Electronic Supplementary Material (ESI) for Chemical Science

Supporting Information: X-ray Crystallographic Tables

Molecular Scaffolds with Remote Directing Groups for Selective Palladium-Catalyzed C-H Bond Functionalizations

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Table 1. Crystal data and structure refinement for **32**.

Identification code	ef02	
Empirical formula	$C_{26}H_{25}N_3O_{3.35}Pd$	
Formula weight	539.88	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P\,2_12_12_1$	
Unit cell dimensions	a = 10.6627(4) Å	α= 90°
	b = 13.0584(5) Å	β= 90°
	c = 17.7049(6) Å	γ = 90°
Volume	2465.19(16) Å^3	
Z	4	
Density (calculated)	1.455 Mg/m^3	
Absorption coefficient	0.786 mm^{-1}	
F(000)	1099.2	
Crystal size	0.20 x 0.20 x 0.20 mm^3	
Theta range for data collection	2.47 to 36.54°.	
Index ranges	-17<=h<=17, -21<=k<=21, -28<=l<=29	
Reflections collected	86426	
Independent reflections	12049 [R(int) = 0.0365]	
Completeness to theta = 36.54°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8587 and 0.8587	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12049 / 0 / 308	
Goodness-of-fit on F^2	1.053	
Final R indices [I>2sigma(I)]	R1 = 0.0231, wR2 = 0.0490	
R indices (all data)	R1 = 0.0263, wR2 = 0.0504	
Absolute structure parameter	-0.005(11)	
Largest diff. peak and hole	0.673 and -0.544 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ef02. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	8809(1)	7697(1)	8655(1)	13(1)
N(2)	10193(1)	8776(1)	8827(1)	14(1)
C(19)	8768(1)	9649(1)	7933(1)	16(1)
N(1)	9696(1)	6715(1)	9459(1)	16(1)
C(7)	10502(1)	8975(1)	9655(1)	14(1)
C(6)	9833(1)	8259(1)	10214(1)	16(1)
N(3)	9528(1)	10427(1)	9148(1)	17(1)
C(8)	11942(1)	8930(1)	9718(1)	19(1)
C(12)	10021(1)	10055(1)	9797(1)	17(1)
C(11)	9824(1)	9801(1)	8483(1)	15(1)
C(24)	8151(1)	8700(1)	7930(1)	16(1)
C(10)	11408(1)	8433(1)	8474(1)	18(1)
C(5)	10117(1)	7139(1)	10107(1)	15(1)
C(9)	12413(1)	9017(1)	8907(1)	21(1)
C(18)	9730(1)	12165(1)	8638(1)	23(1)
C(13)	9097(1)	11465(1)	9087(1)	19(1)
C(4)	10752(1)	6569(1)	10647(1)	19(1)
C(17)	9277(2)	13161(1)	8584(1)	29(1)
C(1)	9895(1)	5711(1)	9341(1)	21(1)
C(20)	8464(1)	10406(1)	7404(1)	22(1)
C(3)	10947(1)	5531(1)	10522(1)	26(1)
C(22)	6894(1)	9292(1)	6875(1)	25(1)
C(21)	7516(1)	10227(1)	6881(1)	26(1)
C(23)	7211(1)	8536(1)	7394(1)	21(1)
C(14)	8044(2)	11753(1)	9492(1)	32(1)
C(2)	10502(1)	5095(1)	9861(1)	27(1)
C(15)	7588(2)	12748(1)	9423(1)	41(1)
C(16)	8202(2)	13446(1)	8967(1)	35(1)
O(1)	10070(1)	10488(1)	10405(1)	24(1)
O(2)	7325(1)	6732(1)	8492(1)	17(1)
C(25)	7422(1)	6005(1)	8005(1)	19(1)

O(3)	8397(1)	5773(1)	7674(1)	33(1)
C(26)	6219(2)	5420(1)	7864(1)	29(1)
O(101)	5211(5)	6845(5)	6183(3)	29(2)
O(102)	4106(5)	7501(4)	7609(3)	18(2)

Table 3. Bond lengths [Å] and angles [°] for ef02.

Pd(1)-C(24)	1.9637(12)
Pd(1)-O(2)	2.0437(9)
Pd(1)-N(2)	2.0627(10)
Pd(1)-N(1)	2.1368(10)
N(2)-C(10)	1.5069(15)
N(2)-C(11)	1.5227(16)
N(2)-C(7)	1.5234(15)
C(19)-C(20)	1.3999(17)
C(19)-C(24)	1.4032(18)
C(19)-C(11)	1.5016(17)
N(1)-C(1)	1.3443(17)
N(1)-C(5)	1.3495(15)
C(7)-C(12)	1.5216(18)
C(7)-C(6)	1.5376(17)
C(7)-C(8)	1.5407(16)
C(6)-C(5)	1.5045(16)
N(3)-C(12)	1.3545(16)
N(3)-C(13)	1.4346(16)
N(3)-C(11)	1.4674(15)
C(8)-C(9)	1.5247(18)
C(12)-O(1)	1.2172(15)
C(24)-C(23)	1.3977(17)
C(10)-C(9)	1.5229(18)
C(5)-C(4)	1.3883(17)
C(18)-C(13)	1.3872(18)
C(18)-C(17)	1.3915(19)
C(13)-C(14)	1.384(2)
C(4)-C(3)	1.389(2)
C(17)-C(16)	1.383(2)
C(1)-C(2)	1.3834(19)
C(20)-C(21)	1.391(2)
C(3)-C(2)	1.384(2)
C(22)-C(21)	1.389(2)
C(22)-C(23)	1.390(2)

C(14)-C(15)	1.393(2)
C(15)-C(16)	1.382(3)
O(2)-C(25)	1.2862(15)
C(25)-O(3)	1.2307(16)
C(25)-C(26)	1.514(2)

C(24)-Pd(1)-O(2)	92.38(4)
C(24)-Pd(1)-N(2)	84.06(5)
O(2)-Pd(1)-N(2)	174.85(4)
C(24)-Pd(1)-N(1)	173.75(5)
O(2)-Pd(1)-N(1)	93.87(4)
N(2)-Pd(1)-N(1)	89.71(4)
C(10)-N(2)-C(11)	108.49(9)
C(10)-N(2)-C(7)	105.30(9)
C(11)-N(2)-C(7)	106.93(9)
C(10)-N(2)-Pd(1)	110.49(7)
C(11)-N(2)-Pd(1)	110.88(7)
C(7)-N(2)-Pd(1)	114.43(7)
C(20)-C(19)-C(24)	120.86(12)
C(20)-C(19)-C(11)	120.96(11)
C(24)-C(19)-C(11)	118.04(10)
C(1)-N(1)-C(5)	118.73(11)
C(1)-N(1)-Pd(1)	123.44(9)
C(5)-N(1)-Pd(1)	117.78(8)
C(12)-C(7)-N(2)	104.14(10)
C(12)-C(7)-C(6)	107.50(10)
N(2)-C(7)-C(6)	114.51(10)
C(12)-C(7)-C(8)	111.04(11)
N(2)-C(7)-C(8)	106.24(10)
C(6)-C(7)-C(8)	113.10(11)
C(5)-C(6)-C(7)	114.60(10)
C(12)-N(3)-C(13)	121.81(11)
C(12)-N(3)-C(11)	113.41(10)
C(13)-N(3)-C(11)	122.34(10)
C(9)-C(8)-C(7)	104.85(10)
O(1)-C(12)-N(3)	126.92(12)

O(1)-C(12)-C(7)	124.23(11)
N(3)-C(12)-C(7)	108.85(10)
N(3)-C(11)-C(19)	115.66(10)
N(3)-C(11)-N(2)	102.95(8)
C(19)-C(11)-N(2)	109.73(9)
C(23)-C(24)-C(19)	118.27(11)
C(23)-C(24)-Pd(1)	126.77(10)
C(19)-C(24)-Pd(1)	114.81(8)
N(2)-C(10)-C(9)	104.28(9)
N(1)-C(5)-C(4)	121.78(11)
N(1)-C(5)-C(6)	116.08(10)
C(4)-C(5)-C(6)	122.12(11)
C(10)-C(9)-C(8)	101.88(10)
C(13)-C(18)-C(17)	119.10(13)
C(14)-C(13)-C(18)	120.84(13)
C(14)-C(13)-N(3)	118.56(12)
C(18)-C(13)-N(3)	120.60(11)
C(5)-C(4)-C(3)	119.11(12)
C(16)-C(17)-C(18)	120.37(15)
N(1)-C(1)-C(2)	122.45(12)
C(21)-C(20)-C(19)	119.68(13)
C(2)-C(3)-C(4)	118.99(13)
C(21)-C(22)-C(23)	120.20(13)
C(22)-C(21)-C(20)	119.99(13)
C(22)-C(23)-C(24)	120.98(13)
C(13)-C(14)-C(15)	119.46(15)
C(1)-C(2)-C(3)	118.93(13)
C(16)-C(15)-C(14)	120.05(15)
C(15)-C(16)-C(17)	120.12(15)
C(25)-O(2)-Pd(1)	119.17(8)
O(3)-C(25)-O(2)	124.67(12)
O(3)-C(25)-C(26)	120.85(12)
O(2)-C(25)-C(26)	114.48(11)

Symmetry transformations used to generate equivalent atoms:

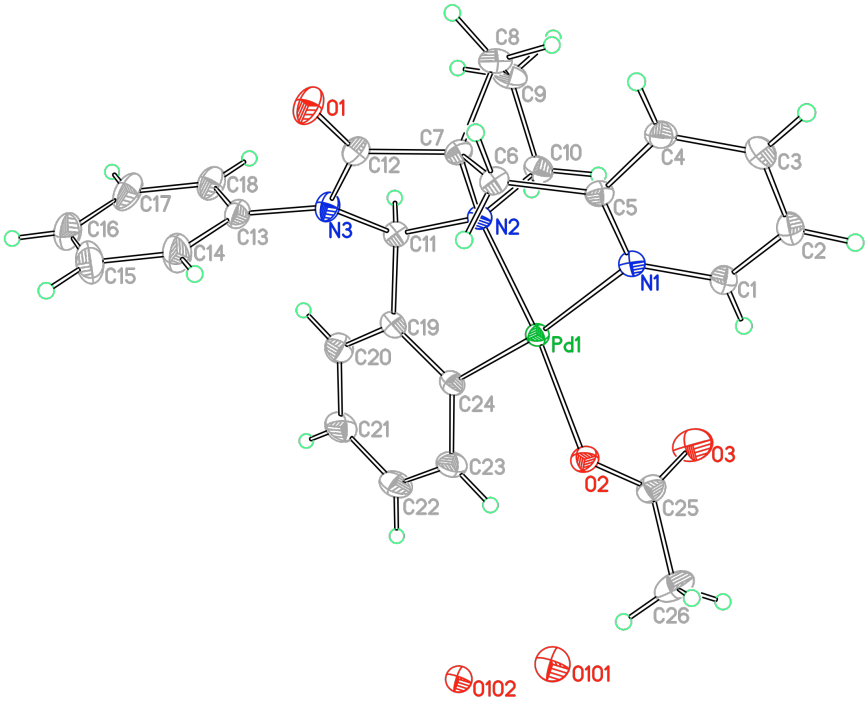
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for ef02. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	13(1)	14(1)	12(1)	-1(1)	-1(1)	0(1)
N(2)	14(1)	15(1)	12(1)	0(1)	0(1)	0(1)
C(19)	16(1)	19(1)	13(1)	1(1)	1(1)	3(1)
N(1)	15(1)	15(1)	17(1)	0(1)	-1(1)	-1(1)
C(7)	16(1)	16(1)	11(1)	-1(1)	0(1)	-2(1)
C(6)	17(1)	16(1)	13(1)	0(1)	1(1)	-2(1)
N(3)	22(1)	14(1)	15(1)	0(1)	1(1)	0(1)
C(8)	16(1)	24(1)	17(1)	2(1)	-2(1)	-4(1)
C(12)	19(1)	16(1)	15(1)	0(1)	2(1)	-2(1)
C(11)	16(1)	16(1)	13(1)	1(1)	1(1)	0(1)
C(24)	15(1)	18(1)	14(1)	-1(1)	-1(1)	2(1)
C(10)	15(1)	24(1)	16(1)	-1(1)	2(1)	2(1)
C(5)	14(1)	16(1)	15(1)	1(1)	0(1)	-2(1)
C(9)	14(1)	30(1)	19(1)	5(1)	1(1)	-3(1)
C(18)	32(1)	18(1)	19(1)	1(1)	1(1)	-2(1)
C(13)	22(1)	14(1)	21(1)	-1(1)	-1(1)	0(1)
C(4)	18(1)	19(1)	20(1)	2(1)	-5(1)	-2(1)
C(17)	49(1)	15(1)	22(1)	1(1)	-6(1)	-2(1)
C(1)	21(1)	17(1)	24(1)	-3(1)	-5(1)	2(1)
C(20)	27(1)	22(1)	19(1)	4(1)	-3(1)	2(1)
C(3)	26(1)	21(1)	31(1)	3(1)	-10(1)	3(1)
C(22)	21(1)	32(1)	22(1)	2(1)	-7(1)	3(1)
C(21)	28(1)	28(1)	22(1)	7(1)	-7(1)	3(1)
C(23)	19(1)	25(1)	21(1)	2(1)	-5(1)	0(1)
C(14)	26(1)	19(1)	51(1)	-2(1)	12(1)	-1(1)
C(2)	29(1)	17(1)	34(1)	-2(1)	-11(1)	5(1)
C(15)	31(1)	24(1)	67(1)	-8(1)	10(1)	6(1)
C(16)	41(1)	16(1)	47(1)	-2(1)	-9(1)	5(1)
O(1)	37(1)	20(1)	16(1)	-4(1)	1(1)	-1(1)
O(2)	16(1)	18(1)	17(1)	-4(1)	1(1)	-1(1)
C(25)	19(1)	19(1)	17(1)	-3(1)	2(1)	-2(1)

O(3)	24(1)	41(1)	35(1)	-20(1)	9(1)	-3(1)
C(26)	28(1)	32(1)	26(1)	-10(1)	4(1)	-12(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ef02.

	x	y	z	U(eq)
H(6A)	10070	8453	10723	19
H(6B)	8935	8359	10166	19
H(8A)	12255	9492	10023	23
H(8B)	12209	8289	9943	23
H(11A)	10547	10095	8219	18
H(10A)	11430	8605	7941	22
H(10B)	11519	7699	8530	22
H(9A)	12459	9725	8746	25
H(9B)	13230	8700	8849	25
H(18A)	10447	11970	8376	27
H(4A)	11043	6878	11086	23
H(17A)	9700	13639	8290	34
H(1A)	9614	5419	8893	25
H(20A)	8894	11026	7402	27
H(3A)	11371	5135	10876	31
H(22A)	6264	9172	6522	30
H(21A)	7298	10733	6535	31
H(23A)	6791	7912	7384	26
H(14A)	7645	11286	9807	38
H(2A)	10609	4400	9769	32
H(15A)	6870	12943	9684	49
H(16A)	7890	14107	8918	42
H(26A)	6367	4893	7497	43
H(26B)	5589	5881	7679	43
H(26C)	5937	5115	8328	43



(Collected data to 0.75Å, but truncated at 1Å due to weak scattering.)

Table 6. Crystal data and structure refinement for **26**.

Identification code	ef05	
Empirical formula	$C_{28}H_{28}N_4O_5$	
Formula weight	500.54	
Temperature	120 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P\,2_1\,2_1\,2_1$	
Unit cell dimensions	a = 8.5307(4) Å	α= 90°.
	b = 9.5523(5) Å	β= 90°.
	c = 30.0128(13) Å	γ = 90°.
Volume	2445.7(2) Å^3	
Z	4	
Density (calculated)	1.359 Mg/m^3	
Absorption coefficient	0.095 mm^{-1}	
F(000)	1056	
Crystal size	0.383 x 0.10 x 0.065 mm^3	
Theta range for data collection	2.24 to 20.82°.	
Index ranges	-8<=h<=8, -9<=k<=9, -30<=l<=28	
Reflections collected	22831	
Independent reflections	2574 [R(int) = 0.0767]	
Completeness to theta = 20.82°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6607	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2574 / 0 / 335	
Goodness-of-fit on F^2	1.183	
Final R indices [I>2sigma(I)]	R1 = 0.0402, wR2 = 0.1084	
R indices (all data)	R1 = 0.0562, wR2 = 0.1404	
Absolute structure parameter	1(2)	
Largest diff. peak and hole	0.404 and -0.456 e.Å^{-3}	

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ef05. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3299(6)	1011(5)	3592(2)	22(1)
C(2)	2788(6)	2290(6)	3451(2)	29(2)
C(3)	3829(7)	24(6)	3303(2)	31(2)
C(4)	2870(6)	2603(6)	2999(2)	29(2)
C(5)	3898(7)	326(5)	2858(2)	26(1)
C(6)	3425(6)	1623(6)	2704(2)	21(1)
C(7)	3578(7)	2035(6)	2227(2)	24(1)
C(8)	4559(7)	1308(6)	1517(2)	27(1)
C(9)	4198(6)	88(6)	1213(2)	20(1)
C(10)	5283(6)	141(6)	807(2)	33(2)
C(11)	2507(6)	35(6)	1043(2)	16(1)
C(12)	1390(6)	-1218(5)	1719(2)	18(1)
C(13)	985(6)	-952(5)	2158(2)	23(1)
C(14)	1927(7)	-2540(5)	1597(2)	25(1)
C(15)	1156(7)	-2005(6)	2474(2)	31(2)
C(16)	2101(7)	-3562(6)	1911(2)	32(2)
C(17)	1729(6)	-3311(6)	2345(2)	30(2)
C(18)	90(6)	811(5)	1351(2)	18(1)
C(19)	523(6)	1838(5)	984(2)	16(1)
C(20)	-643(6)	1839(6)	591(2)	22(1)
C(21)	433(7)	1977(6)	182(2)	31(2)
C(22)	1830(6)	1097(5)	313(2)	22(1)
C(23)	664(6)	3306(5)	1203(2)	18(1)
C(24)	1143(6)	4460(5)	890(2)	18(1)
C(25)	2673(6)	4635(6)	749(2)	23(1)
C(26)	3030(7)	5670(5)	449(2)	26(1)
C(27)	1843(7)	6531(6)	299(2)	25(1)
C(28)	383(7)	6317(6)	463(2)	29(1)
N(1)	3346(5)	714(6)	4069(2)	27(1)
N(2)	1317(5)	-111(4)	1398(1)	17(1)
N(3)	2020(5)	1311(4)	800(1)	18(1)

N(4)	-17(5)	5314(5)	751(1)	27(1)
O(1)	3222(5)	1696(4)	4332(1)	35(1)
O(2)	3580(4)	-500(5)	4188(1)	31(1)
O(3)	3270(5)	3183(4)	2086(1)	38(1)
O(4)	4112(4)	991(4)	1973(1)	27(1)
O(5)	-1121(4)	801(3)	1567(1)	25(1)

Table 8. Bond lengths [Å] and angles [°] for ef05.

C(1)-C(3)	1.358(7)
C(1)-C(2)	1.365(7)
C(1)-N(1)	1.460(7)
C(2)-C(4)	1.388(8)
C(3)-C(5)	1.368(7)
C(4)-C(6)	1.373(7)
C(5)-C(6)	1.383(7)
C(6)-C(7)	1.491(7)
C(7)-O(3)	1.205(6)
C(7)-O(4)	1.336(6)
C(8)-O(4)	1.453(6)
C(8)-C(9)	1.512(7)
C(9)-C(10)	1.530(7)
C(9)-C(11)	1.530(7)
C(11)-N(2)	1.477(6)
C(11)-N(3)	1.481(6)
C(12)-C(13)	1.387(7)
C(12)-C(14)	1.392(7)
C(12)-N(2)	1.432(6)
C(13)-C(15)	1.390(7)
C(14)-C(16)	1.366(7)
C(15)-C(17)	1.394(8)
C(16)-C(17)	1.362(8)
C(18)-O(5)	1.220(6)
C(18)-N(2)	1.375(6)
C(18)-C(19)	1.522(7)
C(19)-N(3)	1.480(6)
C(19)-C(20)	1.544(7)
C(19)-C(23)	1.554(7)
C(20)-C(21)	1.538(7)
C(21)-C(22)	1.510(7)
C(22)-N(3)	1.484(6)
C(23)-C(24)	1.505(7)
C(24)-N(4)	1.349(6)

C(24)-C(25)	1.382(7)
C(25)-C(26)	1.371(7)
C(26)-C(27)	1.380(7)
C(27)-C(28)	1.354(8)
C(28)-N(4)	1.335(6)
N(1)-O(2)	1.230(5)
N(1)-O(1)	1.230(5)

C(3)-C(1)-C(2)	122.0(5)
C(3)-C(1)-N(1)	118.8(5)
C(2)-C(1)-N(1)	119.1(5)
C(1)-C(2)-C(4)	118.6(5)
C(1)-C(3)-C(5)	119.4(5)
C(6)-C(4)-C(2)	120.0(5)
C(3)-C(5)-C(6)	120.1(5)
C(4)-C(6)-C(5)	119.8(5)
C(4)-C(6)-C(7)	118.0(5)
C(5)-C(6)-C(7)	122.1(5)
O(3)-C(7)-O(4)	123.6(5)
O(3)-C(7)-C(6)	124.0(5)
O(4)-C(7)-C(6)	112.4(5)
O(4)-C(8)-C(9)	110.8(4)
C(8)-C(9)-C(10)	109.4(4)
C(8)-C(9)-C(11)	114.7(4)
C(10)-C(9)-C(11)	107.9(4)
N(2)-C(11)-N(3)	103.9(4)
N(2)-C(11)-C(9)	114.3(4)
N(3)-C(11)-C(9)	113.7(4)
C(13)-C(12)-C(14)	119.8(4)
C(13)-C(12)-N(2)	119.6(5)
C(14)-C(12)-N(2)	120.5(4)
C(12)-C(13)-C(15)	119.3(5)
C(16)-C(14)-C(12)	120.2(5)
C(13)-C(15)-C(17)	119.7(5)
C(17)-C(16)-C(14)	120.6(6)
C(16)-C(17)-C(15)	120.2(5)

O(5)-C(18)-N(2)	125.9(4)
O(5)-C(18)-C(19)	126.6(5)
N(2)-C(18)-C(19)	107.5(4)
N(3)-C(19)-C(18)	105.1(4)
N(3)-C(19)-C(20)	105.7(4)
C(18)-C(19)-C(20)	113.4(4)
N(3)-C(19)-C(23)	113.5(4)
C(18)-C(19)-C(23)	107.1(4)
C(20)-C(19)-C(23)	111.9(4)
C(21)-C(20)-C(19)	103.0(4)
C(22)-C(21)-C(20)	102.5(4)
N(3)-C(22)-C(21)	105.4(4)
C(24)-C(23)-C(19)	114.7(4)
N(4)-C(24)-C(25)	121.7(5)
N(4)-C(24)-C(23)	115.9(4)
C(25)-C(24)-C(23)	122.4(5)
C(26)-C(25)-C(24)	119.8(5)
C(25)-C(26)-C(27)	118.8(5)
C(28)-C(27)-C(26)	117.8(5)
N(4)-C(28)-C(27)	125.3(5)
O(2)-N(1)-O(1)	123.2(4)
O(2)-N(1)-C(1)	118.2(5)
O(1)-N(1)-C(1)	118.6(5)
C(18)-N(2)-C(12)	125.0(4)
C(18)-N(2)-C(11)	113.0(4)
C(12)-N(2)-C(11)	121.6(4)
C(19)-N(3)-C(11)	109.8(4)
C(19)-N(3)-C(22)	108.7(4)
C(11)-N(3)-C(22)	113.8(4)
C(28)-N(4)-C(24)	116.6(4)
C(7)-O(4)-C(8)	118.1(4)

Symmetry transformations used to generate equivalent atoms:

Table 9. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for ef05. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	16(3)	27(4)	24(3)	0(3)	0(3)	-1(3)
C(2)	25(4)	28(4)	34(4)	-12(3)	-4(3)	3(3)
C(3)	42(4)	23(3)	27(4)	1(3)	-3(3)	6(3)
C(4)	26(4)	24(3)	37(4)	0(3)	-11(3)	5(3)
C(5)	39(4)	16(3)	23(3)	0(2)	-4(3)	7(3)
C(6)	15(3)	26(3)	23(3)	-6(3)	-11(2)	2(3)
C(7)	22(4)	18(4)	33(4)	-4(3)	-6(3)	-4(3)
C(8)	18(3)	35(3)	28(3)	11(3)	-1(3)	-4(3)
C(9)	17(3)	24(3)	21(3)	4(2)	5(2)	2(3)
C(10)	19(3)	47(4)	34(3)	10(3)	5(3)	12(3)
C(11)	20(3)	11(3)	17(3)	3(2)	9(2)	0(2)
C(12)	14(3)	17(3)	23(3)	7(2)	-3(2)	-6(3)
C(13)	20(3)	26(3)	23(3)	-1(3)	7(2)	2(3)
C(14)	35(4)	16(3)	22(3)	2(3)	1(3)	-5(3)
C(15)	32(4)	43(4)	18(3)	10(3)	0(3)	-14(3)
C(16)	43(4)	21(4)	33(4)	10(3)	-7(3)	-1(3)
C(17)	25(4)	28(4)	37(4)	19(3)	-6(3)	-4(3)
C(18)	20(3)	16(3)	17(3)	0(2)	-1(3)	-8(3)
C(19)	13(3)	18(3)	15(3)	0(2)	-1(2)	1(3)
C(20)	25(4)	20(3)	22(3)	4(2)	-2(3)	-3(3)
C(21)	34(4)	35(4)	23(3)	-2(3)	-6(3)	1(3)
C(22)	28(3)	25(3)	14(3)	5(2)	1(2)	-4(3)
C(23)	17(3)	21(3)	17(3)	1(2)	3(2)	5(3)
C(24)	21(3)	11(3)	22(3)	-3(2)	-2(3)	2(3)
C(25)	23(4)	22(3)	23(3)	1(3)	-1(3)	1(3)
C(26)	25(3)	24(3)	30(3)	-1(3)	5(3)	-1(3)
C(27)	32(4)	24(3)	20(3)	6(3)	3(3)	-5(3)
C(28)	31(4)	26(3)	31(3)	11(3)	-4(3)	1(3)
N(1)	21(3)	33(3)	29(3)	-2(3)	2(2)	-4(3)
N(2)	16(3)	17(2)	18(2)	5(2)	-1(2)	1(2)
N(3)	15(3)	23(3)	17(2)	5(2)	4(2)	3(2)

N(4)	26(3)	23(3)	31(3)	6(2)	2(2)	2(3)
O(1)	37(3)	39(3)	28(2)	-13(2)	-1(2)	-6(2)
O(2)	31(2)	36(3)	27(2)	3(2)	-2(2)	0(2)
O(3)	56(3)	21(2)	37(2)	7(2)	-4(2)	7(2)
O(4)	33(3)	26(2)	22(2)	7(2)	-2(2)	1(2)
O(5)	21(2)	25(2)	27(2)	8(2)	7(2)	1(2)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ef05.

	x	y	z	U(eq)
H(2)	2393	2939	3652	35
H(3)	4142	-850	3407	37
H(4)	2548	3476	2897	35
H(5)	4263	-343	2658	31
H(8A)	5671	1515	1505	32
H(8B)	3994	2130	1416	32
H(9)	4412	-780	1376	24
H(10A)	5170	1028	660	50
H(10B)	5011	-598	605	50
H(10C)	6350	25	902	50
H(11)	2409	-766	841	19
H(13)	603	-78	2241	28
H(14)	2168	-2727	1301	30
H(15)	890	-1840	2770	37
H(16)	2478	-4437	1828	39
H(17)	1857	-4014	2557	36
H(20A)	-1240	975	581	27
H(20B)	-1363	2623	611	27
H(21A)	-68	1613	-84	37
H(21B)	732	2944	132	37
H(22A)	1642	118	246	27
H(22B)	2761	1400	154	27
H(23A)	-339	3548	1334	22
H(23B)	1426	3254	1442	22
H(25)	3458	4051	857	27
H(26)	4053	5790	349	32
H(27)	2039	7235	92	31
H(28)	-405	6918	366	35