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Table 6-ESI *EE*s (eV) and oscillator strengths f for the N 1s excitation spectrum of **II** 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	$4b_{3u}$	Npy	394.21	-	b_{1u}	9.4518	$21b_{2g}^{(100)}$	π_{\perp}^*	A
2	$4b_{2u}$	NpyH	395.95	1.74	b _{1u}	7.1869	$21b_{3g}^{(100)}$	π_{\perp}^*	В
3	$5a_g$	Npy	397.17	2.96	b _{1u}	9.6101	$24b_{1u}^{(98)}$	π_{\perp}^*	C
4	$4b_{3u}$	Npy	397.55	3.34	b_{1u}	4.3849	$23b_{2g}^{(97)}$	π_{\perp}^*	C
5	$4b_{3u}$	Npy	397.95	3.74	b _{1u}	8.8200	$24b_{2a}^{(91)}$	$\pi_{\perp}*$	C