Complexation of Nitrous Oxide by Frustrated Lewis Pairs

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2009

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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^ > 2sigma(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
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H21C H 0.3183 0.8196 0.0368 0.040 Uiso 1 1 calc R . .
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H24B H 0.3089 0.7797 0.2901 0.039 Uiso 1 1 calc R . .
H24C H 0.4563 0.8325 0.2631 0.039 Uiso 1 1 calc R . .
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H25B H 0.4297 0.4809 0.3807 0.039 Uiso 1 1 calc R . .
H25C H 0.2928 0.5629 0.3632 0.039 Uiso 1 1 calc R . .
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H28C H 0.1616 0.6495 0.2536 0.042 Uiso 1 1 calc R . .
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C25 0.0325(9) 0.0276(8) 0.0174(8) -0.0034(6) 0.0026(7) 0.0004(7)
C26 0.0265(8) 0.0327(9) 0.0247(9) -0.0120(7) -0.0064(7) 0.0005(7)
C27 0.0172(7) 0.0189(7) 0.0245(8) -0.0050(6) -0.0032(6) -0.0006(6)
C28 0.0189(8) 0.0257(8) 0.0383(10) -0.0063(7) -0.0010(7) 0.0027(6)
C29 0.0212(8) 0.0204(8) 0.0356(10) -0.0061(7) -0.0010(7) -0.0042(6)
C30 0.0318(9) 0.0275(8) 0.0301(9) -0.0096(7) -0.0113(7) -0.0011(7)
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 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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N2 O1 1.3359(15) . ?
O1 B1 1.5430(18) . ?
B1 C1 1.640(2) . ?
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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F7 F 0.36426(6) -0.34633(5) 0.38861(5) 0.03521(13) Uani 1 1 d . . .
F8 F 0.20169(8) -0.34838(7) 0.26622(7) 0.04812(18) Uani 1 1 d . . .
F9 F 0.06709(8) -0.12687(7) 0.13508(6) 0.04550(16) Uani 1 1 d . . .
F10 F 0.09214(6) 0.08897(6) 0.12413(4) 0.03264(12) Uani 1 1 d . . .
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H20C H -0.2162 0.5629 -0.0120 0.047 Uiso 1 1 calc R . .
C21 C -0.31489(11) 0.32260(9) 0.12558(8) 0.03196(18) Uani 1 1 d . . .
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H21C H -0.3621 0.3264 0.0745 0.048 Uiso 1 1 calc R . .
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H22B H -0.4930 0.5366 0.1833 0.046 Uiso 1 1 calc R . .
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C23 C -0.22928(8) 0.34228(8) 0.32440(6) 0.02305(13) Uani 1 1 d . . .
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C21 0.0367(4) 0.0311(4) 0.0377(5) -0.0089(3) -0.0083(4) -0.0196(4)
C22 0.0197(3) 0.0324(4) 0.0371(4) -0.0039(3) -0.0111(3) -0.0059(3)
C23 0.0182(3) 0.0258(3) 0.0183(3) -0.0012(2) 0.0002(2) -0.0060(2)
C24 0.0192(3) 0.0393(5) 0.0293(4) -0.0035(3) 0.0042(3) -0.0081(3)
C25 0.0251(4) 0.0442(5) 0.0179(3) -0.0077(3) -0.0016(3) -0.0056(3)
C26 0.0293(4) 0.0235(4) 0.0308(4) 0.0046(3) -0.0017(3) -0.0097(3)
C27 0.0188(3) 0.0198(3) 0.0267(3) -0.0105(2) -0.0002(2) -0.0067(2)
C28 0.0317(4) 0.0198(3) 0.0340(4) -0.0021(3) -0.0041(3) -0.0114(3)
C29 0.0240(3) 0.0287(4) 0.0449(5) -0.0218(4) 0.0033(3) -0.0054(3)
C30 0.0235(3) 0.0371(4) 0.0349(4) -0.0199(3) -0.0005(3) -0.0138(3)
B1 0.0161(3) 0.0165(3) 0.0163(3) -0.0041(2) -0.0013(2) -0.0042(2)

_geom_special_details
;
 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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F2 C9 1.3430(11) . ?
F3 C10 1.3394(10) . ?
F4 C11 1.3426(10) . ?
F5 C12 1.3437(9) . ?
F6 C14 1.3488(10) . ?
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F9 C17 1.3456(11) . ?
F10 C18 1.3506(10) . ?
N1 N2 1.2602(8) . ?
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