

Table 5-ESI *EEs* (eV) and oscillator strengths *f* for the N 1s excitation spectrum of **I** from SR ZORA TD-DFT calculations. Only excitations lying at *EE* lower than 398 eV and having $f \geq 10^{-3}$ and contributions $\geq 10\%$ are reported.

	<i>imo</i>	<i>imol</i>	<i>EE</i>	ΔEE	Sym	$f \times 10^3$	<i>fmo</i>	<i>fmo character</i>	<i>Assignment</i>
1	$1b_{3u}$	N ^{py}	394.28	-	b _{1u}	9.9439	$12b_{2g}^{(100)}$	π_{\perp}^*	A
2	$1b_{2u}$	N ^{pyH}	395.98	1.70	b _{1u}	7.7402	$12b_{3g}^{(100)}$	π_{\perp}^*	B
3	$2a_g$	N ^{py} /N ^{pyH}	397.17	2.89	b _{1u}	10.306	$15b_{1u}^{(97)}$	π_{\perp}^*	C
4	$1b_{3u}$	N ^{py}	397.59	3.31	b _{1u}	9.9127	$14b_{2g}^{(97)}$	π_{\perp}^*	C