

Inorganic Chemistry

including bioinorganic chemistry

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C(26)	6133(13)	2551(9)	325(9)	121(9)
C(27)	6786(13)	2963(11)	544(11)	153(12)
C(28)	6569(12)	3369(8)	937(10)	121(10)
C(29)	5698(9)	3413(6)	1124(7)	77(6)
C(30)	5604(9)	3903(6)	1564(7)	92(7)
C(31)	501(11)	3452(8)	3492(8)	104(8)
C(32)	660(12)	2909(9)	3573(8)	113(9)
C(33)	1150(11)	2715(7)	3095(8)	91(7)
C(34)	1542(17)	2140(8)	2971(11)	136(11)
C(34A)	969(17)	1682(10)	2907(14)	230(20)
C(34B)	2218(18)	1940(9)	3574(14)	216(19)
C(35)	-166(12)	4532(7)	1834(9)	114(8)
C(36)	-424(11)	4442(9)	1186(10)	126(10)
C(37)	133(10)	4005(7)	1043(7)	83(7)
C(38)	143(10)	3715(8)	407(8)	101(8)
C(38A)	-798(15)	3455(10)	201(10)	190(14)
C(38B)	204(14)	4091(10)	-156(9)	182(14)
C(39)	1852(11)	4447(6)	2832(7)	80(7)
C(40)	1916(14)	4930(8)	3232(9)	115(9)
C(41)	2676(20)	5227(8)	3346(10)	145(12)
C(42)	3466(14)	5073(8)	3126(9)	115(9)
C(43)	3414(12)	4613(7)	2712(7)	95(8)
C(44)	2649(11)	4302(6)	2565(7)	74(6)
C(45)	923(10)	4177(6)	2715(6)	80(6)
B(1)	3658(8)	301(4)	8499(5)	173(20)
F(1)	3086(15)	69(8)	8794(11)	418(22)
F(2)	4343(13)	416(7)	8888(8)	316(15)
F(3)	3332(12)	740(5)	8240(8)	294(12)
F(4)	3871(10)	-22(5)	8073(6)	214(9)
O(8)	9151(11)	2492(9)	1661(10)	225(12)
C(90)	3790(16)	2074(13)	7064(11)	185(14)
O(10)#	8081(27)	1581(17)	1446(26)	291(31)
O(11)#	7460(32)	858(17)	248(30)	331(38)
O(7)*	2445(17)	225(11)	6836(14)	250(17)
O(9)**	8703(44)	565(36)	2310(34)	320(49)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Occupancy factor 0.5

* Occupancy factor 0.7

** Occupancy factor 0.3

Table 2. Bond lengths (Å)

Co(1)-Co(2)	2.848 (3)	Co(1)-O(3)	2.016 (8)
Co(1)-O(4)	1.998 (9)	Co(1)-O(5)	2.156 (7)
Co(1)-O(6)	2.132 (7)	Co(1)-N(9)	2.125 (12)
Co(1)-N(11)	2.152 (10)	Co(2)-Co(3)	2.915 (2)
Co(2)-O(2)	2.002 (8)	Co(2)-O(3)	2.005 (9)
Co(2)-O(5)	2.160 (7)	Co(2)-O(6)	2.166 (6)
Co(2)-N(6)	2.093 (11)	Co(2)-N(8)	2.123 (10)
Co(3)-O(1)	1.997 (7)	Co(3)-O(2)	2.069 (7)
Co(3)-O(5)	2.166 (6)	Co(3)-O(6)	2.192 (6)
Co(3)-N(2)	2.134 (10)	Co(3)-N(4)	2.140 (11)
O(1)-C(14)	1.314 (14)	O(2)-C(24)	1.387 (15)
O(3)-C(44)	1.354 (16)	N(1)-N(2)	1.351 (16)
N(1)-C(1)	1.367 (19)	N(1)-C(15)	1.465 (16)
N(2)-C(3)	1.342 (18)	N(3)-N(4)	1.334 (15)
N(3)-C(5)	1.369 (20)	N(3)-C(15)	1.447 (16)
N(4)-C(7)	1.281 (19)	N(5)-N(6)	1.364 (17)
N(5)-C(16)	1.405 (22)	N(5)-C(30)	1.451 (19)
N(6)-C(18)	1.327 (21)	N(7)-N(8)	1.335 (14)
N(7)-C(20)	1.330 (21)	N(7)-C(30)	1.455 (17)
N(8)-C(22)	1.364 (16)	N(9)-N(10)	1.349 (16)
N(9)-C(33)	1.336 (20)	N(10)-C(31)	1.324 (20)
N(10)-C(45)	1.450 (18)	N(11)-N(12)	1.355 (15)
N(11)-C(37)	1.283 (16)	N(12)-C(35)	1.255 (20)
N(12)-C(45)	1.433 (16)	C(1)-C(2)	1.368 (27)
C(2)-C(3)	1.349 (25)	C(3)-C(4)	1.505 (26)
C(4)-C(4A)	1.453 (30)	C(4)-C(4B)	1.534 (29)
C(5)-C(6)	1.344 (25)	C(6)-C(7)	1.368 (23)
C(7)-C(8)	1.485 (19)	C(8)-C(8A)	1.532 (21)
C(8)-C(8B)	1.540 (22)	C(9)-C(10)	1.383 (19)
C(9)-C(14)	1.393 (19)	C(9)-C(15)	1.531 (19)
C(10)-C(11)	1.440 (26)	C(11)-C(12)	1.327 (26)
C(12)-C(13)	1.329 (22)	C(13)-C(14)	1.378 (20)
C(16)-C(17)	1.376 (32)	C(17)-C(18)	1.426 (30)
C(18)-C(19)	1.498 (34)	C(19)-C(19A)	1.614 (34)
C(19)-C(19B)	1.486 (36)	C(20)-C(21)	1.388 (28)
C(21)-C(22)	1.367 (24)	C(22)-C(23)	1.478 (21)
C(23)-C(23A)	1.517 (26)	C(23)-C(23B)	1.489 (28)
C(24)-C(25)	1.352 (21)	C(24)-C(29)	1.389 (19)
C(25)-C(26)	1.356 (24)	C(26)-C(27)	1.402 (30)
C(27)-C(28)	1.325 (32)	C(28)-C(29)	1.397 (24)
C(29)-C(30)	1.490 (21)	C(31)-C(32)	1.313 (29)
C(32)-C(33)	1.378 (25)	C(33)-C(34)	1.514 (27)
C(34)-C(34A)	1.372 (32)	C(34)-C(34B)	1.560 (34)
C(35)-C(36)	1.354 (27)	C(36)-C(37)	1.378 (25)
C(37)-C(38)	1.482 (22)	C(38)-C(38A)	1.529 (26)
C(38)-C(38B)	1.473 (27)	C(39)-C(40)	1.405 (24)
C(39)-C(44)	1.409 (24)	C(39)-C(45)	1.507 (22)
C(40)-C(41)	1.320 (34)	C(41)-C(42)	1.359 (36)
C(42)-C(43)	1.379 (25)	C(43)-C(44)	1.350 (23)
B(1)-F(1)	1.236 (26)	B(1)-F(2)	1.236 (20)
B(1)-F(3)	1.236 (17)	B(1)-F(4)	1.236 (17)
O(8)-C(90A)	1.466 (35)	C(90)-O(8A)	1.466 (35)

Table 3. Bond angles ($^{\circ}$)

Co(2)-Co(1)-O(3)	44.8(2)	Co(2)-Co(1)-O(4)	131.0(3)
O(3)-Co(1)-O(4)	175.7(4)	Co(2)-Co(1)-O(5)	48.8(2)
O(3)-Co(1)-O(5)	83.2(3)	O(4)-Co(1)-O(5)	93.2(3)
Co(2)-Co(1)-O(6)	49.0(2)	O(3)-Co(1)-O(6)	82.8(3)
O(4)-Co(1)-O(6)	93.8(4)	O(5)-Co(1)-O(6)	69.8(2)
Co(2)-Co(1)-N(9)	120.3(3)	O(3)-Co(1)-N(9)	89.3(4)
O(4)-Co(1)-N(9)	93.7(4)	O(5)-Co(1)-N(9)	102.0(4)
O(6)-Co(1)-N(9)	169.2(3)	Co(2)-Co(1)-N(11)	120.7(3)
O(3)-Co(1)-N(11)	91.2(4)	O(4)-Co(1)-N(11)	91.8(4)
O(5)-Co(1)-N(11)	167.9(3)	O(6)-Co(1)-N(11)	98.9(3)
N(9)-Co(1)-N(11)	88.6(4)	Co(1)-Co(2)-Co(3)	71.9(1)
Co(1)-Co(2)-O(2)	117.1(2)	Co(3)-Co(2)-O(2)	45.2(2)
Co(1)-Co(2)-O(3)	45.1(2)	Co(3)-Co(2)-O(3)	117.0(2)
O(2)-Co(2)-O(3)	162.0(3)	Co(1)-Co(2)-O(5)	48.6(2)
Co(3)-Co(2)-O(5)	47.7(2)	O(2)-Co(2)-O(5)	83.1(3)
O(3)-Co(2)-O(5)	83.4(3)	Co(1)-Co(2)-O(6)	48.0(2)
Co(3)-Co(2)-O(6)	48.4(2)	O(2)-Co(2)-O(6)	82.0(3)
O(3)-Co(2)-O(6)	82.2(3)	O(5)-Co(2)-O(6)	69.1(2)
Co(1)-Co(2)-N(6)	128.1(3)	Co(3)-Co(2)-N(6)	119.9(3)
O(2)-Co(2)-N(6)	91.7(4)	O(3)-Co(2)-N(6)	102.2(4)
O(5)-Co(2)-N(6)	99.2(3)	O(6)-Co(2)-N(6)	167.2(3)
Co(1)-Co(2)-N(8)	126.7(3)	Co(3)-Co(2)-N(8)	122.9(3)
O(2)-Co(2)-N(8)	92.3(4)	O(3)-Co(2)-N(8)	98.8(4)
O(5)-Co(2)-N(8)	168.9(3)	O(6)-Co(2)-N(8)	100.3(3)
N(6)-Co(2)-N(8)	91.0(4)	Co(2)-Co(3)-O(1)	130.3(2)
Co(2)-Co(3)-O(2)	43.3(2)	O(1)-Co(3)-O(2)	173.5(3)
Co(2)-Co(3)-O(5)	47.5(2)	O(1)-Co(3)-O(5)	93.9(3)
O(2)-Co(3)-O(5)	81.4(3)	Co(2)-Co(3)-O(6)	47.6(2)
O(1)-Co(3)-O(6)	94.3(3)	O(2)-Co(3)-O(6)	79.8(3)
O(5)-Co(3)-O(6)	68.5(2)	Co(2)-Co(3)-N(2)	123.0(3)
O(1)-Co(3)-N(2)	89.3(3)	O(2)-Co(3)-N(2)	95.9(3)
O(5)-Co(3)-N(2)	100.8(4)	O(6)-Co(3)-N(2)	168.9(4)
Co(2)-Co(3)-N(4)	124.7(3)	O(1)-Co(3)-N(4)	87.5(4)
O(2)-Co(3)-N(4)	96.3(4)	O(5)-Co(3)-N(4)	169.2(3)
O(6)-Co(3)-N(4)	100.7(3)	N(2)-Co(3)-N(4)	90.0(4)
Co(3)-O(1)-C(14)	137.3(8)	Co(2)-O(2)-Co(3)	91.5(3)
Co(2)-O(2)-C(24)	134.6(8)	Co(3)-O(2)-C(24)	133.8(8)
Co(1)-O(3)-Co(2)	90.2(3)	Co(1)-O(3)-C(44)	138.4(9)
Co(2)-O(3)-C(44)	131.4(9)	Co(1)-O(5)-Co(2)	82.6(2)
Co(1)-O(5)-Co(3)	103.0(2)	Co(2)-O(5)-Co(3)	84.7(2)
Co(1)-O(6)-Co(2)	83.0(2)	Co(1)-O(6)-Co(3)	103.0(3)
Co(2)-O(6)-Co(3)	84.0(2)	N(2)-N(1)-C(1)	110.1(12)
N(2)-N(1)-C(15)	122.9(10)	C(1)-N(1)-C(15)	126.6(12)
Co(3)-N(2)-N(1)	117.4(8)	Co(3)-N(2)-C(3)	135.4(10)
N(1)-N(2)-C(3)	104.2(11)	N(4)-N(3)-C(5)	110.8(12)
N(4)-N(3)-C(15)	123.7(11)	C(5)-N(3)-C(15)	125.3(12)
Co(3)-N(4)-N(3)	119.1(8)	Co(3)-N(4)-C(7)	134.9(10)
N(3)-N(4)-C(7)	106.0(11)	N(6)-N(5)-C(16)	110.9(13)
N(6)-N(5)-C(30)	124.5(10)	C(16)-N(5)-C(30)	124.1(13)
Co(2)-N(6)-N(5)	114.7(8)	Co(2)-N(6)-C(18)	135.9(12)
N(5)-N(6)-C(18)	107.7(12)	N(8)-N(7)-C(20)	110.5(12)
N(8)-N(7)-C(30)	122.1(10)	C(20)-N(7)-C(30)	127.4(13)
Co(2)-N(8)-N(7)	117.9(7)	Co(2)-N(8)-C(22)	135.9(9)
N(7)-N(8)-C(22)	105.8(10)	Co(1)-N(9)-N(10)	117.9(8)
Co(1)-N(9)-C(33)	132.2(10)	N(10)-N(9)-C(33)	107.2(12)
N(9)-N(10)-C(31)	110.2(12)	N(9)-N(10)-C(45)	122.8(11)

C(31)-N(10)-C(45)	127.0(13)	Co(1)-N(11)-N(12)	117.1(7)
Co(1)-N(11)-C(37)	135.1(10)	N(12)-N(11)-C(37)	107.8(11)
N(11)-N(12)-C(35)	108.4(12)	N(11)-N(12)-C(45)	124.3(10)
C(35)-N(12)-C(45)	127.3(13)	N(1)-C(1)-C(2)	107.7(16)
C(1)-C(2)-C(3)	104.7(16)	N(2)-C(3)-C(2)	113.2(15)
N(2)-C(3)-C(4)	120.5(14)	C(2)-C(3)-C(4)	126.1(15)
C(3)-C(4)-C(4A)	114.8(15)	C(3)-C(4)-C(4B)	110.9(16)
C(4A)-C(4)-C(4B)	110.8(16)	N(3)-C(5)-C(6)	105.1(14)
C(5)-C(6)-C(7)	106.5(15)	N(4)-C(7)-C(6)	111.6(13)
N(4)-C(7)-C(8)	124.0(14)	C(6)-C(7)-C(8)	124.3(14)
C(7)-C(8)-C(8A)	107.9(11)	C(7)-C(8)-C(8B)	113.4(12)
C(8A)-C(8)-C(8B)	108.8(12)	C(10)-C(9)-C(14)	118.6(13)
C(10)-C(9)-C(15)	114.5(12)	C(14)-C(9)-C(15)	126.9(11)
C(9)-C(10)-C(11)	121.5(15)	C(10)-C(11)-C(12)	117.1(15)
C(11)-C(12)-C(13)	120.8(16)	C(12)-C(13)-C(14)	125.2(14)
O(1)-C(14)-C(9)	122.3(12)	O(1)-C(14)-C(13)	121.1(12)
C(9)-C(14)-C(13)	116.5(11)	N(1)-C(15)-N(3)	110.4(10)
N(1)-C(15)-C(9)	113.2(11)	N(3)-C(15)-C(9)	115.0(10)
N(5)-C(16)-C(17)	104.5(16)	C(16)-C(17)-C(18)	108.2(17)
N(6)-C(18)-C(17)	108.7(17)	N(6)-C(18)-C(19)	125.1(17)
C(17)-C(18)-C(19)	126.2(17)	C(18)-C(19)-C(19A)	102.4(20)
C(18)-C(19)-C(19B)	115.3(22)	C(19A)-C(19)-C(19B)	111.2(18)
N(7)-C(20)-C(21)	108.9(17)	C(20)-C(21)-C(22)	104.1(15)
N(8)-C(22)-C(21)	110.7(13)	N(8)-C(22)-C(23)	123.7(12)
C(21)-C(22)-C(23)	125.5(14)	C(22)-C(23)-C(23A)	112.5(14)
C(22)-C(23)-C(23B)	111.0(16)	C(23A)-C(23)-C(23B)	109.0(14)
O(2)-C(24)-C(25)	119.5(12)	O(2)-C(24)-C(29)	119.6(13)
C(25)-C(24)-C(29)	120.8(13)	C(24)-C(25)-C(26)	120.5(14)
C(25)-C(26)-C(27)	120.0(18)	C(26)-C(27)-C(28)	119.2(19)
C(27)-C(28)-C(29)	122.1(17)	C(24)-C(29)-C(28)	117.4(14)
C(24)-C(29)-C(30)	129.5(13)	C(28)-C(29)-C(30)	113.1(13)
N(5)-C(30)-N(7)	107.9(12)	N(5)-C(30)-C(29)	115.3(12)
N(7)-C(30)-C(29)	118.2(11)	N(10)-C(31)-C(32)	106.8(16)
C(31)-C(32)-C(33)	109.7(17)	N(9)-C(33)-C(32)	106.1(15)
N(9)-C(33)-C(34)	121.6(16)	C(32)-C(33)-C(34)	132.1(17)
C(33)-C(34)-C(34A)	118.7(21)	C(33)-C(34)-C(34B)	111.0(17)
C(34A)-C(34)-C(34B)	99.0(18)	N(12)-C(35)-C(36)	111.1(16)
C(35)-C(36)-C(37)	103.4(15)	N(11)-C(37)-C(36)	109.3(14)
N(11)-C(37)-C(38)	122.9(14)	C(36)-C(37)-C(38)	127.8(14)
C(37)-C(38)-C(38A)	108.4(14)	C(37)-C(38)-C(38B)	115.3(16)
C(38A)-C(38)-C(38B)	100.0(14)	C(40)-C(39)-C(44)	115.7(15)
C(40)-C(39)-C(45)	115.3(15)	C(44)-C(39)-C(45)	128.9(13)
C(39)-C(40)-C(41)	121.7(20)	C(40)-C(41)-C(42)	123.3(19)
C(41)-C(42)-C(43)	116.1(19)	C(42)-C(43)-C(44)	122.9(18)
O(3)-C(44)-C(39)	118.5(13)	O(3)-C(44)-C(43)	121.5(15)
C(39)-C(44)-C(43)	120.0(14)	N(10)-C(45)-N(12)	111.1(10)
N(10)-C(45)-C(39)	113.8(11)	N(12)-C(45)-C(39)	116.2(12)
F(1)-B(1)-F(2)	109.5(15)	F(1)-B(1)-F(3)	109.5(15)
F(2)-B(1)-F(3)	109.5(13)	F(1)-B(1)-F(4)	109.5(14)
F(2)-B(1)-F(4)	109.5(14)	F(3)-B(1)-F(4)	109.5(13)

Table 4. Anisotropic displacement coefficients ($\text{\AA}^2 \times 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co(1)	56(1)	63(1)	67(1)	-6(1)	18(1)	-11(1)
Co(2)	48(1)	55(1)	61(1)	-10(1)	0(1)	-2(1)
Co(3)	46(1)	49(1)	60(1)	-1(1)	3(1)	-1(1)
O(1)	53(5)	51(5)	101(7)	-15(4)	18(5)	-21(5)
O(2)	45(5)	56(5)	95(6)	-7(4)	11(4)	-8(5)
O(3)	72(6)	62(5)	68(6)	5(5)	15(4)	-13(4)
O(4)	72(7)	103(8)	167(10)	-33(6)	63(6)	-75(7)
O(5)	43(4)	39(4)	36(4)	-12(3)	0(3)	3(3)
O(6)	34(4)	47(4)	27(4)	-5(3)	7(3)	-2(3)
N(1)	68(8)	64(8)	84(9)	1(7)	3(6)	-16(7)
N(2)	62(8)	49(7)	85(8)	5(6)	13(7)	-5(7)
N(3)	54(7)	43(7)	78(9)	-8(5)	12(6)	-8(6)
N(4)	57(7)	43(7)	75(8)	-4(5)	18(5)	-1(7)
N(5)	64(8)	91(9)	110(10)	0(7)	-26(7)	-30(7)
N(6)	68(8)	84(8)	80(8)	-32(7)	-23(6)	2(6)
N(7)	46(7)	69(8)	139(11)	-17(6)	-13(7)	9(7)
N(8)	48(7)	54(6)	90(8)	-15(5)	-10(6)	5(6)
N(9)	87(9)	85(8)	77(8)	9(7)	29(7)	18(7)
N(10)	79(8)	100(9)	68(8)	16(7)	42(6)	11(7)
N(11)	66(7)	88(8)	56(7)	2(6)	10(6)	-14(6)
N(12)	87(8)	85(8)	68(8)	51(7)	-1(6)	-6(7)
C(1)	101(13)	68(11)	149(19)	51(10)	33(13)	12(11)
C(2)	135(16)	101(14)	120(16)	78(13)	-16(13)	22(12)
C(3)	65(10)	73(11)	107(14)	21(9)	-15(10)	30(10)
C(4)	96(14)	97(13)	114(16)	11(10)	-50(12)	29(12)
C(4A)	189(24)	202(26)	136(20)	13(20)	-48(18)	28(19)
C(4B)	245(31)	140(18)	126(18)	15(20)	-28(18)	4(14)
C(5)	101(12)	114(16)	66(12)	-16(10)	37(9)	-38(10)
C(6)	168(17)	56(11)	96(14)	-17(11)	41(12)	8(10)
C(7)	86(11)	50(10)	69(10)	-14(7)	34(8)	-15(9)
C(8)	101(12)	69(10)	51(8)	4(8)	22(8)	12(7)
C(8A)	130(16)	121(15)	149(18)	8(13)	36(14)	-1(13)
C(8B)	162(17)	72(11)	131(15)	-47(11)	53(13)	-1(10)
C(9)	68(10)	35(7)	75(9)	-35(7)	1(8)	-10(7)
C(10)	125(15)	71(11)	86(11)	4(10)	18(10)	-10(9)
C(11)	100(14)	92(13)	151(17)	-62(12)	39(12)	-15(12)
C(12)	82(12)	85(13)	137(16)	-37(11)	45(11)	-6(11)
C(13)	60(10)	63(10)	111(12)	-30(8)	25(8)	-4(8)
C(14)	58(9)	55(8)	64(8)	-3(8)	1(7)	-6(7)
C(15)	77(10)	52(8)	87(10)	-7(7)	22(8)	-18(7)
C(16)	77(13)	149(18)	142(18)	-6(12)	-37(13)	-36(15)
C(17)	133(21)	269(31)	80(15)	22(20)	-65(14)	-10(17)
C(18)	127(16)	127(15)	92(13)	2(13)	-37(13)	-18(11)
C(19)	165(23)	247(31)	92(17)	-93(22)	-46(15)	83(19)
C(19A)	428(48)	183(24)	108(18)	-27(29)	67(24)	41(18)
C(19B)	109(18)	376(46)	146(24)	34(22)	31(16)	113(27)
C(20)	115(16)	82(13)	243(26)	-43(12)	52(16)	47(14)
C(21)	116(16)	65(12)	210(21)	-32(12)	8(15)	52(12)
C(22)	75(11)	54(9)	87(10)	0(8)	-16(8)	5(7)
C(23)	84(13)	51(10)	162(18)	18(8)	-31(12)	14(10)
C(23A)	127(16)	156(20)	153(19)	24(15)	6(14)	54(16)
C(23B)	199(24)	234(28)	178(24)	147(22)	-110(19)	-94(20)
C(24)	46(9)	83(10)	93(11)	-3(9)	1(8)	13(9)
C(25)	53(10)	99(12)	94(11)	9(8)	27(8)	-41(9)
C(26)	76(13)	161(18)	131(15)	19(13)	29(12)	-37(13)

C(27)	63(13)	226(26)	178(21)	-44(17)	43(13)	-55(19)
C(28)	71(15)	134(17)	156(18)	-12(12)	10(12)	-46(14)
C(29)	32(9)	92(11)	102(11)	-17(8)	-5(8)	5(9)
C(30)	50(9)	115(12)	107(12)	-15(9)	-4(8)	22(10)
C(31)	109(14)	120(14)	84(12)	48(12)	19(10)	11(11)
C(32)	108(14)	163(19)	75(12)	8(14)	42(11)	25(13)
C(33)	98(12)	101(13)	78(11)	0(10)	24(10)	25(9)
C(34)	173(21)	88(16)	164(20)	0(15)	84(17)	41(14)
C(34A)	213(32)	118(20)	366(43)	2(21)	68(29)	44(23)
C(34B)	208(28)	95(17)	348(43)	20(18)	43(29)	43(22)
C(35)	145(16)	127(14)	73(12)	46(12)	29(11)	-6(11)
C(36)	82(13)	178(20)	116(16)	69(13)	1(11)	7(14)
C(37)	71(11)	115(13)	62(10)	-11(10)	2(8)	-3(9)
C(38)	47(9)	173(17)	77(12)	-8(10)	-9(8)	-30(12)
C(38A)	179(23)	255(29)	142(19)	-75(21)	46(17)	-79(19)
C(38B)	162(20)	311(34)	85(15)	-70(21)	64(14)	-52(18)
C(39)	96(14)	67(10)	76(10)	-15(9)	7(9)	-23(8)
C(40)	117(16)	121(16)	106(14)	-3(13)	12(11)	-35(13)
C(41)	194(25)	94(14)	154(20)	-36(17)	43(19)	-77(13)
C(42)	118(16)	114(16)	113(15)	-38(13)	16(13)	-39(12)
C(43)	114(15)	87(12)	82(12)	-20(11)	5(10)	-30(10)
C(44)	84(11)	73(10)	65(10)	-2(10)	16(9)	8(8)
C(45)	105(12)	84(10)	58(9)	13(9)	37(8)	-4(8)
B(1)	174(30)	84(18)	286(45)	70(21)	126(33)	46(25)
F(1)	364(29)	415(36)	556(45)	-111(27)	352(33)	-1(30)
F(2)	275(23)	347(28)	300(25)	-47(22)	-58(19)	11(20)
F(3)	274(20)	142(12)	419(28)	114(13)	-127(19)	-82(15)
F(4)	318(19)	166(12)	169(12)	139(13)	75(12)	14(9)
O(8)	122(13)	291(23)	277(23)	-24(14)	77(13)	-10(18)
C(90)	135(19)	291(33)	137(19)	-33(21)	40(15)	26(20)
O(10)	194(36)	226(41)	457(71)	-119(33)	57(39)	-38(41)
O(11)	277(48)	175(37)	581(92)	-69(35)	207(56)	-41(44)
O(7)	202(25)	221(25)	309(34)	140(22)	-28(22)	-50(22)
O(9)	209(61)	432(108)	271(74)	93(70)	-148(56)	-204(76)

The anisotropic displacement exponent takes the form:

$$-2\pi^2 (h^2 a^{*2} U_{11} + \dots + 2hka^*b^*U_{12})$$

Table 5. H-Atom coordinates ($\times 10^4$) and isotropic displacement coefficients ($\text{\AA}^2 \times 10^3$)

	x	y	z	U
H(4A)	1211	2421	1171	80
H(1A)	4527	690	293	80
H(2A)	5359	853	1426	80
H(4B)	4345	2131	2108	80
H(4AA)	3762	1372	2512	80
H(4AB)	4740	1105	2641	80
H(4AC)	4497	1629	3049	80
H(4BA)	5833	2097	2675	80
H(4BB)	6068	1600	2223	80
H(4BC)	5844	2202	1926	80
H(5A)	3140	1696	-1398	80
H(6A)	3104	2738	-1628	80
H(8A)	2903	3516	-95	80
H(8AA)	2249	4081	-981	80
H(8AB)	2420	3598	-1471	80
H(8AC)	1713	3509	-979	80
H(8BA)	4424	3589	-295	80
H(8BB)	4076	3659	-1043	80
H(8BC)	3898	4137	-549	80
H(10A)	2076	553	-420	80
H(11A)	551	264	-267	80
H(12A)	-202	788	425	80
H(13A)	382	1593	857	80
H(15A)	3171	1131	-377	80
H(16A)	6734	3970	2792	80
H(17A)	6042	3559	3724	80
H(19A)	3683	2938	3124	80
H(19B)	4509	2404	4105	80
H(19C)	5020	2385	3487	80
H(19D)	5376	2779	4077	80
H(19E)	3359	3715	3569	80
H(19F)	3406	3308	4172	80
H(19G)	4277	3642	4038	80
H(20A)	5746	5014	1121	80
H(21A)	4249	5507	720	80
H(23A)	2366	4490	886	80
H(23B)	2371	5157	1701	80
H(23C)	2677	5615	1226	80
H(23D)	1682	5374	1108	80
H(23E)	2656	4692	-121	80
H(23F)	1828	5082	-24	80
H(23G)	2823	5324	93	80
H(25A)	4827	2302	370	80
H(26A)	6248	2252	33	80
H(27A)	7376	2931	402	80
H(28A)	7050	3628	1092	80
H(30A)	6184	4090	1608	80
H(31A)	162	3687	3752	80
H(32A)	460	2672	3904	80
H(34A)	1877	2156	2603	80
H(34B)	565	1770	2516	80
H(34C)	1231	1315	2864	80
H(34D)	634	1683	3275	80
H(34E)	2500	1581	3514	80

H(34F)	2681	2223	3670	80
H(34G)	1864	1914	3930	80
H(35A)	-437	4795	2105	80
H(36A)	-845	4661	892	80
H(38A)	655	3465	427	80
H(38B)	-829	3159	515	80
H(38C)	-1283	3720	227	80
H(38D)	-858	3296	-232	80
H(38E)	237	3923	-576	80
H(38F)	-343	4311	-175	80
H(38G)	724	4330	-39	80
H(40A)	1375	5045	3407	80
H(41A)	2667	5564	3604	80
H(42A)	4024	5272	3264	80
H(43A)	3944	4497	2524	80
H(45A)	553	4392	2974	80

