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Assessment of intercomponent interaction in phenylene bridged dinuclear ruthenium(II) and osmium(II) polypyridyl complexes

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Published in:
Dalton Transactions

DOI:
[10.1039/b409189b](https://doi.org/10.1039/b409189b)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2004

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Guckian, A. L., Doering, M., Ciesielski, M., Walter, O., Hjelm, J., O'Boyle, N. M., Henry, W., Browne, W. R., McGarvey, J. J., & Vos, J. G. (2004). Assessment of intercomponent interaction in phenylene bridged dinuclear ruthenium(II) and osmium(II) polypyridyl complexes. *Dalton Transactions*, (23), 3943-3949. <https://doi.org/10.1039/b409189b>

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Supplementary Material (ESI) for Dalton Transactions
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data_global
_journal_name_full      'Dalton Trans.'
# 1. SUBMISSION DETAILS

_journal_codename_Cambridge 0222

_publ_contact_author_name  'Prof. Johannes G. Vos'
_publ_contact_author_address
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Prof. Johannes G. Vos
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_publ_requested_coeditor_name ?

_publ_contact_letter
;
?
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3. TITLE AND AUTHOR LIST

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;
Electrochemical Tuning of Multiple Emission from Phenyl Bridged
Dinuclear Ruthenium(II) & Osmium(II) containing complexes.
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loop_
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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-
factors based on ALL data will be even larger.
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F23 F -0.1337(5) 0.4616(5) 0.4861(3) 0.120(3) Uani 0.70 d PD . . .
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H34	H	0.5128	0.4307	0.4668	0.059(7)	Uiso	1	calc	R	.	.	.
C35	C	0.4879(4)	0.4270(2)	0.5557(2)	0.0367(13)	Uani	1	d	.	.	.	.
C36	C	0.5785(3)	0.4153(2)	0.5872(2)	0.0331(12)	Uani	1	d	.	.	.	.
C37	C	0.6553(4)	0.4084(2)	0.5573(3)	0.0485(16)	Uani	1	d	.	.	.	.
H37	H	0.6512	0.4102	0.5144	0.059(7)	Uiso	1	calc	R	.	.	.
C38	C	0.7355(4)	0.3992(3)	0.5913(3)	0.0548(17)	Uani	1	d	.	.	.	.
H38	H	0.7866	0.3946	0.5717	0.059(7)	Uiso	1	calc	R	.	.	.
C39	C	0.7415(4)	0.3967(3)	0.6543(3)	0.0523(17)	Uani	1	d	.	.	.	.
H39	H	0.7965	0.3904	0.6776	0.059(7)	Uiso	1	calc	R	.	.	.
C40	C	0.6658(4)	0.4036(2)	0.6825(3)	0.0419(14)	Uani	1	d	.	.	.	.
H40	H	0.6705	0.4016	0.7254	0.059(7)	Uiso	1	calc	R	.	.	.
C41	C	0.5227(4)	0.4398(2)	0.8232(2)	0.0368(13)	Uani	1	d	.	.	.	.
H41	H	0.5162	0.4769	0.8134	0.051(6)	Uiso	1	calc	R	.	.	.
C42	C	0.5460(4)	0.4258(2)	0.8836(3)	0.0440(15)	Uani	1	d	.	.	.	.
H42	H	0.5550	0.4528	0.9139	0.051(6)	Uiso	1	calc	R	.	.	.
C43	C	0.5556(5)	0.3718(3)	0.8987(3)	0.0578(18)	Uani	1	d	.	.	.	.
H43	H	0.5732	0.3612	0.9393	0.051(6)	Uiso	1	calc	R	.	.	.
C44	C	0.5391(4)	0.3328(3)	0.8528(3)	0.0511(17)	Uani	1	d	.	.	.	.
H44	H	0.5439	0.2956	0.8624	0.051(6)	Uiso	1	calc	R	.	.	.
C45	C	0.5155(4)	0.3492(2)	0.7930(2)	0.0354(13)	Uani	1	d	.	.	.	.
C46	C	0.4942(3)	0.3107(2)	0.7399(2)	0.0322(12)	Uani	1	d	.	.	.	.
C47	C	0.5039(4)	0.2544(2)	0.7438(3)	0.0514(17)	Uani	1	d	.	.	.	.
H47	H	0.5244	0.2382	0.7815	0.051(6)	Uiso	1	calc	R	.	.	.
C48	C	0.4833(4)	0.2220(2)	0.6920(3)	0.0448(15)	Uani	1	d	.	.	.	.
H48	H	0.4894	0.1840	0.6948	0.051(6)	Uiso	1	calc	R	.	.	.
C49	C	0.4537(3)	0.2463(2)	0.6367(3)	0.0373(13)	Uani	1	d	.	.	.	.
H49	H	0.4403	0.2253	0.6011	0.051(6)	Uiso	1	calc	R	.	.	.
C50	C	0.4446(3)	0.3027(2)	0.6351(3)	0.0361(13)	Uani	1	d	.	.	.	.
H50	H	0.4238	0.3192	0.5976	0.051(6)	Uiso	1	calc	R	.	.	.
C51	C	-0.0644(4)	0.1867(2)	0.7204(3)	0.0402(14)	Uani	1	d	.	.	.	.
H51	H	-0.0045	0.1761	0.7239	0.058(7)	Uiso	1	calc	R	.	.	.
C52	C	-0.1082(4)	0.1833(2)	0.7715(3)	0.0488(16)	Uani	1	d	.	.	.	.
H52	H	-0.0784	0.1712	0.8089	0.058(7)	Uiso	1	calc	R	.	.	.
C53	C	-0.1973(5)	0.1981(3)	0.7667(3)	0.0580(18)	Uani	1	d	.	.	.	.
H53	H	-0.2287	0.1961	0.8009	0.058(7)	Uiso	1	calc	R	.	.	.
C54	C	-0.2389(4)	0.2158(2)	0.7108(3)	0.0503(16)	Uani	1	d	.	.	.	.
H54	H	-0.2993	0.2253	0.7066	0.058(7)	Uiso	1	calc	R	.	.	.
C55	C	-0.1911(4)	0.2194(2)	0.6605(3)	0.0367(13)	Uani	1	d	.	.	.	.
C56	C	-0.2288(4)	0.2386(2)	0.5990(3)	0.0376(14)	Uani	1	d	.	.	.	.
C57	C	-0.3189(4)	0.2487(3)	0.5814(3)	0.0541(17)	Uani	1	d	.	.	.	.
H57	H	-0.3599	0.2433	0.6095	0.058(7)	Uiso	1	calc	R	.	.	.
C58	C	-0.3482(4)	0.2665(3)	0.5230(4)	0.062(2)	Uani	1	d	.	.	.	.
H58	H	-0.4089	0.2726	0.5109	0.058(7)	Uiso	1	calc	R	.	.	.
C59	C	-0.2861(4)	0.2752(3)	0.4822(3)	0.0618(19)	Uani	1	d	.	.	.	.
H59	H	-0.3044	0.2883	0.4427	0.058(7)	Uiso	1	calc	R	.	.	.
C60	C	-0.1956(4)	0.2641(2)	0.5007(3)	0.0477(16)	Uani	1	d	.	.	.	.
H60	H	-0.1538	0.2697	0.4732	0.058(7)	Uiso	1	calc	R	.	.	.
C61	C	0.0353(4)	0.2080(3)	0.4652(3)	0.0443(15)	Uani	1	d	.	.	.	.
H61	H	0.0214	0.1709	0.4674	0.046(6)	Uiso	1	calc	R	.	.	.
C62	C	0.0744(4)	0.2267(3)	0.4146(3)	0.0522(17)	Uani	1	d	.	.	.	.
H62	H	0.0867	0.2026	0.3836	0.046(6)	Uiso	1	calc	R	.	.	.
C63	C	0.0948(4)	0.2817(3)	0.4115(3)	0.0562(17)	Uani	1	d	.	.	.	.
H63	H	0.1205	0.2954	0.3779	0.046(6)	Uiso	1	calc	R	.	.	.
C64	C	0.0766(4)	0.3168(3)	0.4586(3)	0.0493(16)	Uani	1	d	.	.	.	.
H64	H	0.0896	0.3540	0.4566	0.046(6)	Uiso	1	calc	R	.	.	.
C65	C	0.0389(3)	0.2958(2)	0.5089(3)	0.0350(13)	Uani	1	d	.	.	.	.

C66 C 0.0205(3) 0.3281(2) 0.5623(2) 0.0328(13) Uani 1 d . . .
 C67 C 0.0345(4) 0.3843(2) 0.5676(3) 0.0456(15) Uani 1 d . . .
 H67 H 0.0541 0.4038 0.5351 0.046(6) Uiso 1 calc R . .
 C68 C 0.0193(4) 0.4112(2) 0.6211(3) 0.0477(16) Uani 1 d . . .
 H68 H 0.0279 0.4489 0.6250 0.046(6) Uiso 1 calc R . .
 C69 C -0.0085(4) 0.3814(2) 0.6681(3) 0.0407(14) Uani 1 d . . .
 H69 H -0.0183 0.3984 0.7049 0.046(6) Uiso 1 calc R . .
 C70 C -0.0220(3) 0.3251(2) 0.6605(3) 0.0333(13) Uani 1 d . . .
 H70 H -0.0421 0.3051 0.6925 0.046(6) Uiso 1 calc R . .
 O100 O 0.1219(3) 0.37021(18) 0.2898(2) 0.0594(12) Uani 1 d . . .
 C100 C 0.1210(4) 0.4169(3) 0.3060(3) 0.0499(16) Uani 1 d . . .
 C101 C 0.1842(7) 0.4386(4) 0.3541(5) 0.171(6) Uani 1 d . . .
 H10A H 0.2254 0.4102 0.3695 0.178(19) Uiso 1 calc R . .
 H10B H 0.1530 0.4520 0.3870 0.178(19) Uiso 1 calc R . .
 H10C H 0.2167 0.4682 0.3381 0.178(19) Uiso 1 calc R . .
 C102 C 0.0528(5) 0.4568(3) 0.2775(4) 0.079(2) Uani 1 d . . .
 H10D H 0.0140 0.4388 0.2454 0.178(19) Uiso 1 calc R . .
 H10E H 0.0825 0.4870 0.2602 0.178(19) Uiso 1 calc R . .
 H10F H 0.0180 0.4702 0.3084 0.178(19) Uiso 1 calc R . .
 O200 O 0.1728(4) 0.1011(2) 0.4684(3) 0.0622(19) Uani 0.70 d P . .
 C200 C 0.2496(5) 0.1091(3) 0.4762(4) 0.0359(19) Uani 0.70 d P . .
 C201 C 0.2877(5) 0.1461(3) 0.5239(3) 0.039(2) Uani 0.70 d P . .
 H20A H 0.2410 0.1599 0.5461 0.023(7) Uiso 0.70 calc PR . .
 H20B H 0.3162 0.1762 0.5055 0.023(7) Uiso 0.70 calc PR . .
 H20C H 0.3311 0.1268 0.5518 0.023(7) Uiso 0.70 calc PR . .
 C202 C 0.3119(6) 0.0837(4) 0.4390(4) 0.066(3) Uani 0.70 d P . .
 H20D H 0.2796 0.0600 0.4089 0.023(7) Uiso 0.70 calc PR . .
 H20E H 0.3551 0.0626 0.4651 0.023(7) Uiso 0.70 calc PR . .
 H20F H 0.3421 0.1117 0.4184 0.023(7) Uiso 0.70 calc PR . .

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Ru1 0.0325(2) 0.0235(2) 0.0243(2) 0.00059(18) 0.00576(17) -0.00060(19)
 Ru2 0.0249(2) 0.0288(2) 0.0327(3) 0.00090(19) 0.00489(18) -0.00047(19)
 P1 0.0678(13) 0.0624(12) 0.0544(12) -0.0035(10) 0.0027(10) -0.0063(10)
 F11 0.115(3) 0.060(3) 0.066(3) -0.012(2) 0.012(2) -0.003(2)
 F12 0.140(4) 0.115(4) 0.094(4) -0.038(3) 0.054(3) -0.062(3)
 F13 0.100(3) 0.132(4) 0.059(3) 0.009(3) 0.003(2) 0.036(3)
 F14 0.095(3) 0.095(3) 0.083(3) -0.038(3) 0.008(3) 0.008(3)
 F15 0.074(3) 0.105(4) 0.173(5) -0.016(3) 0.046(3) -0.024(3)
 F16 0.194(6) 0.067(3) 0.095(4) -0.008(3) -0.060(4) 0.025(3)
 P2 0.0504(11) 0.0666(12) 0.0445(11) 0.0105(9) 0.0055(8) 0.0082(9)
 F21 0.053(3) 0.172(5) 0.111(4) 0.048(3) 0.027(3) 0.026(3)
 F24 0.054(2) 0.088(3) 0.093(3) 0.010(2) 0.016(2) -0.002(2)
 F22 0.062(4) 0.073(5) 0.155(7) 0.059(5) 0.024(4) 0.015(3)
 F23 0.092(5) 0.212(10) 0.052(5) -0.047(5) -0.008(4) 0.019(6)
 F25 0.089(6) 0.082(6) 0.255(12) 0.090(7) -0.036(7) -0.010(5)
 F26 0.149(8) 0.204(11) 0.099(7) -0.112(7) -0.039(5) 0.085(8)
 P3 0.0443(9) 0.0393(9) 0.0364(9) -0.0009(7) 0.0041(7) 0.0054(7)
 F32 0.128(4) 0.050(2) 0.100(3) 0.013(2) -0.043(3) 0.012(3)
 F35 0.109(4) 0.051(2) 0.111(4) 0.002(2) -0.028(3) 0.028(2)
 F31 0.094(4) 0.048(3) 0.066(3) -0.004(3) -0.027(3) -0.024(3)
 F33 0.080(4) 0.168(7) 0.094(5) -0.005(5) 0.057(4) 0.006(5)
 F34 0.114(5) 0.058(3) 0.070(4) -0.012(3) -0.045(4) -0.003(3)
 F36 0.121(6) 0.156(7) 0.110(5) -0.031(5) 0.086(5) -0.045(5)

P4 0.0483(10) 0.0484(11) 0.0727(14) 0.0098(10) -0.0025(9) -0.0024(9)
F41 0.065(3) 0.062(3) 0.113(4) 0.035(2) 0.000(2) -0.001(2)
F44 0.090(3) 0.069(3) 0.118(4) 0.026(3) -0.013(3) 0.018(2)
F42 0.078(5) 0.089(6) 0.213(10) 0.083(6) -0.055(6) -0.054(4)
F43 0.137(6) 0.096(5) 0.026(3) -0.008(3) 0.013(3) 0.042(4)
F45 0.054(3) 0.067(4) 0.056(4) -0.015(3) -0.008(3) -0.018(3)
F46 0.084(5) 0.113(6) 0.118(6) 0.016(5) 0.055(5) 0.025(5)
N1 0.030(2) 0.025(2) 0.026(2) 0.0001(18) -0.0018(19) 0.0011(18)
N2 0.033(3) 0.040(3) 0.030(3) -0.001(2) 0.007(2) 0.001(2)
N3 0.039(3) 0.026(2) 0.029(3) -0.0019(19) 0.006(2) -0.003(2)
N4 0.026(2) 0.023(2) 0.034(3) -0.0003(19) 0.0072(19) -0.0058(18)
N5 0.027(2) 0.031(2) 0.033(3) 0.004(2) 0.005(2) 0.0052(19)
N6 0.029(2) 0.043(3) 0.040(3) -0.003(2) 0.007(2) -0.007(2)
N7 0.040(3) 0.025(2) 0.030(3) -0.0039(19) 0.003(2) -0.001(2)
N8 0.035(3) 0.030(2) 0.030(3) 0.002(2) 0.007(2) -0.004(2)
N9 0.028(2) 0.032(2) 0.029(3) 0.0008(19) 0.0071(19) -0.0011(19)
N10 0.029(2) 0.028(2) 0.027(2) -0.003(2) 0.0080(19) 0.0024(19)
N11 0.030(2) 0.033(3) 0.035(3) 0.000(2) 0.007(2) -0.001(2)
N12 0.031(3) 0.034(3) 0.040(3) 0.002(2) 0.002(2) 0.001(2)
N13 0.031(2) 0.038(3) 0.030(3) 0.001(2) 0.005(2) 0.001(2)
N14 0.025(2) 0.026(2) 0.031(3) 0.001(2) 0.0030(19) 0.0042(18)
C1 0.033(3) 0.030(3) 0.021(3) 0.001(2) 0.004(2) 0.004(2)
C2 0.034(3) 0.053(4) 0.032(3) -0.005(3) 0.009(3) -0.004(3)
C3 0.045(4) 0.073(5) 0.049(4) -0.004(4) 0.019(3) 0.000(4)
C4 0.045(4) 0.065(5) 0.053(4) -0.018(3) 0.014(3) 0.019(3)
C5 0.050(4) 0.043(4) 0.046(4) -0.013(3) 0.003(3) 0.004(3)
C6 0.035(3) 0.033(3) 0.033(3) -0.002(2) 0.006(3) 0.004(2)
C7 0.036(3) 0.024(3) 0.025(3) -0.004(2) 0.001(2) 0.001(2)
C8 0.047(3) 0.022(3) 0.025(3) -0.004(2) 0.000(2) -0.005(2)
C9 0.057(4) 0.031(3) 0.040(4) -0.007(3) -0.002(3) 0.001(3)
C10 0.079(5) 0.022(3) 0.055(4) 0.001(3) -0.007(4) -0.006(3)
C11 0.067(5) 0.036(4) 0.047(4) 0.003(3) 0.002(3) -0.019(3)
C12 0.055(4) 0.034(3) 0.036(3) -0.004(3) 0.011(3) -0.008(3)
C13 0.027(3) 0.027(3) 0.036(3) 0.004(2) 0.007(2) -0.003(2)
C14 0.044(3) 0.043(3) 0.025(3) 0.003(3) 0.004(3) -0.012(3)
C15 0.042(3) 0.040(3) 0.028(3) 0.014(3) 0.000(3) -0.007(3)
C16 0.020(3) 0.036(3) 0.032(3) -0.001(2) 0.003(2) -0.002(2)
C17 0.032(3) 0.037(3) 0.025(3) 0.000(2) 0.001(2) -0.002(3)
C18 0.035(3) 0.026(3) 0.035(3) 0.007(2) 0.007(2) -0.006(2)
C19 0.032(3) 0.027(3) 0.035(3) 0.006(2) 0.008(2) 0.000(2)
C20 0.037(4) 0.053(4) 0.056(4) 0.005(3) -0.005(3) 0.005(3)
C21 0.052(4) 0.055(4) 0.069(5) 0.011(4) -0.012(4) 0.018(4)
C22 0.069(5) 0.039(4) 0.075(5) 0.001(3) 0.006(4) 0.023(4)
C23 0.045(4) 0.030(3) 0.056(4) 0.005(3) 0.000(3) 0.006(3)
C24 0.034(3) 0.029(3) 0.038(3) 0.005(2) 0.012(3) 0.001(2)
C25 0.033(3) 0.025(3) 0.035(3) 0.002(2) 0.012(2) 0.001(2)
C26 0.033(3) 0.027(3) 0.037(3) -0.002(2) 0.018(2) -0.005(2)
C27 0.046(4) 0.033(3) 0.044(4) -0.008(3) 0.020(3) -0.003(3)
C28 0.045(4) 0.047(4) 0.056(4) -0.021(3) 0.022(3) -0.018(3)
C29 0.037(4) 0.060(4) 0.061(4) -0.025(3) 0.012(3) -0.016(3)
C30 0.032(3) 0.053(4) 0.046(4) -0.009(3) 0.010(3) -0.008(3)
C31 0.034(3) 0.037(3) 0.030(3) 0.002(2) 0.000(2) 0.000(2)
C32 0.044(4) 0.052(4) 0.031(3) 0.004(3) 0.002(3) 0.002(3)
C33 0.058(4) 0.071(5) 0.027(4) 0.007(3) -0.006(3) -0.010(4)
C34 0.058(4) 0.062(4) 0.027(3) 0.000(3) 0.008(3) -0.010(3)
C35 0.043(3) 0.036(3) 0.032(3) 0.001(3) 0.011(3) 0.001(3)
C36 0.037(3) 0.034(3) 0.030(3) 0.004(2) 0.009(2) -0.002(3)
C37 0.050(4) 0.057(4) 0.042(4) -0.001(3) 0.024(3) 0.000(3)
C38 0.042(4) 0.068(5) 0.059(5) 0.005(4) 0.024(3) 0.009(3)
C39 0.028(3) 0.070(5) 0.060(5) 0.006(3) 0.008(3) 0.003(3)
C40 0.039(3) 0.049(4) 0.036(4) 0.002(3) 0.000(3) -0.005(3)

C41	0.045(3)	0.036(3)	0.030(3)	-0.005(3)	0.003(3)	0.000(3)
C42	0.059(4)	0.046(4)	0.026(3)	-0.003(3)	0.002(3)	-0.002(3)
C43	0.085(5)	0.061(5)	0.024(4)	0.002(3)	-0.004(3)	0.003(4)
C44	0.072(5)	0.044(4)	0.035(4)	0.004(3)	0.001(3)	0.003(3)
C45	0.044(3)	0.028(3)	0.034(3)	0.004(2)	0.002(3)	0.002(3)
C46	0.039(3)	0.029(3)	0.029(3)	0.007(2)	0.006(2)	0.007(2)
C47	0.071(5)	0.030(3)	0.052(4)	0.008(3)	0.003(3)	0.015(3)
C48	0.051(4)	0.024(3)	0.060(4)	-0.007(3)	0.008(3)	-0.001(3)
C49	0.032(3)	0.036(3)	0.045(4)	-0.008(3)	0.009(3)	0.002(3)
C50	0.037(3)	0.035(3)	0.037(3)	-0.003(3)	0.007(3)	0.000(3)
C51	0.036(3)	0.041(3)	0.043(4)	0.009(3)	0.006(3)	-0.001(3)
C52	0.055(4)	0.054(4)	0.039(4)	0.009(3)	0.012(3)	-0.001(3)
C53	0.071(5)	0.060(4)	0.049(4)	0.008(3)	0.031(4)	-0.008(4)
C54	0.033(3)	0.052(4)	0.069(5)	-0.002(3)	0.021(3)	-0.003(3)
C55	0.034(3)	0.030(3)	0.048(4)	0.003(3)	0.013(3)	-0.008(3)
C56	0.030(3)	0.030(3)	0.053(4)	0.000(3)	0.006(3)	0.000(2)
C57	0.031(3)	0.061(4)	0.070(5)	0.008(4)	0.006(3)	0.006(3)
C58	0.025(3)	0.069(5)	0.086(6)	0.002(4)	-0.011(4)	0.001(3)
C59	0.047(4)	0.074(5)	0.058(5)	0.016(4)	-0.019(4)	0.008(4)
C60	0.041(4)	0.054(4)	0.045(4)	0.004(3)	-0.005(3)	0.001(3)
C61	0.047(4)	0.049(4)	0.039(4)	-0.002(3)	0.010(3)	-0.001(3)
C62	0.061(4)	0.059(4)	0.040(4)	-0.006(3)	0.020(3)	0.001(3)
C63	0.064(4)	0.065(5)	0.045(4)	0.008(4)	0.027(3)	0.000(4)
C64	0.060(4)	0.046(4)	0.043(4)	0.008(3)	0.010(3)	0.004(3)
C65	0.033(3)	0.037(3)	0.035(3)	0.010(3)	0.003(2)	0.005(2)
C66	0.033(3)	0.033(3)	0.032(3)	0.002(2)	0.004(2)	0.001(2)
C67	0.056(4)	0.033(3)	0.049(4)	0.008(3)	0.011(3)	-0.002(3)
C68	0.058(4)	0.025(3)	0.061(4)	-0.003(3)	0.010(3)	0.002(3)
C69	0.042(3)	0.037(3)	0.043(4)	-0.004(3)	0.005(3)	0.006(3)
C70	0.030(3)	0.032(3)	0.037(3)	-0.001(3)	0.002(2)	0.003(2)
O100	0.066(3)	0.046(3)	0.065(3)	-0.008(2)	0.005(2)	-0.003(2)
C100	0.055(4)	0.048(4)	0.046(4)	-0.002(3)	0.001(3)	0.001(3)
C101	0.192(12)	0.076(7)	0.205(12)	-0.037(7)	-0.133(10)	0.007(7)
C102	0.082(6)	0.072(5)	0.084(6)	0.010(4)	0.013(5)	0.031(4)
O200	0.031(3)	0.035(3)	0.116(6)	-0.022(3)	-0.007(4)	-0.003(3)
C200	0.036(5)	0.019(4)	0.051(5)	-0.006(4)	0.000(4)	0.004(3)
C201	0.040(5)	0.048(5)	0.031(5)	0.000(4)	0.011(4)	-0.015(4)
C202	0.049(6)	0.079(7)	0.060(7)	-0.023(6)	-0.025(5)	0.005(5)

_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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loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_distance

_geom_bond_site_symmetry_2

_geom_bond_publ_flag

Ru1 N7 2.045(4) . ?

Ru1 N10 2.054(4) . ?

Ru1 N8 2.059(4) . ?

Ru1 N9 2.068(4) . ?

Ru1 N3 2.072(4) . ?

Ru1 N1 2.080(4) . ?

Ru2 N12 2.049(4) . ?
 Ru2 N11 2.050(4) . ?
 Ru2 N13 2.054(4) . ?
 Ru2 N14 2.067(4) . ?
 Ru2 N6 2.081(4) . ?
 Ru2 N4 2.086(4) . ?
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 P1 F15 1.576(5) . ?
 P1 F14 1.577(4) . ?
 P1 F13 1.585(4) . ?
 P1 F12 1.585(5) . ?
 P1 F11 1.605(4) . ?
 P2 F23X 1.492(12) . ?
 P2 F25X 1.524(12) . ?
 P2 F22X 1.531(12) . ?
 P2 F25 1.539(6) . ?
 P2 F26 1.553(6) . ?
 P2 F21 1.581(4) . ?
 P2 F24 1.587(4) . ?
 P2 F22 1.595(5) . ?
 P2 F26X 1.603(12) . ?
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 F25 F25X 1.080(17) . ?
 F25 F26X 1.151(18) . ?
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 P3 F35 1.559(4) . ?
 P3 F33 1.561(5) . ?
 P3 F34 1.573(4) . ?
 P3 F33X 1.573(14) . ?
 P3 F32 1.574(4) . ?
 P3 F31X 1.576(14) . ?
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 P3 F34X 1.584(14) . ?
 P3 F31 1.601(4) . ?
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 P4 F42 1.583(6) . ?
 P4 F42X 1.586(12) . ?
 P4 F43 1.591(5) . ?
 P4 F43X 1.590(14) . ?
 P4 F46 1.605(6) . ?
 F42 F42X 1.024(15) . ?
 F42 F46X 1.356(16) . ?
 F43 F43X 1.46(3) . ?

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F46 F46X 1.024(16) . ?
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N1 C1 1.335(6) . ?
N1 C7 1.388(6) . ?
N2 C1 1.380(6) . ?
N2 C2 1.385(6) . ?
N2 C6 1.390(6) . ?
N3 C8 1.350(6) . ?
N3 C12 1.359(6) . ?
N4 C19 1.320(6) . ?
N4 C25 1.381(6) . ?
N5 C19 1.376(6) . ?
N5 C20 1.375(6) . ?
N5 C24 1.389(6) . ?
N6 C30 1.345(6) . ?
N6 C26 1.376(6) . ?
N7 C31 1.349(6) . ?
N7 C35 1.362(6) . ?
N8 C40 1.367(6) . ?
N8 C36 1.368(6) . ?
N9 C41 1.336(6) . ?
N9 C45 1.361(6) . ?
N10 C50 1.349(6) . ?
N10 C46 1.365(6) . ?
N11 C51 1.350(6) . ?
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N12 C60 1.353(7) . ?
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N13 C61 1.343(7) . ?
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N14 C70 1.329(6) . ?
N14 C66 1.359(6) . ?
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C2 C3 1.326(8) . ?
C3 C4 1.418(8) . ?
C4 C5 1.343(8) . ?
C5 C6 1.424(7) . ?
C6 C7 1.369(7) . ?
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C8 C9 1.400(7) . ?
C9 C10 1.384(8) . ?
C10 C11 1.381(9) . ?
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C13 C14 1.384(7) . ?
C13 C18 1.396(7) . ?
C14 C15 1.388(7) . ?
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C26 C27 1.386(7) . ?
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 C42 C43 1.358(8) . ?
 C43 C44 1.379(8) . ?
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F23X F23 P2 62.2(6) . . ?
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F22X F26 F26X 137.8(13) . . ?
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P2 F22X F22 62.0(6) . . ?
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F23 F23X P2 72.0(8) . . ?
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F33 P3 F36 177.4(4) . . ?
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F31 F31X F33 130.3(15) . . ?
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F33 F33X F34 132.6(14) . . ?
F33 F33X P3 71.7(10) . . ?
F34 F33X P3 62.4(7) . . ?
F34 F34X F36 132.8(15) . . ?
F34 F34X P3 72.7(10) . . ?
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F41 P4 F42X 86.7(6) . . ?
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F45X F46 P4 65.6(9) . . ?
F42 F42X P4 71.0(8) . . ?
F42 F42X F43 129.6(11) . . ?
P4 F42X F43 59.0(5) . . ?
F45 F43X F43 133.9(14) . . ?
F45 F43X P4 71.1(10) . . ?
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F46 F45X P4 68.5(10) . . ?
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F42 F46X P4 64.7(6) . . ?

C1 N1 C7 107.7(4) . . ?
 C1 N1 Ru1 138.1(3) . . ?
 C7 N1 Ru1 113.0(3) . . ?
 C1 N2 C2 129.6(5) . . ?
 C1 N2 C6 109.1(4) . . ?
 C2 N2 C6 121.3(5) . . ?
 C8 N3 C12 118.5(4) . . ?
 C8 N3 Ru1 116.5(3) . . ?
 C12 N3 Ru1 124.5(4) . . ?
 C19 N4 C25 107.8(4) . . ?
 C19 N4 Ru2 138.6(3) . . ?
 C25 N4 Ru2 113.5(3) . . ?
 C19 N5 C20 129.4(5) . . ?
 C19 N5 C24 108.2(4) . . ?
 C20 N5 C24 122.3(5) . . ?
 C30 N6 C26 116.5(5) . . ?
 C30 N6 Ru2 127.0(4) . . ?
 C26 N6 Ru2 116.5(3) . . ?
 C31 N7 C35 118.7(5) . . ?
 C31 N7 Ru1 125.2(4) . . ?
 C35 N7 Ru1 116.1(3) . . ?
 C40 N8 C36 117.4(5) . . ?
 C40 N8 Ru1 126.8(4) . . ?
 C36 N8 Ru1 115.6(3) . . ?
 C41 N9 C45 117.1(4) . . ?
 C41 N9 Ru1 126.8(4) . . ?
 C45 N9 Ru1 115.7(3) . . ?
 C50 N10 C46 118.1(4) . . ?
 C50 N10 Ru1 126.2(4) . . ?
 C46 N10 Ru1 115.5(3) . . ?
 C51 N11 C55 117.7(5) . . ?
 C51 N11 Ru2 126.3(4) . . ?
 C55 N11 Ru2 115.8(4) . . ?
 C60 N12 C56 119.4(5) . . ?
 C60 N12 Ru2 124.9(4) . . ?
 C56 N12 Ru2 115.4(3) . . ?
 C61 N13 C65 118.7(5) . . ?
 C61 N13 Ru2 126.1(4) . . ?
 C65 N13 Ru2 115.2(3) . . ?
 C70 N14 C66 118.5(4) . . ?
 C70 N14 Ru2 126.0(4) . . ?
 C66 N14 Ru2 114.9(3) . . ?
 N1 C1 N2 108.3(4) . . ?
 N1 C1 C13 127.1(5) . . ?
 N2 C1 C13 123.6(5) . . ?
 C3 C2 N2 119.3(6) . . ?
 C2 C3 C4 121.0(6) . . ?
 C5 C4 C3 121.1(6) . . ?
 C4 C5 C6 118.5(6) . . ?
 C7 C6 N2 105.1(4) . . ?
 C7 C6 C5 136.2(5) . . ?
 N2 C6 C5 118.7(5) . . ?
 C6 C7 N1 109.8(4) . . ?
 C6 C7 C8 134.0(5) . . ?
 N1 C7 C8 116.1(4) . . ?
 N3 C8 C9 121.8(5) . . ?
 N3 C8 C7 113.9(4) . . ?
 C9 C8 C7 124.2(5) . . ?
 C10 C9 C8 117.8(6) . . ?
 C11 C10 C9 120.5(5) . . ?
 C12 C11 C10 118.6(6) . . ?

N3 C12 C11 122.7(6) . . ?
 C14 C13 C18 118.5(5) . . ?
 C14 C13 C1 123.1(5) . . ?
 C18 C13 C1 118.3(4) . . ?
 C13 C14 C15 120.5(5) . . ?
 C16 C15 C14 120.7(5) . . ?
 C15 C16 C17 118.8(5) . . ?
 C15 C16 C19 121.9(5) . . ?
 C17 C16 C19 119.2(5) . . ?
 C18 C17 C16 120.1(5) . . ?
 C17 C18 C13 121.3(5) . . ?
 N4 C19 N5 109.4(4) . . ?
 N4 C19 C16 127.4(4) . . ?
 N5 C19 C16 123.2(4) . . ?
 C21 C20 N5 119.0(6) . . ?
 C20 C21 C22 120.3(6) . . ?
 C23 C22 C21 120.9(6) . . ?
 C22 C23 C24 120.0(6) . . ?
 C25 C24 N5 105.2(4) . . ?
 C25 C24 C23 137.2(5) . . ?
 N5 C24 C23 117.5(5) . . ?
 C24 C25 N4 109.3(4) . . ?
 C24 C25 C26 132.4(5) . . ?
 N4 C25 C26 118.2(4) . . ?
 N6 C26 C27 121.5(5) . . ?
 N6 C26 C25 113.2(4) . . ?
 C27 C26 C25 125.2(5) . . ?
 C28 C27 C26 119.3(6) . . ?
 C29 C28 C27 119.4(6) . . ?
 C28 C29 C30 119.0(6) . . ?
 N6 C30 C29 124.3(6) . . ?
 N7 C31 C32 123.4(5) . . ?
 C31 C32 C33 118.0(5) . . ?
 C34 C33 C32 119.7(5) . . ?
 C33 C34 C35 119.3(6) . . ?
 N7 C35 C34 120.9(5) . . ?
 N7 C35 C36 114.8(5) . . ?
 C34 C35 C36 124.3(5) . . ?
 N8 C36 C37 121.0(5) . . ?
 N8 C36 C35 114.2(5) . . ?
 C37 C36 C35 124.7(5) . . ?
 C38 C37 C36 119.4(6) . . ?
 C37 C38 C39 120.3(6) . . ?
 C40 C39 C38 119.3(6) . . ?
 C39 C40 N8 122.5(5) . . ?
 N9 C41 C42 123.8(5) . . ?
 C43 C42 C41 118.8(5) . . ?
 C42 C43 C44 119.1(6) . . ?
 C45 C44 C43 119.6(6) . . ?
 N9 C45 C44 121.6(5) . . ?
 N9 C45 C46 114.2(4) . . ?
 C44 C45 C46 124.2(5) . . ?
 N10 C46 C47 120.6(5) . . ?
 N10 C46 C45 115.1(4) . . ?
 C47 C46 C45 124.4(5) . . ?
 C46 C47 C48 120.4(6) . . ?
 C49 C48 C47 119.4(5) . . ?
 C48 C49 C50 118.2(5) . . ?
 N10 C50 C49 123.4(5) . . ?
 N11 C51 C52 123.4(5) . . ?
 C51 C52 C53 118.9(6) . . ?

C54	C53	C52	118.9(6)	.	.	?
C53	C54	C55	120.0(6)	.	.	?
N11	C55	C54	121.1(5)	.	.	?
N11	C55	C56	114.5(5)	.	.	?
C54	C55	C56	124.4(5)	.	.	?
N12	C56	C57	120.7(5)	.	.	?
N12	C56	C55	114.8(5)	.	.	?
C57	C56	C55	124.5(6)	.	.	?
C58	C57	C56	120.6(6)	.	.	?
C57	C58	C59	118.9(6)	.	.	?
C58	C59	C60	119.6(6)	.	.	?
N12	C60	C59	120.8(6)	.	.	?
N13	C61	C62	123.0(6)	.	.	?
C63	C62	C61	118.4(6)	.	.	?
C62	C63	C64	119.8(6)	.	.	?
C63	C64	C65	119.6(6)	.	.	?
N13	C65	C64	120.6(5)	.	.	?
N13	C65	C66	114.9(5)	.	.	?
C64	C65	C66	124.5(5)	.	.	?
N14	C66	C67	121.0(5)	.	.	?
N14	C66	C65	115.1(5)	.	.	?
C67	C66	C65	123.8(5)	.	.	?
C68	C67	C66	119.9(5)	.	.	?
C69	C68	C67	118.7(5)	.	.	?
C68	C69	C70	119.2(5)	.	.	?
N14	C70	C69	122.6(5)	.	.	?
O100	C100	C101	122.7(7)	.	.	?
O100	C100	C102	122.0(6)	.	.	?
C101	C100	C102	115.3(7)	.	.	?
O200	C200	C201	120.7(8)	.	.	?
O200	C200	C202	122.9(8)	.	.	?
C201	C200	C202	116.4(7)	.	.	?

_diffn_measured_fraction_theta_max	0.965
_diffn_reflns_theta_full	28.31
_diffn_measured_fraction_theta_full	0.965
_refine_diff_density_max	0.709
_refine_diff_density_min	-1.014
_refine_diff_density_rms	0.104