

## Supplementary Material

### **(OC-6-35-A)-Aquadicarbonylchlorido[2-(2-pyridyl)-1,8-naphthyridine- $\kappa^2N^1,N^2$ ]ruthenium(II) hexafluoridophosphate 2,2'-bipyridine**

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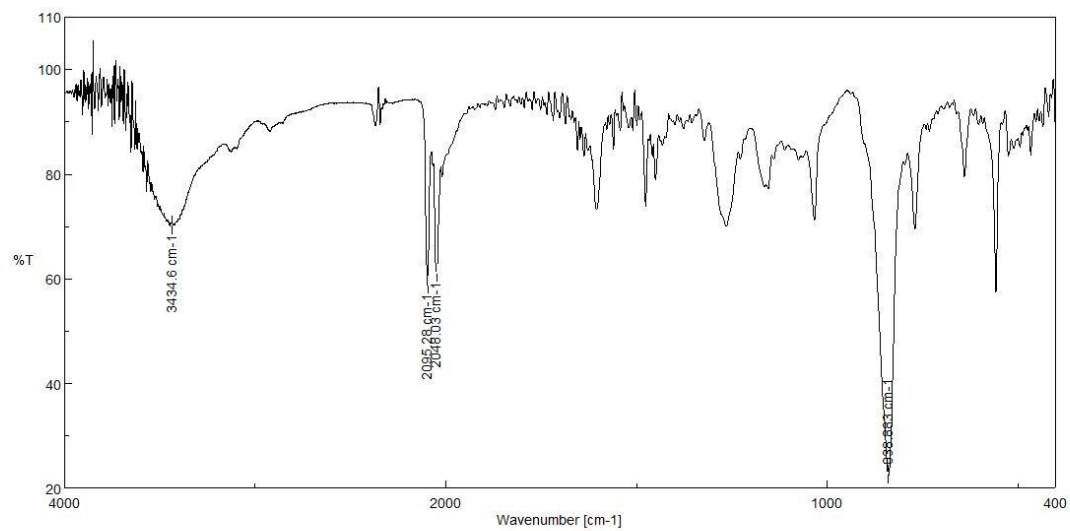


Figure S1. IR spectrum of the title compound (KBr pellet).

Table S1. Comparison between the experimental and DFT-calculated IR peaks for vCO.

	$\nu_s(\text{C}\equiv\text{O})/\text{cm}^{-1}$	$\nu_{as}(\text{C}\equiv\text{O})/\text{cm}^{-1}$
<i>Expt. data (KBr)</i>	2095	2048
<i>Calcd. data (vacuum)*</i>		
<b>(a)</b>	2177	2134
<b>(b)</b>	2173	2126
<b>(c)</b>	2176	2135
<b>(d)</b>	2169	2122
<b>(e)</b>	2173	2129
H-bonded complex**	2167	2125

\*(**a**) to (**e**) correspond to the configurations in Figure 2.

\*\*This is the cation-bpy complex, which is shown in Figure 5.