

# **The influence of electronic modifications on rotational barriers of bis-NHC-complexes as observed by dynamic NMR spectroscopy**

## **Supporting Information**

Andreas Kolmer,<sup>†</sup> Lukas Kaltschnee,<sup>†</sup> Volker Schmidts,<sup>†</sup> Lars H. Peeck,<sup>‡</sup> Herbert  
Plenio,<sup>‡</sup> and Christina M. Thiele<sup>\*,†</sup>

*Clemens-Schöpf-Institut für Organische Chemie und Biochemie, Technische Universität  
Darmstadt, Petersenstrasse 22, 64287 Darmstadt, Germany, and Organometallic Chemistry,  
Technische Universität Darmstadt, Petersenstrasse 18, 64287 Darmstadt, Germany*

E-mail: cthiele@thielelab.de

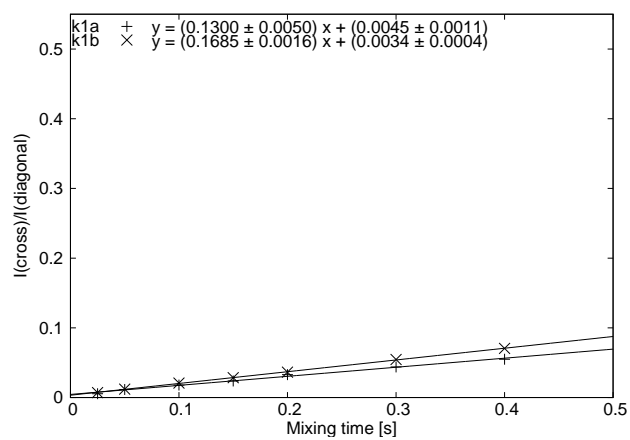
Phone: +49 (0)6151 16 5112. Fax: +49 (0)6151 16 72081

---

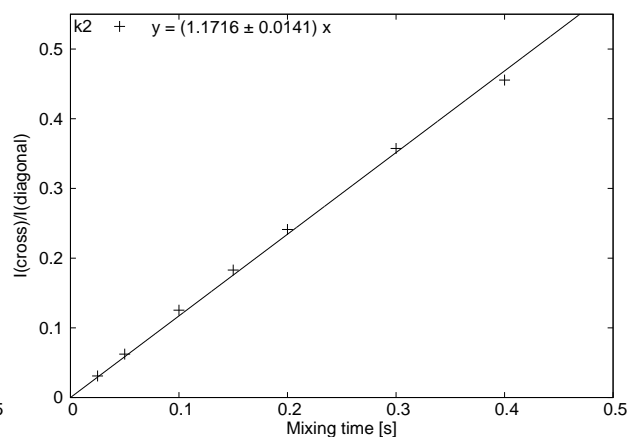
\*To whom correspondence should be addressed

<sup>†</sup>Clemens-Schöpf-Institut für Organische Chemie und Biochemie, Technische Universität Darmstadt, Petersenstrasse 22, 64287 Darmstadt, Germany

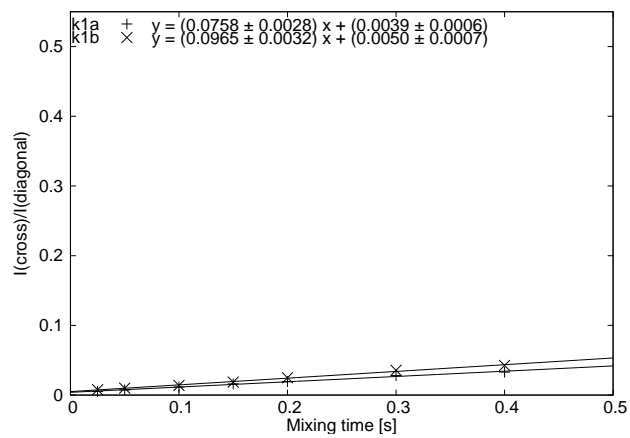
<sup>‡</sup>Organometallic Chemistry, Technische Universität Darmstadt, Petersenstrasse 18, 64287 Darmstadt, Germany



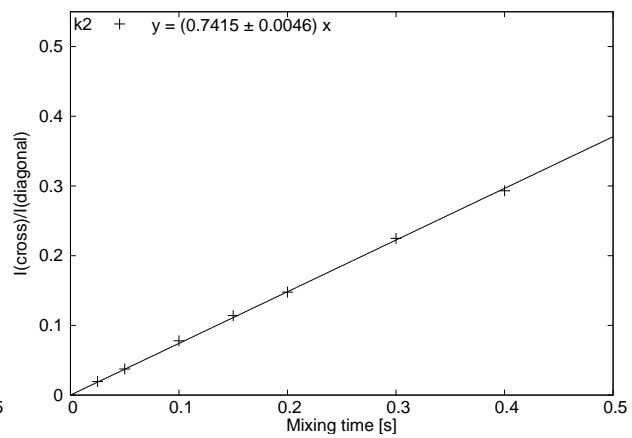
(a) 305K



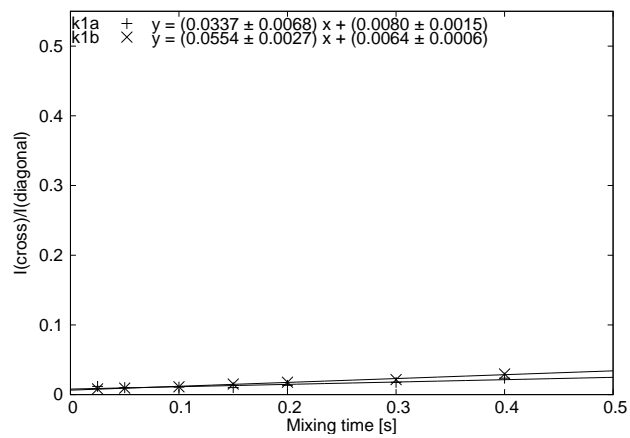
(b) 305K



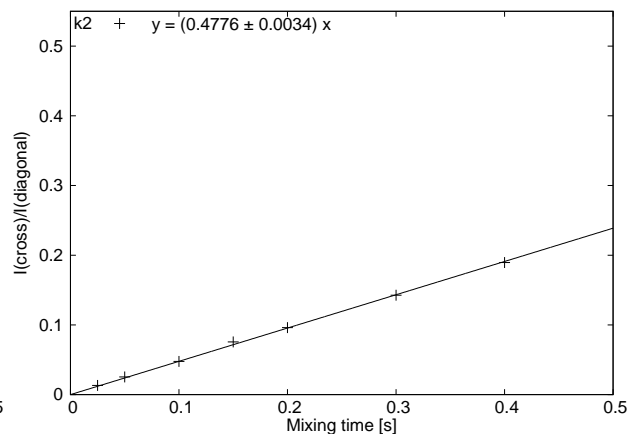
(c) 300K



(d) 300K



(e) 295K



(f) 295K

Figure 1: The PANIC plots for complex 1.

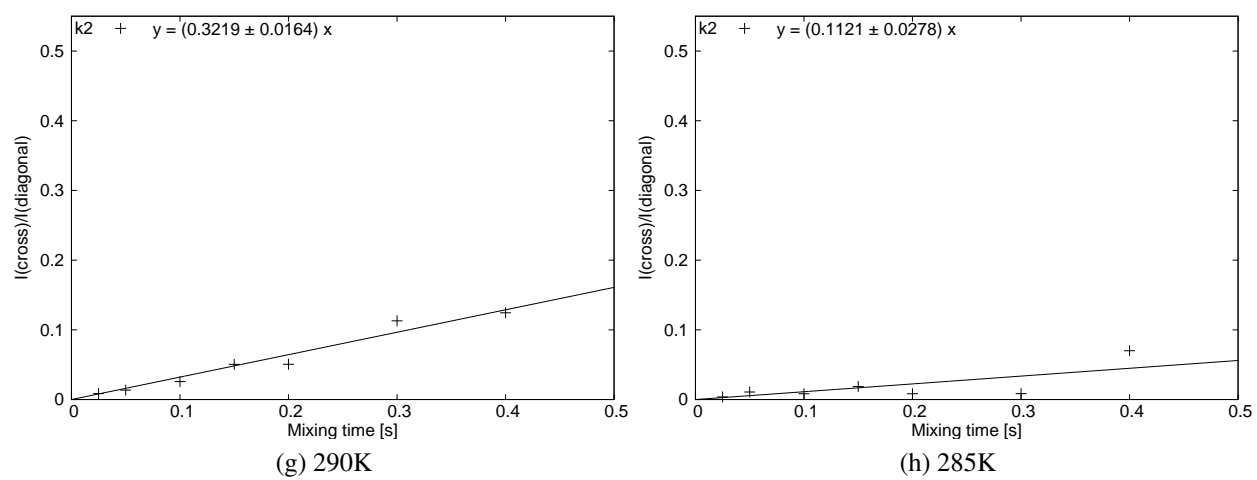
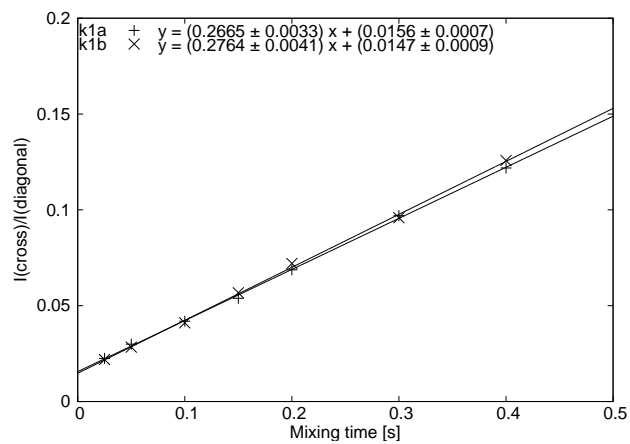
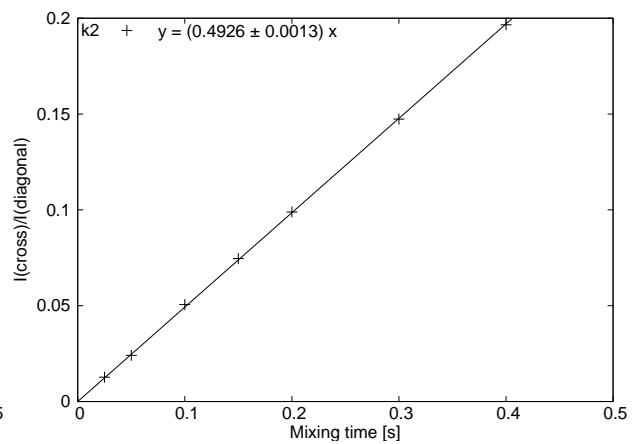


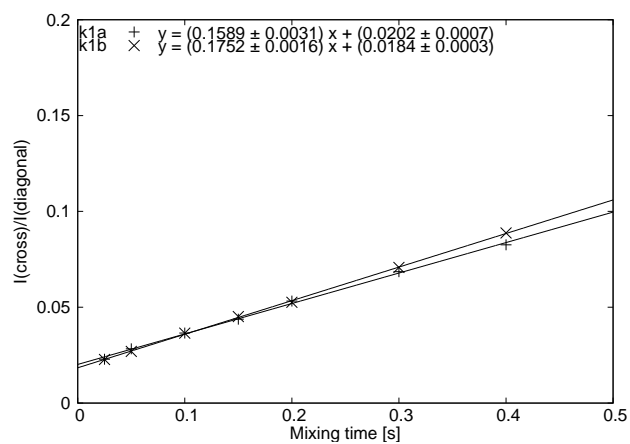
Figure 1: The PANIC plots for complex 1.



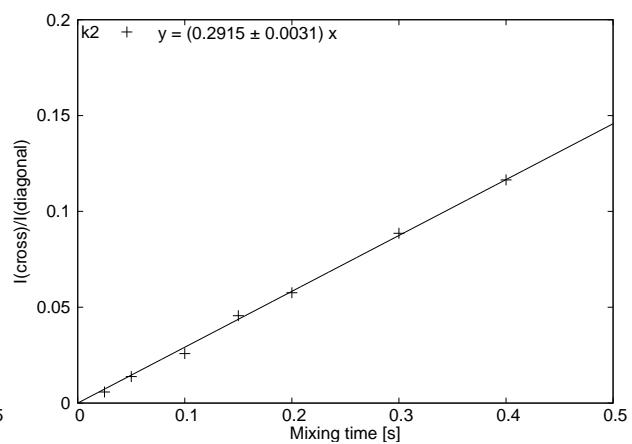
(a) 305K



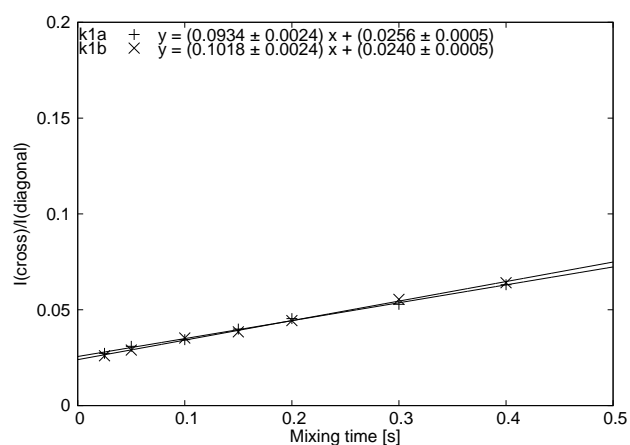
(b) 305K



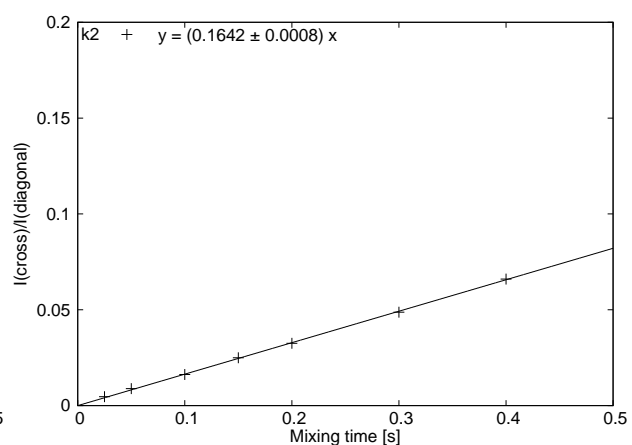
(c) 300K



(d) 300K

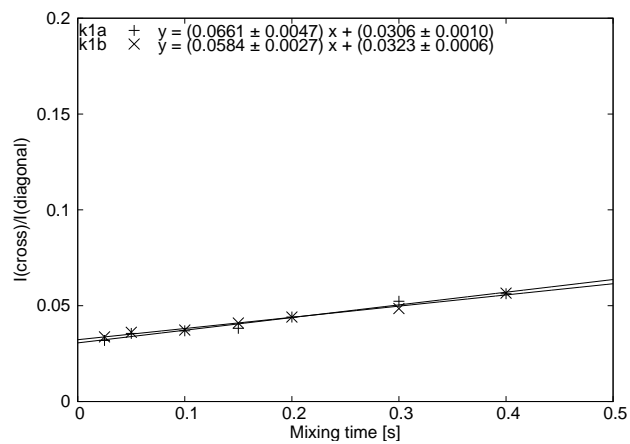


(e) 295K

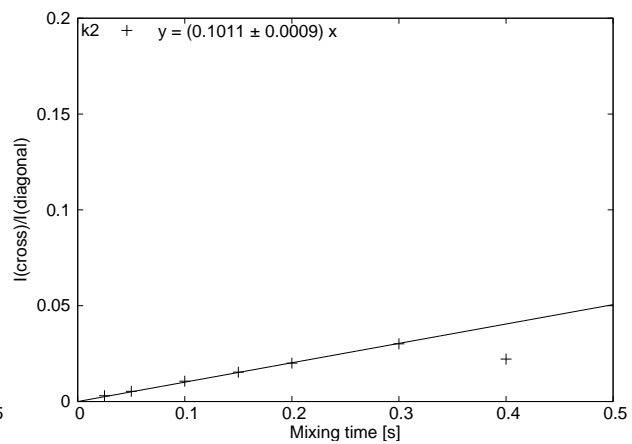


(f) 295K

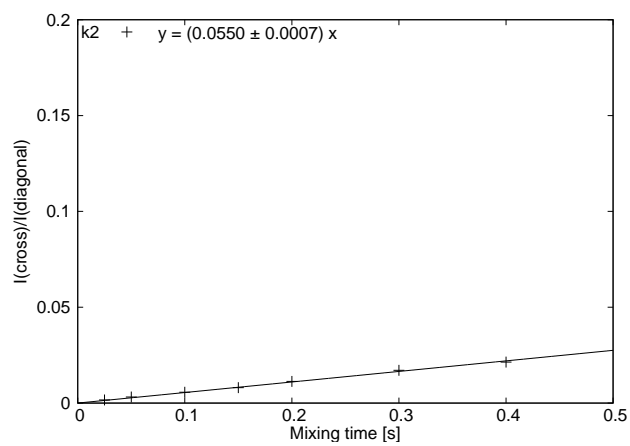
Figure 2: The PANIC plots for complex **2**.



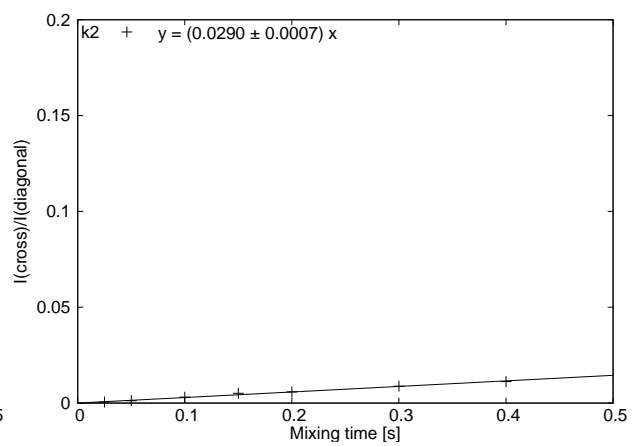
(g) 290K



(h) 290K



(i) 285K



(j) 280K

Figure 2: The PANIC plots for complex **2**.

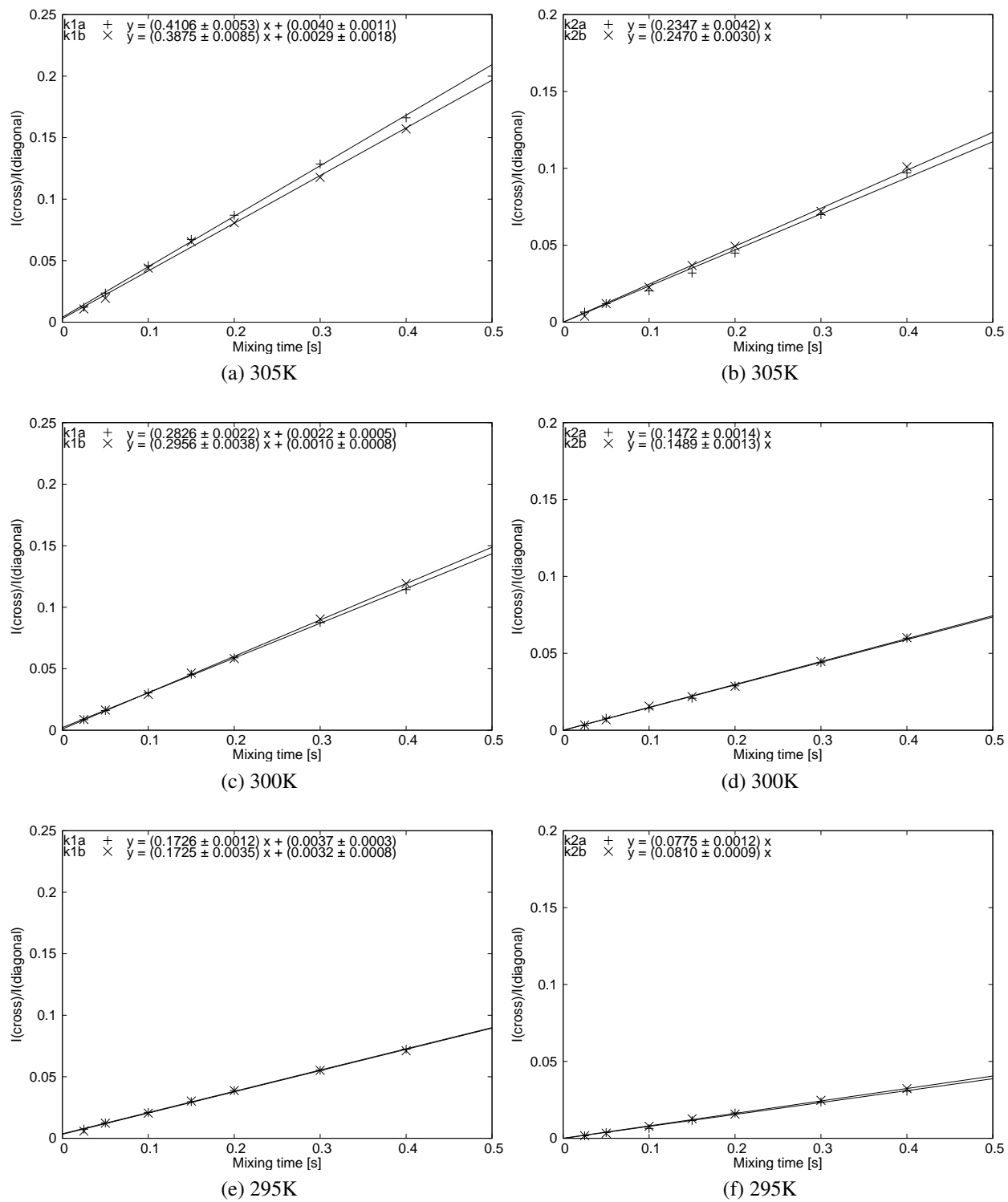


Figure 3: The PANIC plots for complex **3a**.

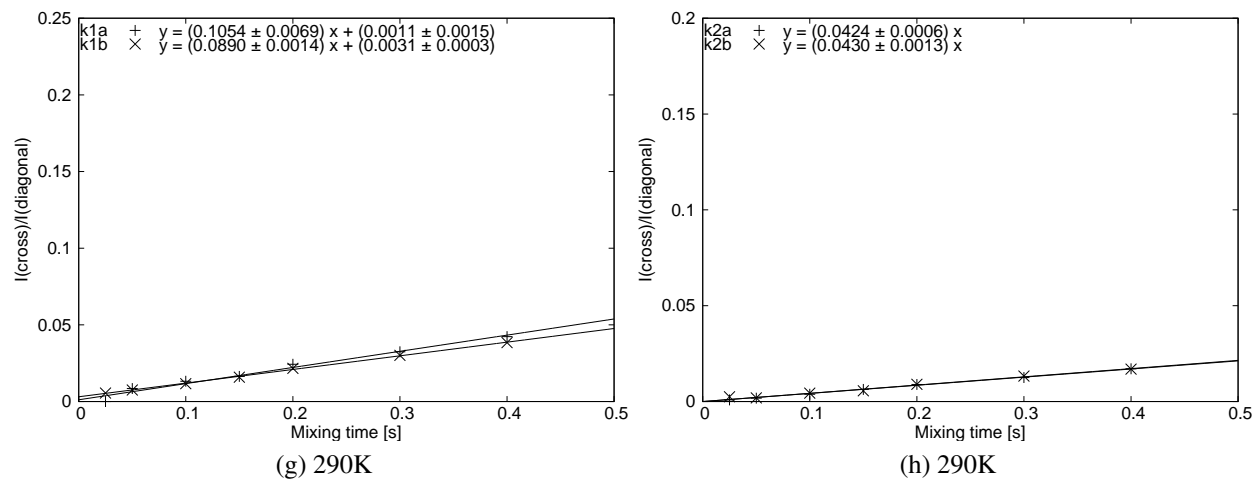


Figure 3: The PANIC plots for complex **3a**.

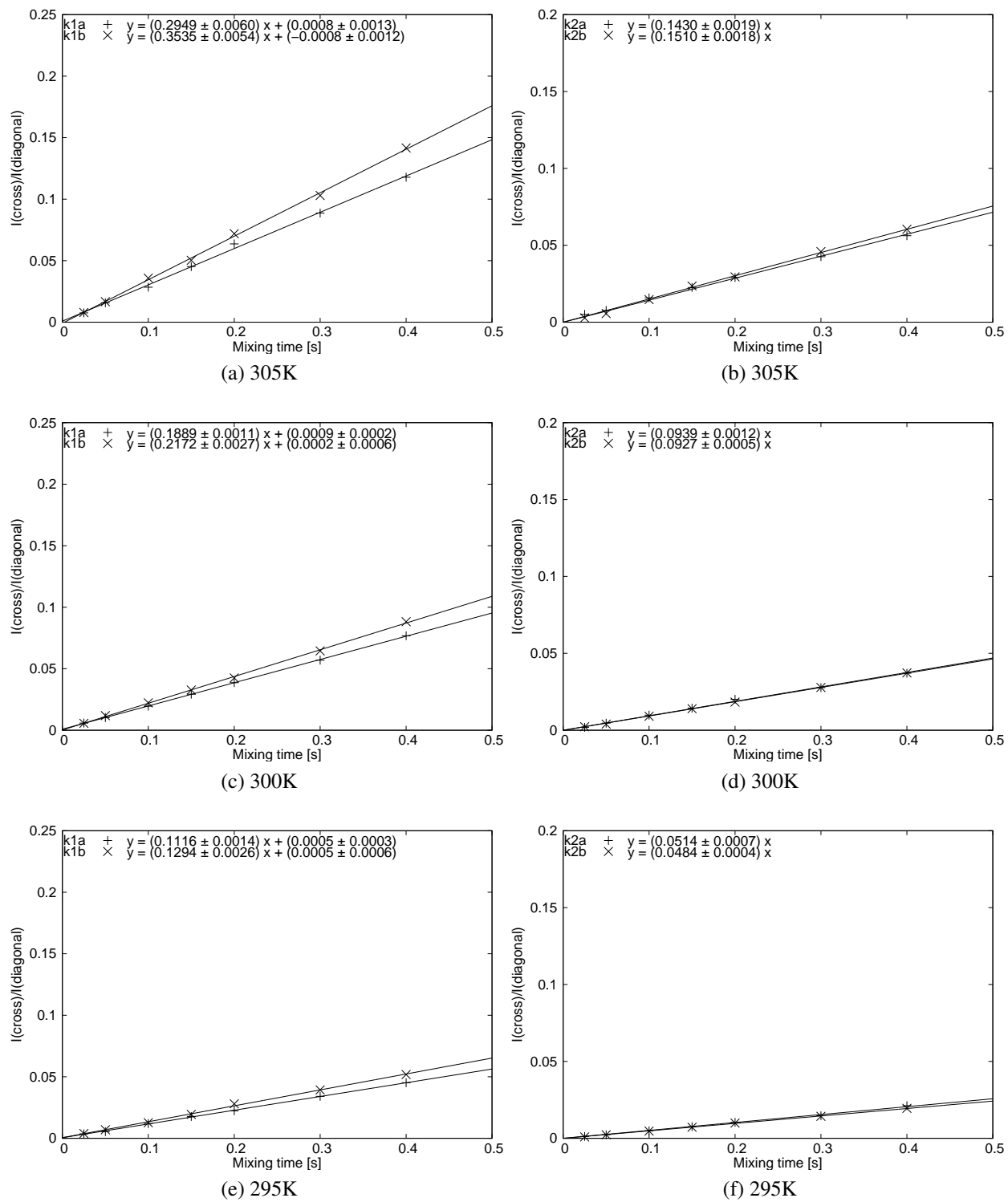


Figure 4: The PANIC plots for complex **3b**.



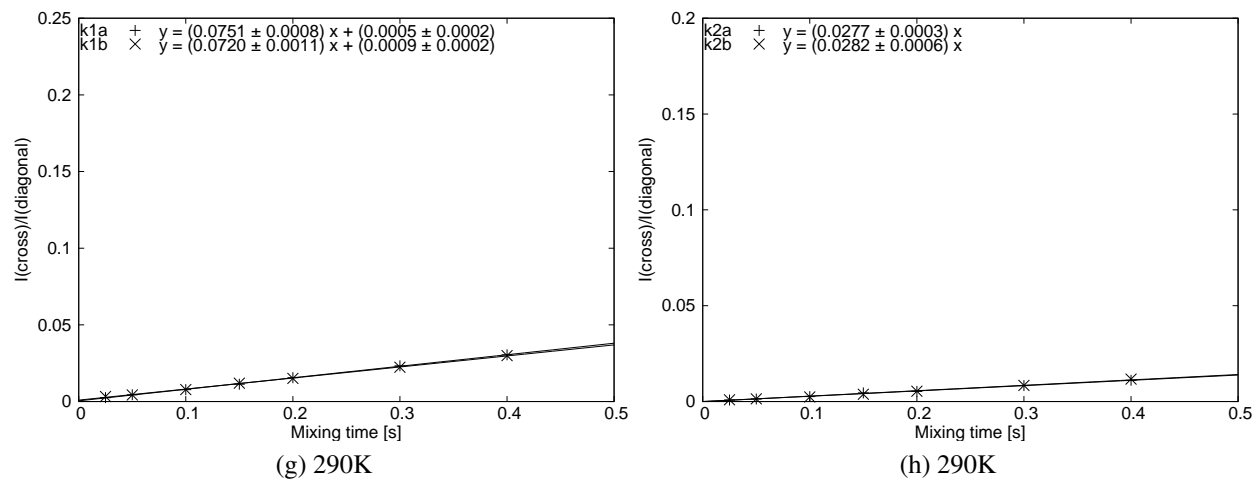


Figure 4: The PANIC plots for complex **3b**.

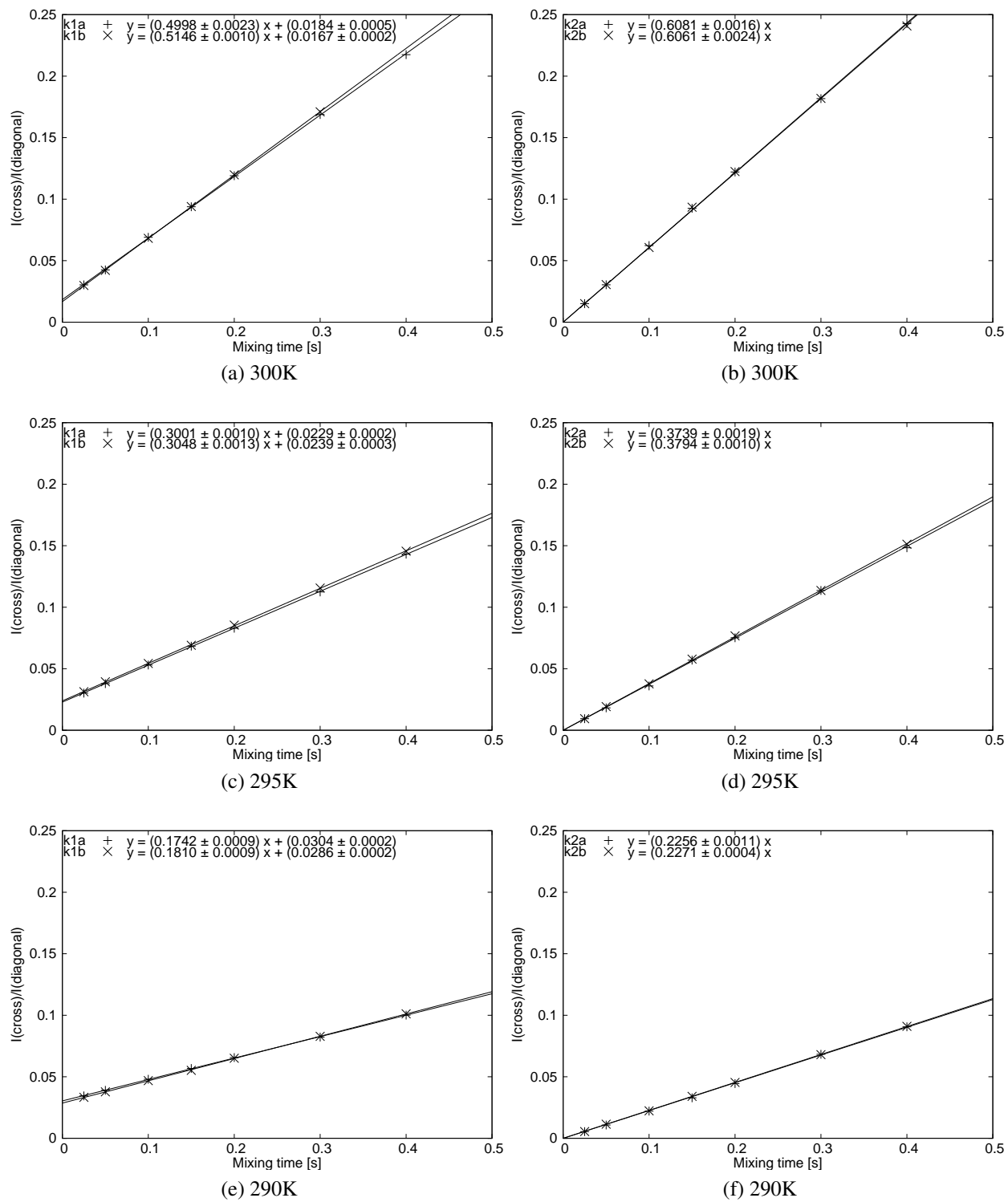


Figure 5: The PANIC plots for complex 4.

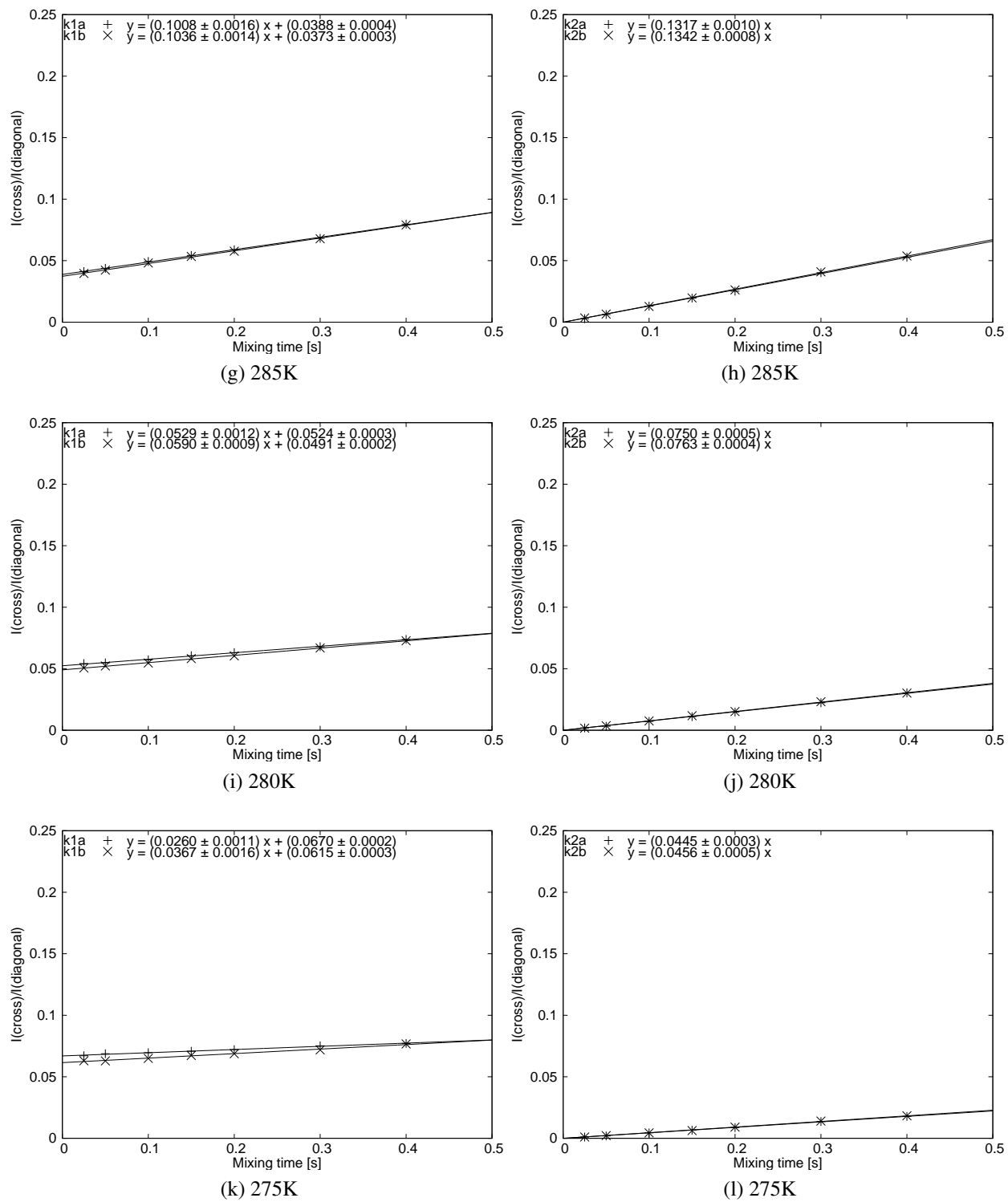


Figure 5: The PANIC plots for complex 4.

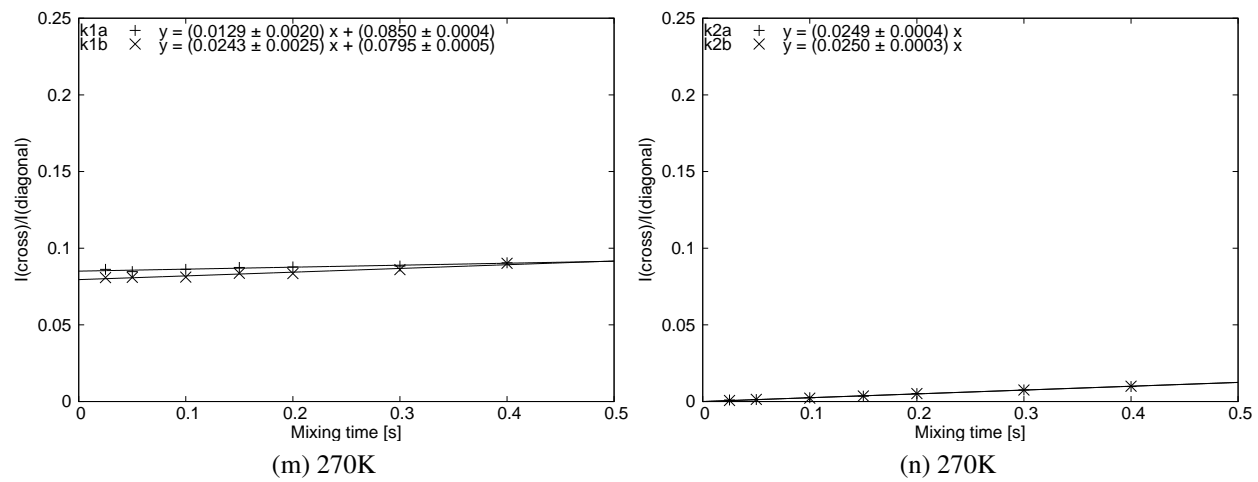
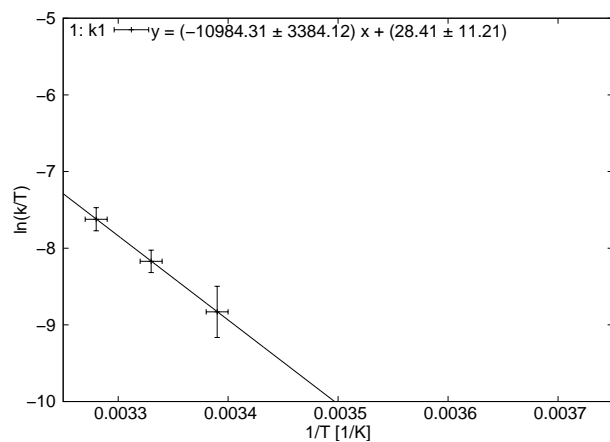
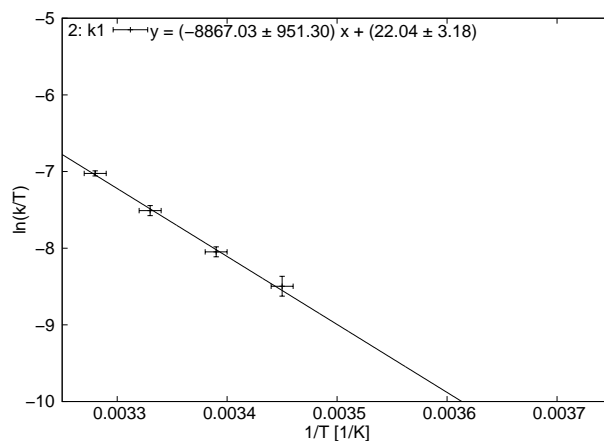


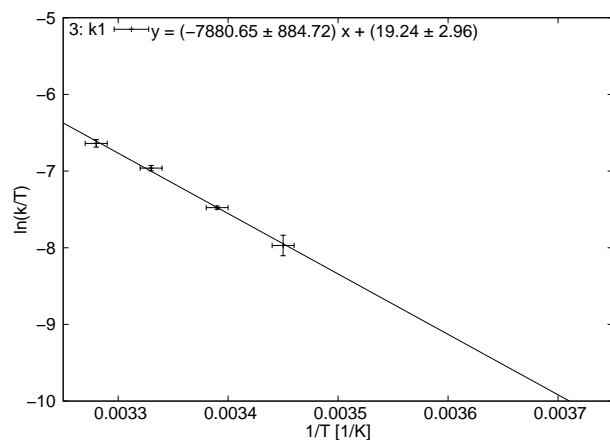
Figure 5: The PANIC plots for complex 4.



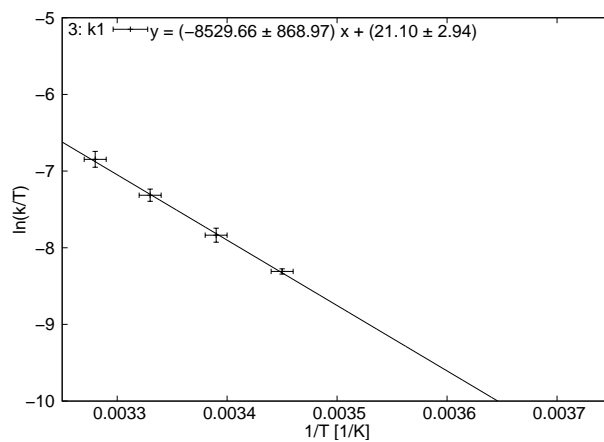
(a) complex 1



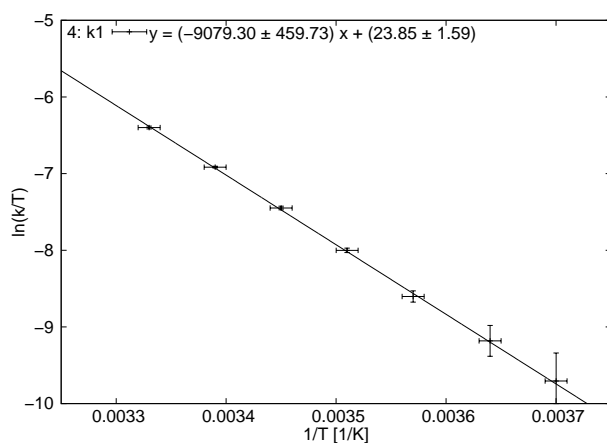
(b) complex 2



(c) complex 3a

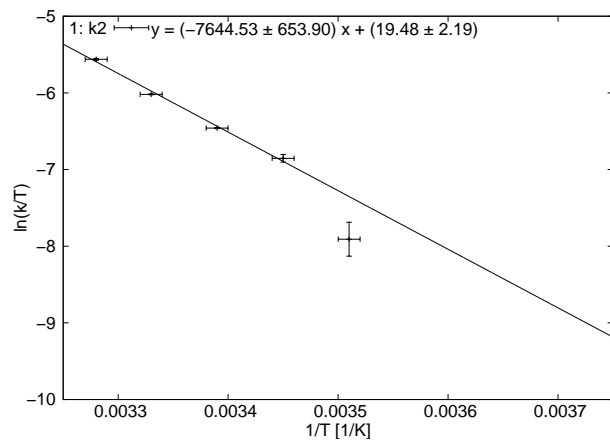


(d) complex 3b

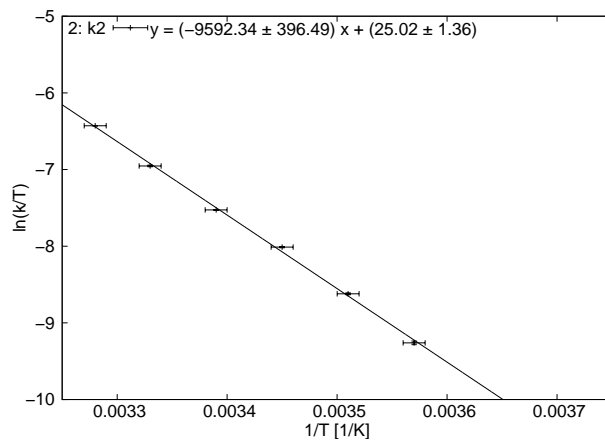


(e) complex 4

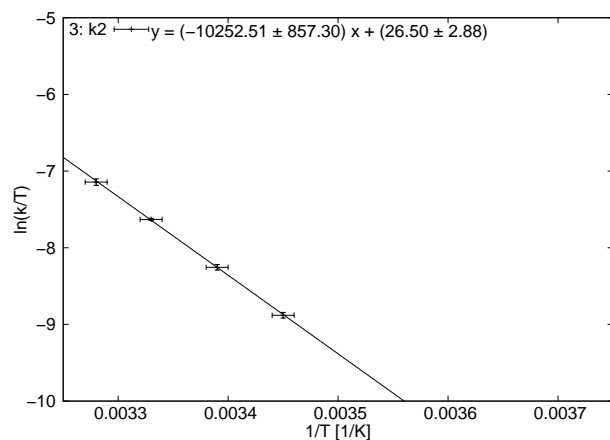
Figure 6: The linearized Eyring plots for  $k_1$ .



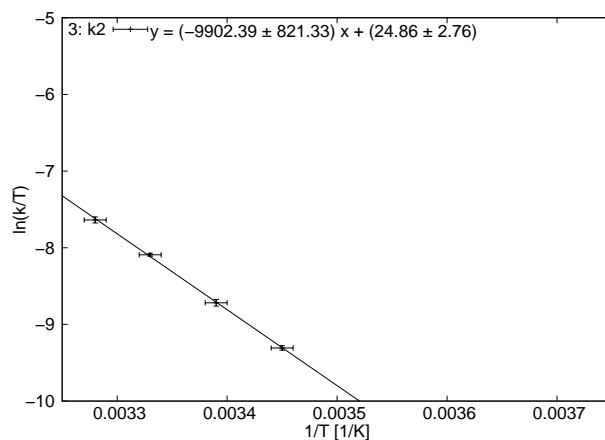
(a) complex 1



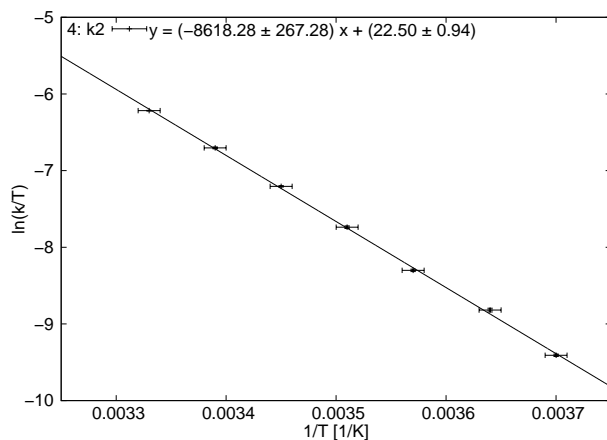
(b) complex 2



(c) complex 3a



(d) complex 3b



(e) complex 4

Figure 7: The linearized Eyring plots for  $k_2$ .