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Efficient catalytic oxidation of primary and secondary alcohols using a non-heme dinuclear iron complex

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The Netherlands
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contribution of the disordered solvent.
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Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F, with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

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N1 0.0338(11) 0.0483(14) 0.0330(11) 0.0062(10) 0.0015(9) -0.0074(10)
N2 0.0339(12) 0.0643(16) 0.0309(12) 0.0007(11) 0.0076(9) -0.0071(11)
N3 0.0297(11) 0.0476(14) 0.0323(11) -0.0053(10) 0.0049(9) -0.0048(10)
N4 0.0384(11) 0.0336(12) 0.0279(10) 0.0019(9) 0.0006(9) -0.0040(9)
C1 0.0416(16) 0.102(3) 0.0284(14) 0.0005(15) 0.0038(12) -0.0084(17)
C2 0.056(2) 0.205(5) 0.0309(17) -0.005(2) 0.0086(15) -0.027(3)
C3 0.064(2) 0.289(8) 0.037(2) -0.007(3) 0.0223(18) -0.042(4)
C4 0.0450(19) 0.201(5) 0.0431(19) -0.004(2) 0.0175(15) -0.027(3)
C5 0.0370(15) 0.084(2) 0.0377(15) 0.0027(15) 0.0100(12) -0.0096(15)
C6 0.0277(13) 0.068(2) 0.0402(15) 0.0030(14) 0.0074(11) -0.0098(13)
C7 0.0313(13) 0.0576(18) 0.0314(13) -0.0087(12) 0.0019(11) -0.0072(12)
C8 0.0312(14) 0.065(2) 0.0502(17) -0.0153(15) 0.0080(12) -0.0052(13)
C9 0.0416(16) 0.0522(19) 0.063(2) -0.0179(16) -0.0001(14) 0.0080(14)
C10 0.0449(16) 0.0400(16) 0.0587(18) -0.0079(14) 0.0008(14) -0.0008(13)
C11 0.0366(14) 0.0387(15) 0.0447(15) -0.0060(12) 0.0058(12) -0.0046(12)
C12 0.0448(15) 0.0416(16) 0.0327(13) 0.0017(11) 0.0066(11) -0.0081(12)
C13 0.0597(18) 0.0503(18) 0.0362(15) -0.0025(13) 0.0143(13) -0.0060(15)
C14 0.0640(19) 0.0528(19) 0.0347(15) -0.0062(13) 0.0028(14) -0.0074(15)
C15 0.0511(17) 0.0459(17) 0.0366(15) -0.0034(12) -0.0052(13) -0.0102(14)
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C17 0.0368(14) 0.0397(15) 0.0390(15) 0.0013(12) -0.0043(11) -0.0079(12)
C18 0.0433(16) 0.0539(18) 0.0505(17) 0.0172(14) 0.0018(13) -0.0156(14)
C19 0.0476(17) 0.0441(17) 0.0470(16) 0.0167(13) -0.0027(13) -0.0066(13)
C20 0.0576(19) 0.0437(18) 0.064(2) 0.0148(16) -0.0061(16) -0.0150(15)
C21 0.082(3) 0.0400(18) 0.073(2) 0.0007(16) 0.003(2) -0.0088(18)
C22 0.078(2) 0.0371(17) 0.075(2) -0.0023(16) 0.0153(19) -0.0019(17)
C23 0.0523(18) 0.0463(18) 0.063(2) 0.0040(15) 0.0068(15) -0.0020(14)
C24 0.0476(16) 0.0387(16) 0.0395(15) 0.0092(12) -0.0032(12) -0.0049(13)
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N1B 0.0356(11) 0.0454(13) 0.0328(11) 0.0036(10) -0.0013(9) -0.0060(10)
N2B 0.0332(11) 0.0440(13) 0.0269(10) 0.0046(9) 0.0040(9) 0.0010(10)
N3B 0.0323(11) 0.0366(12) 0.0307(11) 0.0018(9) 0.0040(9) -0.0025(9)
N4B 0.0406(12) 0.0440(13) 0.0307(11) -0.0022(10) -0.0025(9) 0.0051(10)
C1B 0.0462(15) 0.0444(17) 0.0303(13) 0.0045(12) 0.0081(11) 0.0040(13)
C2B 0.067(2) 0.0501(18) 0.0437(16) 0.0069(14) 0.0129(15) 0.0161(16)
C3B 0.0533(19) 0.071(2) 0.0475(17) 0.0106(16) 0.0155(14) 0.0246(17)

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C4B 0.0370(15) 0.076(2) 0.0384(15) 0.0140(15) 0.0105(12) 0.0083(15)
 C5B 0.0328(14) 0.0567(18) 0.0291(13) 0.0100(12) 0.0033(11) 0.0034(12)
 C6B 0.0274(13) 0.0544(17) 0.0363(14) 0.0073(12) 0.0019(11) -0.0046(12)
 C7B 0.0336(13) 0.0412(15) 0.0360(14) 0.0041(11) 0.0037(11) -0.0037(11)
 C8B 0.0392(15) 0.0541(18) 0.0451(16) 0.0091(14) 0.0105(12) -0.0055(13)
 C9B 0.0500(16) 0.0527(18) 0.0367(15) 0.0100(13) 0.0121(13) -0.0036(14)
 C10B 0.0478(16) 0.0443(16) 0.0331(14) 0.0044(12) 0.0029(12) 0.0017(13)
 C11B 0.0335(13) 0.0367(14) 0.0346(13) -0.0012(11) 0.0026(11) 0.0002(11)
 C12B 0.0501(17) 0.0571(19) 0.0397(16) -0.0044(14) 0.0004(13) 0.0104(14)
 C13B 0.067(2) 0.072(2) 0.0531(19) -0.0093(17) 0.0018(17) 0.0273(19)
 C14B 0.097(3) 0.055(2) 0.060(2) -0.0186(18) -0.005(2) 0.023(2)
 C15B 0.077(2) 0.0452(18) 0.0510(19) -0.0103(15) -0.0106(17) 0.0028(17)
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 C17B 0.0534(17) 0.0421(16) 0.0408(15) 0.0000(13) -0.0045(13) -0.0141(14)
 C18B 0.0360(14) 0.0599(19) 0.0352(14) 0.0068(13) -0.0080(11) -0.0067(13)
 C19B 0.0478(16) 0.0470(17) 0.0318(14) 0.0012(12) -0.0070(12) -0.0030(13)
 C20B 0.065(2) 0.064(2) 0.0392(16) -0.0017(15) -0.0105(15) -0.0180(17)
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 C22B 0.085(3) 0.073(2) 0.0317(15) -0.0125(15) 0.0049(16) 0.011(2)
 C23B 0.0537(17) 0.063(2) 0.0340(15) -0.0044(14) 0.0017(13) 0.0023(15)
 C24B 0.0457(15) 0.0441(16) 0.0261(13) 0.0001(11) -0.0036(11) 0.0019(12)
 P1 0.0411(4) 0.0625(5) 0.0374(4) -0.0026(3) 0.0097(3) 0.0074(4)
 F1 0.0876(16) 0.161(3) 0.0512(12) -0.0118(14) -0.0046(11) 0.0623(16)
 F2 0.0550(10) 0.0564(11) 0.0667(12) -0.0123(9) 0.0211(9) -0.0088(8)
 F3 0.1161(18) 0.0621(13) 0.0916(16) -0.0035(11) 0.0576(14) -0.0097(12)
 F4 0.0546(11) 0.1200(19) 0.0581(12) -0.0109(12) -0.0044(9) 0.0240(12)
 F5 0.0757(13) 0.0982(17) 0.0723(13) -0.0321(12) 0.0168(11) 0.0218(12)
 F6 0.0825(15) 0.1128(19) 0.0842(15) 0.0004(14) 0.0482(13) -0.0184(14)
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 F7 0.0655(13) 0.136(2) 0.0677(14) -0.0287(14) 0.0055(11) -0.0159(13)
 F8 0.0456(10) 0.0605(12) 0.0970(15) 0.0072(11) 0.0153(10) 0.0090(9)
 F9 0.0741(13) 0.0859(15) 0.1063(17) 0.0484(13) 0.0469(13) 0.0261(12)
 F10 0.0434(10) 0.0978(16) 0.0858(14) 0.0153(12) 0.0180(10) 0.0168(10)
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 F12 0.0631(12) 0.0936(16) 0.0787(14) -0.0181(12) 0.0029(11) -0.0133(11)

_geom_special_details

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All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix. The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry. An approximate (isotropic)

treatment of cell esds is used for estimating esds involving l.s. planes.

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_geom_bond_atom_site_label_1

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Fe1 O1 1.9299(18) . ?

Fe1 N4 2.135(2) . ?

Fe1 N2 2.174(2) . ?

Fe1 N3 2.217(2) . ?

Fe1 N1 2.258(2) . ?

Fe2 O2 1.7897(16) . ?

Fe2 O1B 1.9285(17) . ?

Fe2 N4B 2.132(2) . ?

Fe2 N2B 2.179(2) . ?

Fe2 N3B 2.241(2) . ?

Fe2 N1B 2.250(2) . ?

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N1 C6 1.482(4) . ?

N1 C17 1.489(3) . ?

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N2 C1 1.345(4) . ?

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 P2 F8 1.5945(19) . ?
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 C6 N1 C18 113.2(2) . . ?
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 C18B N1B Fe2 110.62(16) . . ?
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C8B C9B H9B 120.3 . . ?
C9B C10B C11B 119.0(2) . . ?
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C11B C10B H10B 120.5 . . ?
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F6 P1 F5 88.80(14) . . ?
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F1 P1 F5 89.37(13) . . ?
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 F10 P2 F8 179.57(14) . . ?
 F7 P2 F12 178.90(15) . . ?
 F9 P2 F12 89.20(14) . . ?
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 F8 P2 F12 89.72(12) . . ?

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 N1B Fe2 O2 Fe1 149.6(3) ?
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 N3 Fe1 N1 C18 -164.2(2) ?
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 N4 Fe1 N2 C5 -14.3(3) ?
 N3 Fe1 N2 C5 53.7(2) ?
 N1 Fe1 N2 C5 -20.6(2) ?
 O2 Fe1 N2 C1 -39.4(3) ?
 O1 Fe1 N2 C1 65.9(3) ?
 N4 Fe1 N2 C1 160.1(3) ?
 N3 Fe1 N2 C1 -131.9(3) ?
 N1 Fe1 N2 C1 153.8(3) ?
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Fe1 N2 C5 C6 -6.0(4) ?
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C3 C4 C5 C6 -178.8(5) ?
C17 N1 C6 C5 -173.5(2) ?
C18 N1 C6 C5 60.7(3) ?
Fe1 N1 C6 C5 -57.0(2) ?
C17 N1 C6 C7 -59.5(3) ?
C18 N1 C6 C7 174.7(2) ?
Fe1 N1 C6 C7 57.0(2) ?
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C4 C5 C6 N1 -136.2(4) ?
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C4 C5 C6 C7 108.4(4) ?
C11 N3 C7 C8 -3.9(4) ?
Fe1 N3 C7 C8 172.1(2) ?
C11 N3 C7 C6 179.3(2) ?
Fe1 N3 C7 C6 -4.8(3) ?
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N3 C7 C8 C9 3.3(4) ?
C6 C7 C8 C9 179.7(3) ?
C7 C8 C9 C10 0.6(4) ?
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C7 N3 C11 C10 0.6(4) ?
Fe1 N3 C11 C10 -174.7(2) ?
C9 C10 C11 N3 3.1(4) ?
C16 N4 C12 C13 -0.6(4) ?
Fe1 N4 C12 C13 158.8(2) ?
N4 C12 C13 C14 0.0(4) ?
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Fe1 N4 C16 C17 21.1(3) ?
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Fe1 N1 C17 C16 30.3(3) ?
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C6 N1 C18 C19 -171.9(2) ?
C17 N1 C18 C19 60.3(3) ?
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C18 C19 C20 C21 178.1(3) ?
C19 C20 C21 C22 1.2(5) ?
C20 C21 C22 C23 -1.0(5) ?
C21 C22 C23 C24 -0.5(5) ?
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Fe1 O1 C24 C19 -52.8(3) ?
C22 C23 C24 O1 -176.3(3) ?
C22 C23 C24 C19 1.9(4) ?
C20 C19 C24 O1 176.4(2) ?
C18 C19 C24 O1 -1.5(4) ?
C20 C19 C24 C23 -1.8(4) ?
C18 C19 C24 C23 -179.7(3) ?
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N3B Fe2 O1B C24B 35.4(4) ?
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N4B Fe2 N1B C6B -134.85(16) ?
N2B Fe2 N1B C6B 39.63(15) ?
N3B Fe2 N1B C6B -43.30(15) ?
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O1B Fe2 N1B C17B -102.36(17) ?
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