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Synthesis, spectroscopic and electrochemical properties of mononuclear and dinuclear bis(bipy)ruthenium(II) complexes containing dimethoxyphenyl(pyridin-2-yl)-1,2,4-triazole ligands

Passaniti, Paolo; Browne, Wesley R.; Lynch, Fiona C.; Hughes, Donal; Nieuwenhuyzen, Mark; James, Paraic; Maestri, Mauro; Vos, Johannes G.

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'Browne, Wesley R.'

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'Lynch, Fiona C.'

'Maestri, M.'

'Nieuwenhuyzen, Mark'

'Passaniti, P.'

'Vos, J.'

_publ_contact_author_name 'Dr J Vos'

_publ_contact_author_address

;

Dr J Vos

School of Chemical Sciences

Dublin City University

Dublin

9

IRELAND

;

_publ_contact_author_email 'JOHANNES.VOS@DCU.IE'

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Synthesis, spectroscopic and electrochemical properties of
mononuclear and dinuclear bis(bipy)ruthenium(II) complexes containing
dimethoxyphenyl-(pyridin-2-yl)1,2,4-triazole ligands.

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on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 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	N	0.1616(6)	0.2807(5)	0.1614(4)	0.0368(15)	Uani	1	1	d	.	.	.	.
C2	C	0.1715(8)	0.1671(7)	0.1783(6)	0.046(2)	Uani	1	1	d	.	.	.	.
H2	H	0.1641	0.1223	0.2372	0.055	Uiso	1	1	calc	R	.	.	.
C3	C	0.1918(9)	0.1146(8)	0.1132(6)	0.055(2)	Uani	1	1	d	.	.	.	.
H3	H	0.1991	0.0354	0.1283	0.066	Uiso	1	1	calc	R	.	.	.
C4	C	0.2014(9)	0.1792(8)	0.0257(7)	0.056(2)	Uani	1	1	d	.	.	.	.
H4	H	0.2159	0.1442	-0.0191	0.067	Uiso	1	1	calc	R	.	.	.
C5	C	0.1892(8)	0.2978(8)	0.0047(6)	0.047(2)	Uani	1	1	d	.	.	.	.
H5	H	0.1942	0.3440	-0.0545	0.057	Uiso	1	1	calc	R	.	.	.
C6	C	0.1694(7)	0.3455(7)	0.0735(5)	0.0373(18)	Uani	1	1	d	.	.	.	.
C7	C	0.1515(7)	0.4726(7)	0.0584(5)	0.0346(17)	Uani	1	1	d	.	.	.	.
C8	C	0.1578(8)	0.5520(8)	-0.0249(5)	0.046(2)	Uani	1	1	d	.	.	.	.
H8	H	0.1743	0.5271	-0.0750	0.055	Uiso	1	1	calc	R	.	.	.
C9	C	0.1397(9)	0.6688(8)	-0.0335(6)	0.053(2)	Uani	1	1	d	.	.	.	.
H9	H	0.1441	0.7231	-0.0892	0.064	Uiso	1	1	calc	R	.	.	.
C10	C	0.1145(8)	0.7036(8)	0.0429(6)	0.051(2)	Uani	1	1	d	.	.	.	.
H10	H	0.1023	0.7814	0.0393	0.062	Uiso	1	1	calc	R	.	.	.
C11	C	0.1082(7)	0.6203(7)	0.1238(6)	0.0431(19)	Uani	1	1	d	.	.	.	.
H11	H	0.0889	0.6452	0.1739	0.052	Uiso	1	1	calc	R	.	.	.
N12	N	0.1285(6)	0.5040(5)	0.1349(4)	0.0354(14)	Uani	1	1	d	.	.	.	.
N13	N	0.1510(6)	0.4567(5)	0.3375(4)	0.0389(15)	Uani	1	1	d	.	.	.	.
C14	C	0.0464(9)	0.5309(7)	0.3666(6)	0.050(2)	Uani	1	1	d	.	.	.	.
H14	H	-0.0349	0.5423	0.3486	0.060	Uiso	1	1	calc	R	.	.	.
C15	C	0.0571(10)	0.5896(8)	0.4219(6)	0.056(2)	Uani	1	1	d	.	.	.	.
H15	H	-0.0164	0.6414	0.4399	0.067	Uiso	1	1	calc	R	.	.	.
C16	C	0.1776(11)	0.5711(8)	0.4506(6)	0.061(3)	Uani	1	1	d	.	.	.	.
H16	H	0.1864	0.6093	0.4889	0.073	Uiso	1	1	calc	R	.	.	.
C17	C	0.2848(9)	0.4955(8)	0.4219(6)	0.055(2)	Uani	1	1	d	.	.	.	.
H17	H	0.3669	0.4816	0.4408	0.066	Uiso	1	1	calc	R	.	.	.
C18	C	0.2683(7)	0.4409(7)	0.3650(5)	0.0384(18)	Uani	1	1	d	.	.	.	.
C19	C	0.3762(7)	0.3644(7)	0.3255(5)	0.0380(18)	Uani	1	1	d	.	.	.	.
C20	C	0.5012(8)	0.3457(8)	0.3380(6)	0.054(2)	Uani	1	1	d	.	.	.	.
H20	H	0.5229	0.3786	0.3755	0.065	Uiso	1	1	calc	R	.	.	.
C21	C	0.5928(9)	0.2792(8)	0.2956(7)	0.058(2)	Uani	1	1	d	.	.	.	.
H21	H	0.6773	0.2662	0.3041	0.070	Uiso	1	1	calc	R	.	.	.
C22	C	0.5592(8)	0.2316(8)	0.2404(6)	0.055(2)	Uani	1	1	d	.	.	.	.
H22	H	0.6199	0.1875	0.2096	0.066	Uiso	1	1	calc	R	.	.	.
C23	C	0.4342(7)	0.2502(7)	0.2314(5)	0.046(2)	Uani	1	1	d	.	.	.	.
H23	H	0.4135	0.2140	0.1962	0.055	Uiso	1	1	calc	R	.	.	.
N24	N	0.3402(6)	0.3174(5)	0.2702(4)	0.0355(14)	Uani	1	1	d	.	.	.	.
N25	N	0.1649(6)	0.2146(5)	0.3723(4)	0.0386(15)	Uani	1	1	d	.	.	.	.
C26	C	0.2754(8)	0.1174(7)	0.4247(6)	0.047(2)	Uani	1	1	d	.	.	.	.

H26 H 0.3538 0.1102 0.4060 0.056 Uiso 1 1 calc R . . .
C27 C 0.2773(9) 0.0283(8) 0.5046(6) 0.059(2) Uani 1 1 d . . .
H27 H 0.3559 -0.0376 0.5393 0.071 Uiso 1 1 calc R . . .
C28 C 0.1628(9) 0.0369(8) 0.5329(6) 0.054(2) Uani 1 1 d . . .
H28 H 0.1632 -0.0223 0.5876 0.065 Uiso 1 1 calc R . . .
C29 C 0.0490(9) 0.1324(8) 0.4808(6) 0.052(2) Uani 1 1 d . . .
H29 H -0.0293 0.1382 0.4987 0.063 Uiso 1 1 calc R . . .
C30 C 0.0505(7) 0.2211(7) 0.4005(5) 0.0386(18) Uani 1 1 d . . .
C31 C -0.0620(7) 0.3306(7) 0.3379(5) 0.0360(18) Uani 1 1 d . . .
N32 N -0.0432(6) 0.4060(5) 0.2624(4) 0.0317(14) Uani 1 1 d . . .
N33 N -0.1623(6) 0.5042(6) 0.2197(4) 0.0386(15) Uani 1 1 d . . .
C34 C -0.2447(7) 0.4793(7) 0.2739(5) 0.0371(18) Uani 1 1 d . . .
N35 N -0.1880(6) 0.3714(6) 0.3492(4) 0.0405(15) Uani 1 1 d . . .
C36 C -0.3856(7) 0.5682(7) 0.2605(5) 0.0410(19) Uani 1 1 d . . .
C37 C -0.4363(7) 0.5914(8) 0.3364(6) 0.044(2) Uani 1 1 d . . .
H37 H -0.3823 0.5488 0.3931 0.053 Uiso 1 1 calc R . . .
C38 C -0.5636(8) 0.6750(8) 0.3315(6) 0.048(2) Uani 1 1 d . . .
C39 C -0.6459(8) 0.7349(9) 0.2493(7) 0.061(3) Uani 1 1 d . . .
H39 H -0.7327 0.7905 0.2454 0.073 Uiso 1 1 calc R . . .
C40 C -0.5978(8) 0.7114(9) 0.1715(7) 0.065(3) Uani 1 1 d . . .
H40 H -0.6531 0.7523 0.1155 0.078 Uiso 1 1 calc R . . .
C41 C -0.4681(8) 0.6273(9) 0.1766(6) 0.054(2) Uani 1 1 d . . .
O42 O -0.6005(6) 0.6893(6) 0.4128(5) 0.0686(18) Uani 1 1 d . . .
C43 C -0.7124(10) 0.8002(10) 0.4075(9) 0.086(4) Uani 1 1 d . . .
H43A H -0.7270 0.7984 0.4686 0.129 Uiso 1 1 calc R . . .
H43B H -0.7860 0.8064 0.3761 0.129 Uiso 1 1 calc R . . .
H43C H -0.7000 0.8712 0.3741 0.129 Uiso 1 1 calc R . . .
O44 O -0.4149(6) 0.6000(7) 0.1034(4) 0.077(2) Uani 1 1 d . . .
C45 C -0.4997(12) 0.6575(16) 0.0180(8) 0.130(6) Uani 1 1 d . . .
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H45B H -0.5385 0.7468 -0.0013 0.195 Uiso 1 1 calc R . . .
H45C H -0.5663 0.6326 0.0257 0.195 Uiso 1 1 calc R . . .
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H2SB H -0.2347 0.7920 0.3472 0.179 Uiso 1 1 calc R . . .
H2SC H -0.2999 0.7059 0.3616 0.179 Uiso 1 1 calc R . . .
C3S C -0.4287(15) 0.9069(15) 0.1974(10) 0.124(5) Uiso 1 1 d . . .
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C3 0.066(6) 0.041(5) 0.065(6) -0.025(5) 0.009(5) -0.028(5)
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C9 0.060(6) 0.041(5) 0.051(5) -0.007(4) 0.015(4) -0.026(4)
C10 0.057(6) 0.037(5) 0.058(6) -0.010(4) 0.009(4) -0.026(4)
C11 0.043(5) 0.035(4) 0.051(5) -0.022(4) 0.004(4) -0.013(4)
N12 0.032(3) 0.031(3) 0.044(4) -0.016(3) 0.008(3) -0.014(3)
N13 0.044(4) 0.031(3) 0.035(3) -0.010(3) 0.006(3) -0.014(3)
C14 0.054(5) 0.040(5) 0.052(5) -0.021(4) 0.014(4) -0.016(4)
C15 0.072(7) 0.048(5) 0.057(5) -0.032(5) 0.020(5) -0.028(5)
C16 0.095(8) 0.051(5) 0.048(5) -0.024(4) 0.008(5) -0.039(6)
C17 0.062(6) 0.058(6) 0.055(5) -0.022(5) 0.008(5) -0.036(5)
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C43 0.069(7) 0.075(7) 0.121(10) -0.064(7) 0.040(7) -0.020(6)
O44 0.045(4) 0.118(6) 0.056(4) -0.041(4) 0.009(3) -0.023(4)
C45 0.069(8) 0.213(17) 0.066(8) -0.061(10) -0.004(6) -0.026(10)
P1 0.0534(17) 0.0439(16) 0.079(2) -0.0193(13) 0.0194(13) -0.0233(13)
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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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N25	C26	C27	122.7(8)	.	.	?
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C28	C29	C30	119.4(8)	.	.	?
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C29	C30	C31	126.5(7)	.	.	?
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F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 are statistically about twice as large as those based on F, and R-
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H21B H 0.1272 -0.0908 1.0822 0.129 Uiso 1 1 calc R . .
H21C H 0.1971 -0.0158 1.1140 0.129 Uiso 1 1 calc R . .
N1B N 0.0313(4) -0.1768(2) 0.9166(3) 0.0476(11) Uani 1 1 d . . .
C2B C -0.0781(5) -0.1718(3) 0.9501(4) 0.0619(16) Uani 1 1 d . . .
H2B H -0.1340 -0.1338 0.9285 0.074 Uiso 1 1 calc R . .
C3B C -0.1135(5) -0.2191(3) 1.0145(4) 0.0651(17) Uani 1 1 d . . .
H3B H -0.1911 -0.2131 1.0360 0.078 Uiso 1 1 calc R . .
C4B C -0.0326(5) -0.2755(3) 1.0465(4) 0.0622(16) Uani 1 1 d . . .
H4B H -0.0540 -0.3087 1.0901 0.075 Uiso 1 1 calc R . .
C5B C 0.0812(5) -0.2819(3) 1.0130(3) 0.0490(13) Uani 1 1 d . . .
H5B H 0.1381 -0.3196 1.0339 0.059 Uiso 1 1 calc R . .
C6B C 0.1101(4) -0.2320(2) 0.9482(3) 0.0362(11) Uani 1 1 d . . .
C7B C 0.2305(4) -0.2365(3) 0.9099(3) 0.0345(11) Uani 1 1 d . . .
N8B N 0.3011(4) -0.2981(2) 0.9172(3) 0.0491(11) Uani 1 1 d . . .
N9B N 0.3999(4) -0.2781(2) 0.8737(3) 0.0441(10) Uani 1 1 d . . .
H9B H 0.4705 -0.3206 0.8608 0.053 Uiso 1 1 d R . .
N10B N 0.2772(3) -0.1791(2) 0.8641(2) 0.0341(9) Uani 1 1 d . . .
C11B C 0.3853(4) -0.2072(2) 0.8418(3) 0.0344(11) Uani 1 1 d . . .
C12B C 0.4734(4) -0.1633(2) 0.7949(3) 0.0344(11) Uani 1 1 d . . .
C13B C 0.4367(4) -0.0915(3) 0.7659(3) 0.0393(12) Uani 1 1 d . . .
H13B H 0.3575 -0.0736 0.7757 0.047 Uiso 1 1 calc R . .
C14B C 0.5154(5) -0.0459(3) 0.7225(3) 0.0411(12) Uani 1 1 d . . .
C15B C 0.6342(5) -0.0714(3) 0.7103(3) 0.0534(14) Uani 1 1 d . . .
H15B H 0.6886 -0.0407 0.6826 0.064 Uiso 1 1 calc R . .
C16B C 0.6719(5) -0.1426(3) 0.7393(4) 0.0557(15) Uani 1 1 d . . .
H16B H 0.7528 -0.1593 0.7322 0.067 Uiso 1 1 calc R . .
C17B C 0.5915(5) -0.1897(3) 0.7788(3) 0.0470(13) Uani 1 1 d . . .
O18B O 0.4652(4) 0.0226(2) 0.6935(3) 0.0657(11) Uani 1 1 d . . .
C19B C 0.5334(6) 0.0671(4) 0.6411(5) 0.103(3) Uani 1 1 d . . .
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H19E H 0.5488 0.0394 0.5887 0.155 Uiso 1 1 calc R . .
H19F H 0.6125 0.0808 0.6746 0.155 Uiso 1 1 calc R . .
O20B O 0.6216(4) -0.2613(2) 0.8068(3) 0.0786(13) Uani 1 1 d . . .
C21B C 0.7210(6) -0.2988(4) 0.7715(5) 0.101(3) Uani 1 1 d . . .
H21D H 0.8004 -0.2785 0.7979 0.152 Uiso 1 1 calc R . .
H21E H 0.7128 -0.2916 0.7078 0.152 Uiso 1 1 calc R . .
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C3A 0.049(3) 0.070(4) 0.051(3) -0.006(3) -0.020(3) 0.007(3)
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C5A 0.035(3) 0.042(3) 0.046(3) -0.008(2) 0.003(2) -0.010(2)
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N8A 0.038(2) 0.042(2) 0.048(3) 0.002(2) -0.006(2) -0.008(2)
N9A 0.041(2) 0.041(3) 0.045(3) 0.008(2) -0.002(2) -0.002(2)
N10A 0.036(2) 0.034(2) 0.037(2) 0.0005(19) -0.0033(18) -0.0055(19)
C11A 0.034(3) 0.036(3) 0.038(3) -0.001(2) 0.001(2) 0.006(2)
C12A 0.037(3) 0.045(3) 0.036(3) -0.002(2) -0.005(2) 0.011(2)
C13A 0.047(3) 0.049(3) 0.048(3) -0.001(3) -0.007(3) -0.001(3)
C14A 0.044(3) 0.066(4) 0.057(4) -0.004(3) -0.010(3) -0.005(3)
C15A 0.056(4) 0.084(5) 0.052(4) -0.008(3) -0.013(3) -0.001(3)
C16A 0.068(4) 0.073(4) 0.035(3) -0.001(3) -0.012(3) 0.017(3)
C17A 0.051(3) 0.048(3) 0.037(3) 0.000(3) -0.001(3) 0.011(3)
O18A 0.067(3) 0.113(4) 0.097(3) 0.029(3) -0.030(3) -0.037(3)
C19A 0.105(6) 0.106(6) 0.097(6) 0.014(5) 0.007(5) -0.029(5)
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C6B 0.039(3) 0.032(3) 0.037(3) -0.001(2) 0.003(2) -0.007(2)
C7B 0.028(3) 0.037(3) 0.038(3) 0.003(2) 0.001(2) 0.000(2)
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C15B 0.043(3) 0.065(4) 0.053(3) 0.009(3) 0.008(3) -0.011(3)
C16B 0.031(3) 0.072(4) 0.066(4) 0.010(3) 0.012(3) 0.006(3)
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C19B 0.084(5) 0.078(5) 0.150(7) 0.059(5) 0.021(5) -0.013(4)
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C21B 0.090(5) 0.082(5) 0.143(7) 0.033(5) 0.061(5) 0.053(4)

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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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 O18A C14A C15A 116.3(5) . . ?
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Refinement of F2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F2, conventional R-factors R are based on F, with F set to zero for negative F2. The threshold expression of F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F2 are statistically about twice as large as those based on F, and R-

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factors based on ALL data will be even larger.

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C2 C -0.3419(7) 1.0630(5) -0.3973(5) 0.0511(18) Uani 1 1 d . . .
H2 H -0.3186 1.0612 -0.4972 0.061 Uiso 1 1 d R . .
C3 C -0.4262(6) 1.1516(4) -0.3665(5) 0.0399(14) Uani 1 1 d . . .
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C4 C -0.4620(6) 1.1470(5) -0.2437(5) 0.0377(14) Uani 1 1 d . . .
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C5 C -0.4169(5) 1.0535(4) -0.1579(5) 0.0281(13) Uani 1 1 d . . .
H5 H -0.4254 1.0396 -0.0564 0.034 Uiso 1 1 d R . .
C6 C -0.3318(5) 0.9678(4) -0.1971(4) 0.0228(12) Uani 1 1 d . . .
C7 C -0.2719(5) 0.8688(4) -0.1058(4) 0.0233(12) Uani 1 1 d . . .
N8 N -0.2796(4) 0.8651(3) 0.0244(4) 0.0231(10) Uani 1 1 d . . .
N9 N -0.2032(4) 0.7658(3) 0.0724(3) 0.0230(10) Uani 1 1 d . . .
H9 H -0.1888 0.7422 0.1830 0.028 Uiso 1 1 d R . .
C10 C -0.1564(5) 0.7149(4) -0.0278(4) 0.0211(12) Uani 1 1 d . . .
N11 N -0.2004(4) 0.7785(3) -0.1443(3) 0.0202(10) Uani 1 1 d . . .
C12 C -0.0747(5) 0.6055(4) -0.0131(4) 0.0215(12) Uani 1 1 d . . .
C13 C -0.0998(5) 0.5318(4) -0.1266(5) 0.0204(12) Uani 1 1 d . . .
H13 H -0.1862 0.5590 -0.2264 0.025 Uiso 1 1 d R . .
C14 C 0.0263(5) 0.5740(4) 0.1142(4) 0.0229(12) Uani 1 1 d . . .
O15 O 0.0482(4) 0.6536(3) 0.2173(3) 0.0319(9) Uani 1 1 d . . .
```

```

C16 C 0.1358(6) 0.6192(5) 0.3532(4) 0.0434(16) Uani 1 1 d . . .
H16A H 0.2498 0.6020 0.3457 0.052 Uiso 1 1 d R . .
H16B H 0.0681 0.5418 0.3802 0.052 Uiso 1 1 d R . .
H16C H 0.1396 0.7016 0.4086 0.052 Uiso 1 1 d R . .

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_atom_site_aniso_U_12
N1 0.054(3) 0.037(3) 0.036(3) 0.010(2) 0.026(2) 0.013(3)
C2 0.071(5) 0.049(4) 0.041(3) 0.025(3) 0.028(3) 0.026(4)
C3 0.049(4) 0.032(3) 0.038(3) 0.014(3) 0.011(3) 0.016(3)
C4 0.044(4) 0.029(3) 0.040(3) 0.002(3) 0.011(3) 0.006(3)
C5 0.035(3) 0.025(3) 0.026(3) 0.000(2) 0.010(3) 0.008(3)
C6 0.022(3) 0.024(3) 0.020(3) 0.001(2) 0.003(2) 0.005(3)
C7 0.027(3) 0.026(3) 0.018(3) 0.000(2) 0.007(2) -0.002(3)
N8 0.027(3) 0.020(2) 0.023(2) 0.000(2) 0.0074(19) 0.003(2)
N9 0.031(3) 0.021(2) 0.018(2) 0.0015(19) 0.0091(19) 0.007(2)
C10 0.024(3) 0.020(3) 0.021(3) -0.001(2) 0.008(2) -0.001(3)
N11 0.031(3) 0.016(2) 0.017(2) -0.002(2) 0.0116(19) 0.000(2)
C12 0.025(3) 0.021(3) 0.022(3) -0.001(2) 0.012(2) 0.000(3)
C13 0.025(3) 0.018(3) 0.017(3) 0.006(2) 0.003(2) 0.004(3)
C14 0.030(3) 0.022(3) 0.018(3) -0.003(2) 0.008(2) -0.005(3)
O15 0.042(2) 0.025(2) 0.0233(18) -0.0053(17) 0.0007(17) 0.0124(18)
C16 0.053(4) 0.042(4) 0.026(3) -0.010(3) -0.005(3) 0.015(3)

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_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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N1 C2 1.348(6) . ?
C2 C3 1.380(7) . ?
C3 C4 1.372(7) . ?
C4 C5 1.380(6) . ?
C5 C6 1.395(6) . ?
C6 C7 1.480(6) . ?
C7 N8 1.338(5) . ?
C7 N11 1.356(5) . ?
N8 N9 1.369(5) . ?
N9 C10 1.344(5) . ?
C10 N11 1.350(5) . ?
C10 C12 1.466(6) . ?
C12 C13 1.397(6) . ?
C12 C14 1.406(6) . ?

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C13 C14 1.394(6) 3_565 ?
 C14 O15 1.365(5) . ?
 C14 C13 1.394(6) 3_565 ?
 O15 C16 1.439(5) . ?

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 _geom_angle_atom_site_label_2
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 _geom_angle_site_symmetry_3
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C6 N1 C2 116.8(5) . . ?
 N1 C2 C3 124.1(5) . . ?
 C4 C3 C2 118.0(5) . . ?
 C3 C4 C5 119.4(5) . . ?
 C4 C5 C6 118.7(4) . . ?
 N1 C6 C5 122.9(4) . . ?
 N1 C6 C7 115.7(4) . . ?
 C5 C6 C7 121.4(4) . . ?
 N8 C7 N11 115.0(4) . . ?
 N8 C7 C6 121.5(4) . . ?
 N11 C7 C6 123.5(4) . . ?
 C7 N8 N9 102.1(3) . . ?
 C10 N9 N8 110.4(3) . . ?
 N9 C10 N11 109.4(4) . . ?
 N9 C10 C12 124.9(4) . . ?
 N11 C10 C12 125.7(4) . . ?
 C10 N11 C7 103.1(3) . . ?
 C13 C12 C14 120.2(4) . . ?
 C13 C12 C10 119.2(4) . . ?
 C14 C12 C10 120.6(4) . . ?
 C14 C13 C12 120.3(4) 3_565 . ?
 O15 C14 C13 124.6(4) . 3_565 ?
 O15 C14 C12 115.9(4) . . ?
 C13 C14 C12 119.5(4) 3_565 . ?
 C14 O15 C16 117.4(4) . . ?

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