Table 4-ESI *EE*s (eV) and oscillator strengths *f* for the C 1s excitation spectrum of **II** from SR ZORA TD-DFT calculations. Only excitations lying at *EE* lower than 288 eV and having $f \geq 10 \times 10^{-3}$ and contributions ≥ 20% are reported.

	imo	imol	*EE*	Δ*EE*	sym	$f \times 10^3$	*fmo*(%)	*fmo character*	*Assignment*
1	$13b_{2u}$	C^7	281.07		b_{1u}	15.410	$21b_{3g}^{(96)}$	$\pi_\perp^*$	**S**
2	$12b_{3u} + 12b_{2u}$	C^2	281.50		b_{1u}	18.646	$21b_{2g}^{(70)} + 21b_{3g}^{(30)}$	$\pi_\perp^*$	**S**
3	$11b_{2u}$	C^6	282.22		b_{1u}	22.399	$21b_{3g}^{(94)}$	$\pi_\perp^*$	**A**
4	$10b_{3u} + 10b_{2u}$	C^5	282.30		b_{1u}	38.531	$21b_{2g}^{(51)} + 21b_{3g}^{(48)}$	$\pi_\perp^*$	**A**
5	$12b_{1g}$	C^7	282.33		b_{1u}	17.901	$20a_u^{(99)}$	$\pi_\perp^*$	**A**
6	$9b_{2u} + 9b_{3u}$	C^1	282.71		b_{1u}	18.698	$21b_{3g}^{(52)} + 21b_{2g}^{(48)}$	$\pi_\perp^*$	**A**
7	$11b_{1g}$	C^2	282.75		b_{1u}	18.838	$20a_u^{(99)}$	$\pi_\perp^*$	**A**
8	$9b_{1g}$	C^5	283.52		b_{1u}	25.435	$20a_u^{(97)}$	$\pi_\perp^*$	**B**
9	$8b_{3u} + 9a_g + 7b_{1g}$	C^{25}	284.17		b_{2u}	52.176	$38b_{1g}^{(32)} + 41b_{2u}^{(24)} + 41b_{3u}^{(24)}$	$\pi_\parallel^*$ (e_{2u}^2)	**B**
10	$8b_{2u} + 7b_{1g} + 9a_g$	C^{25}	284.17		b_{3u}	49.018	$38b_{1g}^{(32)} + 41b_{2u}^{(24)} + 41b_{3u}^{(24)}$	$\pi_\parallel^*$ (e_{2u}^2)	**B**
11	$13b_{2u}$	C^7	284.46		b_{1u}	23.683	$23b_{3g}^{(88)}$	$\pi_\perp^*$	**B**
12	$12b_{3u}$	C^2	284.90		b_{1u}	19.241	$23b_{2g}^{(70)}$	$\pi_\perp^*$	**C**
13	$12b_{1g}$	C^7	284.90		b_{1u}	37.911	$23a_u^{(94)}$	$\pi_\perp^*$	**C**
14	$11b_{1g}$	C^2	285.33		b_{1u}	50.465	$23a_u^{(86)}$	$\pi_\perp^*$	**C**
15	$10a_g$	C^1	285.67		b_{1u}	16.093	$24b_{1u}^{(96)}$	$\pi_\perp^*$	**C**
16	$6b_{3u}$	C^{37}	285.79		b_{2u}	11.504	$38b_{1g}^{(79)}$	$\pi_\parallel^*$ (e_{2u}^2)	**C**
17	$6b_{2u}$	C^{37}	285.79		b_{3u}	10.454	$38b_{1g}^{(79)}$	$\pi_\parallel^*$ (e_{2u}^2)	**C**
18	$10b_{1g+}11b_{3u}$	C^6	285.99		b_{1u}	21.738	$23a_u^{(73)} + 24b_{2g}^{(20)}$	$\pi_\perp^*$	**C**
19	$9b_{3u} + 9b_{2u}$	C^1	286.11		b_{1u}	22.657	$23b_{2g}^{(43)} + 23b_{3g}^{(41)}$	$\pi_\perp^*$	**C**
20	$13b_{2u}$	C^7	286.11		b_{1u}	24.690	$25b_{3g}^{(85)}$	$\pi_\perp^*$	**C**
21	$5b_{3u} + 6a_g + 4b_{1g}$	C^{45}	286.13		b_{2u}	48.934	$38b_{1g+}^{(32)}41b_{2u}^{(24)} + 41b_{3u}^{(24)}$	$\pi_\parallel^*$ (e_{2u}^2)	**C**
22	$5b_{2u} + 4b_{1g} + 6a_g$	C^{45}	286.13		b_{3u}	46.893	$38b_{1g+}^{(32)}41b_{2u}^{(24)} + 41b_{3u}^{(24)}$	$\pi_\parallel^*$ (e_{2u}^2)	**C**
23	$4b_{1u} + 4a_u + 4b_{2g+}4b_{3g}$	C^{29}	286.17		b_{2u}	122.23	$22b_{3g}^{(23)} + 22b_{2g}^{(23)} + 21a_u^{(22)} + 23b_{1u}^{(20)}$	$\pi_\parallel^*$ (e_{2u}^1)	**C**
24	$4a_u + 4b_{1u} + 4b_{3g} + 4b_{2g}$	C^{29}	286.17		b_{3u}	116.80	$22b_{3g}^{(23)} + 22b_{2g}^{(23)} + 21a_u^{(22)} + 23b_{1u}^{(20)}$	$\pi_\parallel^*$ (e_{2u}^1)	**C**
25	$7a_g$	C^{37}	286.17		b_{2u}	43.467	$42b_{2u}^{(20)}$	σ^*	**C**
26	$5b_{1g}$	C^{37}	286.17		b_{3u}	40.486	$42b_{2u}^{(20)}$	σ^*	**C**
27	$5b_{1g} + 7a_g$	C^{37}	286.18		b_{2u}	30.613	$42b_{3u}^{(32)} + 42b_{2u}^{(30)}$	σ^*	**C**
28	$7a_g + 5b_{1g}$	C^{37}	286.18		b_{3u}	28.404	$42b_{3u}^{(32)} + 42b_{2u}^{(30)}$	σ^*	**C**

29	$3a_u + 3b_{3g} + 3b_{2g}$	C^{37}	286.26		b_{1u}	31.910	$39b_{1g}^{(41)} + 42b_{2u}^{(23)} + 42b_{3u}^{(23)}$	σ*	**C**
30	$5b_{3u} + 6a_g + 4b_{1g}$	C^{45}	286.38		b_{2u}	13.782	$39b_{1g}^{(38)} + 42b_{2u}^{(24)} + 42b_{3u}^{(23)}$	σ*	**C**
31	$5b_{2u} + 4b_{1g} + 6a_g$	C^{45}	286.38		b_{3u}	13.426	$39b_{1g}^{(38)} + 42b_{2u}^{(24)} + 42b_{3u}^{(23)}$	σ*	**C**
32	$8b_{1g}$	C^{1}	286.49		b_{1u}	28.257	$23a_u^{(90)}$	$\pi_\perp$*	**C**
33	$12b_{3u}$	C^{2}	286.65		b_{1u}	12.126	$25b_{2g}^{(98)}$	$\pi_\perp$*	**C**
34	$11b_{2u} + 11b_{3u}$	C^{6}	287.26		b_{1u}	15.799	$25b_{3g}^{(50)} + 25b_{2g}^{(32)}$	$\pi_\perp$*	**D**
35	$10b_{2u} + 10b_{3u}$	C^{5}	287.28		b_{1u}	11.113	$25b_{3g}^{(66)} + 25b_{2g}^{(20)}$	$\pi_\perp$*	**D**
36	$10b_{3u}$	C^{5}	287.47		b_{1u}	38.628	$25b_{2g}^{(78)}$	$\pi_\perp$*	**D**
37	$11b_{3u}$	C^{6}	287.51		b_{1u}	115.32	$25b_{2g}^{(65)}$	$\pi_\perp$*	**D**
38	$9b_{2u} + 9b_{3u}$	C^{1}	287.75		b_{1u}	17.137	$25b_{3g}^{(65)} + 25b_{2g}^{(20)}$	$\pi_\perp$*	**D**
39	$8b_{3u}$	C^{25}	287.84		b_{2u}	29.101	$42b_{1g}^{(41)}$	σ*	**D**
40	$8b_{2u}$	C^{25}	287.84		b_{3u}	29.054	$42b_{1g}^{(41)}$	σ*	**D**
41	$9b_{3u}$	C^{1}	287.94		b_{1u}	58.707	$25b_{2g}^{(78)}$	$\pi_\perp$*	**D**