Supplementary data for article:

Milenković, M. R.; Bacchi, A.; Cantoni, G.; Radulović, S. S.; Gligorijević, N.; Aranđelović, S.; Sladić, D.; Vujčić, M.; Mitić, D.; Anđelković, K. K. Synthesis, Characterisation and Biological Activity of Co(III) Complex with the Condensation Product of 2-(Diphenylphosphino)Benzaldehyde and Ethyl Carbazate. *Inorganica Chimica Acta* **2013**, *395*, 33–43. https://doi.org/10.1016/j.ica.2012.09.043

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##########################################
# Synthesis, characterisation and biological activity of Co(III)
# complex with the condensation product of
# 2-(diphenylphosphino)benzaldehyde and ethyl carbazate
#
# Milica Milenkovic, Alessia Bacchi, Giulia Cantoni, Katarina
# Andjelkovic, Nevenka Gligorijevic, Sandra Aranjdelovic,
# Dusan Sladic, Miroslava Vujcic, Dragana Mitic, Sinisa Radulovic
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and
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 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
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based
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R-
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O2 O -0.12630(6) 0.56581(12) 0.79786(4) 0.0655(3) Uani 1 1 d . . .
C1 C -0.01544(6) 0.24844(15) 0.93846(4) 0.0423(3) Uani 1 1 d . . .
C2 C -0.00875(7) 0.28240(17) 0.97643(4) 0.0492(3) Uani 1 1 d . . .
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C7 C -0.07123(6) 0.27378(16) 0.87470(4) 0.0471(3) Uani 1 1 d . . .
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H9A H -0.1835 0.5062 0.7236 0.103 Uiso 1 1 calc R . .
H9B H -0.1240 0.5733 0.7304 0.103 Uiso 1 1 calc R . .
C10 C -0.13253(17) 0.4179(5) 0.69162(7) 0.1411(15) Uani 1 1 d . . .
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H10B H -0.1471 0.4769 0.6706 0.212 Uiso 1 1 calc R . .
H10C H -0.1491 0.3238 0.6890 0.212 Uiso 1 1 calc R . .
C11 C 0.08907(6) 0.11325(16) 0.95755(4) 0.0445(3) Uani 1 1 d . . .
C12 C 0.09381(7) -0.01670(19) 0.97713(5) 0.0556(4) Uani 1 1 d . . .
H12 H 0.0689 -0.0909 0.9701 0.067 Uiso 1 1 calc R . .
C13 C 0.13520(9) -0.0366(2) 1.00698(6) 0.0713(5) Uani 1 1 d . . .
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C14 C 0.17247(9) 0.0720(3) 1.01751(6) 0.0769(6) Uani 1 1 d . . .
H14 H 0.2003 0.0583 1.0376 0.092 Uiso 1 1 calc R . .
C15 C 0.16839(8) 0.2010(3) 0.99826(6) 0.0725(5) Uani 1 1 d . . .
H15 H 0.1934 0.2747 1.0055 0.087 Uiso 1 1 calc R . .
C16 C 0.12751(7) 0.2215(2) 0.96841(5) 0.0576(4) Uani 1 1 d . . .
H16 H 0.1255 0.3085 0.9553 0.069 Uiso 1 1 calc R . .
C17 C 0.00461(6) -0.02674(17) 0.90770(4) 0.0481(3) Uani 1 1 d . . .
C18 C 0.02178(9) -0.1097(2) 0.87931(5) 0.0680(5) Uani 1 1 d . . .
H18 H 0.0488 -0.0748 0.8660 0.082 Uiso 1 1 calc R . .
C19 C -0.00161(13) -0.2449(3) 0.87087(7) 0.0924(8) Uani 1 1 d . . .
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H19 H 0.0100 -0.3002 0.8519 0.111 Uiso 1 1 calc R . .
C20 C -0.04139(13) -0.2976(2) 0.89003(8) 0.0918(8) Uani 1 1 d . . .
H20 H -0.0567 -0.3881 0.8842 0.110 Uiso 1 1 calc R . .
C21 C -0.05841(10) -0.2169(2) 0.91775(7) 0.0803(6) Uani 1 1 d . . .
H21 H -0.0854 -0.2528 0.9309 0.096 Uiso 1 1 calc R . .
C22 C -0.03591(8) -0.08181(19) 0.92655(5) 0.0601(4) Uani 1 1 d . . .
H22 H -0.0482 -0.0274 0.9454 0.072 Uiso 1 1 calc R . .
P2 P -0.228429(15) -0.37546(4) 0.880902(10) 0.04257(12) Uani 1 1 d . . .
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O4 O -0.06313(6) 0.07385(13) 0.78670(4) 0.0675(4) Uani 1 1 d . . .
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C23 C -0.24112(6) -0.17975(15) 0.88244(4) 0.0395(3) Uani 1 1 d . . .
C24 C -0.28199(7) -0.12189(17) 0.90117(4) 0.0482(3) Uani 1 1 d . . .
H24 H -0.3061 -0.1838 0.9110 0.058 Uiso 1 1 calc R . .
C25 C -0.28729(8) 0.02562(19) 0.90546(5) 0.0574(4) Uani 1 1 d . . .
H25 H -0.3148 0.0622 0.9180 0.069 Uiso 1 1 calc R . .
C26 C -0.25168(9) 0.11849(18) 0.89117(6) 0.0634(5) Uani 1 1 d . . .
H26 H -0.2548 0.2177 0.8945 0.076 Uiso 1 1 calc R . .
C27 C -0.21149(7) 0.06488(17) 0.87208(5) 0.0557(4) Uani 1 1 d . . .
H27 H -0.1881 0.1285 0.8622 0.067 Uiso 1 1 calc R . .
C28 C -0.20539(6) -0.08388(15) 0.86737(4) 0.0418(3) Uani 1 1 d . . .
C29 C -0.16399(6) -0.14077(15) 0.84587(4) 0.0419(3) Uani 1 1 d . . .
H29 H -0.1585 -0.2402 0.8452 0.050 Uiso 1 1 calc R . .
C30 C -0.06922(6) -0.05532(17) 0.78702(5) 0.0481(3) Uani 1 1 d . . .
C31 C -0.01147(10) -0.0926(3) 0.74038(7) 0.0852(7) Uani 1 1 d . . .
H31A H 0.0197 -0.1557 0.7389 0.102 Uiso 1 1 calc R . .
H31B H 0.0026 0.0018 0.7487 0.102 Uiso 1 1 calc R . .
C32 C -0.04389(18) -0.0800(7) 0.70367(11) 0.172(2) Uani 1 1 d . . .
H32A H -0.0542 -0.1746 0.6942 0.259 Uiso 1 1 calc R . .
H32B H -0.0226 -0.0327 0.6869 0.259 Uiso 1 1 calc R . .
H32C H -0.0764 -0.0243 0.7055 0.259 Uiso 1 1 calc R . .
C33 C -0.28375(7) -0.45660(16) 0.90307(5) 0.0520(4) Uani 1 1 d . . .
C34 C -0.26980(10) -0.5227(2) 0.93740(5) 0.0706(5) Uani 1 1 d . . .
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C35 C -0.30840(17) -0.6017(3) 0.95343(8) 0.1010(10) Uani 1 1 d . . .
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H37 H -0.4114 -0.5553 0.8899 0.131 Uiso 1 1 calc R . .
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C39 C -0.25272(6) -0.42238(16) 0.83204(4) 0.0435(3) Uani 1 1 d . . .
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C41 C -0.26440(10) -0.6122(2) 0.78592(6) 0.0751(6) Uani 1 1 d . . .
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C44 C -0.27769(8) -0.32847(19) 0.80499(5) 0.0573(4) Uani 1 1 d . . .
H44 H -0.2826 -0.2322 0.8111 0.069 Uiso 1 1 calc R . .
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O4 0.0787(8) 0.0398(6) 0.0937(9) -0.0049(6) 0.0452(7) -0.0063(5)
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C31 0.0868(14) 0.0794(14) 0.1032(18) -0.0057(13) 0.0602(14) -0.0039(12)
C32 0.142(3) 0.279(6) 0.103(2) 0.074(3) 0.039(2) 0.004(4)
C33 0.0734(10) 0.0356(7) 0.0507(8) -0.0030(6) 0.0218(7) -0.0082(7)
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C36 0.159(3) 0.0651(14) 0.122(2) -0.0224(14) 0.100(2) -0.0416(16)
C37 0.1062(19) 0.118(2) 0.117(2) -0.0415(18) 0.0604(17) -0.0637(18)
C38 0.0784(13) 0.0944(16) 0.0727(12) -0.0068(11) 0.0255(10) -0.0347(12)
C39 0.0495(7) 0.0371(7) 0.0461(7) -0.0019(6) 0.0146(6) -0.0020(6)
C40 0.0898(12) 0.0398(8) 0.0571(10) -0.0016(7) 0.0241(9) 0.0052(8)
C41 0.1103(16) 0.0504(10) 0.0700(12) -0.0198(9) 0.0315(12) -0.0044(10)
C42 0.0833(13) 0.0762(13) 0.0568(10) -0.0199(10) 0.0105(9) -0.0085(10)
C43 0.0791(12) 0.0705(12) 0.0567(10) -0.0022(9) -0.0061(9) 0.0033(10)
C44 0.0680(10) 0.0443(8) 0.0565(9) -0.0039(7) -0.0020(8) 0.0057(7)

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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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O1 C9 1.444(2) . ?
O2 C8 1.2042(19) . ?
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C15 C16 1.375(3) . ?
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C5 C6 C1 119.23(14) . . ?
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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
 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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P2 P 0.69604(2) 0.28308(3) 1.082497(17) 0.03027(8) Uani 1 1 d . . .
O1 O 0.55055(6) 0.28796(7) 0.98816(5) 0.0362(2) Uani 1 1 d . . .
O2 O 0.42784(7) 0.31955(9) 1.03181(7) 0.0490(3) Uani 1 1 d . . .
O3 O 0.59106(6) 0.13305(8) 0.91518(5) 0.0385(2) Uani 1 1 d . . .
O4 O 0.57622(9) 0.14899(11) 0.80585(6) 0.0563(3) Uani 1 1 d . . .
N1 N 0.56937(7) 0.12033(9) 1.04683(6) 0.0336(2) Uani 1 1 d . . .
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N3 N 0.69964(8) 0.27450(9) 0.92857(6) 0.0340(2) Uani 1 1 d . . .
N4 N 0.66861(9) 0.25450(11) 0.86289(6) 0.0428(3) Uani 1 1 d . . .
C1 C 0.63948(10) -0.04247(11) 1.06904(8) 0.0397(3) Uani 1 1 d . . .
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C4 C 0.75532(17) -0.20184(16) 1.07046(14) 0.0751(7) Uani 1 1 d . . .
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C5 C 0.68055(16) -0.20960(15) 1.10406(13) 0.0710(6) Uani 1 1 d . . .
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C9 C 0.36647(12) 0.29514(15) 1.08140(13) 0.0640(6) Uani 1 1 d . . .
H9A H 0.3952 0.2860 1.1252 0.077 Uiso 1 1 calc R . .
H9B H 0.3362 0.2342 1.0691 0.077 Uiso 1 1 calc R . .
C10 C 0.30561(16) 0.3812(2) 1.08257(18) 0.0966(10) Uani 1 1 d . . .
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C12 C 0.89224(12) 0.05194(19) 1.07848(10) 0.0624(5) Uani 1 1 d . . .
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C14 C 1.02382(13) 0.1384(2) 1.06910(14) 0.0813(8) Uani 1 1 d . . .
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C15 C 0.98880(14) 0.19291(18) 1.01569(14) 0.0701(6) Uani 1 1 d . . .
H15 H 1.0213 0.2409 0.9951 0.084 Uiso 1 1 calc R . .
C16 C 0.90412(11) 0.17550(14) 0.99279(11) 0.0530(4) Uani 1 1 d . . .
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C17 C 0.75537(10) 0.02846(11) 0.90575(8) 0.0386(3) Uani 1 1 d . . .
C18 C 0.81645(12) 0.06013(17) 0.86287(9) 0.0569(5) Uani 1 1 d . . .
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C20 C 0.76021(17) -0.0514(2) 0.77756(11) 0.0764(7) Uani 1 1 d . . .
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C21 C 0.69749(17) -0.08081(16) 0.81866(11) 0.0681(6) Uani 1 1 d . . .
H21 H 0.6569 -0.1274 0.8035 0.082 Uiso 1 1 calc R . .
C22 C 0.69446(12) -0.04132(13) 0.88266(9) 0.0509(4) Uani 1 1 d . . .
H22 H 0.6517 -0.0613 0.9104 0.061 Uiso 1 1 calc R . .
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C24 C 0.77867(9) 0.36941(11) 1.05942(7) 0.0351(3) Uani 1 1 d . . .
C25 C 0.81824(11) 0.42638(13) 1.11077(9) 0.0470(4) Uani 1 1 d . . .
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C31 C 0.60675(18) 0.1886(2) 0.74416(10) 0.0747(7) Uani 1 1 d . . .
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H31B H 0.5921 0.2587 0.7396 0.090 Uiso 1 1 calc R . .
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H32B H 0.5037 0.1364 0.6897 0.159 Uiso 1 1 calc R . .
H32C H 0.5802 0.0610 0.6930 0.159 Uiso 1 1 calc R . .
C33 C 0.61935(9) 0.37022(11) 1.11648(7) 0.0347(3) Uani 1 1 d . . .
C34 C 0.58396(11) 0.35816(13) 1.17858(9) 0.0470(4) Uani 1 1 d . . .
H34 H 0.5992 0.3036 1.2054 0.056 Uiso 1 1 calc R . .
C35 C 0.52575(13) 0.42793(15) 1.20040(10) 0.0592(5) Uani 1 1 d . . .
H35 H 0.5021 0.4195 1.2418 0.071 Uiso 1 1 calc R . .
C36 C 0.50299(12) 0.50890(15) 1.16154(11) 0.0570(5) Uani 1 1 d . . .
H36 H 0.4636 0.5547 1.1764 0.068 Uiso 1 1 calc R . .
C37 C 0.53837(12) 0.52248(13) 1.10047(10) 0.0517(4) Uani 1 1 d . . .
H37 H 0.5232 0.5777 1.0743 0.062 Uiso 1 1 calc R . .
C38 C 0.59647(10) 0.45410(12) 1.07810(8) 0.0421(3) Uani 1 1 d . . .
H38 H 0.6206 0.4641 1.0370 0.051 Uiso 1 1 calc R . .
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C39 C 0.73811(10) 0.20957(11) 1.15322(7) 0.0373(3) Uani 1 1 d . . .
C40 C 0.68150(11) 0.14820(12) 1.18597(8) 0.0452(3) Uani 1 1 d . . .
H40 H 0.6240 0.1468 1.1718 0.054 Uiso 1 1 calc R . .
C41 C 0.71069(14) 0.08937(15) 1.23948(9) 0.0575(5) Uani 1 1 d . . .
H41 H 0.6728 0.0481 1.2607 0.069 Uiso 1 1 calc R . .
C42 C 0.79552(15) 0.09167(17) 1.26138(10) 0.0646(5) Uani 1 1 d . . .
H42 H 0.8148 0.0526 1.2976 0.077 Uiso 1 1 calc R . .
C43 C 0.85173(13) 0.15206(19) 1.22934(10) 0.0644(5) Uani 1 1 d . . .
H43 H 0.9090 0.1536 1.2442 0.077 Uiso 1 1 calc R . .
C44 C 0.82385(11) 0.21041(15) 1.17539(9) 0.0500(4) Uani 1 1 d . . .
H44 H 0.8625 0.2503 1.1538 0.060 Uiso 1 1 calc R . .
B1 B 0.4750(2) 0.2035(3) 0.32032(18) 0.0831(9) Uani 1 1 d . . .
F4 F 0.51382(17) 0.1506(2) 0.27533(13) 0.1622(10) Uani 1 1 d . A .
F1 F 0.5366(5) 0.2613(8) 0.3415(3) 0.261(5) Uani 0.705(7) 1 d P A 1
F2 F 0.4142(3) 0.2513(3) 0.2845(2) 0.141(2) Uani 0.705(7) 1 d P A 1
F3 F 0.4455(5) 0.1432(5) 0.3643(4) 0.216(5) Uani 0.705(7) 1 d P A 1
F12 F 0.4736(11) 0.3063(6) 0.3288(7) 0.165(8) Uani 0.295(7) 1 d P A 2
F11 F 0.5076(15) 0.1888(12) 0.3828(5) 0.204(9) Uani 0.295(7) 1 d P A 2
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0.00344(13)
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0.00016(12)
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N2 0.0302(6) 0.0403(6) 0.0561(8) 0.0042(6) 0.0119(5) 0.0018(5)
N3 0.0353(6) 0.0381(6) 0.0290(5) 0.0027(4) 0.0042(4) 0.0011(5)
N4 0.0484(7) 0.0511(8) 0.0287(6) 0.0033(5) -0.0001(5) -0.0047(6)
C1 0.0411(7) 0.0359(7) 0.0419(8) 0.0070(6) 0.0008(6) -0.0013(6)
C2 0.0465(8) 0.0360(7) 0.0415(8) 0.0059(6) 0.0059(6) 0.0065(6)
C3 0.0650(12) 0.0502(10) 0.0689(12) 0.0130(9) 0.0178(9) 0.0212(9)
C4 0.0834(16) 0.0497(11) 0.0936(17) 0.0230(11) 0.0163(13) 0.0260(10)
C5 0.0796(15) 0.0472(10) 0.0863(16) 0.0306(10) 0.0070(12) 0.0082(10)
C6 0.0555(10) 0.0472(9) 0.0640(11) 0.0194(8) 0.0052(8) -0.0012(8)
C7 0.0343(7) 0.0380(7) 0.0469(8) 0.0070(6) 0.0066(6) -0.0044(6)
C8 0.0293(6) 0.0387(7) 0.0461(8) -0.0006(6) 0.0035(5) 0.0021(5)
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C11 0.0325(7) 0.0525(9) 0.0476(8) -0.0099(7) 0.0023(6) 0.0089(6)
C12 0.0452(9) 0.0880(15) 0.0534(10) 0.0012(10) -0.0012(8) 0.0135(10)
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C16 0.0395(8) 0.0490(9) 0.0705(12) -0.0106(8) 0.0018(8) 0.0009(7)
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F31 0.185(13) 0.187(15) 0.32(2) -0.064(14) 0.188(14) -0.064(11)

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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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loop_
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