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Solid-State NMR Crystallographic and Density Functional Theory Investigation of Fe-CO and Fe-CO Analog Metalloporphyrins and Metalloproteins

Supporting Information

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Table S1. Crystal data and structure refinement for Fe(OEP)(CO)(1-MeIm).

Empirical formula	C44 H57 Fe N6 O
Formula weight	741.81
Temperature	198(2) K
Wavelength	.71073 A
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 11.872(2) A alpha = 84.19(3) deg
	b = 13.192(3) A beta = 69.72(3) deg
from 2783 reflns with	
	c = 14.305(3) A gamma = 69.85(3) deg
4<=theta<=28	
	V = 1972.5(7) A^3 Z = 2
Density (calculated)	1.249 Mg/m^3
Absorption coefficient	0.424 mm^-1
Crystal size	0.23 x 0.16 x 0.08 mm
Crystal color	Red
Theta range for data collection	1.52 to 25.00 deg
Index ranges	-13<=h<=14, -11<=k<=16, -15<=l<=17
Collection method	\w scans
Reflections collected	10326 [R(int) = 0.0413]
Independent reflections	6785 [3873 obs, I >2sigma(I)]
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.9295 and 0.8470
Refinement (shift/err=0.001)	Full-matrix least-squares on F^2
Data / restraints / parameters	6519 / 72 / 496
Goodness-of-fit on F^2	1.025
Final R indices (obs data)	R1 = 0.0594, wR2 = 0.1283
R indices (all data)	R1 = 0.1227, wR2 = 0.1673
calc w=1/[\s^2^(Fo^2^)+(0.0610P)^2^+0.9241P] where P=(Fo^2^+2Fc^2^)/3	
Largest diff. peak and hole	.665 and -.592 e.A^-3

Crystal preparation and structure refinement summary for Fe(OEP)(CO)(1-MeIm).

Crystals were grown from hexane. The data crystal was mounted using oil (Paratone-N, Exxon) to a thin glass fiber with the (1 0 1) scattering planes roughly normal to the spindle axis.

Systematic conditions suggested the ambiguous space group. The structure was solved by direct methods (Sheldrick, 1990). The hexane exhibited disorder about an inversion center and was refined by imposing DFIX, SIMU and DELU restraints. All H-atom positions have been calculated and refined isotropically. The space group choice was confirmed by successful convergence of the full-matrix least-squares refinement on F^2^ (Sheldrick, 1993). The highest peaks in the final difference Fourier map were in the vicinity of the disordered hexane; the final map had no other significant features. A final analysis of variance between observed and calculated structure factors showed no dependence on amplitude or resolution.

Methyl H atom positions, R-CH~3~, were optimized by rotation about R-C bonds with idealized C-H, R--H and H--H distances. Remaining H atoms were included as fixed idealized contributors.

Sheldrick, G.M. (1990). SHELXS-86. Acta Cryst. A46, 467-473.

Sheldrick, G.M. (1993). SHELXL-93. Program for crystal structure refinement. Institute fur anorg chemie, G\"ottingen, Germany.

Siemens Industrial Automation, Incorporated. (1994). SAINT V4; SHELXTL V5; SMART V4. Madison, Wisconsin, USA.

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Fe(OEP)(CO)(1-MeIm). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	9622(1)	7477(1)	7870(1)	28(1)
O(1)	9892(3)	5315(3)	7355(2)	61(1)
N(1)	8323(3)	7375(2)	9178(2)	29(1)
N(2)	11006(3)	6770(2)	8451(2)	28(1)
N(3)	10927(3)	7624(2)	6573(2)	27(1)
N(4)	8232(3)	8226(2)	7303(2)	28(1)
N(5)	9498(3)	8963(3)	8339(2)	29(1)
N(6)	8943(3)	10395(3)	9288(3)	38(1)
C(1)	8531(4)	6914(3)	10037(3)	28(1)
C(2)	9731(4)	6451(3)	10129(3)	30(1)
C(3)	10877(4)	6371(3)	9400(3)	29(1)
C(4)	12103(4)	5838(3)	9519(3)	30(1)
C(5)	12988(4)	5901(3)	8629(3)	31(1)
C(6)	12304(4)	6481(3)	7969(3)	28(1)
C(7)	12863(4)	6693(3)	6984(3)	33(1)
C(8)	12230(4)	7230(3)	6331(3)	31(1)
C(9)	12840(4)	7476(3)	5303(3)	34(1)
C(10)	11891(4)	8000(3)	4933(3)	36(1)
C(11)	10710(4)	8090(3)	5721(3)	31(1)
C(12)	9517(4)	8572(3)	5637(3)	36(1)
C(13)	8362(4)	8630(3)	6357(3)	31(1)
C(14)	7125(4)	9112(3)	6225(3)	36(1)
C(15)	6257(4)	8993(3)	7084(3)	37(1)
C(16)	6944(4)	8447(3)	7760(3)	32(1)
C(17)	6399(4)	8189(3)	8740(3)	32(1)
C(18)	7025(4)	7706(3)	9401(3)	30(1)
C(19)	6405(4)	7456(3)	10428(3)	32(1)
C(20)	7352(4)	6969(3)	10815(3)	33(1)
C(21)	12311(4)	5317(3)	10453(3)	37(1)
C(22)	12087(5)	6111(3)	11256(3)	48(1)
C(23)	14413(4)	5491(3)	8363(3)	40(1)
C(24)	14927(5)	6243(4)	8676(4)	62(2)
C(25)	14249(4)	7121(4)	4771(3)	48(1)
C(26)	14732(5)	6117(4)	4126(4)	67(2)
C(27)	12001(5)	8393(4)	3889(3)	44(1)
C(28)	11836(5)	7639(4)	3251(3)	54(1)
C(29)	6936(5)	9625(3)	5282(3)	43(1)
C(30)	7253(5)	8796(4)	4471(3)	63(2)
C(31)	4836(4)	9369(4)	7339(4)	48(1)
C(32)	4381(5)	8686(4)	6852(4)	73(2)
C(33)	4997(4)	7724(3)	10923(3)	37(1)
C(34)	4306(4)	8893(4)	11263(4)	54(1)
C(35)	7247(4)	6551(3)	11849(3)	41(1)
C(36)	7377(5)	7304(4)	12520(3)	60(2)
C(37)	9760(4)	6195(4)	7530(3)	32(1)
C(38)	8783(4)	9455(3)	9204(3)	36(1)
C(39)	9806(5)	10520(4)	8418(4)	49(1)
C(40)	10146(5)	9642(4)	7836(3)	47(1)

C(41)	8264(5)	11158(4)	10145(4)	56(1)
C(51)	-2558(19)	5681(14)	6054(12)	143(5)
C(52)	-1603(17)	5406(16)	5017(11)	164(5)
C(53)	-215(16)	4758(12)	5087(17)	127(4)
C(54)	477(17)	5553(12)	4871(20)	147(5)
C(55)	1912(16)	4964(12)	4792(11)	128(4)
C(56)	2464(22)	3960(12)	4141(13)	150(5)

Table S3. Anisotropic displacement parameters (A^2 x 10^3) for Fe(OEP)(CO)(1-MeIm). The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Fe(1)	33(1)	31(1)	23(1)	1(1)	-11(1)	-11(1)
O(1)	89(3)	42(2)	53(2)	-5(2)	-19(2)	-28(2)
N(1)	31(2)	30(2)	27(2)	-1(2)	-10(2)	-11(2)
N(2)	32(2)	27(2)	26(2)	3(2)	-12(2)	-10(2)
N(3)	33(2)	30(2)	22(2)	1(2)	-10(2)	-13(2)
N(4)	37(2)	28(2)	22(2)	0(2)	-13(2)	-13(2)
N(5)	33(2)	30(2)	29(2)	2(2)	-16(2)	-10(2)
N(6)	45(2)	32(2)	41(2)	-2(2)	-19(2)	-11(2)
C(1)	40(3)	24(2)	22(2)	-1(2)	-10(2)	-13(2)
C(2)	40(3)	34(2)	19(2)	4(2)	-12(2)	-14(2)
C(3)	37(3)	24(2)	29(2)	1(2)	-16(2)	-7(2)
C(4)	38(3)	26(2)	29(2)	-2(2)	-16(2)	-9(2)
C(5)	35(3)	26(2)	38(3)	-4(2)	-22(2)	-7(2)
C(6)	36(3)	25(2)	25(2)	-1(2)	-11(2)	-12(2)
C(7)	33(3)	30(2)	37(3)	-2(2)	-13(2)	-9(2)
C(8)	36(3)	34(2)	23(2)	-8(2)	-6(2)	-13(2)
C(9)	37(3)	35(3)	26(2)	-5(2)	0(2)	-17(2)
C(10)	52(3)	34(3)	24(2)	0(2)	-11(2)	-19(2)
C(11)	39(3)	31(2)	24(2)	1(2)	-12(2)	-13(2)
C(12)	60(3)	29(2)	28(3)	5(2)	-21(2)	-19(2)
C(13)	43(3)	27(2)	30(3)	0(2)	-17(2)	-15(2)
C(14)	49(3)	30(3)	37(3)	2(2)	-26(2)	-11(2)
C(15)	44(3)	36(3)	39(3)	-1(2)	-22(2)	-14(2)
C(16)	34(3)	32(2)	38(3)	1(2)	-20(2)	-13(2)
C(17)	28(2)	35(2)	34(3)	-5(2)	-9(2)	-13(2)
C(18)	37(3)	29(2)	30(2)	-1(2)	-14(2)	-14(2)
C(19)	40(3)	32(2)	27(2)	-2(2)	-9(2)	-17(2)
C(20)	41(3)	32(2)	27(2)	-4(2)	-7(2)	-18(2)
C(21)	47(3)	32(3)	36(3)	3(2)	-24(2)	-8(2)
C(22)	68(3)	41(3)	42(3)	-2(2)	-31(3)	-13(2)
C(23)	39(3)	37(3)	42(3)	1(2)	-20(2)	-4(2)
C(24)	46(3)	65(4)	84(4)	-4(3)	-36(3)	-15(3)
C(25)	55(3)	56(3)	32(3)	4(2)	-7(2)	-24(3)
C(26)	67(4)	62(4)	52(3)	-9(3)	3(3)	-17(3)
C(27)	57(3)	43(3)	31(3)	2(2)	-10(2)	-21(2)
C(28)	78(4)	55(3)	35(3)	3(2)	-22(3)	-28(3)
C(29)	57(3)	44(3)	41(3)	7(2)	-33(2)	-16(2)
C(30)	96(4)	65(4)	46(3)	7(3)	-47(3)	-25(3)
C(31)	39(3)	56(3)	55(3)	4(2)	-29(2)	-12(2)
C(32)	69(4)	82(4)	100(5)	13(3)	-52(4)	-42(3)
C(33)	36(3)	43(3)	32(2)	-1(2)	-4(2)	-19(2)
C(34)	44(3)	53(3)	54(3)	-4(3)	-4(2)	-15(2)
C(35)	50(3)	44(3)	26(2)	5(2)	-7(2)	-20(2)
C(36)	92(4)	62(3)	30(3)	-6(2)	-24(3)	-23(3)
C(37)	36(3)	43(3)	21(2)	-1(2)	-11(2)	-14(2)
C(38)	39(3)	32(3)	43(3)	-1(2)	-17(2)	-14(2)
C(39)	68(4)	36(3)	51(3)	5(2)	-23(3)	-26(3)
C(40)	64(3)	41(3)	37(3)	5(2)	-15(2)	-22(3)
C(41)	67(4)	36(3)	61(3)	-19(2)	-28(3)	1(2)

C(51)	245(10)	123(9)	104(8)	36(8)	-63(8)	-120(8)
C(52)	257(10)	142(9)	109(7)	40(8)	-69(8)	-90(8)
C(53)	239(10)	133(9)	83(6)	35(7)	-83(7)	-132(7)
C(54)	260(10)	119(9)	97(6)	46(7)	-70(8)	-107(7)
C(55)	237(10)	121(9)	88(7)	53(6)	-70(8)	-133(7)
C(56)	260(11)	120(9)	89(8)	48(7)	-60(8)	-97(8)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Fe(OEP)(CO)(1-MeIm). Treatment of hydrogen atoms not specifically described in the refinement summary was "noref."

	x	y	z	U(eq)
H(2A)	9762(4)	6160(3)	10758(3)	36
H(7A)	13767(4)	6448(3)	6729(3)	40
H(12A)	9487(4)	8898(3)	5020(3)	44
H(17A)	5500(4)	8364(3)	8979(3)	38
H(21A)	13196(4)	4811(3)	10281(3)	44
H(21B)	11734(4)	4888(3)	10731(3)	44
H(22A)	12241(5)	5713(3)	11841(3)	72
H(22B)	11206(5)	6604(3)	11446(3)	72
H(22C)	12670(5)	6527(3)	10996(3)	72
H(23A)	14667(4)	4786(3)	8682(3)	48
H(23B)	14805(4)	5369(3)	7632(3)	48
H(24A)	15855(5)	5928(4)	8481(4)	93
H(24B)	14561(5)	6355(4)	9401(4)	93
H(24C)	14699(5)	6938(4)	8350(4)	93
H(25A)	14689(4)	6978(4)	5269(3)	58
H(25B)	14465(4)	7715(4)	4347(3)	58
H(26A)	15655(5)	5923(4)	3797(4)	101
H(26B)	14315(5)	6258(4)	3620(4)	101
H(26C)	14539(5)	5521(4)	4542(4)	101
H(27A)	12847(5)	8478(4)	3565(3)	53
H(27B)	11349(5)	9113(4)	3924(3)	53
H(28A)	11917(5)	7937(4)	2584(3)	81
H(28B)	10992(5)	7565(4)	3558(3)	81
H(28C)	12491(5)	6929(4)	3199(3)	81
H(29A)	7481(5)	10084(3)	5025(3)	52
H(29B)	6039(5)	10099(3)	5434(3)	52
H(30A)	7114(5)	9175(4)	3874(3)	95
H(30B)	6703(5)	8350(4)	4715(3)	95
H(30C)	8146(5)	8335(4)	4306(3)	95
H(31A)	4546(4)	10126(4)	7128(4)	57
H(31B)	4436(4)	9358(4)	8071(4)	57
H(32A)	3451(5)	8972(4)	7047(4)	110
H(32B)	4644(5)	7938(4)	7070(4)	110
H(32C)	4754(5)	8707(4)	6126(4)	110
H(33A)	4837(4)	7257(3)	11508(3)	45
H(33B)	4638(4)	7554(3)	10452(3)	45
H(34A)	3394(4)	9010(4)	11579(4)	80
H(34B)	4439(4)	9361(4)	10687(4)	80
H(34C)	4638(4)	9064(4)	11744(4)	80
H(35A)	7917(4)	5839(3)	11802(3)	49
H(35B)	6412(4)	6442(3)	12161(3)	49
H(36A)	7300(5)	6987(4)	13180(3)	91
H(36B)	6704(5)	8005(4)	12584(3)	91
H(36C)	8210(5)	7401(4)	12226(3)	91
H(38A)	8214(4)	9175(3)	9714(3)	44
H(39A)	10117(5)	11112(4)	8246(4)	58
H(40A)	10742(5)	9517(4)	7179(3)	56

H(41A)	8567(5)	11779(4)	10009(4)	84
H(41B)	8426(5)	10796(4)	10742(4)	84
H(41C)	7348(5)	11406(4)	10256(4)	84
H(51A)	-3405(19)	6076(14)	6013(12)	214
H(51B)	-2316(19)	6131(14)	6403(12)	214
H(51C)	-2573(19)	5014(14)	6421(12)	214
H(52A)	-1590(17)	6077(16)	4640(11)	196
H(52B)	-1848(17)	4957(16)	4659(11)	196
H(53A)	-286(16)	4463(12)	5762(17)	152
H(53B)	239(16)	4152(12)	4594(17)	152
H(54A)	66(17)	6112(12)	5409(20)	176
H(54B)	438(17)	5915(12)	4237(20)	176
H(55A)	2407(16)	5457(12)	4504(11)	153
H(55B)	1965(16)	4766(12)	5465(11)	153
H(56A)	3354(22)	3598(12)	4095(13)	225
H(56B)	2419(22)	4159(12)	3473(13)	225
H(56C)	1978(22)	3470(12)	4432(13)	225

Table S5. Bond lengths [A] and angles [deg] for Fe(OEP)(CO)(1-MeIm).

Fe(1)-C(37)	1.744(5)
Fe(1)-N(1)	1.998(3)
Fe(1)-N(2)	1.998(3)
Fe(1)-N(4)	2.000(3)
Fe(1)-N(3)	2.005(3)
Fe(1)-N(5)	2.077(3)
O(1)-C(37)	1.158(5)
N(1)-C(18)	1.375(5)
N(1)-C(1)	1.377(5)
N(2)-C(6)	1.381(5)
N(2)-C(3)	1.382(5)
N(3)-C(11)	1.374(5)
N(3)-C(8)	1.377(5)
N(4)-C(16)	1.375(5)
N(4)-C(13)	1.381(5)
N(5)-C(38)	1.314(5)
N(5)-C(40)	1.368(5)
N(6)-C(38)	1.340(5)
N(6)-C(39)	1.348(5)
N(6)-C(41)	1.474(5)
C(1)-C(2)	1.391(5)
C(1)-C(20)	1.438(5)
C(2)-C(3)	1.374(5)
C(3)-C(4)	1.444(5)
C(4)-C(5)	1.358(5)
C(4)-C(21)	1.499(5)
C(5)-C(6)	1.447(5)
C(5)-C(23)	1.504(6)
C(6)-C(7)	1.380(5)
C(7)-C(8)	1.387(5)
C(8)-C(9)	1.456(5)
C(9)-C(10)	1.353(6)
C(9)-C(25)	1.499(6)
C(10)-C(11)	1.438(6)
C(10)-C(27)	1.507(5)
C(11)-C(12)	1.380(6)
C(12)-C(13)	1.382(6)
C(13)-C(14)	1.457(6)
C(14)-C(15)	1.339(6)
C(14)-C(29)	1.500(5)
C(15)-C(16)	1.455(5)
C(15)-C(31)	1.503(6)
C(16)-C(17)	1.388(5)
C(17)-C(18)	1.375(5)
C(18)-C(19)	1.459(5)
C(19)-C(20)	1.359(6)
C(19)-C(33)	1.498(6)
C(20)-C(35)	1.505(5)
C(21)-C(22)	1.526(5)
C(23)-C(24)	1.501(6)
C(25)-C(26)	1.514(6)
C(27)-C(28)	1.518(6)
C(29)-C(30)	1.534(6)
C(31)-C(32)	1.520(6)

C(33)-C(34)	1.514(6)
C(35)-C(36)	1.527(6)
C(39)-C(40)	1.356(6)
C(51)-C(52)	1.510(10)
C(52)-C(53)	1.608(9)
C(53)-C(54)	1.492(9)
C(54)-C(55)	1.578(9)
C(55)-C(56)	1.510(10)

C(37)-Fe(1)-N(1)	89.8(2)
C(37)-Fe(1)-N(2)	88.3(2)
N(1)-Fe(1)-N(2)	90.03(14)
C(37)-Fe(1)-N(4)	93.4(2)
N(1)-Fe(1)-N(4)	89.86(14)
N(2)-Fe(1)-N(4)	178.31(13)
C(37)-Fe(1)-N(3)	92.0(2)
N(1)-Fe(1)-N(3)	178.11(13)
N(2)-Fe(1)-N(3)	89.79(14)
N(4)-Fe(1)-N(3)	90.26(13)
C(37)-Fe(1)-N(5)	176.8(2)
N(1)-Fe(1)-N(5)	88.73(13)
N(2)-Fe(1)-N(5)	88.80(13)
N(4)-Fe(1)-N(5)	89.52(13)
N(3)-Fe(1)-N(5)	89.39(13)
C(18)-N(1)-C(1)	105.0(3)
C(18)-N(1)-Fe(1)	127.3(3)
C(1)-N(1)-Fe(1)	127.7(3)
C(6)-N(2)-C(3)	104.7(3)
C(6)-N(2)-Fe(1)	127.7(3)
C(3)-N(2)-Fe(1)	127.3(3)
C(11)-N(3)-C(8)	105.4(3)
C(11)-N(3)-Fe(1)	127.2(3)
C(8)-N(3)-Fe(1)	127.3(3)
C(16)-N(4)-C(13)	104.7(3)
C(16)-N(4)-Fe(1)	128.1(3)
C(13)-N(4)-Fe(1)	127.2(3)
C(38)-N(5)-C(40)	104.3(4)
C(38)-N(5)-Fe(1)	127.2(3)
C(40)-N(5)-Fe(1)	128.5(3)
C(38)-N(6)-C(39)	106.2(4)
C(38)-N(6)-C(41)	126.6(4)
C(39)-N(6)-C(41)	127.1(4)
N(1)-C(1)-C(2)	123.9(4)
N(1)-C(1)-C(20)	111.2(4)
C(2)-C(1)-C(20)	124.9(4)
C(3)-C(2)-C(1)	126.6(4)
C(2)-C(3)-N(2)	124.4(4)
C(2)-C(3)-C(4)	124.4(4)
N(2)-C(3)-C(4)	111.2(3)
C(5)-C(4)-C(3)	106.4(3)
C(5)-C(4)-C(21)	128.3(4)
C(3)-C(4)-C(21)	125.2(4)
C(4)-C(5)-C(6)	107.0(4)
C(4)-C(5)-C(23)	127.8(4)
C(6)-C(5)-C(23)	125.2(4)
C(7)-C(6)-N(2)	124.2(4)
C(7)-C(6)-C(5)	125.0(4)
N(2)-C(6)-C(5)	110.7(3)

C(6)-C(7)-C(8)	126.2(4)
N(3)-C(8)-C(7)	124.5(4)
N(3)-C(8)-C(9)	110.3(4)
C(7)-C(8)-C(9)	125.2(4)
C(10)-C(9)-C(8)	106.4(4)
C(10)-C(9)-C(25)	128.5(4)
C(8)-C(9)-C(25)	124.9(4)
C(9)-C(10)-C(11)	107.2(4)
C(9)-C(10)-C(27)	128.1(4)
C(11)-C(10)-C(27)	124.6(4)
N(3)-C(11)-C(12)	124.3(4)
N(3)-C(11)-C(10)	110.7(4)
C(12)-C(11)-C(10)	125.0(4)
C(11)-C(12)-C(13)	127.0(4)
N(4)-C(13)-C(12)	124.0(4)
N(4)-C(13)-C(14)	110.8(4)
C(12)-C(13)-C(14)	125.2(4)
C(15)-C(14)-C(13)	106.7(4)
C(15)-C(14)-C(29)	129.2(4)
C(13)-C(14)-C(29)	124.1(4)
C(14)-C(15)-C(16)	107.0(4)
C(14)-C(15)-C(31)	127.7(4)
C(16)-C(15)-C(31)	125.3(4)
N(4)-C(16)-C(17)	123.3(4)
N(4)-C(16)-C(15)	110.9(4)
C(17)-C(16)-C(15)	125.8(4)
C(18)-C(17)-C(16)	126.8(4)
N(1)-C(18)-C(17)	124.6(4)
N(1)-C(18)-C(19)	110.8(4)
C(17)-C(18)-C(19)	124.6(4)
C(20)-C(19)-C(18)	106.1(4)
C(20)-C(19)-C(33)	128.9(4)
C(18)-C(19)-C(33)	125.0(4)
C(19)-C(20)-C(1)	107.0(4)
C(19)-C(20)-C(35)	128.5(4)
C(1)-C(20)-C(35)	124.5(4)
C(4)-C(21)-C(22)	114.2(3)
C(24)-C(23)-C(5)	113.7(4)
C(9)-C(25)-C(26)	113.0(4)
C(10)-C(27)-C(28)	113.3(3)
C(14)-C(29)-C(30)	112.9(4)
C(15)-C(31)-C(32)	113.5(4)
C(19)-C(33)-C(34)	113.8(3)
C(20)-C(35)-C(36)	113.4(3)
O(1)-C(37)-Fe(1)	175.1(4)
N(5)-C(38)-N(6)	112.8(4)
N(6)-C(39)-C(40)	107.0(4)
C(39)-C(40)-N(5)	109.7(4)
C(51)-C(52)-C(53)	109.4(9)
C(54)-C(53)-C(52)	106.2(7)
C(53)-C(54)-C(55)	110.2(7)
C(56)-C(55)-C(54)	109.9(8)

Table S6. Torsion angles [deg] for Fe(OEP)(CO)(1-MeIm).

C(37)-Fe(1)-N(1)-C(18)	-90.7(3)
N(2)-Fe(1)-N(1)-C(18)	-179.0(3)
N(4)-Fe(1)-N(1)-C(18)	2.6(3)
N(3)-Fe(1)-N(1)-C(18)	97(4)
N(5)-Fe(1)-N(1)-C(18)	92.2(3)
C(37)-Fe(1)-N(1)-C(1)	85.9(3)
N(2)-Fe(1)-N(1)-C(1)	-2.4(3)
N(4)-Fe(1)-N(1)-C(1)	179.3(3)
N(3)-Fe(1)-N(1)-C(1)	-87(4)
N(5)-Fe(1)-N(1)-C(1)	-91.2(3)
C(37)-Fe(1)-N(2)-C(6)	86.8(3)
N(1)-Fe(1)-N(2)-C(6)	176.7(3)
N(4)-Fe(1)-N(2)-C(6)	-97(5)
N(3)-Fe(1)-N(2)-C(6)	-5.2(3)
N(5)-Fe(1)-N(2)-C(6)	-94.6(3)
C(37)-Fe(1)-N(2)-C(3)	-86.5(3)
N(1)-Fe(1)-N(2)-C(3)	3.4(3)
N(4)-Fe(1)-N(2)-C(3)	90(5)
N(3)-Fe(1)-N(2)-C(3)	-178.5(3)
N(5)-Fe(1)-N(2)-C(3)	92.1(3)
C(37)-Fe(1)-N(3)-C(11)	93.0(3)
N(1)-Fe(1)-N(3)-C(11)	-94(4)
N(2)-Fe(1)-N(3)-C(11)	-178.7(3)
N(4)-Fe(1)-N(3)-C(11)	-.4(3)
N(5)-Fe(1)-N(3)-C(11)	-89.9(3)
C(37)-Fe(1)-N(3)-C(8)	-83.2(3)
N(1)-Fe(1)-N(3)-C(8)	90(4)
N(2)-Fe(1)-N(3)-C(8)	5.0(3)
N(4)-Fe(1)-N(3)-C(8)	-176.6(3)
N(5)-Fe(1)-N(3)-C(8)	93.8(3)
C(37)-Fe(1)-N(4)-C(16)	86.9(3)
N(1)-Fe(1)-N(4)-C(16)	-3.0(3)
N(2)-Fe(1)-N(4)-C(16)	-89(5)
N(3)-Fe(1)-N(4)-C(16)	178.9(3)
N(5)-Fe(1)-N(4)-C(16)	-91.7(3)
C(37)-Fe(1)-N(4)-C(13)	-92.7(3)
N(1)-Fe(1)-N(4)-C(13)	177.5(3)
N(2)-Fe(1)-N(4)-C(13)	91(5)
N(3)-Fe(1)-N(4)-C(13)	-.6(3)
N(5)-Fe(1)-N(4)-C(13)	88.8(3)
C(37)-Fe(1)-N(5)-C(38)	-63(3)
N(1)-Fe(1)-N(5)-C(38)	.9(3)
N(2)-Fe(1)-N(5)-C(38)	-89.1(3)
N(4)-Fe(1)-N(5)-C(38)	90.8(3)
N(3)-Fe(1)-N(5)-C(38)	-178.9(3)
C(37)-Fe(1)-N(5)-C(40)	116(3)
N(1)-Fe(1)-N(5)-C(40)	179.8(4)
N(2)-Fe(1)-N(5)-C(40)	89.8(4)
N(4)-Fe(1)-N(5)-C(40)	-90.3(4)
N(3)-Fe(1)-N(5)-C(40)	.0(3)
C(18)-N(1)-C(1)-C(2)	178.7(4)
Fe(1)-N(1)-C(1)-C(2)	1.4(5)
C(18)-N(1)-C(1)-C(20)	-.9(4)
Fe(1)-N(1)-C(1)-C(20)	-178.1(2)

N(1)-C(1)-C(2)-C(3)	-.4(6)
C(20)-C(1)-C(2)-C(3)	179.1(4)
C(1)-C(2)-C(3)-N(2)	1.5(6)
C(1)-C(2)-C(3)-C(4)	-177.1(4)
C(6)-N(2)-C(3)-C(2)	-178.0(4)
Fe(1)-N(2)-C(3)-C(2)	-3.5(5)
C(6)-N(2)-C(3)-C(4)	.7(4)
Fe(1)-N(2)-C(3)-C(4)	175.2(2)
C(2)-C(3)-C(4)-C(5)	177.9(4)
N(2)-C(3)-C(4)-C(5)	-.7(4)
C(2)-C(3)-C(4)-C(21)	-1.5(6)
N(2)-C(3)-C(4)-C(21)	179.8(3)
C(3)-C(4)-C(5)-C(6)	.5(4)
C(21)-C(4)-C(5)-C(6)	179.9(4)
C(3)-C(4)-C(5)-C(23)	178.6(4)
C(21)-C(4)-C(5)-C(23)	-2.0(7)
C(3)-N(2)-C(6)-C(7)	177.9(4)
Fe(1)-N(2)-C(6)-C(7)	3.4(5)
C(3)-N(2)-C(6)-C(5)	-.3(4)
Fe(1)-N(2)-C(6)-C(5)	-174.8(2)
C(4)-C(5)-C(6)-C(7)	-178.3(4)
C(23)-C(5)-C(6)-C(7)	3.5(6)
C(4)-C(5)-C(6)-N(2)	-.1(4)
C(23)-C(5)-C(6)-N(2)	-178.3(3)
N(2)-C(6)-C(7)-C(8)	.8(6)
C(5)-C(6)-C(7)-C(8)	178.8(4)
C(11)-N(3)-C(8)-C(7)	-180.0(4)
Fe(1)-N(3)-C(8)-C(7)	-3.1(6)
C(11)-N(3)-C(8)-C(9)	1.0(4)
Fe(1)-N(3)-C(8)-C(9)	177.9(2)
C(6)-C(7)-C(8)-N(3)	-1.0(7)
C(6)-C(7)-C(8)-C(9)	177.9(4)
N(3)-C(8)-C(9)-C(10)	-1.0(5)
C(7)-C(8)-C(9)-C(10)	180.0(4)
N(3)-C(8)-C(9)-C(25)	-176.7(4)
C(7)-C(8)-C(9)-C(25)	4.3(6)
C(8)-C(9)-C(10)-C(11)	.6(4)
C(25)-C(9)-C(10)-C(11)	176.1(4)
C(8)-C(9)-C(10)-C(27)	-177.2(4)
C(25)-C(9)-C(10)-C(27)	-1.7(7)
C(8)-N(3)-C(11)-C(12)	179.0(4)
Fe(1)-N(3)-C(11)-C(12)	2.1(6)
C(8)-N(3)-C(11)-C(10)	-.7(4)
Fe(1)-N(3)-C(11)-C(10)	-177.5(2)
C(9)-C(10)-C(11)-N(3)	.0(5)
C(27)-C(10)-C(11)-N(3)	177.9(3)
C(9)-C(10)-C(11)-C(12)	-179.7(4)
C(27)-C(10)-C(11)-C(12)	-1.8(6)
N(3)-C(11)-C(12)-C(13)	-3.1(7)
C(10)-C(11)-C(12)-C(13)	176.6(4)
C(16)-N(4)-C(13)-C(12)	-179.6(4)
Fe(1)-N(4)-C(13)-C(12)	.0(5)
C(16)-N(4)-C(13)-C(14)	-.1(4)
Fe(1)-N(4)-C(13)-C(14)	179.6(2)
C(11)-C(12)-C(13)-N(4)	1.9(7)
C(11)-C(12)-C(13)-C(14)	-177.6(4)
N(4)-C(13)-C(14)-C(15)	-.3(4)
C(12)-C(13)-C(14)-C(15)	179.2(4)

N(4)-C(13)-C(14)-C(29)	179.8(3)
C(12)-C(13)-C(14)-C(29)	-.6(6)
C(13)-C(14)-C(15)-C(16)	.6(4)
C(29)-C(14)-C(15)-C(16)	-179.6(4)
C(13)-C(14)-C(15)-C(31)	178.9(4)
C(29)-C(14)-C(15)-C(31)	-1.2(7)
C(13)-N(4)-C(16)-C(17)	-178.7(3)
Fe(1)-N(4)-C(16)-C(17)	1.7(6)
C(13)-N(4)-C(16)-C(15)	.4(4)
Fe(1)-N(4)-C(16)-C(15)	-179.2(2)
C(14)-C(15)-C(16)-N(4)	-.6(5)
C(31)-C(15)-C(16)-N(4)	-179.1(4)
C(14)-C(15)-C(16)-C(17)	178.5(4)
C(31)-C(15)-C(16)-C(17)	.1(7)
N(4)-C(16)-C(17)-C(18)	1.3(6)
C(15)-C(16)-C(17)-C(18)	-177.7(4)
C(1)-N(1)-C(18)-C(17)	-178.3(4)
Fe(1)-N(1)-C(18)-C(17)	-1.1(6)
C(1)-N(1)-C(18)-C(19)	.6(4)
Fe(1)-N(1)-C(18)-C(19)	177.9(2)
C(16)-C(17)-C(18)-N(1)	-1.6(7)
C(16)-C(17)-C(18)-C(19)	179.6(4)
N(1)-C(18)-C(19)-C(20)	-.1(4)
C(17)-C(18)-C(19)-C(20)	178.8(4)
N(1)-C(18)-C(19)-C(33)	178.8(4)
C(17)-C(18)-C(19)-C(33)	-2.3(6)
C(18)-C(19)-C(20)-C(1)	-.4(4)
C(33)-C(19)-C(20)-C(1)	-179.3(4)
C(18)-C(19)-C(20)-C(35)	179.6(4)
C(33)-C(19)-C(20)-C(35)	.7(7)
N(1)-C(1)-C(20)-C(19)	.8(4)
C(2)-C(1)-C(20)-C(19)	-178.7(4)
N(1)-C(1)-C(20)-C(35)	-179.2(3)
C(2)-C(1)-C(20)-C(35)	1.3(6)
C(5)-C(4)-C(21)-C(22)	103.4(5)
C(3)-C(4)-C(21)-C(22)	-77.3(5)
C(4)-C(5)-C(23)-C(24)	-82.2(5)
C(6)-C(5)-C(23)-C(24)	95.6(5)
C(10)-C(9)-C(25)-C(26)	-76.8(6)
C(8)-C(9)-C(25)-C(26)	97.9(5)
C(9)-C(10)-C(27)-C(28)	99.2(5)
C(11)-C(10)-C(27)-C(28)	-78.3(5)
C(15)-C(14)-C(29)-C(30)	-102.3(5)
C(13)-C(14)-C(29)-C(30)	77.5(5)
C(14)-C(15)-C(31)-C(32)	74.7(6)
C(16)-C(15)-C(31)-C(32)	-107.2(5)
C(20)-C(19)-C(33)-C(34)	100.1(5)
C(18)-C(19)-C(33)-C(34)	-78.6(5)
C(19)-C(20)-C(35)-C(36)	-101.6(5)
C(1)-C(20)-C(35)-C(36)	78.4(5)
N(1)-Fe(1)-C(37)-O(1)	-70(5)
N(2)-Fe(1)-C(37)-O(1)	21(5)
N(4)-Fe(1)-C(37)-O(1)	-159(5)
N(3)-Fe(1)-C(37)-O(1)	110(5)
N(5)-Fe(1)-C(37)-O(1)	-6(7)
C(40)-N(5)-C(38)-N(6)	-.7(5)
Fe(1)-N(5)-C(38)-N(6)	178.4(2)
C(39)-N(6)-C(38)-N(5)	.7(5)

C(41)-N(6)-C(38)-N(5)	178.2(4)
C(38)-N(6)-C(39)-C(40)	-.3(5)
C(41)-N(6)-C(39)-C(40)	-177.8(4)
N(6)-C(39)-C(40)-N(5)	-.1(5)
C(38)-N(5)-C(40)-C(39)	.5(5)
Fe(1)-N(5)-C(40)-C(39)	-178.6(3)
C(51)-C(52)-C(53)-C(54)	-102(2)
C(52)-C(53)-C(54)-C(55)	-173(2)
C(53)-C(54)-C(55)-C(56)	47(2)

Table S7. Crystal data and structure refinement for Ru(OEP)(CO)(1-MeIm).

Empirical formula	C42 H52 Cl2 N6 O Ru
Formula weight	828.87
Temperature	198(2) K
Wavelength	.71073 A
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 10.4568(2) A alpha = 80.6950(10) deg
	b = 12.98060(10) A beta = 76.9820(10) deg
from 5798 reflns with 4<=theta<=28	c = 15.9683(2) A gamma = 72.0180(10) deg
	V = 1998.65(5) A^3 Z = 2
Density (calculated)	1.378 Mg/m^3
Absorption coefficient	1.133 mm^-1
Crystal size	0.10 x 0.12 x 0.12 mm
Crystal color	Red
Theta range for data collection	1.32 to 28.23 deg
Index ranges	-13<=h<=13, -16<=k<=9, -21<=l<=20
Collection method	\w scans
Reflections collected	13046 [R(int) = 0.0332]
Independent reflections	9023 [7172 obs, I >2sigma(I)]
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.6729 and 0.5694
Refinement (shift/err=0.002)	Full-matrix least-squares on F^2
Data / restraints / parameters	9019 / 6 / 564
Goodness-of-fit on F^2	1.142
Final R indices (obs data)	R1 = 0.0593, wR2 = 0.1216
R indices (all data)	R1 = 0.0837, wR2 = 0.1433
calc w=1/[\s^2^(Fo^2^)+(0.0366P)^2^+4.9543P] where P=(Fo^2^+2Fc^2^)/3	
Largest diff. peak and hole	.638 and -.801 e.A^-3

Crystal preparation and structure refinement summary for Ru(OEP)(CO)(1-MeIm).

Crystals were grown from methylene-chloride / methanol. The data crystal was mounted using oil (Paratone-N, Exxon) to a thin glass fiber with the (1 -2 1) scattering planes roughly normal to the spindle axis.

Systematic conditions suggested the ambiguous space group. The structure was solved by direct methods (Sheldrick, 1990). Two ethyl groups (C27-C28; C35-C36) exhibited disorder and thus, same atomic distance restraints (SADI) were placed on the disordered pairs. All H-atom positions have been calculated and refined isotropically. The space group choice was confirmed by successful convergence of the full-matrix least-squares refinement on F^2^ (Sheldrick, 1993). The highest peaks in the final difference Fourier map were in the vicinity of the Ru atom; the final map had no other significant features. A final analysis of variance between observed and calculated structure factors showed no dependence on amplitude or resolution.

Methyl H atom positions, R-CH-3~, were optimized by rotation about R-C bonds with idealized C-H, R--H and H--H distances. Remaining H atoms were included as fixed idealized contributors.

Sheldrick, G.M. (1990). SHELXS-86. Acta Cryst. A46, 467-473.

Sheldrick, G.M. (1993). SHELXL-93. Program for crystal structure refinement. Institute fur anorg chemie, G\"ottingen, Germany.

Siemens Industrial Automation, Incorporated. (1994). SAINT V4; SHELXTL V5; SMART V4. Madison, Wisconsin, USA.

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Ru(OEP)(CO)(1-MeIm). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	7598(1)	2287(1)	7399(1)	25(1)
N(1)	9225(3)	1249(3)	6684(2)	25(1)
N(2)	7735(3)	1146(3)	8458(2)	27(1)
N(3)	6070(3)	3372(3)	8147(2)	28(1)
N(4)	7567(3)	3474(3)	6371(2)	30(1)
N(5)	9106(4)	2885(3)	7782(2)	31(1)
N(6)	11093(4)	3076(4)	7901(3)	47(1)
O(1)	5650(4)	1376(3)	6858(2)	51(1)
C(1)	9809(4)	1451(3)	5835(2)	26(1)
C(2)	10915(4)	496(3)	5560(3)	27(1)
C(3)	10970(4)	-271(3)	6253(3)	26(1)
C(4)	9909(4)	203(3)	6961(3)	25(1)
C(5)	9628(4)	-303(3)	7785(3)	27(1)
C(6)	8627(4)	115(3)	8484(2)	27(1)
C(7)	8344(5)	-457(4)	9334(3)	36(1)
C(8)	7295(6)	236(4)	9811(3)	51(1)
C(9)	6908(5)	1249(3)	9259(3)	35(1)
C(10)	5886(5)	2189(4)	9500(3)	39(1)
C(11)	5498(4)	3172(3)	8998(3)	29(1)
C(12)	4441(4)	4147(3)	9287(3)	31(1)
C(13)	4415(4)	4922(3)	8605(3)	31(1)
C(14)	5438(4)	4439(3)	7888(3)	28(1)
C(15)	5769(4)	4958(3)	7068(3)	34(1)
C(16)	6739(5)	4529(3)	6370(3)	34(1)
C(17)	7033(5)	5109(4)	5516(3)	46(1)
C(18)	8010(5)	4379(4)	5013(3)	51(1)
C(19)	8367(5)	3359(4)	5564(3)	36(1)
C(20)	9394(4)	2425(3)	5323(3)	33(1)
C(21)	11834(4)	424(4)	4688(3)	34(1)
C(22)	13065(6)	819(7)	4629(4)	67(2)
C(23)	11942(4)	-1401(3)	6306(3)	33(1)
C(24)	13173(5)	-1484(4)	6685(4)	53(1)
C(25)	9144(5)	-1597(3)	9619(3)	40(1)
C(26)	10483(6)	-1650(4)	9867(3)	51(1)
C(27A)	6359(12)	-93(9)	10661(6)	33(3)
C(28A)	6955(14)	52(11)	11401(7)	56(4)
C(27B)	6900(11)	141(9)	10810(7)	37(3)
C(28B)	5625(12)	-249(9)	11022(8)	53(4)
C(29)	3570(5)	4240(4)	10172(3)	38(1)
C(30)	2323(7)	3870(7)	10281(4)	77(2)
C(31)	3505(5)	6077(3)	8568(3)	37(1)
C(32)	2206(6)	6213(5)	8236(4)	59(2)
C(33)	6371(6)	6299(4)	5266(4)	61(2)
C(34)	5037(7)	6506(5)	4974(5)	75(2)
C(35A)	8567(7)	4521(5)	4036(4)	39(2)
C(36A)	9889(9)	4834(7)	3908(4)	58(3)
C(35B)	8972(20)	4773(16)	4242(12)	28(5)
C(36B)	8338(24)	4576(20)	3514(13)	48(7)

C(37)	6381(4)	1752(3)	7068(3)	30(1)
C(38)	10466(5)	2510(4)	7576(3)	44(1)
C(39)	10074(6)	3872(5)	8333(3)	51(1)
C(40)	8883(5)	3744(4)	8241(3)	42(1)
C(41)	12581(6)	2893(5)	7782(5)	64(2)
C(200)	2672(6)	1683(5)	2278(4)	60(2)
Cl(1)	1138(2)	2649(1)	2657(1)	69(1)
Cl(2)	4093(2)	2118(2)	2214(1)	79(1)

Table S9. Anisotropic displacement parameters (A^2 x 10^3) for Ru(OEP)(CO)(1-MeIm). The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ru(1)	27(1)	21(1)	20(1)	2(1)	-3(1)	-1(1)
N(1)	27(2)	24(2)	21(2)	3(1)	-7(1)	-3(1)
N(2)	32(2)	22(2)	21(2)	2(1)	-3(1)	-1(1)
N(3)	28(2)	22(2)	25(2)	-3(1)	-1(1)	3(1)
N(4)	30(2)	26(2)	25(2)	4(1)	-3(1)	-1(1)
N(5)	36(2)	27(2)	27(2)	0(1)	-7(2)	-5(2)
N(6)	43(2)	44(2)	56(3)	2(2)	-15(2)	-14(2)
O(1)	47(2)	64(2)	48(2)	-12(2)	-9(2)	-21(2)
C(1)	26(2)	26(2)	22(2)	1(2)	-2(2)	-4(2)
C(2)	23(2)	30(2)	24(2)	-3(2)	-2(2)	-5(2)
C(3)	26(2)	26(2)	25(2)	-3(2)	-7(2)	-5(2)
C(4)	28(2)	21(2)	25(2)	-3(2)	-6(2)	-4(2)
C(5)	32(2)	18(2)	27(2)	3(2)	-9(2)	-2(2)
C(6)	37(2)	20(2)	20(2)	3(2)	-6(2)	-5(2)
C(7)	47(3)	28(2)	21(2)	6(2)	-6(2)	0(2)
C(8)	69(4)	33(3)	23(2)	10(2)	9(2)	4(2)
C(9)	50(3)	25(2)	18(2)	3(2)	0(2)	1(2)
C(10)	48(3)	35(2)	18(2)	0(2)	3(2)	1(2)
C(11)	33(2)	24(2)	23(2)	-4(2)	-2(2)	0(2)
C(12)	36(2)	27(2)	26(2)	-7(2)	-6(2)	-3(2)
C(13)	28(2)	28(2)	33(2)	-8(2)	-5(2)	-1(2)
C(14)	29(2)	22(2)	30(2)	-3(2)	-7(2)	1(2)
C(15)	34(2)	25(2)	33(2)	5(2)	-7(2)	1(2)
C(16)	37(2)	25(2)	30(2)	7(2)	-2(2)	-1(2)
C(17)	44(3)	32(2)	42(3)	17(2)	0(2)	2(2)
C(18)	51(3)	37(3)	38(3)	15(2)	3(2)	8(2)
C(19)	37(2)	31(2)	25(2)	12(2)	0(2)	-1(2)
C(20)	34(2)	33(2)	23(2)	6(2)	0(2)	-3(2)
C(21)	30(2)	40(3)	26(2)	-2(2)	-2(2)	-5(2)
C(22)	53(4)	109(6)	48(3)	-5(4)	4(3)	-46(4)
C(23)	35(2)	29(2)	29(2)	-3(2)	-2(2)	-1(2)
C(24)	44(3)	41(3)	68(4)	6(3)	-22(3)	2(2)
C(25)	55(3)	26(2)	26(2)	7(2)	-2(2)	-2(2)
C(26)	63(3)	38(3)	44(3)	5(2)	-18(3)	-1(3)
C(27A)	41(7)	35(6)	20(5)	6(4)	-3(5)	-11(5)
C(28A)	77(9)	75(9)	25(7)	6(6)	-8(6)	-42(8)
C(27B)	40(6)	32(5)	35(8)	4(4)	-8(5)	-5(4)
C(28B)	52(7)	49(7)	50(7)	13(5)	-7(6)	-14(6)
C(29)	45(3)	35(2)	27(2)	-10(2)	-2(2)	0(2)
C(30)	82(5)	127(7)	37(3)	-15(4)	15(3)	-67(5)
C(31)	40(3)	22(2)	38(3)	-6(2)	-4(2)	3(2)
C(32)	47(3)	40(3)	81(5)	-1(3)	-22(3)	4(3)
C(33)	66(4)	38(3)	46(3)	20(3)	4(3)	9(3)
C(34)	75(5)	53(4)	71(5)	12(4)	-20(4)	11(3)
C(35A)	50(4)	32(3)	28(3)	8(3)	-4(3)	-8(3)
C(36A)	79(6)	67(5)	33(4)	2(3)	-1(4)	-36(5)
C(37)	33(2)	31(2)	20(2)	0(2)	-4(2)	-3(2)
C(38)	42(3)	33(2)	56(3)	-6(2)	-9(2)	-7(2)

C(39)	58(3)	50(3)	47(3)	-12(2)	-9(3)	-19(3)
C(40)	44(3)	47(3)	35(3)	-12(2)	-1(2)	-12(2)
C(41)	38(3)	61(4)	93(5)	6(4)	-23(3)	-13(3)
C(200)	49(3)	70(4)	59(4)	-8(3)	-12(3)	-12(3)
Cl(1)	53(1)	76(1)	68(1)	-15(1)	5(1)	-11(1)
Cl(2)	56(1)	114(2)	75(1)	-10(1)	-10(1)	-38(1)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Ru(OEP)(CO)(1-MeIm). Treatment of hydrogen atoms not specifically described in the refinement summary was "noref."

	x	y	z	U(eq)
H(5)	10174(4)	-1011(3)	7886(3)	42(14)
H(10)	5406(5)	2155(4)	10065(3)	40(13)
H(15)	5276(4)	5684(3)	6977(3)	35(12)
H(20)	9858(4)	2454(3)	4754(3)	50(15)
H(21A)	11311(4)	852(4)	4256(3)	74(19)
H(21B)	12142(4)	-327(4)	4556(3)	56(16)
H(22A)	13633(21)	719(30)	4068(10)	70(19)
H(22B)	13576(23)	412(23)	5063(17)	90(24)
H(22C)	12771(6)	1577(10)	4716(25)	84(24)
H(23A)	12255(4)	-1638(3)	5731(3)	52(15)
H(23B)	11451(4)	-1893(3)	6656(3)	31(12)
H(24A)	13744(18)	-2222(7)	6703(20)	49(15)
H(24B)	12875(5)	-1265(26)	7261(9)	101(27)
H(24C)	13682(20)	-1016(21)	6334(13)	47(15)
H(25A)	9338(5)	-2051(3)	9153(3)	28(11)
H(25B)	8583(5)	-1893(3)	10109(3)	48(14)
H(26A)	10930(16)	-2389(5)	10054(19)	52(15)
H(26B)	10301(6)	-1203(19)	10328(13)	44(14)
H(26C)	11063(13)	-1391(23)	9377(6)	49(15)
H(27A)	5426(12)	370(9)	10692(6)	31(25)
H(27B)	6358(12)	-843(9)	10681(6)	77(43)
H(28A)	6429(51)	-161(63)	11940(7)	106(54)
H(28B)	6927(74)	801(15)	11381(30)	83(47)
H(28C)	7886(29)	-394(48)	11351(29)	53(35)
H(27C)	7632(11)	-378(9)	11066(7)	70(43)
H(27D)	6711(11)	841(9)	11024(7)	33(25)
H(28D)	5316(38)	-314(49)	11636(8)	78(41)
H(28E)	5834(20)	-945(25)	10810(36)	37(27)
H(28F)	4919(24)	265(27)	10752(34)	48(30)
H(29A)	4116(5)	3812(4)	10592(3)	54(16)
H(29B)	3292(5)	4993(4)	10295(3)	52(15)
H(30A)	1749(19)	4316(20)	9890(17)	49(16)
H(30B)	1831(22)	3930(30)	10864(8)	63(17)
H(30C)	2587(7)	3125(11)	10158(24)	129(36)
H(31A)	4014(5)	6542(3)	8197(3)	55(16)
H(31B)	3258(5)	6316(3)	9143(3)	75(20)
H(32A)	1688(19)	6966(6)	8209(22)	68(18)
H(32B)	1669(18)	5788(24)	8619(13)	69(20)
H(32C)	2441(6)	5971(28)	7669(10)	71(20)
H(33A)	6213(6)	6703(4)	5758(4)	47(15)
H(33B)	6998(6)	6573(4)	4805(4)	52(15)
H(34A)	4682(24)	7270(7)	4811(28)	101(25)
H(34B)	4394(16)	6271(34)	5436(11)	87(24)
H(34C)	5183(11)	6109(30)	4486(19)	113(31)
H(35A)	8740(7)	3846(5)	3786(4)	23(14)
H(35B)	7904(7)	5084(5)	3753(4)	30(16)
H(36A)	10535(19)	4274(19)	4194(26)	59(23)

H(36B)	9705(12)	5508(20)	4148(28)	67(25)
H(36C)	10260(27)	4916(39)	3302(5)	91(30)
H(38)	10924(5)	1929(4)	7248(3)	61(17)
H(39)	10184(6)	4392(5)	8628(3)	93(24)
H(40)	8022(5)	4184(4)	8461(3)	54(16)
H(41A)	12854(11)	2718(49)	8335(6)	180(46)
H(41B)	12812(9)	3539(17)	7499(36)	112(28)
H(41C)	13046(6)	2300(33)	7434(33)	174(46)
H(20A)	2748(6)	1014(5)	2660(4)	132(33)
H(20B)	2648(6)	1523(5)	1709(4)	72(20)

Table S11. Bond lengths [A] and angles [deg] for Ru(OEP)(CO)(1-MeIm).

Ru(1)-C(37)	1.829(5)
Ru(1)-N(1)	2.054(3)
Ru(1)-N(4)	2.060(3)
Ru(1)-N(2)	2.060(3)
Ru(1)-N(3)	2.063(3)
Ru(1)-N(5)	2.192(4)
N(1)-C(1)	1.375(5)
N(1)-C(4)	1.378(5)
N(2)-C(9)	1.373(5)
N(2)-C(6)	1.375(5)
N(3)-C(11)	1.374(5)
N(3)-C(14)	1.378(5)
N(4)-C(19)	1.371(5)
N(4)-C(16)	1.376(5)
N(5)-C(38)	1.334(6)
N(5)-C(40)	1.363(6)
N(6)-C(38)	1.347(6)
N(6)-C(39)	1.377(7)
N(6)-C(41)	1.472(7)
O(1)-C(37)	1.156(5)
C(1)-C(20)	1.394(5)
C(1)-C(2)	1.459(5)
C(2)-C(3)	1.362(5)
C(2)-C(21)	1.501(5)
C(3)-C(4)	1.458(5)
C(3)-C(23)	1.507(5)
C(4)-C(5)	1.384(5)
C(5)-C(6)	1.399(6)
C(6)-C(7)	1.452(5)
C(7)-C(8)	1.352(6)
C(7)-C(25)	1.512(6)
C(8)-C(9)	1.459(6)
C(8)-C(27B)	1.550(11)
C(8)-C(27A)	1.567(11)
C(9)-C(10)	1.393(6)
C(10)-C(11)	1.390(6)
C(11)-C(12)	1.461(5)
C(12)-C(13)	1.357(6)
C(12)-C(29)	1.500(6)
C(13)-C(14)	1.454(6)
C(13)-C(31)	1.507(6)
C(14)-C(15)	1.393(6)
C(15)-C(16)	1.387(6)
C(16)-C(17)	1.465(6)
C(17)-C(18)	1.365(7)
C(17)-C(33)	1.513(6)
C(18)-C(19)	1.461(6)
C(18)-C(35B)	1.53(2)
C(18)-C(35A)	1.541(7)
C(19)-C(20)	1.390(6)
C(21)-C(22)	1.505(7)
C(23)-C(24)	1.510(7)
C(25)-C(26)	1.518(7)
C(27A)-C(28A)	1.515(13)

C(27B)-C(28B)	1.518(14)
C(29)-C(30)	1.489(7)
C(31)-C(32)	1.517(7)
C(33)-C(34)	1.502(9)
C(35A)-C(36A)	1.519(10)
C(35B)-C(36B)	1.55(2)
C(39)-C(40)	1.348(7)
C(200)-Cl(2)	1.723(6)
C(200)-Cl(1)	1.755(6)

C(37)-Ru(1)-N(1)	91.4(2)
C(37)-Ru(1)-N(4)	93.5(2)
N(1)-Ru(1)-N(4)	89.75(13)
C(37)-Ru(1)-N(2)	90.9(2)
N(1)-Ru(1)-N(2)	90.17(12)
N(4)-Ru(1)-N(2)	175.6(2)
C(37)-Ru(1)-N(3)	92.9(2)
N(1)-Ru(1)-N(3)	175.66(14)
N(4)-Ru(1)-N(3)	90.11(13)
N(2)-Ru(1)-N(3)	89.64(13)
C(37)-Ru(1)-N(5)	178.3(2)
N(1)-Ru(1)-N(5)	86.94(13)
N(4)-Ru(1)-N(5)	86.95(13)
N(2)-Ru(1)-N(5)	88.60(13)
N(3)-Ru(1)-N(5)	88.72(14)
C(1)-N(1)-C(4)	107.1(3)
C(1)-N(1)-Ru(1)	126.7(3)
C(4)-N(1)-Ru(1)	126.2(3)
C(9)-N(2)-C(6)	107.0(3)
C(9)-N(2)-Ru(1)	126.5(3)
C(6)-N(2)-Ru(1)	126.4(3)
C(11)-N(3)-C(14)	107.0(3)
C(11)-N(3)-Ru(1)	126.6(3)
C(14)-N(3)-Ru(1)	126.4(3)
C(19)-N(4)-C(16)	107.5(3)
C(19)-N(4)-Ru(1)	126.4(3)
C(16)-N(4)-Ru(1)	126.1(3)
C(38)-N(5)-C(40)	104.5(4)
C(38)-N(5)-Ru(1)	126.9(3)
C(40)-N(5)-Ru(1)	128.5(3)
C(38)-N(6)-C(39)	106.6(4)
C(38)-N(6)-C(41)	125.9(5)
C(39)-N(6)-C(41)	127.4(5)
N(1)-C(1)-C(20)	124.5(4)
N(1)-C(1)-C(2)	109.7(3)
C(20)-C(1)-C(2)	125.8(4)
C(3)-C(2)-C(1)	106.6(3)
C(3)-C(2)-C(21)	128.0(4)
C(1)-C(2)-C(21)	125.3(4)
C(2)-C(3)-C(4)	107.4(3)
C(2)-C(3)-C(23)	127.6(4)
C(4)-C(3)-C(23)	125.0(4)
N(1)-C(4)-C(5)	124.8(4)
N(1)-C(4)-C(3)	109.2(3)
C(5)-C(4)-C(3)	126.0(4)
C(4)-C(5)-C(6)	128.2(4)
N(2)-C(6)-C(5)	124.2(3)
N(2)-C(6)-C(7)	109.5(3)

C(5)-C(6)-C(7)	126.3(4)
C(8)-C(7)-C(6)	107.1(4)
C(8)-C(7)-C(25)	127.8(4)
C(6)-C(7)-C(25)	124.9(4)
C(7)-C(8)-C(9)	107.1(4)
C(7)-C(8)-C(27B)	126.1(5)
C(9)-C(8)-C(27B)	123.9(5)
C(7)-C(8)-C(27A)	125.8(5)
C(9)-C(8)-C(27A)	124.2(5)
N(2)-C(9)-C(10)	124.7(4)
N(2)-C(9)-C(8)	109.2(4)
C(10)-C(9)-C(8)	126.1(4)
C(11)-C(10)-C(9)	127.8(4)
N(3)-C(11)-C(10)	124.6(4)
N(3)-C(11)-C(12)	109.6(3)
C(10)-C(11)-C(12)	125.8(4)
C(13)-C(12)-C(11)	106.6(4)
C(13)-C(12)-C(29)	128.1(4)
C(11)-C(12)-C(29)	125.3(4)
C(12)-C(13)-C(14)	107.5(4)
C(12)-C(13)-C(31)	127.7(4)
C(14)-C(13)-C(31)	124.8(4)
N(3)-C(14)-C(15)	124.2(4)
N(3)-C(14)-C(13)	109.2(3)
C(15)-C(14)-C(13)	126.5(4)
C(16)-C(15)-C(14)	128.3(4)
N(4)-C(16)-C(15)	124.9(4)
N(4)-C(16)-C(17)	109.1(4)
C(15)-C(16)-C(17)	126.0(4)
C(18)-C(17)-C(16)	107.0(4)
C(18)-C(17)-C(33)	127.9(4)
C(16)-C(17)-C(33)	125.1(4)
C(17)-C(18)-C(19)	106.8(4)
C(17)-C(18)-C(35B)	120.3(9)
C(19)-C(18)-C(35B)	125.7(8)
C(17)-C(18)-C(35A)	128.6(4)
C(19)-C(18)-C(35A)	124.4(5)
N(4)-C(19)-C(20)	124.9(4)
N(4)-C(19)-C(18)	109.6(4)
C(20)-C(19)-C(18)	125.5(4)
C(19)-C(20)-C(1)	127.6(4)
C(2)-C(21)-C(22)	113.5(4)
C(3)-C(23)-C(24)	113.8(4)
C(7)-C(25)-C(26)	113.5(4)
C(28A)-C(27A)-C(8)	106.3(9)
C(28B)-C(27B)-C(8)	105.3(9)
C(30)-C(29)-C(12)	113.9(4)
C(13)-C(31)-C(32)	113.5(4)
C(34)-C(33)-C(17)	113.6(5)
C(36A)-C(35A)-C(18)	108.1(6)
C(18)-C(35B)-C(36B)	97.9(13)
O(1)-C(37)-Ru(1)	177.3(4)
N(5)-C(38)-N(6)	111.7(5)
C(40)-C(39)-N(6)	105.9(5)
C(39)-C(40)-N(5)	111.2(5)
Cl(2)-C(200)-Cl(1)	112.7(4)

Table S12. Torsion angles [deg] for Ru(OEP)(CO)(1-MeIm).

C(37)-Ru(1)-N(1)-C(1)	89.9(4)
N(4)-Ru(1)-N(1)-C(1)	-3.7(3)
N(2)-Ru(1)-N(1)-C(1)	-179.2(3)
N(3)-Ru(1)-N(1)-C(1)	-92(2)
N(5)-Ru(1)-N(1)-C(1)	-90.6(3)
C(37)-Ru(1)-N(1)-C(4)	-88.0(3)
N(4)-Ru(1)-N(1)-C(4)	178.4(3)
N(2)-Ru(1)-N(1)-C(4)	2.9(3)
N(3)-Ru(1)-N(1)-C(4)	90(2)
N(5)-Ru(1)-N(1)-C(4)	91.5(3)
C(37)-Ru(1)-N(2)-C(9)	-88.0(4)
N(1)-Ru(1)-N(2)-C(9)	-179.5(4)
N(4)-Ru(1)-N(2)-C(9)	92(2)
N(3)-Ru(1)-N(2)-C(9)	4.9(4)
N(5)-Ru(1)-N(2)-C(9)	93.6(4)
C(37)-Ru(1)-N(2)-C(6)	88.5(4)
N(1)-Ru(1)-N(2)-C(6)	-3.0(4)
N(4)-Ru(1)-N(2)-C(6)	-92(2)
N(3)-Ru(1)-N(2)-C(6)	-178.6(4)
N(5)-Ru(1)-N(2)-C(6)	-89.9(4)
C(37)-Ru(1)-N(3)-C(11)	87.7(4)
N(1)-Ru(1)-N(3)-C(11)	-91(2)
N(4)-Ru(1)-N(3)-C(11)	-178.8(4)
N(2)-Ru(1)-N(3)-C(11)	-3.2(4)
N(5)-Ru(1)-N(3)-C(11)	-91.8(4)
C(37)-Ru(1)-N(3)-C(14)	-92.9(4)
N(1)-Ru(1)-N(3)-C(14)	89(2)
N(4)-Ru(1)-N(3)-C(14)	.6(4)
N(2)-Ru(1)-N(3)-C(14)	176.2(4)
N(5)-Ru(1)-N(3)-C(14)	87.5(4)
C(37)-Ru(1)-N(4)-C(19)	-86.7(4)
N(1)-Ru(1)-N(4)-C(19)	4.8(4)
N(2)-Ru(1)-N(4)-C(19)	94(2)
N(3)-Ru(1)-N(4)-C(19)	-179.6(4)
N(5)-Ru(1)-N(4)-C(19)	91.7(4)
C(37)-Ru(1)-N(4)-C(16)	93.5(4)
N(1)-Ru(1)-N(4)-C(16)	-175.1(4)
N(2)-Ru(1)-N(4)-C(16)	-86(2)
N(3)-Ru(1)-N(4)-C(16)	.5(4)
N(5)-Ru(1)-N(4)-C(16)	-88.2(4)
C(37)-Ru(1)-N(5)-C(38)	13(5)
N(1)-Ru(1)-N(5)-C(38)	-3.7(4)
N(4)-Ru(1)-N(5)-C(38)	-93.6(4)
N(2)-Ru(1)-N(5)-C(38)	86.6(4)
N(3)-Ru(1)-N(5)-C(38)	176.2(4)
C(37)-Ru(1)-N(5)-C(40)	-171(5)
N(1)-Ru(1)-N(5)-C(40)	172.7(4)
N(4)-Ru(1)-N(5)-C(40)	82.8(4)
N(2)-Ru(1)-N(5)-C(40)	-97.0(4)
N(3)-Ru(1)-N(5)-C(40)	-7.4(4)
C(4)-N(1)-C(1)-C(20)	179.7(4)
Ru(1)-N(1)-C(1)-C(20)	1.5(6)
C(4)-N(1)-C(1)-C(2)	-.2(5)
Ru(1)-N(1)-C(1)-C(2)	-178.4(3)

N(1)-C(1)-C(2)-C(3)	.3(5)
C(20)-C(1)-C(2)-C(3)	-179.6(4)
N(1)-C(1)-C(2)-C(21)	-177.0(4)
C(20)-C(1)-C(2)-C(21)	3.1(7)
C(1)-C(2)-C(3)-C(4)	-.3(5)
C(21)-C(2)-C(3)-C(4)	176.9(4)
C(1)-C(2)-C(3)-C(23)	-179.6(4)
C(21)-C(2)-C(3)-C(23)	-2.3(7)
C(1)-N(1)-C(4)-C(5)	179.6(4)
Ru(1)-N(1)-C(4)-C(5)	-2.2(6)
C(1)-N(1)-C(4)-C(3)	.0(4)
Ru(1)-N(1)-C(4)-C(3)	178.2(3)
C(2)-C(3)-C(4)-N(1)	.2(5)
C(23)-C(3)-C(4)-N(1)	179.5(4)
C(2)-C(3)-C(4)-C(5)	-179.4(4)
C(23)-C(3)-C(4)-C(5)	-.1(7)
N(1)-C(4)-C(5)-C(6)	.4(7)
C(3)-C(4)-C(5)-C(6)	179.9(4)
C(9)-N(2)-C(6)-C(5)	179.4(4)
Ru(1)-N(2)-C(6)-C(5)	2.4(6)
C(9)-N(2)-C(6)-C(7)	.5(5)
Ru(1)-N(2)-C(6)-C(7)	-176.5(3)
C(4)-C(5)-C(6)-N(2)	-.5(7)
C(4)-C(5)-C(6)-C(7)	178.2(4)
N(2)-C(6)-C(7)-C(8)	-.5(6)
C(5)-C(6)-C(7)-C(8)	-179.4(5)
N(2)-C(6)-C(7)-C(25)	-177.8(4)
C(5)-C(6)-C(7)-C(25)	3.3(8)
C(6)-C(7)-C(8)-C(9)	.3(6)
C(25)-C(7)-C(8)-C(9)	177.5(5)
C(6)-C(7)-C(8)-C(27B)	-160.9(7)
C(25)-C(7)-C(8)-C(27B)	16.2(11)
C(6)-C(7)-C(8)-C(27A)	161.6(7)
C(25)-C(7)-C(8)-C(27A)	-21.3(11)
C(6)-N(2)-C(9)-C(10)	178.4(5)
Ru(1)-N(2)-C(9)-C(10)	-4.6(7)
C(6)-N(2)-C(9)-C(8)	-.3(5)
Ru(1)-N(2)-C(9)-C(8)	176.7(3)
C(7)-C(8)-C(9)-N(2)	.0(6)
C(27B)-C(8)-C(9)-N(2)	161.8(7)
C(27A)-C(8)-C(9)-N(2)	-161.6(7)
C(7)-C(8)-C(9)-C(10)	-178.7(5)
C(27B)-C(8)-C(9)-C(10)	-16.9(10)
C(27A)-C(8)-C(9)-C(10)	19.7(10)
N(2)-C(9)-C(10)-C(11)	.8(9)
C(8)-C(9)-C(10)-C(11)	179.3(5)
C(14)-N(3)-C(11)-C(10)	-178.4(4)
Ru(1)-N(3)-C(11)-C(10)	1.1(7)
C(14)-N(3)-C(11)-C(12)	1.1(5)
Ru(1)-N(3)-C(11)-C(12)	-179.5(3)
C(9)-C(10)-C(11)-N(3)	1.1(8)
C(9)-C(10)-C(11)-C(12)	-178.3(5)
N(3)-C(11)-C(12)-C(13)	-1.0(5)
C(10)-C(11)-C(12)-C(13)	178.5(5)
N(3)-C(11)-C(12)-C(29)	178.8(4)
C(10)-C(11)-C(12)-C(29)	-1.7(8)
C(11)-C(12)-C(13)-C(14)	.4(5)
C(29)-C(12)-C(13)-C(14)	-179.3(4)
C(11)-C(12)-C(13)-C(31)	-179.9(4)

C(29)-C(12)-C(13)-C(31)	.4(8)
C(11)-N(3)-C(14)-C(15)	178.1(4)
Ru(1)-N(3)-C(14)-C(15)	-1.4(6)
C(11)-N(3)-C(14)-C(13)	-.8(5)
Ru(1)-N(3)-C(14)-C(13)	179.7(3)
C(12)-C(13)-C(14)-N(3)	.2(5)
C(31)-C(13)-C(14)-N(3)	-179.5(4)
C(12)-C(13)-C(14)-C(15)	-178.7(4)
C(31)-C(13)-C(14)-C(15)	1.6(7)
N(3)-C(14)-C(15)-C(16)	1.0(8)
C(13)-C(14)-C(15)-C(16)	179.7(5)
C(19)-N(4)-C(16)-C(15)	179.1(5)
Ru(1)-N(4)-C(16)-C(15)	-1.1(7)
C(19)-N(4)-C(16)-C(17)	.1(5)
Ru(1)-N(4)-C(16)-C(17)	180.0(3)
C(14)-C(15)-C(16)-N(4)	.3(8)
C(14)-C(15)-C(16)-C(17)	179.2(5)
N(4)-C(16)-C(17)-C(18)	1.6(6)
C(15)-C(16)-C(17)-C(18)	-177.4(5)
N(4)-C(16)-C(17)-C(33)	-177.7(5)
C(15)-C(16)-C(17)-C(33)	3.4(9)
C(16)-C(17)-C(18)-C(19)	-2.4(6)
C(33)-C(17)-C(18)-C(19)	176.8(6)
C(16)-C(17)-C(18)-C(35B)	-154.3(9)
C(33)-C(17)-C(18)-C(35B)	24.9(12)
C(16)-C(17)-C(18)-C(35A)	172.2(6)
C(33)-C(17)-C(18)-C(35A)	-8.6(11)
C(16)-N(4)-C(19)-C(20)	176.1(5)
Ru(1)-N(4)-C(19)-C(20)	-3.8(7)
C(16)-N(4)-C(19)-C(18)	-1.6(6)
Ru(1)-N(4)-C(19)-C(18)	178.5(3)
C(17)-C(18)-C(19)-N(4)	2.6(6)
C(35B)-C(18)-C(19)-N(4)	152.5(10)
C(35A)-C(18)-C(19)-N(4)	-172.3(5)
C(17)-C(18)-C(19)-C(20)	-175.1(5)
C(35B)-C(18)-C(19)-C(20)	-25.2(13)
C(35A)-C(18)-C(19)-C(20)	10.0(9)
N(4)-C(19)-C(20)-C(1)	-.3(8)
C(18)-C(19)-C(20)-C(1)	177.1(5)
N(1)-C(1)-C(20)-C(19)	1.5(8)
C(2)-C(1)-C(20)-C(19)	-178.7(5)
C(3)-C(2)-C(21)-C(22)	-89.9(6)
C(1)-C(2)-C(21)-C(22)	86.8(6)
C(2)-C(3)-C(23)-C(24)	96.1(5)
C(4)-C(3)-C(23)-C(24)	-83.0(5)
C(8)-C(7)-C(25)-C(26)	-97.3(7)
C(6)-C(7)-C(25)-C(26)	79.4(6)
C(7)-C(8)-C(27A)-C(28A)	96.1(10)
C(9)-C(8)-C(27A)-C(28A)	-105.7(9)
C(27B)-C(8)-C(27A)-C(28A)	-5.9(10)
C(7)-C(8)-C(27B)-C(28B)	-105.2(9)
C(9)-C(8)-C(27B)-C(28B)	96.4(9)
C(27A)-C(8)-C(27B)-C(28B)	-4.7(9)
C(13)-C(12)-C(29)-C(30)	94.0(7)
C(11)-C(12)-C(29)-C(30)	-85.7(6)
C(12)-C(13)-C(31)-C(32)	-93.4(6)
C(14)-C(13)-C(31)-C(32)	86.2(6)
C(18)-C(17)-C(33)-C(34)	94.9(8)

C(16)-C(17)-C(33)-C(34)	-86.0(7)
C(17)-C(18)-C(35A)-C(36A)	97.2(8)
C(19)-C(18)-C(35A)-C(36A)	-89.1(7)
C(35B)-C(18)-C(35A)-C(36A)	14(2)
C(17)-C(18)-C(35B)-C(36B)	-107.0(14)
C(19)-C(18)-C(35B)-C(36B)	106.8(14)
C(35A)-C(18)-C(35B)-C(36B)	8.9(12)
N(1)-Ru(1)-C(37)-O(1)	31(8)
N(4)-Ru(1)-C(37)-O(1)	121(8)
N(2)-Ru(1)-C(37)-O(1)	-59(8)
N(3)-Ru(1)-C(37)-O(1)	-149(8)
N(5)-Ru(1)-C(37)-O(1)	15(12)
C(40)-N(5)-C(38)-N(6)	1.5(5)
Ru(1)-N(5)-C(38)-N(6)	178.6(3)
C(39)-N(6)-C(38)-N(5)	-.8(6)
C(41)-N(6)-C(38)-N(5)	-178.7(5)
C(38)-N(6)-C(39)-C(40)	-.2(6)
C(41)-N(6)-C(39)-C(40)	177.6(5)
N(6)-C(39)-C(40)-N(5)	1.2(6)
C(38)-N(5)-C(40)-C(39)	-1.7(5)
Ru(1)-N(5)-C(40)-C(39)	-178.7(3)

Table S13. Crystal data and structure refinement for Os(OEP)(CO)(1-MeIM).

Empirical formula	C42 H52 Cl2 N6 O Os
Formula weight	918.00
Temperature	198(2) K
Wavelength	.71073 A
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 10.3677(3) A alpha = 80.6350(10) deg
	b = 12.9871(4) A beta = 76.7310(10) deg
from 3856 reflns with 4<=theta<=28	c = 15.9564(5) A gamma = 72.2190(10) deg
	V = 1981.25(10) A^3 Z = 2
Density (calculated)	1.539 Mg/m^3
Absorption coefficient	3.394 mm^-1
Crystal size	0.11 x 0.09 x 0.01 mm
Crystal Color	Dark red
Theta range for data collection	1.32 to 25.02 deg
Index ranges	-12<=h<=11, -9<=k<=15, -18<=l<=17
Collection method	\w scans
Reflections collected	10705 [R(int) = 0.0733]
Independent reflections	6916 [5297 obs, I >2sigma(I)]
Absorption correction	integration
Max. and min. transmission	0.9595 and 0.6561
Refinement (shift/err=0.001)	Full-matrix least-squares on F^2
Data / restraints / parameters	6914 / 2 / 488
Goodness-of-fit on F^2	1.147
Final R indices (obs data)	R1 = 0.0653, wR2 = 0.1228
R indices (all data)	R1 = 0.1000, wR2 = 0.1449
calc w=1/[\s^2^(Fo^2^)+(0.0249P)^2^+17.0365P] where P=(Fo^2^+2Fc^2^)/3	
Largest diff. peak and hole	1.316 and -1.525 e.A^-3

Crystal preparation and structure refinement summary for Os(OEP)(CO)(1-MeIM).

Crystals were grown from methylene-chloride / methanol.
The data crystal was mounted using oil (Paratone-N, Exxon) to a thin glass fiber with the (1 1 0) scattering planes roughly normal to the spindle axis.

Systematic conditions suggested the ambiguous space group. The structure was solved by direct methods (Sheldrick, 1990). One ethyl group (C35-C36) exhibited a disorder. Delta-U (delu) restraints have been applied to the C35-C36 disordered pair. All the positions of the H-atoms have been calculated and refined isotropically. The space group choice was confirmed by successful convergence of the full-matrix least-squares refinement on F^2^ (Sheldrick, 1993). The highest peaks in the final difference Fourier map were in the vicinity of the Os atom; the final map had no other significant features. A final analysis of variance between observed and calculated structure factors showed no dependence on amplitude or resolution.

Methyl H atom positions, R-CH~3~, were optimized by rotation about R-C bonds with idealized C-H, R--H and H--H distances. Remaining H atoms were included as fixed idealized contributors. H atom U's were assigned as 1.2 times Ueq of adjacent non-H atoms.

Sheldrick, G.M. (1990). SHELXS-86. Acta Cryst. A46, 467-473.

Sheldrick, G.M. (1993). SHELXL-93. Program for crystal structure refinement. Institute fur anorg chemie, G\"ottingen, Germany.

Siemens Industrial Automation, Incorporated. (1994). SAINT V4; SHELXTL V5; SMART V4. Madison, Wisconsin, USA.

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Os(OEP)(CO)(1-MeIM). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor

	x	y	z	U(eq)
Os(1)	7425(1)	7732(1)	7614(1)	27(1)
O(1)	9386(9)	8657(7)	8148(5)	48(2)
N(1)	8938(8)	6630(6)	6866(5)	27(2)
N(2)	7420(8)	6550(7)	8643(5)	31(2)
N(3)	5771(8)	8766(6)	8327(5)	25(2)
N(4)	7268(9)	8864(6)	6548(5)	27(2)
N(5)	5907(9)	7140(6)	7242(5)	28(2)
N(6)	3909(10)	6946(7)	7119(6)	42(2)
C(1)	9532(10)	6838(8)	6006(6)	29(2)
C(2)	10557(11)	5857(8)	5719(7)	31(3)
C(3)	10595(11)	5080(8)	6409(7)	30(3)
C(4)	9586(10)	5567(8)	7122(7)	31(3)
C(5)	9229(11)	5047(9)	7950(7)	35(3)
C(6)	8256(12)	5492(9)	8664(7)	39(3)
C(7)	7947(13)	4920(10)	9510(8)	51(4)
C(8)	6971(13)	5643(10)	10001(8)	52(4)
C(9)	6623(11)	6664(9)	9455(7)	36(3)
C(10)	5574(11)	7607(9)	9691(7)	38(3)
C(11)	5182(10)	8566(8)	9185(6)	27(2)
C(12)	4063(10)	9522(8)	9453(7)	28(2)
C(13)	4010(10)	10279(8)	8760(6)	25(2)
C(14)	5094(11)	9799(8)	8056(6)	27(2)
C(15)	5365(11)	10306(8)	7215(6)	31(3)
C(16)	6390(10)	9883(8)	6513(7)	27(2)
C(17)	6670(12)	10462(9)	5665(6)	37(3)
C(18)	7738(13)	9765(10)	5193(7)	47(3)
C(19)	8111(11)	8757(8)	5741(6)	32(3)
C(20)	9135(12)	7813(8)	5495(7)	38(3)
C(21)	11427(12)	5742(9)	4828(7)	38(3)
C(22)	12738(17)	6077(14)	4711(9)	80(5)
C(23)	11498(11)	3928(8)	6436(8)	39(3)
C(24)	12799(13)	3798(10)	6756(10)	62(4)
C(25)	8602(14)	3716(10)	9744(9)	67(5)
C(26)	9916(16)	3499(11)	10049(10)	78(5)
C(27)	6383(15)	5479(11)	10991(10)	80(6)
C(28)	5089(22)	5209(14)	11093(10)	102(7)
C(29)	3137(11)	9591(9)	10323(6)	32(3)
C(30)	1905(13)	9179(12)	10380(8)	61(4)
C(31)	3039(11)	11414(8)	8696(7)	36(3)
C(32)	1801(12)	11490(10)	8326(9)	55(4)
C(33)	5860(13)	11607(8)	5374(7)	44(3)
C(34)	4522(14)	11647(10)	5115(9)	59(4)
C(35A)	8101(34)	9846(25)	4204(21)	36(9)
C(36A)	9414(37)	10231(23)	3953(22)	48(9)
C(35B)	8716(32)	10066(21)	4334(19)	34(7)
C(36B)	8099(24)	9937(20)	3593(17)	50(8)
C(37)	4561(12)	7494(9)	7442(8)	45(3)

C(38)	4927(14)	6171(10)	6677(8)	50(3)
C(39)	6141(13)	6286(10)	6764(7)	38(3)
C(40)	2421(12)	7115(11)	7238(9)	60(4)
C(41)	8640(11)	8267(8)	7943(6)	30(3)
C(42)	7741(15)	1665(13)	7244(11)	73(4)
Cl(1)	6139(4)	2622(4)	7660(3)	84(1)
Cl(2)	9099(5)	2143(4)	7196(3)	93(1)

Table S15. Anisotropic displacement parameters (A^2 x 10^3) for Os(OEP)(CO)(1-MeIM). The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Os(1)	28(1)	21(1)	22(1)	-1(1)	-1(1)	2(1)
O(1)	36(5)	61(6)	47(5)	-16(4)	-2(4)	-12(4)
N(1)	26(5)	21(5)	22(4)	7(4)	-3(4)	4(4)
N(2)	22(5)	30(5)	28(5)	4(4)	-3(4)	3(4)
N(3)	27(5)	20(4)	24(5)	-2(4)	-8(4)	3(4)
N(4)	31(5)	25(5)	22(5)	-6(4)	-5(4)	-1(4)
N(5)	31(5)	15(4)	32(5)	2(4)	-9(4)	0(4)
N(6)	36(6)	33(5)	53(6)	-4(5)	-7(5)	-6(5)
C(1)	28(6)	27(6)	24(6)	-4(5)	-6(5)	4(5)
C(2)	32(6)	24(6)	30(6)	-10(5)	-4(5)	7(5)
C(3)	27(6)	21(6)	36(6)	-7(5)	-5(5)	4(5)
C(4)	23(6)	26(6)	40(7)	-13(5)	0(5)	1(5)
C(5)	33(6)	26(6)	33(6)	3(5)	-2(5)	4(5)
C(6)	38(7)	30(6)	38(7)	4(5)	3(6)	-5(5)
C(7)	55(8)	33(7)	37(7)	15(6)	8(6)	8(6)
C(8)	52(8)	37(7)	43(8)	9(6)	8(6)	5(6)
C(9)	26(6)	44(7)	26(6)	12(5)	-5(5)	1(5)
C(10)	39(7)	39(7)	23(6)	1(5)	14(5)	-8(6)
C(11)	26(6)	26(6)	21(5)	5(4)	-9(5)	2(5)
C(12)	21(5)	33(6)	33(6)	-4(5)	-7(5)	-9(5)
C(13)	21(5)	33(6)	18(5)	-5(5)	-3(4)	-4(5)
C(14)	32(6)	25(6)	25(6)	-3(5)	-9(5)	-6(5)
C(15)	36(6)	21(5)	31(6)	-14(5)	-6(5)	4(5)
C(16)	31(6)	15(5)	30(6)	4(4)	-11(5)	1(4)
C(17)	45(7)	30(6)	18(5)	2(5)	5(5)	6(5)
C(18)	59(8)	36(7)	27(6)	0(5)	4(6)	6(6)
C(19)	43(7)	22(6)	17(5)	3(4)	-4(5)	5(5)
C(20)	44(7)	29(6)	31(6)	-8(5)	0(5)	2(5)
C(21)	45(7)	27(6)	34(6)	-12(5)	-2(5)	3(5)
C(22)	102(13)	110(14)	43(8)	-22(9)	12(8)	-64(11)
C(23)	39(7)	24(6)	43(7)	-11(5)	-4(6)	9(5)
C(24)	49(8)	41(8)	87(11)	-7(7)	-18(8)	7(6)
C(25)	64(9)	47(8)	54(9)	30(7)	5(7)	8(7)
C(26)	80(11)	52(9)	69(10)	8(8)	-22(9)	27(8)
C(27)	57(9)	34(8)	95(12)	30(8)	33(9)	10(7)
C(28)	155(20)	90(14)	53(10)	21(10)	-18(12)	-39(13)
C(29)	34(6)	31(6)	23(6)	-4(5)	2(5)	-3(5)
C(30)	50(8)	95(11)	41(8)	-7(8)	7(6)	-36(8)
C(31)	37(7)	26(6)	38(6)	-11(5)	1(5)	0(5)
C(32)	37(7)	48(8)	74(9)	9(7)	-29(7)	2(6)
C(33)	70(9)	14(5)	36(7)	-4(5)	3(6)	-4(6)
C(34)	64(9)	48(8)	53(8)	11(7)	-17(7)	-4(7)
C(35A)	46(20)	38(17)	17(19)	12(12)	-16(14)	-1(14)
C(36A)	51(20)	30(16)	47(20)	-3(14)	7(16)	-1(13)
C(35B)	34(18)	37(14)	28(17)	6(11)	-9(12)	-7(13)
C(36B)	55(16)	77(18)	23(15)	21(12)	-16(11)	-34(13)
C(37)	32(7)	30(6)	69(9)	-8(6)	-12(6)	-2(5)

C(38)	64(9)	48(8)	38(7)	-23(6)	-1(6)	-15(7)
C(39)	39(7)	45(7)	34(7)	-11(6)	-4(5)	-15(6)
C(40)	31(7)	68(10)	75(10)	1(8)	-9(7)	-12(6)
C(41)	28(6)	25(6)	20(6)	-1(5)	2(5)	9(5)
C(42)	60(9)	76(11)	85(11)	-17(9)	-28(9)	-5(8)
Cl(1)	64(3)	89(3)	84(3)	-16(2)	8(2)	-10(2)
Cl(2)	70(3)	122(4)	92(3)	-13(3)	-12(2)	-36(3)

Table S16. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Os(OEP)(CO)(1-MeIM). Treatment of hydrogen atoms not specifically described in the refinement summary was "noref."

	x	y	z	U(eq)
H(5A)	9696(11)	4315(9)	8037(7)	42
H(10A)	5087(11)	7578(9)	10257(7)	46
H(15A)	4802(11)	11005(8)	7108(6)	37
H(20A)	9605(12)	7840(8)	4924(7)	46
H(21A)	10886(12)	6183(9)	4409(7)	46
H(21B)	11668(12)	4990(9)	4708(7)	46
H(22A)	13247(17)	5984(14)	4131(9)	96
H(22B)	13291(17)	5633(14)	5114(9)	96
H(22C)	12508(17)	6826(14)	4813(9)	96
H(23A)	11739(11)	3693(8)	5860(8)	47
H(23B)	10984(11)	3462(8)	6811(8)	47
H(24A)	13339(13)	3052(10)	6761(10)	75
H(24B)	12567(13)	4014(10)	7332(10)	75
H(24C)	13321(13)	4247(10)	6380(10)	75
H(25A)	7957(14)	3433(10)	10193(9)	81
H(25B)	8774(14)	3331(10)	9239(9)	81
H(26A)	10279(16)	2731(11)	10185(10)	94
H(26B)	9751(16)	3864(11)	10556(10)	94
H(26C)	10568(16)	3761(11)	9602(10)	94
H(27A)	7033(15)	4896(11)	11270(10)	96
H(27B)	6227(15)	6139(11)	11256(10)	96
H(28A)	4708(22)	5100(14)	11698(10)	122
H(28B)	5254(22)	4556(14)	10829(10)	122
H(28C)	4450(22)	5793(14)	10820(10)	122
H(29A)	2816(11)	10341(9)	10453(6)	38
H(29B)	3662(11)	9170(9)	10756(6)	38
H(30A)	1348(13)	9241(12)	10950(8)	73
H(30B)	2214(13)	8430(12)	10264(8)	73
H(30C)	1369(13)	9602(12)	9961(8)	73
H(31A)	2727(11)	11663(8)	9269(7)	43
H(31B)	3542(11)	11898(8)	8336(7)	43
H(32A)	1231(12)	12228(10)	8302(9)	66
H(32B)	1282(12)	11029(10)	8687(9)	66
H(32C)	2098(12)	11262(10)	7753(9)	66
H(33A)	5649(13)	12061(8)	5841(7)	53
H(33B)	6433(13)	11906(8)	4885(7)	53
H(34A)	4060(14)	12385(10)	4938(9)	71
H(34B)	3939(14)	11369(10)	5599(9)	71
H(34C)	4723(14)	11213(10)	4643(9)	71
H(35A)	8271(34)	9144(25)	4000(21)	44
H(35B)	7356(34)	10362(25)	3956(21)	44
H(36A)	9693(37)	10299(23)	3335(22)	58
H(36B)	10139(37)	9712(23)	4205(22)	58
H(36C)	9230(37)	10924(23)	4164(22)	58
H(35C)	8754(32)	10807(21)	4308(19)	41
H(35D)	9643(32)	9583(21)	4306(19)	41

H(36D)	8661(24)	10109(20)	3052(17)	60
H(36E)	7183(24)	10420(20)	3630(17)	60
H(36F)	8063(24)	9200(20)	3630(17)	60
H(37A)	4101(12)	8070(9)	7775(8)	53
H(38A)	4807(14)	5663(10)	6375(8)	59
H(39A)	7007(13)	5852(10)	6535(7)	46
H(40A)	2246(12)	6607(11)	6935(9)	72
H(40B)	1997(12)	7843(11)	7015(9)	72
H(40C)	2044(12)	7007(11)	7844(9)	72
H(42A)	7844(15)	985(13)	7613(11)	88
H(42B)	7722(15)	1523(13)	6669(11)	88