



Figure 45. Multifrequency EPR and DFT Calculations (ORCA) for $\text{Tp}^*\text{Mo}^{\text{V}}\text{S}(\text{cat})$; cat = catecholate. (a) x-ray crystal structure of $\text{Tp}^*\text{Mo}^{\text{V}}\text{S}(\text{cat})$. Experimental spectra: (b) S-band, (d) X-band, (f) Q-band recorded at 130 K. (c,e,g) Computer-simulated spectra. $g_{xx} = 1.9646$, $g_{yy} = 1.9595$, $g_{zz} = 1.8970$, $A_{xx} = 30.0$, $A_{yy} = 29.0$, $A_{zz} = 67.5 \times 10^{-4} \text{ cm}^{-1}$, $\alpha = 0^\circ$, $\beta = 34.5^\circ$, $\gamma = 0^\circ$. (h) ORCA calculations of the HOMO and LUMO for $\text{Tp}^*\text{Mo}^{\text{V}}\text{S}(\text{cat})$ and the orientation of the principal components of the g - and A -matrices [52].