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Table 5-ESI *EE*s (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 $f \ge 10^{-3}$ and contributions $\ge 10\%$ are reported.

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