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End-on and side-on peroxy derivatives of non-heme iron complexes with pentadentate ligands

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O8A O 0.2622(15) 0.5203(6) 0.0572(5) 0.099(4) Uani 0.65 1 d PDU . .
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H12B H 0.0400 0.2499 0.2387 0.041 Uiso 1 1 calc R . .
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H13A H -0.0370 0.1431 0.3112 0.075 Uiso 1 1 calc R . .
H13B H 0.1388 0.1413 0.2847 0.075 Uiso 1 1 calc R . .
C14 C 0.0630(10) 0.1746(4) 0.4320(4) 0.052(2) Uani 1 1 d . . .
H14A H -0.0555 0.1891 0.4076 0.062 Uiso 1 1 calc R . .
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C15 C 0.1241(11) 0.2338(5) 0.4818(4) 0.062(2) Uani 1 1 d . . .
H15A H 0.2083 0.2090 0.5191 0.075 Uiso 1 1 calc R . .
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C16 C 0.0699(13) 0.3556(5) 0.4201(4) 0.067(3) Uani 1 1 d . . .
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H18B H 0.1724 0.0451 0.3678 0.082 Uiso 1 1 calc R . .
H18C H 0.2765 0.0709 0.4407 0.082 Uiso 1 1 calc R . .
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are estimated using the full covariance matrix. The cell esds are taken
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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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C1 N2 Fe1 132.0(4) . . ?
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C11 N3 Fe1 131.8(4) . . ?
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C14 N4 Fe1 108.5(4) . . ?
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C14 C15 H15B 108.7 . . ?
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H21A C21 H21B 109.5 . . ?
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H21A C21 H21C 109.5 . . ?
H21B C21 H21C 109.5 . . ?
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O2 C11 O1 113.0(3) . . ?
O4A C11 O1 117.6(4) . . ?
O3B C11 O4B 100.3(10) . . ?
O2 C11 O4B 89.1(6) . . ?
O1 C11 O4B 94.4(6) . . ?
O2 C11 O3A 99.3(4) . . ?
O4A C11 O3A 103.5(5) . . ?
O1 C11 O3A 102.5(4) . . ?
O6 C12 O8A 126.1(6) . . ?

O6 C12 O5 108.6(5) . . ?
O8A C12 O5 108.6(6) . . ?
O6 C12 O8B 88.3(9) . . ?
O5 C12 O8B 104.8(7) . . ?
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C1 N2 C5 C6 -171.9(5) ?
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