AE-441: Determination of absorption coefficient of [Ru(CO)(OH)2(PNP)] with UV/Vis

Date: 2025-02-05 **Tags:** Dihydroxo PNP P(tBu)N(py)P(tBu)
[Ru(CO)(OH)2(PNP)] AE UV/Vis

Category: Two-photon Status: Done

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Reaction scheme/sample structure

Literature/reference experiments

Literature	https://doi.org/10.1039/D1EE01053K
Reproduction	
Similar experiments	PBDF - NB-JSC-143: Testing of BFD2 (MZ-124-6) DMSO and DMSO-H2O solutions

Reagents

Name	CAS Number / Experiment Number	Inventory number	Amount [μmol]	Equivalents	Mass _{theo} [mg]	Mass _{exp} [mg]	Molar mass [g/mol]	Density (g/ml)	Volume [ml]
[Ru(CO)(OH)2(PNP)]	Two-photon - AE-382: Synthesis of [Ru(CO)(OH)2(PNPtBu)] using Ag2O, 5 h (AE-382-3)	/	4.47 + 4.0	1	2.5 + 2.233	2.58 + 2.22	558.65	1	/
water	Prep work - AE-442: Degassing of Milli-Q water	1	1	/	1	I	1	1	2.5 + 4.0 + 1.5 + 1.4 + 1.5 + 1.8

Procedure/observations

All steps (unless stated otherwise) were carried out under argon using either standard Protocol - Schlenk Technique or in an nitrogen filled glovebox (MBRAUN).

The synthesis/reactions were performed in the dark by either wrapping the reaction flasks in aluminum foil or turning the lab light and light in the fume hood off, when the flasks were uncovered.

Date	Time	Step	Pictures	Observations
05.02		2 10 mL Schlenk flask were set under argon		
	10:10	To flask 1 [Ru] (2.58 mg) and to flask 2 [Ru] (2.22 mg) were added in air		
	10:20	Both flasks were set under argon: flask 1: AE-441-1 , flask 2: AE-441-2		

11:53 - 11:56	To -1 water (2.5 mL) and to -2 water (4.0 mL) was added		
- 12:16	The obtained solutions were stirred at 500 rpm	left: -2, right -1.jpg	left: clear, yellow solution, right: cloudy, yellow- orange suspension
	The Equipment - Avantes UV/vis spectrophotometer was turned on and allow to warm up for approx. 10 min		
	Both lamps were tuned on and the device was connected to the computer		
	A dark refernce spectra was measured to assure, that the light intesitiy is fitting		
12:12	A reference spectra of water was measured.	water.jpg	clear
	The water was discarded and the cuvette was dried by shaking off most of the water		
	From here on AE-441-1		
	The suspension was taken into a 5 mL syringe		
	From now work under air for -1:		
	The suspension was filtered through a PA syringe filter (pore diameter = 0.2 µm) into the quartz cuvette used for the reference measurement of water.		
12:21	An UV/Vis was recorded AE-441-1-1	-1-1.jpg	To concentrated
	The sample was pured in a 50 mL beaker		
	The cuvette was washed once with water and dried by shaking off most of the water		
	from AE-441-1-1 0.5 mL were taken off and transferrred into the cuvette using a 1 mL Eppendorf syringe		
	To the cuvette water (1.5 mL) was added using a 1 mL Eppendorf syringe		
12:25	An UV/Vis was recorded AE-441-1-2	-1-2.jpg	Better, still to concentrated
	The sample was pured in a 10 mL snap on cap vial		
	The cuvette was washed once with water and dried by shaking off most of the water		

	from AE-441-1-2 0.7 mL were taken off and transferrred into the cuvette using a 1 mL Eppendorf syringe		
	To the cuvette water (1.4 mL) was added using a 1 mL Eppendorf syringe		
12:28	An UV/Vis was recorded AE-441-1-3		Good intensity
	The sample was pured in a 10 mL snap on cap vial		
	The cuvette was washed once with water and dried by shaking off most of the water		
12:32	From here on AE-441-2 and work under air. The flask was kept closed, when not in use	-2 before takeing sample.jpg	no change
	0.5 mL of AE-441-2 were transferred into the cuvette using a 1 mL Eppendorf syringe		
	To the cuvette water (1.5 mL) was added using a 1 mL Eppendorf syringe		
12:35	An UV/Vis was recorded AE-441-2-1	-2-1.jpg	Looks ok, bit to concentrated
	The sample was pured in a 10 mL snap on cap vial		
	The cuvette was washed once with water and dried by shaking off most of the water		
	0.3 mL of AE-441-2 were transferred into the cuvette using a 1 mL Eppendorf syringe		
	To the cuvette water (1.8 mL) was added using a 1 mL Eppendorf syringe		
12:38	An UV/Vis was recorded AE-441-2-2	-2-2.jpg	Good intensity

Analysis

Date	Time		Analysis method	Analytical device	Solvent	Raw Data	Processed Data	Comparative Data	Used for evalutaion	Interpretation
05.02	12:21	AE-441-1-1	UV/Vis	Equipment - Avantes UV/vis spectrophotometer	H2O	AE-441-1-1.ABS8	AE-441-1-1_7420287SP.TXT AE-441-1-1.png	KRA-092: Radiation of [Ru(CO)(OH)2(PNPtBu)], 365 nm and white	UV_Vis_plotting_a.py	A[365 nm]: 2.645 Storng absorbtion, no clear bands observed
05.02	12:25	AE-441-1-2	UV/Vis	Equipment - Avantes UV/vis spectrophotometer	H2O	Ae-441-1-2.ABS8	Ae-441-1-2_7420287SP.TXT AE-441-1-2.png	KRA-092: Radiation of [Ru(CO)(OH)2(PNPtBu)], 365 nm and white	UV_Vis_plotting_a.py	A[365 nm]: 0.741 Stong absorprtion, 2 weak bands observed. For detailed discussion see -2-2

05.02	12:28	AE-441-1-3	UV/Vis	Equipment - Avantes UV/vis spectrophotometer	H2O	AE-441-1-3.ABS8	AE-441-1-3_7420287SP.TXT AE-441-1-3.png	KRA-092: Radiation of [Ru(CO)(OH)2(PNPtBu)], 365 nm and white	UV_Vis_plotting_a.py	A[365 nm]: 0.261 1 peak and 2 bands observed. For detailed discussion see -2-2
05.02	12:35	AE-441-2-1	UV/Vis	Equipment - Avantes UV/vis spectrophotometer	H2O	AE-441-2-1.ABS8	AE-441-2-1_7420287SP.TXT AE-441-2-1.png	KRA-092: Radiation of [Ru(CO)(OH)2(PNPtBu)], 365 nm and white	UV_Vis_plotting_a.py	A[365 nm]: 0.504 1 peak and 2 bands observed. For detailed discussion see -2-2
05.02	12:38	AE-441-2-2	UV/Vis	Equipment - Avantes UV/vis spectrophotometer	H2O	AE-441-2-2.ABS8	AE-441-2-2_7420287SP.TXT AE-441-2-2.png	KRA-092: Radiation of [Ru(CO)(OH)2(PNPtBu)], 365 nm and white	UV_Vis_plotting_a.py	A[365 nm]: 0.315 1 peak at 229 nm (A = 2.269). 1 band at 275 nm (A = 0.916) 1band at approx. 365 nm (A = 0.315)

Results

Result	File
Absorption coefficient: 2110 +- 100 M*cm^-1	AE-441_abostpiton_coeffientsaturated_conc.xlsx
Saturation concnetration: 1.44 +- 0.04 mM	AE-441_abostpiton_coeffientsaturated_conc.xlsx

Linked experiments

- KRA-092: Radiation of [Ru(CO)(OH)2(PNPtBu)], 365 nm and white

PBDF - NB-JSC-143: Testing of BFD2 (MZ-124-6) DMSO and DMSO-H2O solutions

Prep work - AE-442: Degassing of Milli-Q water

Two-photon - AE-382: Synthesis of [Ru(CO)(OH)2(PNPtBu)] using Ag2O, 5 h

Linked resource

Equipment - Avantes UV/vis spectrophotometer

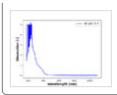
Attached files

AE-441_abostpiton_coeffientsaturated_conc.xlsx

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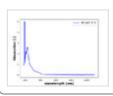
AE-441-1-2.png

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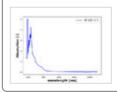
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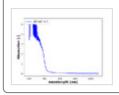
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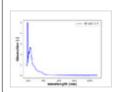
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AE-441-2-2.png

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UV_Vis_plotting_a.py

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water.jpg

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1-2.jpg

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left-2-right-1.jpg

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1-1.jpg

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2-before-takeing-sample.jpg

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2-1.jpg

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2-2.jpg

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Unique eLabID: 20250205-abfeea3185aff5d7554811f3afa6144d09c46eb9 Link: https://elab.water-splitting.org/experiments.php?mode=view&id=1707