



<b>Experiment title:</b> Study of the laser induced excited state of the $Na_2[Ru(NO_2)_4(OH)(NO)]2H_2O$ compound	<b>Experiment number:</b> CH419/420	
<b>Beamline:</b> ID11	<b>Date of Experiment:</b> from: 22-6-98                      to: 28-6-98	<b>Date of Report:</b>
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**Report:**

The experiment consisted of X-ray diffraction data collection on a  $Na_2[Ru(NO_2)_4(NO)(OH)]2H_2O$  monocrystal at 48KeV before and after laser excitation in order to determine laser-induced structural changes. A full data set was measured at 110K on the non-excited sample with the CCD Brucker area detector system. The indexing of the data allowed the optimization of the excitation by irradiating the crystal with the polarization direction of the laser light perpendicular to the NO-Ru-OH molecular axis. The crystal was excited for 8 hours with the 457.9nm argon laser line with a power density of 40mW/cm<sup>2</sup>. A full data collection was collected after irradiation. Afterwards the sample was de-excited by rising the temperature upto 230K for 30 minutes. A last data collection was performed at 110K on the de-excited sample.

We observed broadening of the Bragg peaks after excitation as well as significant differences in some integrated intensities. The X-ray diffraction data showed significant differences between the excited and non-excited crystal for the **Ru** - NO, N - O and one of the **Ru** -  $NO_2$  bonds (see table 1). The analysis of the data set collected on the de-excited sample demonstrated the structural changes are not due to any sample damage since we could reproduce the structural results preceding the excitation.

# Synchrotron X-ray single-crystal diffraction

	<b>Non-excited Sample</b>	<b>Excited Sample</b>	<b>De-excited Sample</b>
<b>Ru-N1</b>	1.746(8)	1.667(11)	1.756(11)
<b>Ru-OH</b>	1.930(7)	1.844( 10)	1.934(10)
<b>Ru-N2</b>	2.061(7)	2.119(11)	2.047( 10)
<b>Ru-N3</b>	2.056(8)	2.105(11)	2.062(10)
<b>Ru-N4</b>	2.060(9)	2.071(15)	2.046(13)
<b>Ru-NS</b>	2.086(9)	2.105(12)	2.075( 11)
<b>N1-09</b>	1.132(12)	1.081(17)	1.123(17)
<b>Ru-N1-09</b>	177.41(79)	176( 1)	175(1)
<b>R factor</b>	<b>0.066</b>	<b>0.078</b>	<b>0.086</b>
<b>Isotropic</b>	1892 ref.	1806 ref.	1766 ref.
<b>Refinement</b>	82 param.	82 param.	82 param.

Table 1. Na<sub>2</sub>[Ru(NO<sub>2</sub>)<sub>4</sub>NOOH]H<sub>2</sub>O most significant bond distances (in Å)