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data_global

# Cooperative Bimetallic Effects on New Iridium(III) Pyrazolate Complexes:
# Hydrogen-Hydrogen, Carbon-Hydrogen and Carbon-Chlorine Bond Activations
# by Eduardo Sola, Vladimir I. Bakhmutov, Francisco Torres, Anabel Elduque,
# José A. López, Fernando J. Lahoz, Helmut Werner and Luis A. Oro
#
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#-------------------------------------------------------------
# Publication details
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      'Sola, E.'
      'Bakhmutov, V.I.'
      'Torres, F.'
      'Elduque, A.'
      'L\´opez J.A.'
      'Lahoz, F.J.'
      'Werner, H.'
      'Oro, L.A.'
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# Data for compound 2 (local labelling as edu1psi)

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 bis(tricyclohexylphosphine)-di-iridium(iii)
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 Due to the highly anisotropic shape of the measured crystal, a semi-
 empirical absorption correction specially designed for thin plates was
 applied (XPREP program, v 5.03, Siemens Analytical X-Ray Instruments, Inc.
 1994, Madison, WI, USA). The procedure refines three 'shape' factors (\mt
 and two edge factors) and requires the Miller index of the principal
 face of the crystal (1 0 0), the minimun glancing angles (3 deg, used
 to eliminate difficul-to-correct reflections) and a set of psi-scan
 measurements (11 reflcts. measured at psi intervals of 10 deg)
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 The selected crystal is a twinned crystal with a principal component.
 A photographic analysis of several samples showed to be, in all cases, more
 complicated twins.
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 Refinement on F^2^ for ALL reflections except for 328 with very negative
 F^2^ or flagged by the user for potential systematic errors. Weighted
 R-factors wR and all goodnesses 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
 observed criterion of F^2^ > 2sigma(F^2^) is used only for calculating
 _R_factor_obs 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.

 Number of data use in the analysis.- A total of 7801 reflections were
 measured (an independent set -1≤h≤17, -1≤k≤15, -18≤l≤17 and some symmetry
 equivalent reflections -1≤h≤17, -14≤k≤-2, -18≤l≤17). After the elimination
 of the reflections clearly affected by the second component of the twinned
 crystal (asymmetric or double peaks, bad background, off-center
 reflections) and those almost parallel to the plane of the lamina
 (absorption correction), a total of 5862 non-unique reflections remains
 in the data set.
 First run with SHELXL-93 rejects 224 reflections (systematic absences and
 very negative reflections, Fo^2^<-3\sFo^2^), to give 5638 reflections
 before merging. Merging procedure gives 4587 reflections. Due to the
 twinned nature of the crystal, 328 negative reflections were automatically
 (Fo^2^<-1\sFo^2^) treated as unobserved. The final number of reflections
 used in the refinement were 4259.

 All the restraints included in the refinement affect exclusively to the
 displacement parameters of anisotropic atoms. Probably due to the bad
 quality of data (twinned and highly anisotropic shaped crystal) the
 obtained thermal parameters for some atoms gave -without restraints-
 unreasonable parameters. A rigid bond restraint has been applied to all
 bonds between non-hydrogen atoms (DELU instruction in SHELXL-93).

 Hydrogen atoms (except hydrides) were included in calculated positions,
 refined riding on the corresponding carbon atoms, and with isotropic thermal
 parameters set at 20% or 50% greater than those for the carbons to which
 they are attached.
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N2 N 0.4147(11) 0.1637(13) 0.0584(10) 0.033(3) Uani 1 d U .
C1 C 0.4608(15) 0.3202(18) 0.0852(14) 0.043(4) Uani 1 d U .
H1 H 0.4640(15) 0.3895(18) 0.1026(14) 0.051 Uiso 1 calc R .
C2 C 0.5209(14) 0.2697(18) 0.0492(14) 0.044(5) Uani 1 d U .
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C3 C 0.4876(14) 0.1721(18) 0.0301(13) 0.040(4) Uani 1 d U .
H3 H 0.5133(14) 0.1204(18) 0.0013(13) 0.047 Uiso 1 calc R .
N3 N 0.3720(11) 0.1619(13) 0.2453(9) 0.032(3) Uani 1 d U .
N4 N 0.3890(11) 0.0678(13) 0.2125(10) 0.034(3) Uani 1 d U .
C4 C 0.4107(14) 0.1675(17) 0.3263(12) 0.037(4) Uani 1 d U .
H4 H 0.4113(14) 0.2258(17) 0.3620(12) 0.045 Uiso 1 calc R .
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H5 H 0.4786(14) 0.0616(18) 0.4086(13) 0.049 Uiso 1 calc R .
C6 C 0.4376(14) 0.0191(17) 0.2791(13) 0.040(4) Uani 1 d U .
H6 H 0.4608(14) -0.0473(17) 0.2765(13) 0.048 Uiso 1 calc R .
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C7 C 0.3624(14) 0.4336(16) 0.2786(13) 0.038(4) Uani 1 d U .
C8 C 0.4006(17) 0.5085(17) 0.3392(13) 0.047(6) Uani 1 d U .
H8A H 0.3607(17) 0.5252(17) 0.3778(13) 0.070 Uiso 1 calc R .
H8B H 0.4126(17) 0.5699(17) 0.3082(13) 0.070 Uiso 1 calc R .
H8C H 0.4549(17) 0.4821(17) 0.3735(13) 0.070 Uiso 1 calc R .
P1 P 0.1881(4) 0.3366(5) 0.0629(4) 0.0368(13) Uani 1 d U .
C9 C 0.1468(16) 0.2695(18) -0.0402(13) 0.046(4) Uani 1 d U .
H9 H 0.1304(16) 0.1997(18) -0.0242(13) 0.055 Uiso 1 calc R .
C10 C 0.2254(16) 0.2557(21) -0.0891(13) 0.052(5) Uani 1 d U .
H10A H 0.2198(16) 0.1903(21) -0.1197(13) 0.078 Uiso 1 calc R .
H10B H 0.2802(16) 0.2571(21) -0.0469(13) 0.078 Uiso 1 calc R .
H10C H 0.2247(16) 0.3110(21) -0.1309(13) 0.078 Uiso 1 calc R .
C11 C 0.0708(17) 0.3114(22) -0.0967(15) 0.062(7) Uani 1 d U .
H11A H 0.0224(17) 0.3134(22) -0.0659(15) 0.093 Uiso 1 calc R .
H11B H 0.0552(17) 0.2687(22) -0.1484(15) 0.093 Uiso 1 calc R .
H11C H 0.0835(17) 0.3805(22) -0.1139(15) 0.093 Uiso 1 calc R .
C12 C 0.0855(15) 0.3551(20) 0.1069(14) 0.048(4) Uani 1 d U .
H12 H 0.0450(15) 0.3943(20) 0.0616(14) 0.058 Uiso 1 calc R .
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C13 C 0.0411(14) 0.2599(22) 0.1183(18) 0.064(6) Uani 1 d U .
H13A H 0.0399(14) 0.2163(22) 0.0676(18) 0.096 Uiso 1 calc R .
H13B H -0.0184(14) 0.2745(22) 0.1248(18) 0.096 Uiso 1 calc R .
H13C H 0.0720(14) 0.2249(22) 0.1702(18) 0.096 Uiso 1 calc R .
C14 C 0.1045(16) 0.4244(19) 0.1872(14) 0.055(5) Uani 1 d U .
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H14C H 0.0703(16) 0.4017(19) 0.2294(14) 0.082 Uiso 1 calc R .
C15 C 0.2195(16) 0.4675(17) 0.0424(18) 0.053(5) Uani 1 d U .
H15 H 0.2437(16) 0.4973(17) 0.1006(18) 0.063 Uiso 1 calc R .
C16 C 0.1418(15) 0.5357(18) 0.0023(16) 0.054(6) Uani 1 d U .
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H16B H 0.1171(15) 0.5118(18) -0.0563(16) 0.081 Uiso 1 calc R .
H16C H 0.1615(15) 0.6061(18) -0.0005(16) 0.081 Uiso 1 calc R .
C17 C 0.2882(16) 0.4783(18) -0.0087(19) 0.063(6) Uani 1 d U .
H17A H 0.3320(16) 0.4253(18) 0.0083(19) 0.095 Uiso 1 calc R .
H17B H 0.3153(16) 0.5454(18) 0.0021(19) 0.095 Uiso 1 calc R .
H17C H 0.2628(16) 0.4715(18) -0.0704(19) 0.095 Uiso 1 calc R .
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H19B H 0.2247(15) -0.0402(16) 0.2734(14) 0.061 Uiso 1 calc R .
H19C H 0.1314(15) 0.0078(16) 0.2737(14) 0.061 Uiso 1 calc R .
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H20B H 0.0200(16) -0.0466(19) 0.1070(17) 0.082 Uiso 1 calc R .
H20C H 0.0534(16) -0.0993(19) 0.1991(17) 0.082 Uiso 1 calc R .
C21 C 0.2898(16) -0.1768(17) 0.1787(14) 0.044(4) Uani 1 d U .
H21 H 0.3059(16) -0.1432(17) 0.2366(14) 0.053 Uiso 1 calc R .
C22 C 0.2300(15) -0.2616(16) 0.1919(15) 0.052(5) Uani 1 d U .
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H22B H 0.1820(15) -0.2341(16) 0.2163(15) 0.078 Uiso 1 calc R .
H22C H 0.2619(15) -0.3118(16) 0.2319(15) 0.078 Uiso 1 calc R .
C23 C 0.3744(16) -0.2157(17) 0.1597(17) 0.055(6) Uani 1 d U .
H23A H 0.4147(16) -0.2295(17) 0.2143(17) 0.082 Uiso 1 calc R .
H23B H 0.3995(16) -0.1644(17) 0.1267(17) 0.082 Uiso 1 calc R .
H23C H 0.3639(16) -0.2785(17) 0.1257(17) 0.082 Uiso 1 calc R .
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H24 H 0.1434(16) -0.1910(18) 0.0237(14) 0.058 Uiso 1 calc R .
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H25B H 0.0821(16) -0.1044(21) -0.0936(14) 0.083 Uiso 1 calc R .
H25C H 0.1622(16) -0.0278(21) -0.0868(14) 0.083 Uiso 1 calc R .
C26 C 0.2447(17) -0.1910(18) -0.0409(14) 0.053(5) Uani 1 d U .
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N2 0.040(7) 0.025(7) 0.035(8) -0.013(8) 0.012(9) -0.011(8)
C1 0.042(9) 0.039(8) 0.048(13) 0.008(11) 0.011(12) -0.015(11)
C2 0.034(8) 0.048(11) 0.049(13) 0.011(11) 0.007(11) 0.001(11)
C3 0.034(8) 0.050(9) 0.042(12) 0.013(11) 0.025(10) 0.016(11)
N3 0.037(9) 0.041(7) 0.022(6) -0.009(8) 0.019(7) 0.009(9)
N4 0.032(9) 0.040(8) 0.028(6) -0.006(8) -0.002(8) 0.010(8)
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C5 0.038(13) 0.053(11) 0.025(7) 0.005(10) -0.010(10) -0.002(11)
C6 0.045(13) 0.038(9) 0.035(8) 0.002(10) 0.005(10) 0.026(11)
N5 0.042(11) 0.042(7) 0.031(8) -0.017(9) -0.012(9) 0.002(10)
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C21 0.064(11) 0.038(9) 0.036(10) 0.004(10) 0.020(11) 0.012(12)
C22 0.060(11) 0.022(9) 0.071(16) 0.025(12) 0.009(13) 0.008(12)
C23 0.057(10) 0.026(12) 0.080(18) -0.018(12) 0.011(15) 0.007(12)
C24 0.053(13) 0.038(12) 0.046(9) -0.015(11) -0.010(12) -0.008(12)
C25 0.050(14) 0.078(16) 0.034(10) -0.023(13) 0.000(11) -0.014(15)
C26 0.074(14) 0.045(15) 0.041(10) -0.015(11) 0.011(13) 0.001(14)

_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.
;

loop_
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 _geom_bond_atom_site_label_2
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 _geom_bond_site_symmetry_2
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Ir1 N3 2.08(2) . ?
Ir1 N1 2.12(2) . ?
Ir1 P1 2.252(6) . ?
Ir1 Ir2 2.9817(14) . ?
Ir2 N2 2.08(2) . ?
Ir2 N4 2.102(15) . ?
Ir2 P2 2.216(6) . ?
N1 C1 1.33(3) . ?
N1 N2 1.37(2) . ?
N2 C3 1.31(2) . ?
C1 C2 1.37(3) . ?
C2 C3 1.40(3) . ?
N3 C4 1.30(2) . ?
N3 N4 1.39(2) . ?
N4 C6 1.33(2) . ?
C4 C5 1.33(3) . ?
C5 C6 1.38(3) . ?
N5 C7 1.13(2) . ?
C7 C8 1.42(3) . ?
P1 C15 1.84(2) . ?
P1 C9 1.85(2) . ?
P1 C12 1.89(2) . ?
C9 C11 1.45(3) . ?
C9 C10 1.59(3) . ?
C12 C13 1.46(3) . ?
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C15 C17 1.48(3) . ?
C15 C16 1.55(3) . ?
P2 C18 1.84(2) . ?
P2 C24 1.85(2) . ?
P2 C21 1.88(2) . ?
C18 C20 1.46(3) . ?
C18 C19 1.52(3) . ?
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C21 C23 1.51(3) . ?
C24 C25 1.48(3) . ?
C24 C26 1.51(3) . ?

loop_
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N5 Ir1 N1 91.3(7) . . ?
N3 Ir1 N1 84.2(6) . . ?
N5 Ir1 P1 96.0(5) . . ?
N3 Ir1 P1 173.1(5) . . ?
N1 Ir1 P1 102.0(5) . . ?
N5 Ir1 Ir2 147.2(5) . . ?
N3 Ir1 Ir2 67.9(4) . . ?
N1 Ir1 Ir2 66.7(5) . . ?
P1 Ir1 Ir2 111.63(15) . . ?
N2 Ir2 N4 85.3(7) . . ?
N2 Ir2 P2 178.1(5) . . ?
N4 Ir2 P2 95.9(5) . . ?
N2 Ir2 Ir1 68.3(4) . . ?
N4 Ir2 Ir1 67.1(5) . . ?
P2 Ir2 Ir1 113.53(15) . . ?
C1 N1 N2 108.4(18) . . ?
C1 N1 Ir1 137.8(16) . . ?
N2 N1 Ir1 112.8(13) . . ?
C3 N2 N1 108.2(18) . . ?
C3 N2 Ir2 139.0(16) . . ?
N1 N2 Ir2 112.2(12) . . ?
N1 C1 C2 108.7(21) . . ?
C1 C2 C3 105.9(20) . . ?
N2 C3 C2 108.6(20) . . ?
C4 N3 N4 109.1(17) . . ?
C4 N3 Ir1 138.2(15) . . ?
N4 N3 Ir1 112.6(11) . . ?
C6 N4 N3 105.0(15) . . ?
C6 N4 Ir2 142.7(14) . . ?
N3 N4 Ir2 112.3(12) . . ?
N3 C4 C5 110.1(19) . . ?
C4 C5 C6 105.7(18) . . ?
N4 C6 C5 109.9(18) . . ?
C7 N5 Ir1 173.5(18) . . ?
N5 C7 C8 176.6(24) . . ?
C15 P1 C9 110.7(11) . . ?
C15 P1 C12 102.8(12) . . ?
C9 P1 C12 101.8(11) . . ?
C15 P1 Ir1 113.8(8) . . ?
C9 P1 Ir1 114.2(8) . . ?
C12 P1 Ir1 112.3(7) . . ?
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C13 C12 C14 115.2(21) . . ?
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C24 P2 C21 105.4(11) . . ?
C18 P2 Ir2 114.7(7) . . ?
C24 P2 Ir2 116.2(9) . . ?
C21 P2 Ir2 115.6(8) . . ?
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C20 C18 P2 123.7(18) . . ?
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C22 C21 C23 112.2(19) . . ?
C22 C21 P2 115.7(17) . . ?
C23 C21 P2 113.3(16) . . ?
C25 C24 C26 110.7(19) . . ?
C25 C24 P2 111.1(16) . . ?
C26 C24 P2 110.5(17) . . ?
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