

Table 2: Selected calculated and experimental electronic transitions of ETRP.

Transition	Calculated	Experimental		
#	λ / nm	λ / nm	$\text{MO}_i \rightarrow \text{MO}_f$	Assignment
5	703.3	648	$416 \rightarrow 430$	Q_x
10	627.6	552	$416 \rightarrow 431$	Q_y
40	520.0	—	$429 \rightarrow 430$	MLCT (Ru $\rightarrow$ P)
49	502.1	450	$429 \rightarrow 448$	MLCT (Ru $\rightarrow$ Cl-Phen)
62	488.3	—	$423 \rightarrow 430$	MLCT (Ru $\rightarrow$ P)
183	373.3	—	$429 \rightarrow 456$	MLCT (Ru $\rightarrow$ Py)
215	345.2	419	$399 \rightarrow 431$	Soret
229	338.1	295	$425 \rightarrow 457$	MLCT (Ru $\rightarrow$ Cl-Phen)