
C (42)–C (41)–Fe (2)	70.4 (6)
C (45)–C (41)–Fe (2)	69.9 (5)
P (6)–C (41)–Fe (2)	122.1 (5)
C (41)–C (42)–C (43)	108.8 (10)
C (41)–C (42)–Fe (2)	69.6 (6)
C (43)–C (42)–Fe (2)	69.9 (6)
C (44)–C (43)–C (42)	105.2 (10)
C (44)–C (43)–Fe (2)	69.6 (6)
C (42)–C (43)–Fe (2)	68.4 (6)
C (45)–C (44)–C (43)	110.8 (10)
C (45)–C (44)–Fe (2)	69.9 (6)
C (43)–C (44)–Fe (2)	70.0 (6)
C (44)–C (45)–C (41)	107.1 (9)
C (44)–C (45)–Fe (2)	70.6 (6)
C (41)–C (45)–Fe (2)	68.5 (5)
C (50)–C (46)–C (47)	107.3 (8)
C (50)–C (46)–P (5)	125.1 (7)
C (47)–C (46)–P (5)	127.4 (7)
C (50)–C (46)–Fe (2)	68.9 (5)
C (47)–C (46)–Fe (2)	69.5 (5)
P (5)–C (46)–Fe (2)	123.5 (5)
C (48)–C (47)–C (46)	108.8 (9)
C (48)–C (47)–Fe (2)	71.1 (6)
C (46)–C (47)–Fe (2)	68.5 (5)



C (47)–C (48)–C (49)	106.1 (10)
C (47)–C (48)–Fe (2)	69.0 (6)
C (49)–C (48)–Fe (2)	67.7 (6)
C (50)–C (49)–C (48)	109.0 (9)
C (50)–C (49)–Fe (2)	68.8 (6)
C (48)–C (49)–Fe (2)	70.6 (6)
C (46)–C (50)–C (49)	108.7 (9)
C (46)–C (50)–Fe (2)	70.5 (6)
C (49)–C (50)–Fe (2)	70.5 (6)
C (56)–C (51)–C (52)	115.5 (9)
C (56)–C (51)–P (5)	119.8 (8)
C (52)–C (51)–P (5)	124.6 (8)
C (51)–C (52)–C (53)	121.8 (10)
C (54)–C (53)–C (52)	119.0 (11)
C (55)–C (54)–C (53)	120.4 (11)
C (54)–C (55)–C (56)	119.6 (11)
C (55)–C (56)–C (51)	123.7 (11)
C (58)–C (57)–C (62)	114.0 (9)
C (58)–C (57)–P (5)	125.3 (8)
C (62)–C (57)–P (5)	120.7 (8)
C (57)–C (58)–C (59)	123.7 (10)
C (60)–C (59)–C (58)	119.7 (11)
C (59)–C (60)–C (61)	120.2 (11)
C (60)–C (61)–C (62)	119.9 (11)
C (57)–C (62)–C (61)	122.4 (11)
C (68)–C (63)–C (64)	117.6 (10)
C (68)–C (63)–P (6)	123.6 (8)
C (64)–C (63)–P (6)	118.8 (8)
C (63)–C (64)–C (65)	121.0 (11)
C (66)–C (65)–C (64)	120.6 (12)
C (65)–C (66)–C (67)	118.3 (12)
C (66)–C (67)–C (68)	122.2 (12)
C (63)–C (68)–C (67)	120.2 (12)
C (74)–C (69)–C (70)	116.0 (10)
C (74)–C (69)–P (6)	125.8 (8)
C (70)–C (69)–P (6)	117.9 (8)
C (71)–C (70)–C (69)	122.1 (12)
C (72)–C (71)–C (70)	116.8 (12)
C (71)–C (72)–C (73)	121.7 (12)
C (74)–C (73)–C (72)	119.2 (12)
C (73)–C (74)–C (69)	124.3 (12)
P (2)–Co (1)–P (1)	110.19 (11)
P (2)–Co (1)–P (3)	106.47 (12)
P (1)–Co (1)–P (3)	107.43 (12)

P(2)-Co(1)-P(4)	114.25(12)
P(1)-Co(1)-P(4)	114.58(12)
P(3)-Co(1)-P(4)	103.12(14)
P(6)-Co(2)-P(5)	106.51(11)
P(6)-Co(2)-P(7)	109.09(12)
P(5)-Co(2)-P(7)	112.05(11)
P(6)-Co(2)-P(8)	112.68(11)
P(5)-Co(2)-P(8)	110.28(11)
P(7)-Co(2)-P(8)	106.32(12)
C(10)-Fe(1)-C(5)	110.2(4)
C(10)-Fe(1)-C(2)	138.6(4)
C(5)-Fe(1)-C(2)	68.4(4)
C(10)-Fe(1)-C(9)	41.0(4)
C(5)-Fe(1)-C(9)	111.0(5)
C(2)-Fe(1)-C(9)	179.2(5)
C(10)-Fe(1)-C(6)	42.1(4)
C(5)-Fe(1)-C(6)	140.1(4)
C(2)-Fe(1)-C(6)	111.4(4)
C(9)-Fe(1)-C(6)	68.7(4)
C(10)-Fe(1)-C(1)	109.7(4)
C(5)-Fe(1)-C(1)	41.0(4)
C(2)-Fe(1)-C(1)	40.9(3)
C(9)-Fe(1)-C(1)	138.3(5)
C(6)-Fe(1)-C(1)	111.4(4)
C(10)-Fe(1)-C(4)	138.5(5)
C(5)-Fe(1)-C(4)	40.4(4)
C(2)-Fe(1)-C(4)	68.3(4)
C(9)-Fe(1)-C(4)	111.6(5)
C(6)-Fe(1)-C(4)	179.4(5)
C(1)-Fe(1)-C(4)	68.7(4)
C(10)-Fe(1)-C(3)	178.0(5)
C(5)-Fe(1)-C(3)	67.8(5)
C(2)-Fe(1)-C(3)	41.0(4)
C(9)-Fe(1)-C(3)	139.5(5)
C(6)-Fe(1)-C(3)	139.4(4)
C(1)-Fe(1)-C(3)	68.8(4)
C(4)-Fe(1)-C(3)	40.0(4)
C(10)-Fe(1)-C(7)	68.6(4)
C(5)-Fe(1)-C(7)	178.4(4)
C(2)-Fe(1)-C(7)	113.3(4)
C(9)-Fe(1)-C(7)	67.3(5)
C(6)-Fe(1)-C(7)	39.7(4)
C(1)-Fe(1)-C(7)	140.3(4)
C(4)-Fe(1)-C(7)	139.8(4)

C(3)–Fe(1)–C(7)	113.4(5)
C(10)–Fe(1)–C(8)	68.9(4)
C(5)–Fe(1)–C(8)	138.9(4)
C(2)–Fe(1)–C(8)	140.4(4)
C(9)–Fe(1)–C(8)	40.4(4)
C(6)–Fe(1)–C(8)	67.8(4)
C(1)–Fe(1)–C(8)	178.5(4)
C(4)–Fe(1)–C(8)	112.1(4)
C(3)–Fe(1)–C(8)	112.6(5)
C(7)–Fe(1)–C(8)	39.7(4)
C(41)–Fe(2)–C(50)	108.3(4)
C(41)–Fe(2)–C(42)	40.0(3)
C(50)–Fe(2)–C(42)	135.7(4)
C(41)–Fe(2)–C(45)	41.6(4)
C(50)–Fe(2)–C(45)	110.2(4)
C(42)–Fe(2)–C(45)	68.5(4)
C(41)–Fe(2)–C(46)	109.2(4)
C(50)–Fe(2)–C(46)	40.6(4)
C(42)–Fe(2)–C(46)	109.8(4)
C(45)–Fe(2)–C(46)	138.4(4)
C(41)–Fe(2)–C(49)	136.8(4)
C(50)–Fe(2)–C(49)	40.7(4)
C(42)–Fe(2)–C(49)	176.1(5)
C(45)–Fe(2)–C(49)	110.5(5)
C(46)–Fe(2)–C(49)	68.3(4)
C(41)–Fe(2)–C(44)	67.9(4)
C(50)–Fe(2)–C(44)	139.9(4)
C(42)–Fe(2)–C(44)	67.9(4)
C(45)–Fe(2)–C(44)	39.5(4)
C(46)–Fe(2)–C(44)	177.1(4)
C(49)–Fe(2)–C(44)	113.8(4)
C(41)–Fe(2)–C(43)	69.1(4)
C(50)–Fe(2)–C(43)	177.3(4)
C(42)–Fe(2)–C(43)	41.7(4)
C(45)–Fe(2)–C(43)	68.5(4)
C(46)–Fe(2)–C(43)	138.9(4)
C(49)–Fe(2)–C(43)	141.8(5)
C(44)–Fe(2)–C(43)	40.4(4)
C(41)–Fe(2)–C(47)	139.7(4)
C(50)–Fe(2)–C(47)	69.4(4)
C(42)–Fe(2)–C(47)	112.8(4)
C(45)–Fe(2)–C(47)	178.6(4)
C(46)–Fe(2)–C(47)	42.0(4)
C(49)–Fe(2)–C(47)	68.3(4)

C(44)-Fe(2)-C(47)	140.1(4)
C(43)-Fe(2)-C(47)	112.0(4)
C(41)-Fe(2)-C(48)	178.0(4)
C(50)-Fe(2)-C(48)	69.7(4)
C(42)-Fe(2)-C(48)	141.5(4)
C(45)-Fe(2)-C(48)	138.8(4)
C(46)-Fe(2)-C(48)	69.3(4)
C(49)-Fe(2)-C(48)	41.7(4)
C(44)-Fe(2)-C(48)	113.6(4)
C(43)-Fe(2)-C(48)	112.9(5)
C(47)-Fe(2)-C(48)	39.9(4)
C(6)-P(1)-C(11)	97.8(4)
C(6)-P(1)-C(23)	98.6(5)
C(11)-P(1)-C(23)	97.5(5)
C(6)-P(1)-Co(1)	116.9(3)
C(11)-P(1)-Co(1)	121.3(4)
C(23)-P(1)-Co(1)	120.1(3)
C(17)-P(2)-C(29)	96.9(4)
C(17)-P(2)-C(1)	97.5(4)
C(29)-P(2)-C(1)	100.3(4)
C(17)-P(2)-Co(1)	117.8(3)
C(29)-P(2)-Co(1)	119.6(3)
C(1)-P(2)-Co(1)	120.1(3)
C(40)-P(3)-C(38)	97.7(6)
C(40)-P(3)-C(39)	99.1(7)
C(38)-P(3)-C(39)	100.7(6)
C(40)-P(3)-Co(1)	119.6(5)
C(38)-P(3)-Co(1)	117.0(4)
C(39)-P(3)-Co(1)	118.8(5)
C(35)-P(4)-C(36)	99.3(6)
C(35)-P(4)-C(37)	95.8(6)
C(36)-P(4)-C(37)	97.9(7)
C(35)-P(4)-Co(1)	117.6(4)
C(36)-P(4)-Co(1)	122.0(5)
C(37)-P(4)-Co(1)	119.2(5)
C(51)-P(5)-C(46)	103.2(5)
C(51)-P(5)-C(57)	96.8(4)
C(46)-P(5)-C(57)	99.1(4)
C(51)-P(5)-Co(2)	112.1(3)
C(46)-P(5)-Co(2)	120.2(3)
C(57)-P(5)-Co(2)	121.6(3)
C(41)-P(6)-C(63)	99.4(4)
C(41)-P(6)-C(69)	100.5(4)
C(63)-P(6)-C(69)	99.3(4)

C(41)–P(6)–Co(2)	118.6(3)
C(63)–P(6)–Co(2)	121.5(3)
C(69)–P(6)–Co(2)	113.8(3)
C(80)–P(7)–C(79)	98.7(6)
C(80)–P(7)–C(78)	98.3(6)
C(79)–P(7)–C(78)	99.1(5)
C(80)–P(7)–Co(2)	117.8(4)
C(79)–P(7)–Co(2)	122.8(4)
C(78)–P(7)–Co(2)	115.7(4)
C(76)–P(8)–C(77)	97.0(5)
C(76)–P(8)–C(75)	99.6(5)
C(77)–P(8)–C(75)	98.7(6)
C(76)–P(8)–Co(2)	123.6(4)
C(77)–P(8)–Co(2)	117.1(4)
C(75)–P(8)–Co(2)	116.2(3)

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for Complex 8.  
 The anisotropic displacement factor exponent takes the form:  
 $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$

	U11	U22	U33	U23	U13	U12
C(1)	52(6)	24(5)	35(6)	-7(4)	1(5)	-11(5)
C(2)	35(6)	30(5)	58(7)	-14(5)	11(5)	-4(5)
C(3)	78(9)	42(6)	50(7)	-6(6)	-18(6)	8(6)
C(4)	47(7)	73(8)	32(6)	0(6)	-13(5)	-20(6)
C(5)	78(8)	51(7)	35(6)	-14(5)	-10(6)	-12(6)
C(6)	52(7)	42(6)	32(6)	-3(5)	1(5)	-23(5)
C(7)	28(6)	62(7)	59(7)	-16(6)	-2(5)	-16(5)
C(8)	43(7)	64(8)	66(8)	-12(7)	-16(6)	-12(6)
C(9)	125(12)	48(7)	45(7)	-18(6)	-18(7)	-24(8)
C(10)	62(7)	39(6)	39(6)	-10(5)	-3(5)	-14(5)
C(11)	64(7)	36(6)	40(6)	-3(5)	-5(5)	-9(5)
C(12)	69(8)	59(8)	65(8)	-12(7)	-5(6)	-21(7)
C(13)	106(11)	52(8)	72(10)	-11(7)	9(8)	-42(8)
C(14)	113(12)	43(7)	52(8)	4(6)	26(8)	-4(8)
C(15)	88(10)	57(8)	63(9)	-10(7)	-9(7)	-1(7)
C(16)	77(9)	54(7)	52(8)	-4(6)	4(6)	-10(6)
C(17)	47(6)	36(6)	35(6)	-12(5)	-2(5)	1(5)
C(18)	54(7)	51(7)	57(7)	-30(6)	1(5)	-2(6)
C(19)	49(7)	54(7)	78(9)	-24(7)	8(6)	0(6)
C(20)	69(9)	75(9)	87(10)	-60(8)	-21(7)	20(7)
C(21)	72(8)	76(9)	46(7)	-20(7)	3(6)	12(7)
C(22)	28(6)	58(7)	74(8)	-28(6)	3(5)	5(5)
C(23)	37(6)	52(7)	38(6)	-17(5)	7(5)	-4(5)
C(24)	121(12)	55(8)	64(9)	-14(7)	37(8)	6(8)
C(25)	131(13)	54(8)	78(10)	-20(7)	27(9)	5(8)
C(26)	98(12)	67(10)	135(15)	-36(10)	0(11)	26(9)
C(27)	183(19)	103(13)	112(14)	-10(11)	87(13)	45(13)
C(28)	108(12)	63(8)	105(12)	-15(8)	60(10)	12(8)
C(29)	44(6)	45(6)	45(6)	-24(5)	3(5)	-15(5)
C(30)	57(8)	71(8)	57(8)	-10(6)	-6(6)	-21(7)
C(31)	76(10)	144(15)	78(10)	-49(11)	-7(8)	-51(11)
C(32)	140(15)	54(9)	70(10)	-30(8)	31(10)	-51(10)
C(33)	54(8)	68(8)	63(8)	-27(7)	12(7)	-8(7)
C(34)	62(7)	39(6)	52(7)	-13(5)	14(6)	-16(6)

C(35)	57(8)	95(10)	86(10)	-6(8)	-6(7)	15(7)
C(36)	115(12)	36(7)	132(13)	-8(8)	20(10)	2(7)
C(37)	112(12)	103(11)	60(9)	-4(8)	-23(8)	3(9)
C(38)	104(11)	112(11)	60(8)	-48(8)	24(8)	-51(9)
C(39)	80(10)	124(12)	105(12)	-62(10)	7(8)	-44(9)
C(40)	240(20)	42(8)	78(10)	-31(7)	18(11)	-26(10)
C(41)	27(5)	52(6)	43(6)	-27(5)	1(4)	-4(5)
C(42)	55(7)	56(7)	49(7)	-28(6)	2(5)	-20(6)
C(43)	60(8)	76(9)	77(9)	-51(8)	-4(6)	10(7)
C(44)	78(9)	36(6)	73(9)	-27(6)	-21(7)	11(6)
C(45)	38(6)	40(6)	78(8)	-32(6)	3(6)	-4(5)
C(46)	45(6)	30(5)	44(6)	-15(5)	-6(5)	-10(5)
C(47)	49(7)	39(6)	62(7)	-25(5)	-5(5)	-10(5)
C(48)	65(8)	53(7)	76(9)	-37(7)	-14(7)	7(6)
C(49)	80(9)	45(7)	53(7)	-9(6)	-33(7)	5(6)
C(50)	54(7)	39(6)	51(7)	-16(5)	-9(5)	-1(5)
C(51)	39(6)	44(6)	41(6)	-21(5)	10(5)	-14(5)
C(52)	63(7)	58(7)	39(6)	-16(6)	6(5)	-8(6)
C(53)	80(9)	75(9)	48(7)	-28(7)	-3(6)	4(7)
C(54)	41(7)	104(11)	74(9)	-60(8)	10(6)	-20(7)
C(55)	62(8)	66(8)	71(9)	-49(7)	-5(6)	5(6)
C(56)	48(6)	46(6)	53(7)	-26(5)	-5(5)	0(5)
C(57)	45(6)	32(5)	44(6)	-15(5)	1(5)	2(5)
C(58)	67(8)	76(8)	46(7)	-31(6)	5(6)	-31(7)
C(59)	58(8)	68(8)	66(8)	-33(7)	19(6)	-38(6)
C(60)	49(7)	76(9)	63(9)	-21(7)	17(6)	-14(6)
C(61)	102(11)	93(10)	39(7)	-13(7)	44(7)	-29(9)
C(62)	76(8)	71(8)	53(8)	-33(7)	2(6)	-31(7)
C(63)	29(5)	54(7)	53(7)	-19(6)	0(5)	-13(5)
C(64)	43(6)	61(7)	58(8)	-21(6)	4(5)	-1(6)
C(65)	115(12)	88(10)	33(7)	-4(7)	11(7)	21(9)
C(66)	89(10)	56(9)	94(12)	-13(8)	27(9)	-21(8)
C(67)	74(9)	58(8)	99(11)	-19(8)	1(8)	-26(7)
C(68)	56(7)	55(7)	77(9)	-18(7)	-1(6)	-24(6)
C(69)	27(5)	43(6)	60(7)	-24(5)	5(5)	-16(5)
C(70)	76(9)	93(10)	75(9)	-46(8)	-9(7)	-4(8)
C(71)	61(8)	92(10)	89(10)	-44(9)	-34(7)	9(7)
C(72)	117(12)	71(9)	74(10)	-29(8)	-51(9)	-20(9)
C(73)	54(8)	132(13)	81(10)	-62(9)	-10(7)	-2(8)
C(74)	57(8)	90(9)	75(9)	-54(8)	-9(7)	-5(7)
C(75)	35(6)	98(9)	63(8)	-41(7)	12(5)	-9(6)
C(76)	95(9)	66(8)	43(7)	-28(6)	9(6)	-14(7)
C(77)	94(10)	46(7)	94(10)	-34(7)	-5(8)	18(7)
C(78)	143(12)	28(6)	54(8)	-5(5)	13(8)	4(7)

C (79)	77 (9)	86 (9)	41 (7)	-29 (6)	1 (6)	2 (7)
C (80)	89 (10)	101 (10)	61 (9)	-15 (8)	-7 (7)	22 (8)
Co (1)	42 (1)	39 (1)	37 (1)	-10 (1)	-4 (1)	-5 (1)
Co (2)	38 (1)	40 (1)	38 (1)	-16 (1)	0 (1)	-3 (1)
Fe (1)	43 (1)	42 (1)	38 (1)	-13 (1)	-5 (1)	-6 (1)
Fe (2)	43 (1)	36 (1)	51 (1)	-19 (1)	-3 (1)	-2 (1)
P (1)	50 (2)	42 (2)	34 (2)	-11 (1)	-2 (1)	-9 (1)
P (2)	36 (2)	37 (1)	38 (2)	-11 (1)	0 (1)	-6 (1)
P (3)	75 (2)	54 (2)	51 (2)	-23 (2)	7 (2)	-20 (2)
P (4)	58 (2)	54 (2)	55 (2)	-3 (2)	-11 (2)	4 (2)
P (5)	39 (2)	33 (1)	34 (1)	-14 (1)	0 (1)	-7 (1)
P (6)	40 (2)	43 (2)	41 (2)	-19 (1)	-2 (1)	-7 (1)
P (7)	63 (2)	47 (2)	41 (2)	-12 (1)	-3 (1)	5 (2)
P (8)	42 (2)	55 (2)	47 (2)	-21 (1)	2 (1)	-3 (1)

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Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for Complex 8.

	x	y	z	U(eq)
H(2)	2828	-122	3310	50
H(3)	4384	-277	4311	71
H(4)	3495	504	5050	65
H(5)	1400	1144	4522	65
H(7)	5394	1155	2688	61
H(8)	5796	1543	3749	72
H(9)	3902	2380	3905	85
H(10)	2309	2528	2919	56
H(12)	4600	2976	1697	79
H(13)	5100	4103	833	94
H(14)	4232	4445	-263	91
H(15)	2776	3702	-483	87
H(16)	2092	2653	419	77
H(18)	-117	2500	2884	62
H(19)	-1166	3237	3428	72
H(20)	-2281	2704	4446	83
H(21)	-2303	1409	4971	79
H(22)	-1233	655	4410	63
H(24)	3719	231	2345	100
H(25)	4904	-624	2034	108
H(26)	5998	-250	955	121
H(27)	5761	979	222	173
H(28)	4529	1826	598	118
H(30)	-2035	627	2807	77
H(31)	-3368	-386	3143	114
H(32)	-2646	-1537	3920	102
H(33)	-713	-1659	4377	73
H(34)	596	-650	4036	62
H(35A)	-2225	2221	2256	130
H(35B)	-2545	1973	1616	130
H(35C)	-2620	2827	1534	130
H(36A)	-787	3739	1059	151
H(36B)	601	3503	1322	151
H(36C)	-530	3436	1874	151
H(37A)	-1203	2231	435	147

H(37B)	-54	2768	228	147
H(37C)	-1420	3083	344	147
H(38A)	1999	1111	547	130
H(38B)	694	1058	224	130
H(38C)	1544	329	565	130
H(39A)	-1631	1018	1059	144
H(39B)	-1655	254	1696	144
H(39C)	-1195	267	938	144
H(40A)	861	-599	1589	173
H(40B)	443	-541	2329	173
H(40C)	1837	-358	2031	173
H(42)	5387	5755	1621	60
H(43)	7273	4765	1710	78
H(44)	6630	3555	2717	72
H(45)	4458	3756	3230	59
H(47)	7911	5993	2683	57
H(48)	8653	4640	3417	73
H(49)	6763	4047	4313	73
H(50)	4925	5030	4120	57
H(52)	5823	6181	4464	64
H(53)	5652	6756	5322	79
H(54)	4810	7969	5025	78
H(55)	4127	8595	3900	72
H(56)	4347	8039	3058	56
H(58)	7081	7671	3012	72
H(59)	8391	8518	2205	73
H(60)	8522	8576	1061	77
H(61)	7351	7794	699	97
H(62)	5943	6995	1485	75
H(64)	2629	5214	4108	64
H(65)	1664	4340	5110	101
H(66)	974	3223	5061	99
H(67)	1163	3004	4001	94
H(68)	2065	3874	2986	76
H(70)	368	5630	2392	92
H(71)	-1020	5684	1494	92
H(72)	-198	5368	543	100
H(73)	1933	5033	471	99
H(74)	3230	5007	1335	80
H(75A)	-427	6677	3641	93
H(75B)	180	5943	3546	93
H(75C)	-174	6639	2877	93
H(76A)	1166	6731	4499	99
H(76B)	2596	6947	4351	99

H(76C)	2217	6115	4499	99
H(77A)	1003	8056	2628	114
H(77B)	2038	8127	3137	114
H(77C)	649	7917	3430	114
H(78A)	3505	8546	843	117
H(78B)	4180	8289	1573	117
H(78C)	2758	8586	1524	117
H(79A)	3149	6727	698	100
H(79B)	4424	7085	771	100
H(79C)	3324	7593	326	100
H(80A)	1230	7940	824	132
H(80B)	786	7728	1623	132
H(80C)	867	7113	1262	132

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Table 6. Torsion angles [deg] for Complex 8.

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