

Supporting Information

Blue-Green Luminescent Rhenium(I) Tricarbonyl Complexes with Pyridine-Functionalized N-heterocyclic Carbene Ligands

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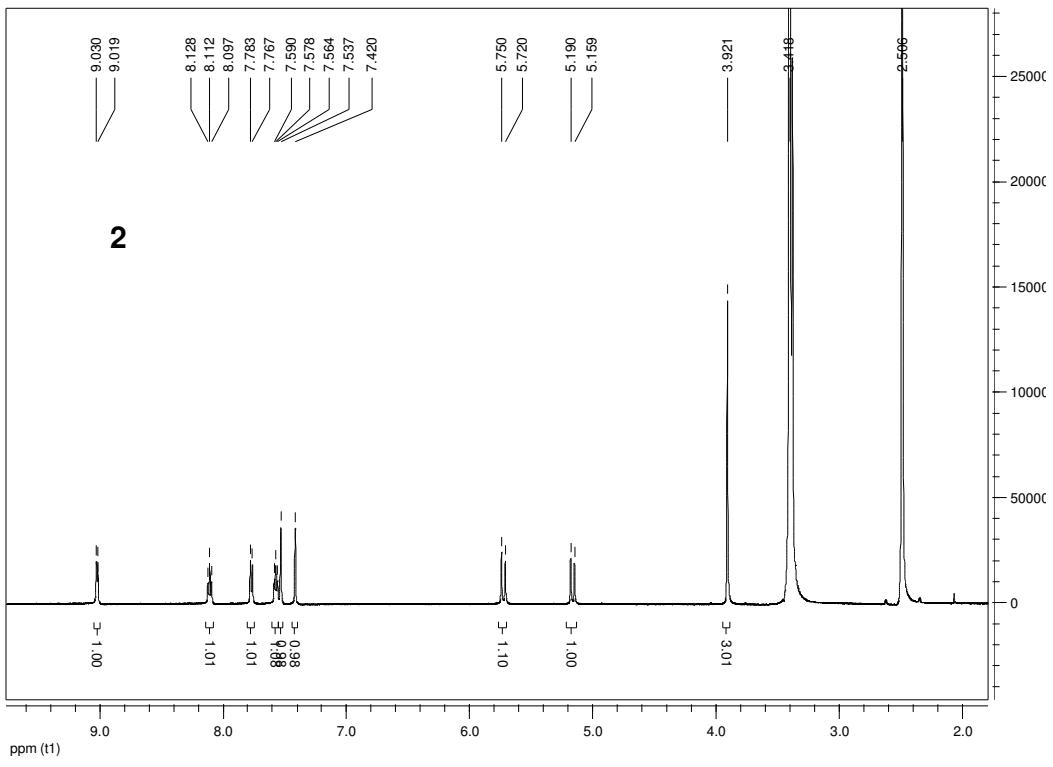
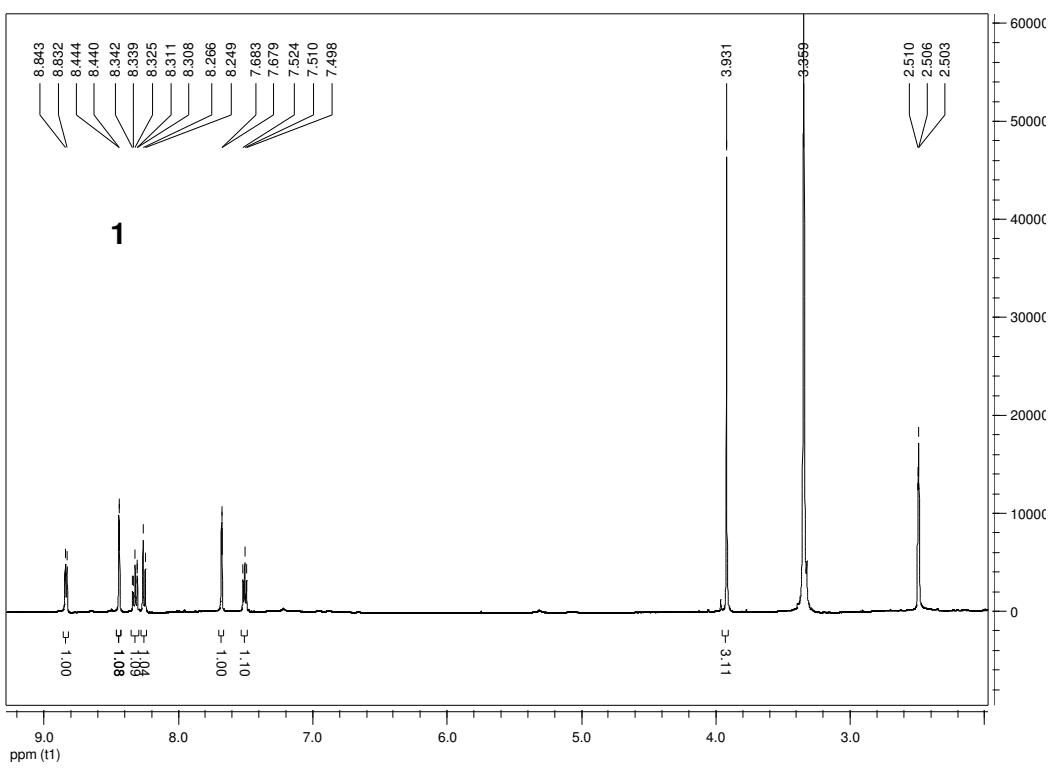
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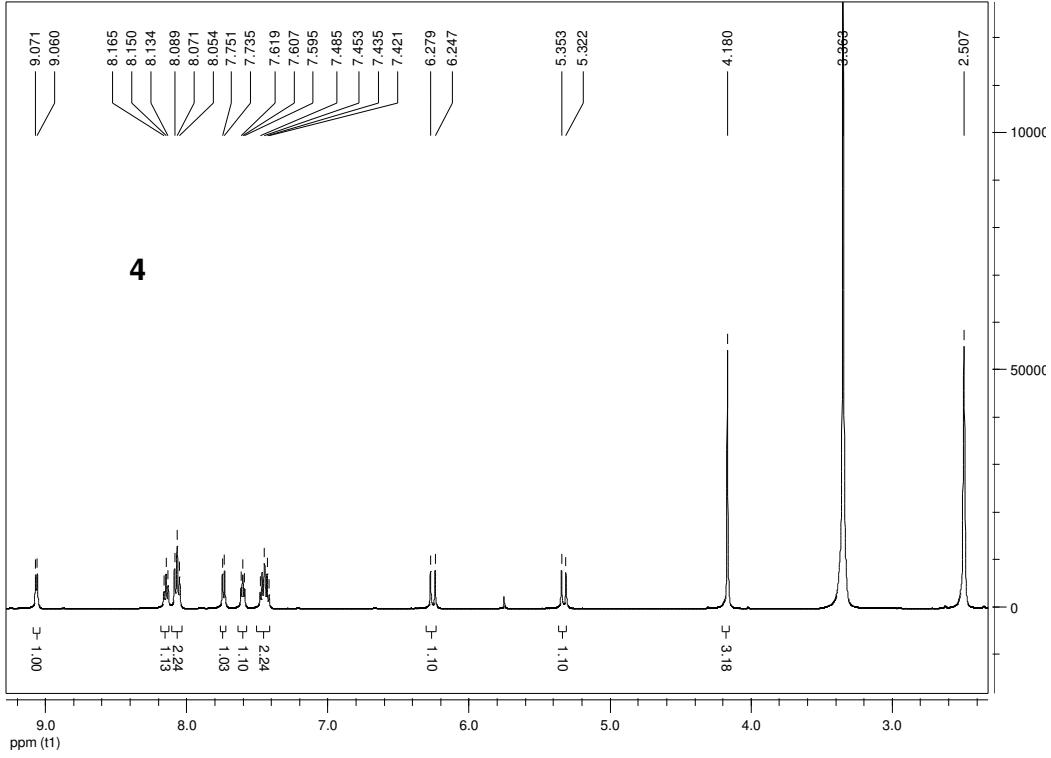
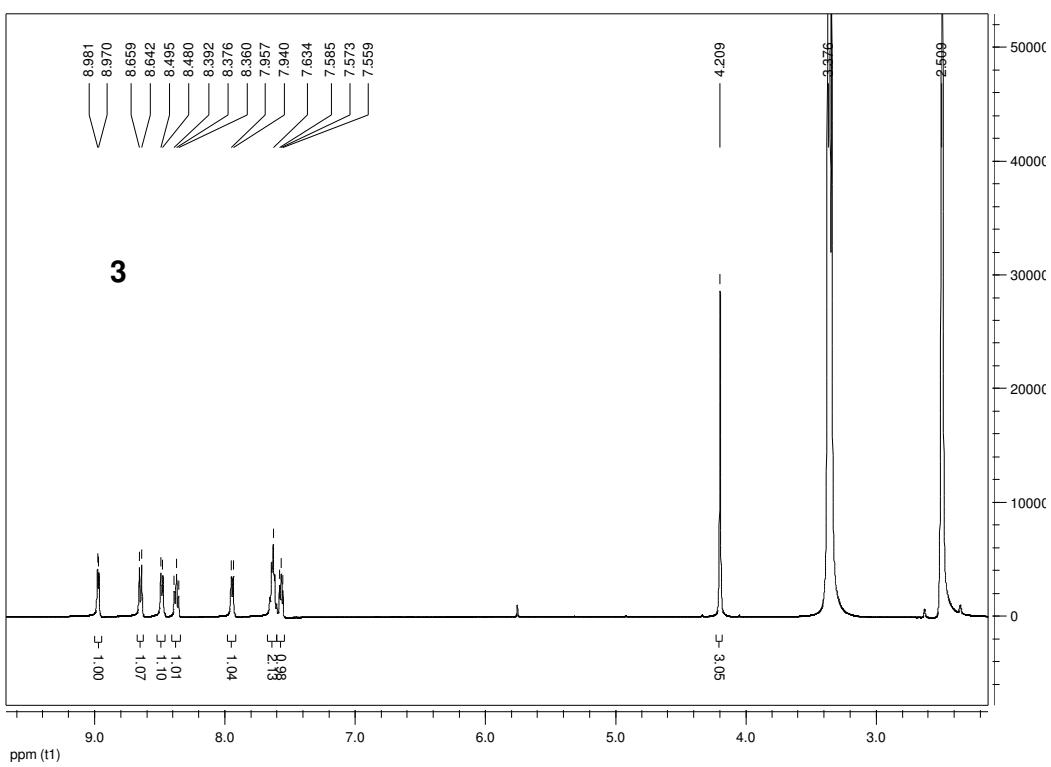
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Figure 5S. Photoluminescence lifetime decay curves of **1**, **3** and **5** in solid state at room temperature (a-c) and in deaerated CH₂Cl₂ (d-f) at 77 K.

Table S1. Summary of crystallographic data for complexes **3**, **4**, and **5**

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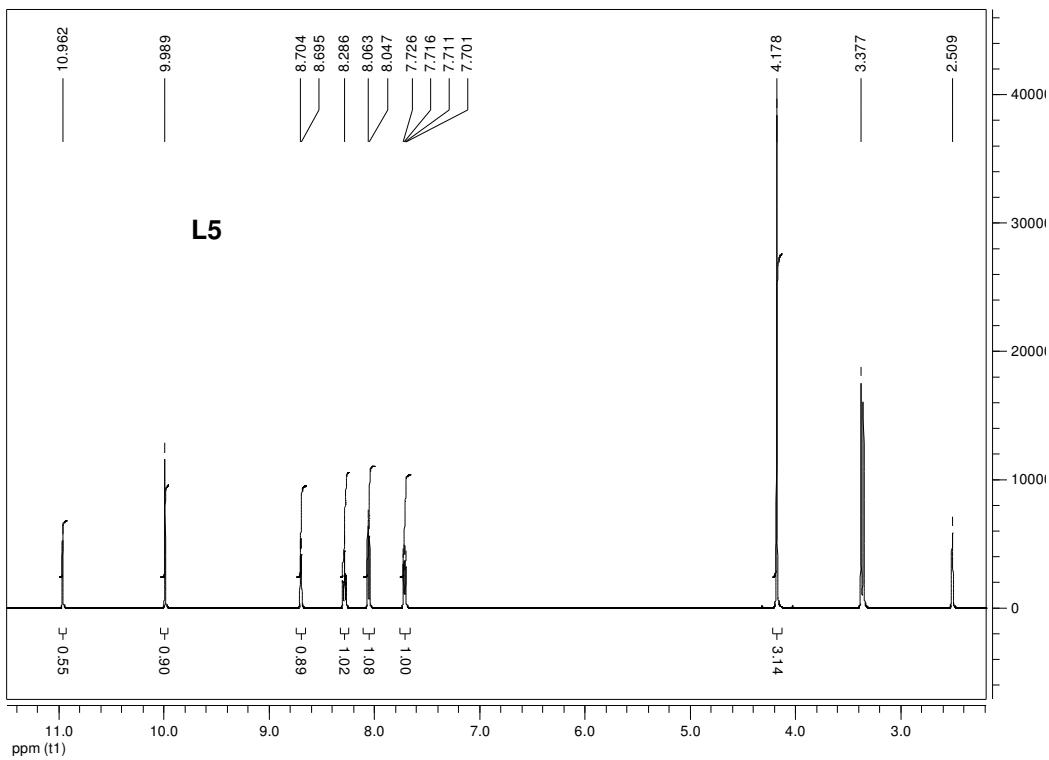
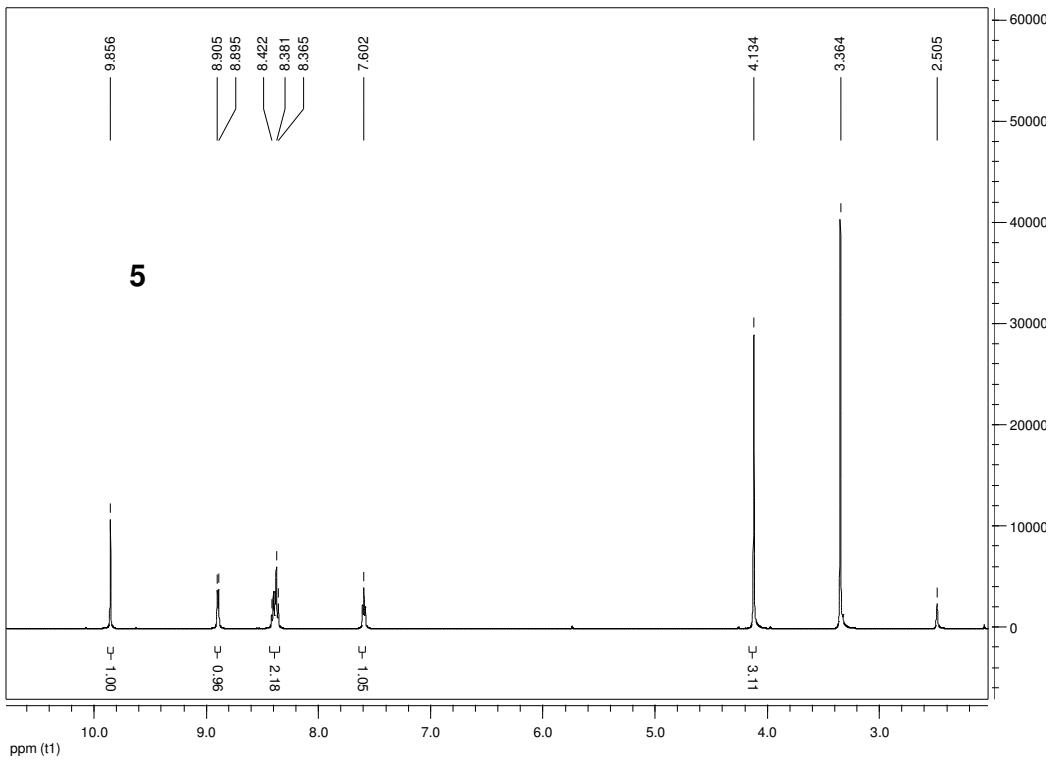


Figure 1S. ^1H NMR spectra of complexes **1-5** and ligand **L5** in $\text{d}^6\text{-DMSO}$ at room temperature

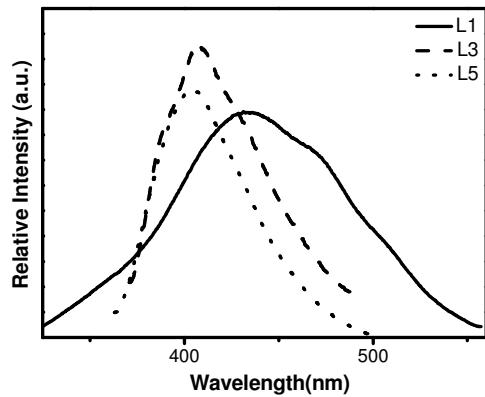


Figure 2S. Emission spectra of ligands **L1**, **L3** and **L5** in degassed CH_2Cl_2 solution (1×10^{-3} M) under ambient conditions.

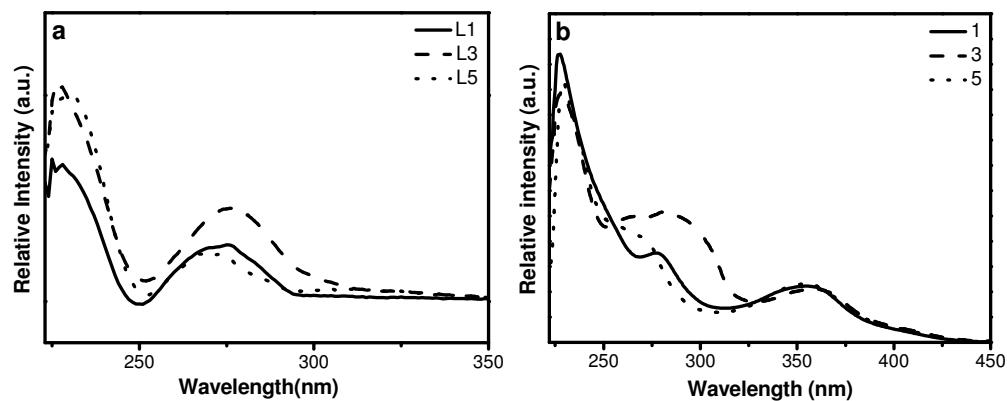


Figure 3S. Absorption spectra of (a) ligands **L1**, **L3**, **L5** and (b) complexes **1**, **3**, **5** in CH_2Cl_2 solution (1×10^{-5} M) at room temperature.

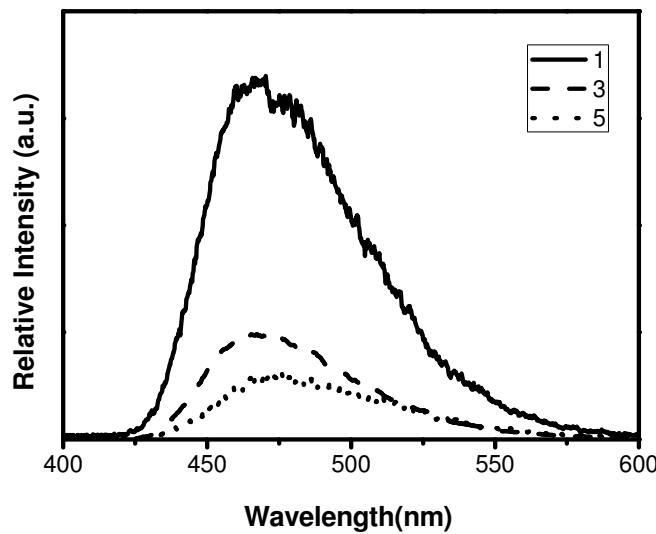


Figure 4S. The emission spectra of complexes **1**, **3**, and **5** in deaerated CH_2Cl_2 at 77 K.

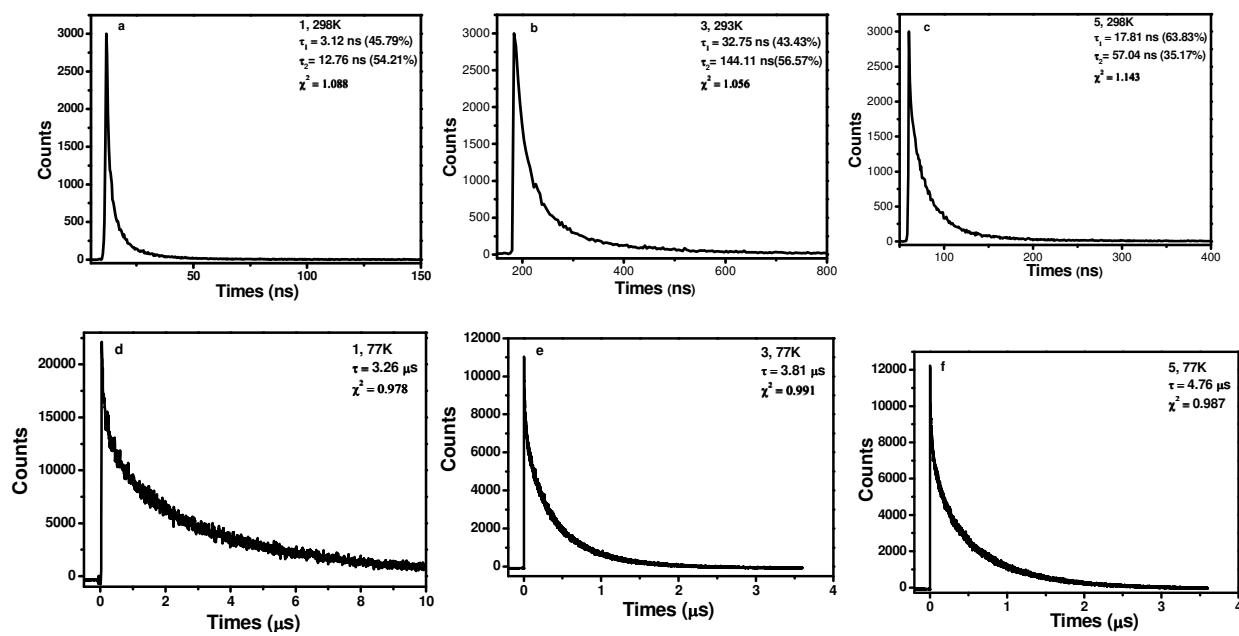


Figure 5S. Photoluminescence lifetime decay curve of **1**, **3** and **5** in solid state at room temperature (a-c) and in deaerated CH_2Cl_2 at 77 K (d-f).

Table S1. Summary of crystallographic data for complexes **3**, **4**, and **5**

Compound	3 ·CH ₂ Cl ₂	4 ·CH ₂ Cl ₂	5
Formula	C ₁₇ H ₁₃ Cl ₃ N ₃ O ₃ Re	C ₁₈ H ₁₅ Cl ₃ N ₃ O ₃ Re	C ₁₁ H ₈ ClN ₄ O ₃ Re
Formula weight	599.85	613.88	465.86
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	P $\bar{1}$	P2 ₁ /n	P2 ₁ /n
<i>a</i> (Å)	9.7810(12)	8.451(3)	8.2452(6)
<i>b</i> (Å)	10.0970(18)	13.371(5)	17.1482(13)
<i>c</i> (Å)	11.4850(14)	18.280(7)	9.6324(7)
α (deg)	87.557(2)	90	90
β (deg)	68.459(3)	95.183(5)	93.0670(10)
γ (deg)	68.542(2)	90	90
<i>V</i> (Å ³)	976.4(2)	2057.2(14)	1359.98(17)
<i>D</i> _(calc) (g/cm ³)	2.040	1.982	2.275
<i>Z</i>	2	4	4
<i>T</i> (K)	298.3	298.3	298.3
Radiation (MoKa)	0.71073	0.71073	0.71073
<i>F</i> (000)	572	1176	872
Absorpt coefficient(mm ⁻¹)	6.656	6.321	9.143
θ range for data collection (deg)	2.42-26.0	1.89-26.0	2.43-25.99
Data/restr/paras	3735/0/245	4037/0/254	2661/0/182
Reflections collected	5293	10900	7315
Reflections unique	3735	4037	2661
Completeness to θ (deg)	26.0(97.2%)	26.0(99.8%)	25.99(99.9%)
<i>R</i> _{int}	0.0242	0.0408	0.0479
Max. and min. transmission	0.3222, 0.2573	0.3958, 0.2903	0.2176, 0.1701
Goodness-of-fit on <i>F</i> ²	1.014	1.082	1.050
<i>R</i> _I , <i>wR</i> ₂ [<i>I</i> >2σ(<i>I</i>)] ^a	0.0425, 0.0923	0.0396, 0.0952	0.0402, 0.0825
<i>R</i> _I , <i>wR</i> ₂ (all data)	0.0500, 0.0936	0.0574, 0.1014	0.0589, 0.0870
CCDC NO.	828916	828917	828918

^a $R_1 = \sum |F_o| - |F_c| / \sum |F_o|$; $wR_2 = [\sum w(|F_o| - |F_c|)^2 / \sum w|F_o|^2]^{1/2}$