

Table 2-ESI. Γ_{XS} representation products corresponding to electric dipole allowed transitions in D_{2h} symmetry.^{a,b}

\otimes	a_g	b_{1g}	b_{2g}	b_{3g}	a_u	b_{1u}	b_{2u}	b_{3u}
	a_g					b_{1u}	b_{2u}	b_{3u}
	b_{1g}				b_{1u}	b_{3u}	b_{2u}	
	b_{2g}				b_{2u}	b_{3u}	b_{1u}	
	b_{3g}				b_{3u}	b_{2u}	b_{1u}	
	a_u	b_{1u}	b_{2u}	b_{3u}				
	b_{1u}	b_{1u}	b_{3u}	b_{2u}				
	b_{2u}	b_{2u}	b_{3u}	b_{1u}				
	b_{3u}	b_{3u}	b_{2u}	b_{1u}				

^a $\Gamma_{XS} = b_{1u}$ implies 1s π^* transitions involving *pcm*-based π_{\perp}^* MOs. ^b $\Gamma_{XS} = b_{2u}$ or b_{3u} implies 1s π^* transitions involving Ph- and F-based π_{\parallel}^* .
