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Fine Tuning of Molecular Rotor Function in Photochemical Molecular Switches

Supplementary Information

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Mixing Times

Mixing Times - t_{mix} (s) - used for the rotor *cis-1* (S,S) at various temperatures

t_{mix} (s)	0.05	0.1	0.2	0.3	0.5	0.7	1.0	1.5
25°C			x	x	x	x	x	x
35°C		x	x	x	x			
45°C	x	x	x	x				
55°C	x	x	x	x				

Mixing Times - t_{mix} (s) - used for the rotor *trans-1* (S,S) at various temperatures

t_{mix} (s)	0.05	0.1	0.2	0.3	0.5	0.7	1.0	1.5
25°C				x	x	x	x	
35°C				x	x	x	x	
45°C		x	x	x	x			
55°C	x	x	x	x				

Mixing Times - t_{mix} (s) - used for the rotor *cis-2* (C,S) at various temperatures

t_{mix} (s)	0.05	0.1	0.2	0.3	0.5	0.7	1.0	1.5
25°C				x	x	x		
35°C			x	x	x			
45°C	x	x	x					
55°C	x	x						

Mixing Times - t_{mix} (s) - used for the rotor *trans-2* (C,S) at various temperatures

t_{mix} (s)	0.05	0.1	0.2	0.3	0.5	0.7	1.0	1.5
25°C				x	x	x		
35°C			x		x			
45°C	x	x	x	x				
55°C	x	x	x					

Mixing Times - t_{mix} (s) - used for the rotor *cis-3* (O,S) at various temperatures

t_{mix} (s)	0.05	0.1	0.2	0.3	0.5	0.7	1.0	1.5
25°C		x	x	x	x	x		
35°C		x	x	x	x			
45°C	x	x	x					
55°C	x	x						

Mixing Times - t_{mix} (s) - used for the rotor *trans-3* (O,S) at various temperatures

t_{mix} (s)	0.05	0.1	0.2	0.3	0.5	0.7	1.0	1.5
25°C		x				x	x	x
35°C		x	x	x	x			
45°C	x	x	x	x				
55°C	x	x						

Mixing Times - t_{mix} (s) - used for the rotor *cis-4* (S,O) at various temperatures

t_{mix} (s)	0.05	0.1	0.2	0.3	0.5	0.7	1.0	1.5
25°C				x	x	x	x	
35°C				x	x			
45°C	x	x	x					
55°C	x	x						

Mixing Times - t_{mix} (s) - used for the rotor *cis-5* (C,O) at various temperatures

t_{mix} (s)	0.05	0.1	0.2	0.3	0.5	0.7	1.0	1.5
25°C				x	x	x	x	x
35°C								
45°C	x	x	x	x				
55°C	x	x						

Mixing Times - t_{mix} (s) - used for the rotor *cis-6* (O,O) at various temperatures

t_{mix} (s)	0.05	0.1	0.2	0.3	0.5	0.7	1.0	1.5
25°C					x	x		
35°C		x	x	x	x	x		
45°C	x	x	x	x				
55°C	x	x						

Mixing Times - t_{mix} (s) - used for the rotor *trans-6* (O,O) at various temperatures

t_{mix} (s)	0.05	0.1	0.2	0.3	0.5	0.7	1.0	1.5
25°C					x	x		
35°C			x	x	x			
45°C	x	x	x					
55°C	x	x						

Rate Constants of the Rotation

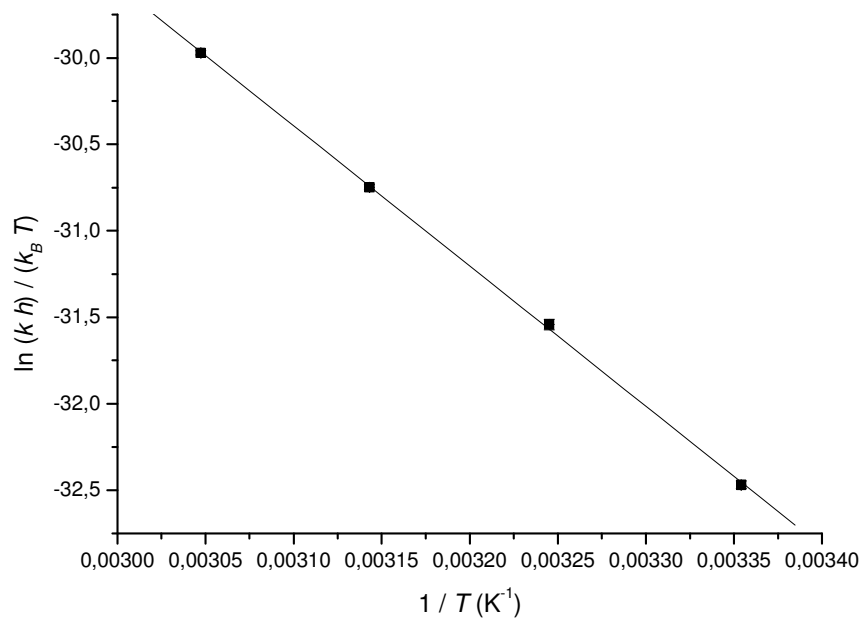
	<i>cis-1</i> (S,S)	<i>trans-1</i> (S,S)	<i>cis-2</i> (C,S)	<i>trans-2</i> (C,S)
T (°C)	k (s ⁻¹)	k (s ⁻¹)	k (s ⁻¹)	k (s ⁻¹)
25°C	$4.9 \pm 0.1 \cdot 10^{-2}$	$2.0 \pm 0.1 \cdot 10^{-2}$	$4.4 \pm 0.3 \cdot 10^{-2}$	$3.0 \pm 0.1 \cdot 10^{-2}$
35°C	$1.28 \pm 0.04 \cdot 10^{-1}$	$4.6 \pm 0.1 \cdot 10^{-2}$	$1.11 \pm 0.02 \cdot 10^{-1}$	$7.8 \pm 0.2 \cdot 10^{-2}$
45°C	$2.93 \pm 0.04 \cdot 10^{-1}$	$1.09 \pm 0.05 \cdot 10^{-1}$	$2.63 \pm 0.06 \cdot 10^{-1}$	$1.65 \pm 0.05 \cdot 10^{-1}$
55°C	$6.58 \pm 0.08 \cdot 10^{-1}$	$2.49 \pm 0.09 \cdot 10^{-1}$	$5.94 \pm 0.07 \cdot 10^{-1}$	$3.74 \pm 0.07 \cdot 10^{-1}$

	<i>cis-3</i> (O,S)	<i>trans-3</i> (O,S)	<i>cis-4</i> (S,O)	<i>cis-5</i> (C,O)
T (°C)	k (s ⁻¹)	k (s ⁻¹)	k (s ⁻¹)	k (s ⁻¹)
25°C	$4.09 \pm 0.06 \cdot 10^{-2}$	$3.91 \pm 0.03 \cdot 10^{-2}$	$5.9 \pm 0.1 \cdot 10^{-2}$	$4.94 \pm 0.08 \cdot 10^{-2}$
35°C	$1.01 \pm 0.01 \cdot 10^{-1}$	$1.00 \pm 0.02 \cdot 10^{-1}$	$1.47 \pm 0.03 \cdot 10^{-1}$	$9.9 \pm 0.2 \cdot 10^{-2}$
45°C	$2.36 \pm 0.04 \cdot 10^{-1}$	$2.26 \pm 0.04 \cdot 10^{-1}$	$3.39 \pm 0.08 \cdot 10^{-1}$	$2.83 \pm 0.02 \cdot 10^{-1}$
55°C	$5.20 \pm 0.03 \cdot 10^{-1}$	$5.0 \pm 0.2 \cdot 10^{-1}$	$7.75 \pm 0.08 \cdot 10^{-1}$	$6.55 \pm 0.02 \cdot 10^{-1}$

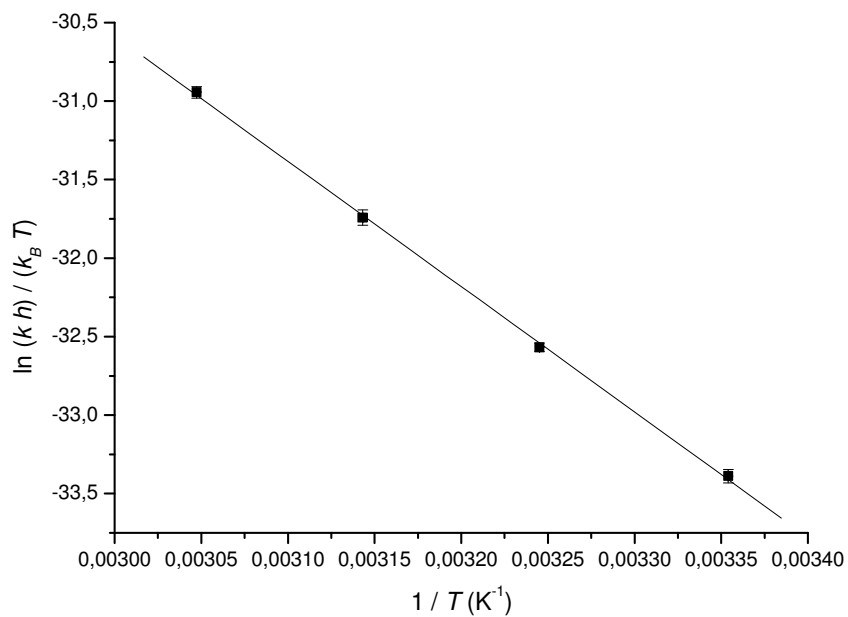
	<i>cis-6</i> (O,O)	<i>trans-6</i> (O,O)
T (°C)	k (s ⁻¹)	k (s ⁻¹)
25°C	$5.89 \pm 0.01 \cdot 10^{-2}$	$3.6 \pm 0.1 \cdot 10^{-2}$
35°C	$1.49 \pm 0.03 \cdot 10^{-1}$	$9.5 \pm 0.1 \cdot 10^{-2}$
45°C	$3.47 \pm 0.05 \cdot 10^{-1}$	$2.23 \pm 0.03 \cdot 10^{-1}$
55°C	$7.61 \pm 0.09 \cdot 10^{-1}$	$5.0 \pm 0.7 \cdot 10^{-1}$

Eyring Plots

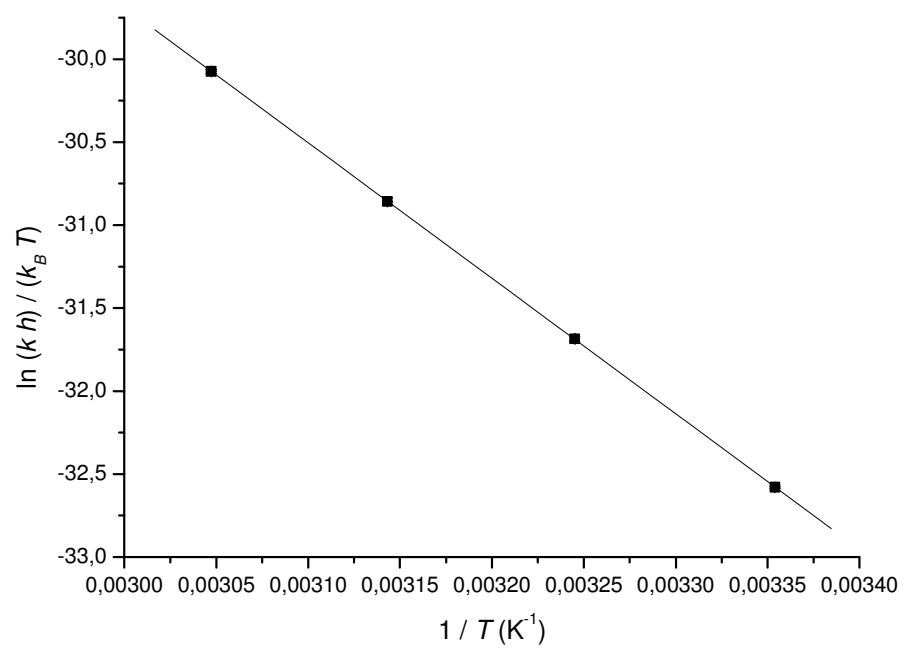
Eyring plot for the *cis*-SS-1 rotor:



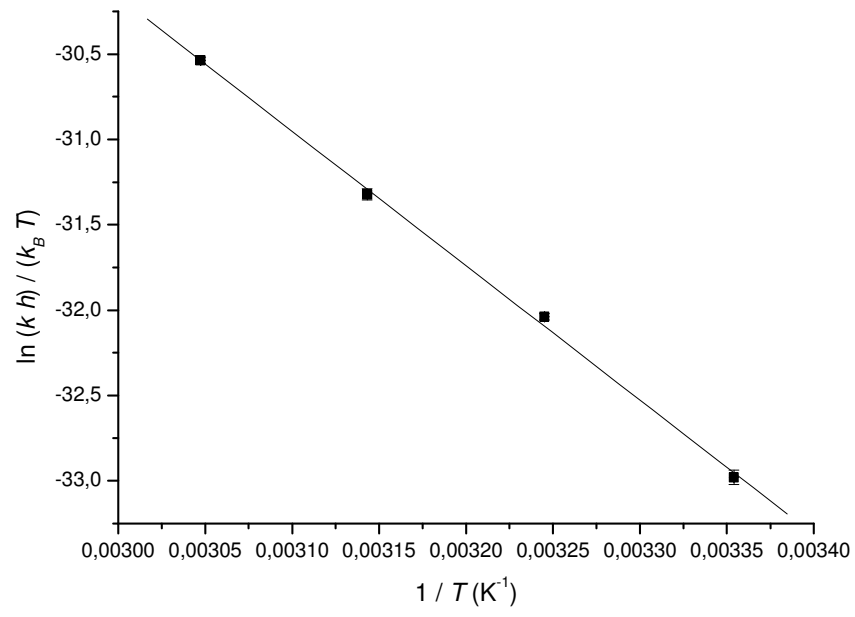
Eyring plot for the *trans*-SS-1 rotor:



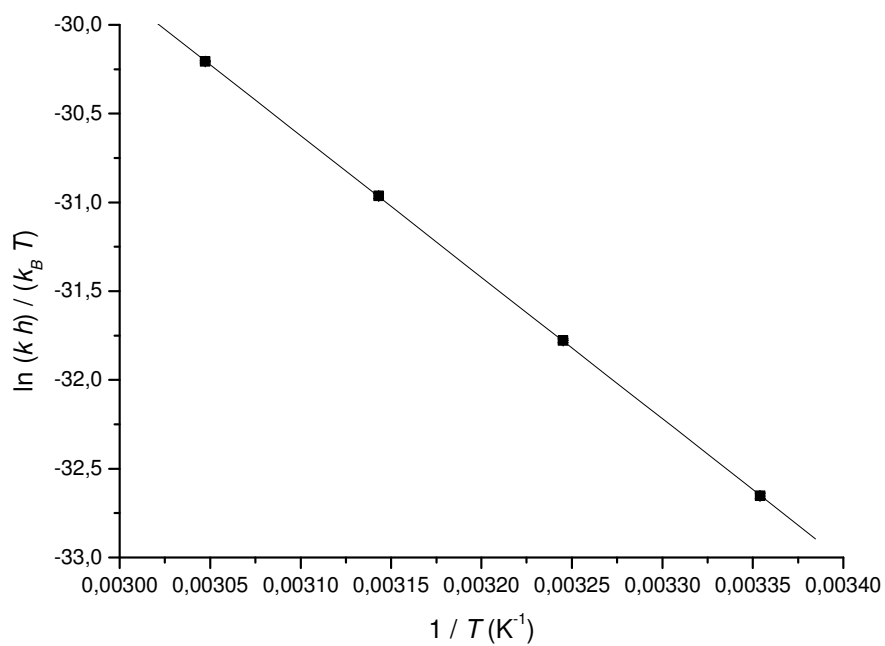
Eyring plot for the *cis*-CS-2 rotor:



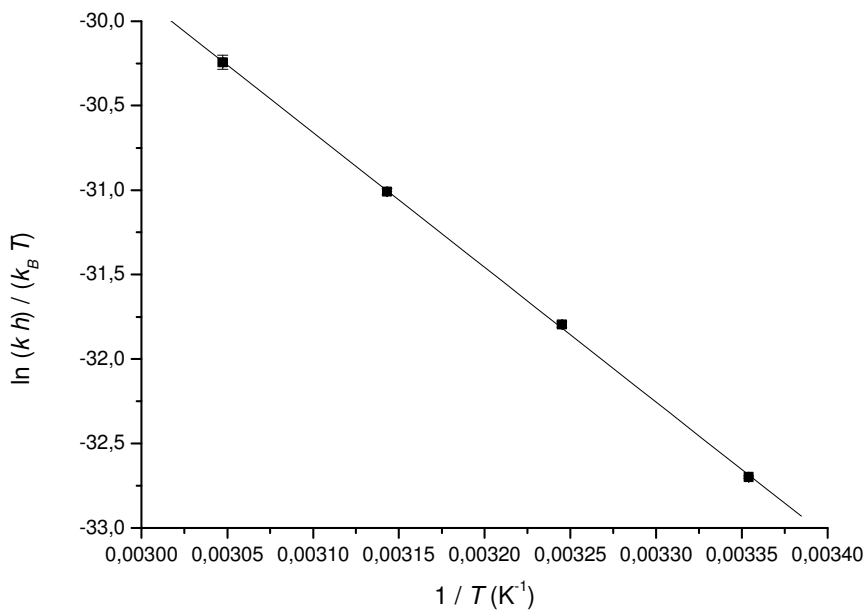
Eyring plot for the *trans*-CS-2 rotor:



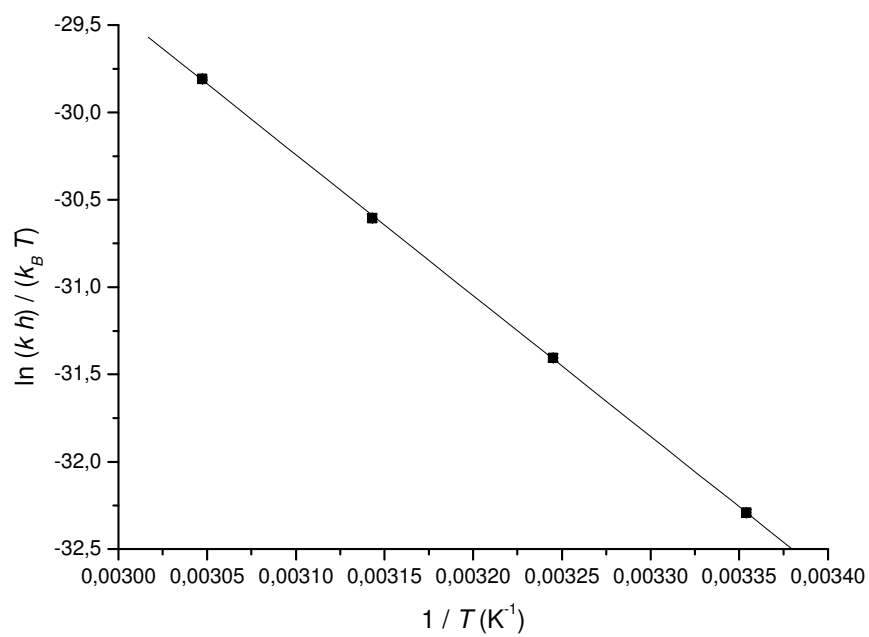
Eyring plot for the *cis*-OS-3 rotor:



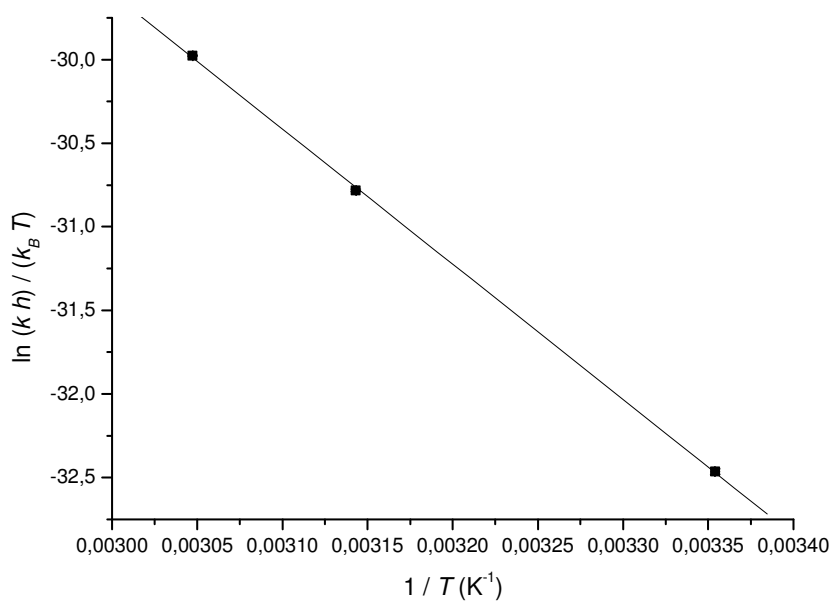
Eyring plot for the *trans*-OS-3 rotor:



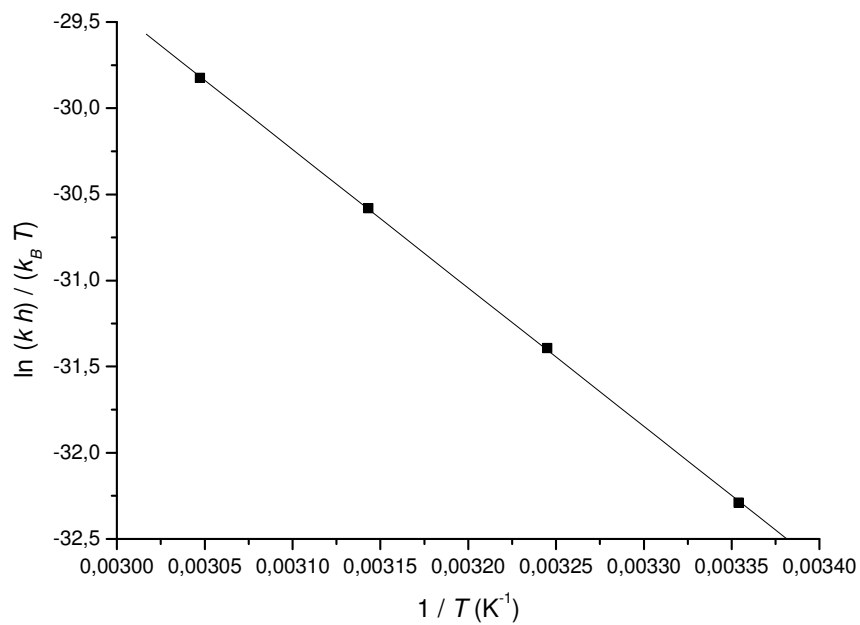
Eyring plot for the *cis*-SO-4 rotor:



Eyring plot for the *cis*-CO-5 rotor:



Eyring plot for the *cis*-OO-6 rotor:



Eyring plot for the *trans*-OO-6 rotor:

