

Table 6-ESI *EEs* (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 $f \geq 10^{-3}$ 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	$4b_{3u}$	N ^{py}	394.21	-	b _{1u}	9.4518	$21b_{2g}^{(100)}$	π_{\perp}^*	A
2	$4b_{2u}$	N ^{pyH}	395.95	1.74	b _{1u}	7.1869	$21b_{3g}^{(100)}$	π_{\perp}^*	B
3	$5a_g$	N ^{py}	397.17	2.96	b _{1u}	9.6101	$24b_{1u}^{(98)}$	π_{\perp}^*	C
4	$4b_{3u}$	N ^{py}	397.55	3.34	b _{1u}	4.3849	$23b_{2g}^{(97)}$	π_{\perp}^*	C
5	$4b_{3u}$	N ^{py}	397.95	3.74	b _{1u}	8.8200	$24b_{2g}^{(91)}$	π_{\perp}^*	C