

Table 3-ESI *EEs* (eV) and oscillator strengths *f* for the C 1s excitation spectrum of **I** from SR ZORA TD-DFT calculations. Only excitations lying at *EE* lower than 288 eV and having *f* ≥ 10 × 10⁻³ and contributions ≥ 20% are reported.

	<i>imo</i>	<i>imol</i>	<i>EE</i>	ΔEE	Sym	<i>f</i> × 10 ³	<i>fmo</i>	<i>fmo character</i>	<i>Assignment</i>
1	10 <i>b</i> _{2u} + 10 <i>b</i> _{3u}	C ⁷	281.14	-	b _{1u}	15.234	12 <i>b</i> _{3g} ⁽⁸²⁾ + 12 <i>b</i> _{2g} ⁽¹⁸⁾	$\pi_{\perp}^*$	S
2	7 <i>b</i> _{3u}	C ²⁹	281.58	0.44	b _{1u}	17.500	12 <i>b</i> _{2g} ⁽¹⁰⁰⁾	$\pi_{\perp}^*$	S
3	4 <i>b</i> _{3u} + 4 <i>b</i> _{2u}	C ⁵	282.06	0.92	b _{1u}	41.465	12 <i>b</i> _{2g} ⁽⁶⁷⁾ + 12 <i>b</i> _{3g} ⁽³³⁾	$\pi_{\perp}^*$	A
4	3 <i>b</i> _{2u} + 3 <i>b</i> _{2u}	C ⁶	282.18	1.04	b _{1u}	18.044	12 <i>b</i> _{3g} ⁽⁷⁴⁾ + 12 <i>b</i> _{2g} ⁽²⁶⁾	$\pi_{\perp}^*$	A
5	9 <i>b</i> _{1g}	C ⁷	282.41	1.27	b _{1u}	18.978	11 <i>a</i> _u ⁽¹⁰⁰⁾	$\pi_{\perp}^*$	A
6	2 <i>b</i> _{2u} + 2 <i>b</i> _{2u}	C ¹	282.70	1.56	b _{1u}	17.116	12 <i>b</i> _{2g} ⁽⁷⁴⁾ + 12 <i>b</i> _{3g} ⁽²⁶⁾	$\pi_{\perp}^*$	A
7	6 <i>b</i> _{1g}	C ²⁹	282.84	1.70	b _{1u}	23.263	11 <i>a</i> _u ⁽¹⁰⁰⁾	$\pi_{\perp}^*$	A
8	8 <i>a</i> _g + 8 <i>b</i> _{3u}	C ²	283.23	2.09	b _{2u}	14.217	30 <i>b</i> _{2u} ⁽⁵²⁾ + 27 <i>b</i> _{1g} ⁽³⁴⁾	$\pi_{\parallel}^* (e_{2u}^2)$	B
9	3 <i>b</i> _{1g}	C ⁵	283.27	2.13	b _{1u}	30.038	11 <i>a</i> _u ⁽⁹⁹⁾	$\pi_{\perp}^*$	B
10	8 <i>b</i> _{3u} + 7 <i>b</i> _{1g}	C ²	283.32	2.18	b _{2u}	29.164	27 <i>b</i> _{1g} ⁽⁴⁹⁾ + 30 <i>b</i> _{3u} ⁽²⁵⁾	$\pi_{\parallel}^* (e_{2u}^2)$	B
11	7 <i>b</i> _{2u} + 7 <i>b</i> _{1g} + 8 <i>a</i> _g	C ²	283.32	2.18	b _{3u}	40.018	27 <i>b</i> _{1g} ⁽⁴²⁾ + 30 <i>b</i> _{2u} ⁽²³⁾ + 30 <i>b</i> _{3u} ⁽²¹⁾	$\pi_{\parallel}^* (e_{2u}^2)$	B
12	2 <i>b</i> _{1u} + 2 <i>a</i> _u + 2 <i>b</i> _{2g}	C ²⁹	283.41	2.27	b _{2u}	146.69	13 <i>b</i> _{3g} ⁽²⁵⁾ + 13 <i>b</i> _{2g} ⁽²⁵⁾ + 12 <i>a</i> _u ⁽²¹⁾	$\pi_{\parallel}^* (e_{2u}^1)$	B
13	2 <i>a</i> _u + 2 <i>b</i> _{1u} + 2 <i>b</i> _{3g}	C ²⁹	283.42	2.28	b _{3u}	147.97	13 <i>b</i> _{3g} ⁽²³⁾ + 13 <i>b</i> _{2g} ⁽²³⁾ + 12 <i>a</i> _u ⁽²⁰⁾	$\pi_{\parallel}^* (e_{2u}^1)$	B
14	9 <i>b</i> _{3u} + 10 <i>a</i> _g + 8 <i>b</i> _{1g}	C ⁴⁵	283.42	2.28	b _{2u}	52.508	27 <i>b</i> _{1g} ⁽³⁴⁾ + 30 <i>b</i> _{2u} ⁽²⁴⁾ + 30 <i>b</i> _{3u} ⁽²⁴⁾	$\pi_{\parallel}^* (e_{2u}^2)$	B
15	9 <i>b</i> _{2u} + 8 <i>b</i> _{1g} + 10 <i>a</i> _g	C ⁴⁵	283.42	2.28	b _{3u}	51.139	27 <i>b</i> _{1g} ⁽³⁴⁾ + 30 <i>b</i> _{2u} ⁽²⁴⁾ + 30 <i>b</i> _{3u} ⁽²⁴⁾	$\pi_{\parallel}^* (e_{2u}^2)$	B
16	1 <i>b</i> _{1u} + 1 <i>a</i> _u	C ³⁷	283.45	2.31	b _{2u}	50.337	13 <i>b</i> _{3g} ⁽²²⁾ + 13 <i>b</i> _{2g} ⁽²²⁾	$\pi_{\parallel}^* (e_{2u}^1)$	B
17	1 <i>a</i> _u + 1 <i>b</i> _{1u}	C ³⁷	283.45	2.31	b _{3u}	48.995	13 <i>b</i> _{3g} ⁽²²⁾ + 13 <i>b</i> _{2g} ⁽²²⁾	$\pi_{\parallel}^* (e_{2u}^1)$	B
18	5 <i>b</i> _{3u} + 6 <i>a</i> _g + 4 <i>b</i> _{1g}	C ²⁵	283.77	2.63	b _{2u}	50.581	27 <i>b</i> _{1g} ⁽³³⁾ + 30 <i>b</i> _{2u} ⁽²⁴⁾ + 30 <i>b</i> _{3u} ⁽²⁴⁾	$\pi_{\parallel}^* (e_{2u}^2)$	B
19	5 <i>b</i> _{2u} + 4 <i>b</i> _{1g} + 6 <i>a</i> _g	C ²⁵	283.77	2.63	b _{3u}	49.090	27 <i>b</i> _{1g} ⁽³³⁾ + 30 <i>b</i> _{2u} ⁽²⁴⁾ + 30 <i>b</i> _{3u} ⁽²⁴⁾	$\pi_{\parallel}^* (e_{2u}^2)$	B
20	10 <i>b</i> _{2u} + 10 <i>b</i> _{3u}	C ⁷	284.46	3.32	b _{1u}	22.872	14 <i>b</i> _{3g} ⁽⁶⁸⁾ + 14 <i>b</i> _{2g} ⁽²⁸⁾	$\pi_{\perp}^*$	C
21	9 <i>b</i> _{1g}	C ⁷	284.86	3.72	b _{1u}	33.752	13 <i>a</i> _u ⁽⁹⁵⁾	$\pi_{\perp}^*$	C
22	7 <i>b</i> _{3u}	C ²⁹	284.94	3.80	b _{1u}	25.316	14 <i>b</i> _{2g} ⁽⁹³⁾	$\pi_{\perp}^*$	C
23	4 <i>a</i> _g	C ⁶	285.05	3.91	b _{1u}	10.667	15 <i>b</i> _{1u} ⁽⁹⁹⁾	$\pi_{\perp}^*$	C
24	6 <i>b</i> _{1g}	C ²⁹	285.32	4.18	b _{1u}	54.004	13 <i>a</i> _u ⁽⁹²⁾	$\pi_{\perp}^*$	C
25	3 <i>b</i> _{3u}	C ⁶	285.50	4.36	b _{1u}	14.832	14 <i>b</i> _{2g} ⁽⁹¹⁾	$\pi_{\perp}^*$	C
26	3 <i>a</i> _g	C ¹	285.60	4.46	b _{1u}	15.770	15 <i>b</i> _{1u} ⁽⁹⁶⁾	$\pi_{\perp}^*$	C
27	10 <i>b</i> _{2u}	C ⁷	285.93	4.79	b _{1u}	20.361	16 <i>b</i> _{3g} ⁽⁹³⁾	$\sigma^* + \pi_{\perp}^*$	D
28	2 <i>b</i> _{3u} + 2 <i>b</i> _{2u}	C ¹	286.04	4.90	b _{1u}	29.220	14 <i>b</i> _{2g} ⁽⁶⁵⁾ + 14 <i>b</i> _{3g} ⁽²⁸⁾	$\pi_{\perp}^*$	D

29	$5b_{1g}$	C^{37}	286.19	5.05	b_{1u}	13.632	$15a_u^{(76)}$	$\pi_{\perp}^*$	D
30	$1b_{1g}$	C^1	286.38	5.24	b_{1u}	24.560	$13a_u^{(95)}$	$\pi_{\perp}^*$	D
31	$7b_{1g}$	C^2	286.59	5.45	b_{2u}	13.829	$34b_{3u}^{(96)}$	σ^*	D
32	$8b_{3u} + 8b_{3u}$	C^2	286.66	5.52	b_{3u}	24.517	$38a_g^{(61)} + 39a_g^{(22)}$	$\sigma^* + \pi_{\parallel}^* (b_{2g})$	D
33	$8b_{3u}$	C^2	286.68	5.54	b_{3u}	22.294	$39a_g^{(75)}$	$\pi_{\parallel}^* (b_{2g})$	D
34	$8b_{3u}$	C^2	286.73	5.59	b_{2u}	20.974	$31b_{1g}^{(92)}$	$\sigma^* + \pi_{\parallel}^* (b_{2g})$	D
35	$4b_{2u}$	C^5	286.77	5.63	b_{1u}	15.696	$16b_{3g}^{(81)}$	$\sigma^* + \pi_{\perp}^*$	D
36	$10a_g + 8b_{1g}$	C^{45}	286.84	5.70	b_{2u}	13.061	$35b_{2u}^{(49)} + 35b_{3u}^{(24)}$	σ^*	D
37	$8b_{1g} + 10a_g$	C^{45}	286.84	5.70	b_{3u}	13.037	$35b_{2u}^{(49)} + 35b_{3u}^{(24)}$	σ^*	D
38	$7b_{1g}$	C^2	286.86	5.72	b_{2u}	26.208	$35b_{3u}^{(94)}$	σ^*	D
39	$10a_g$	C^{45}	286.90	5.76	b_{2u}	11.382	$36b_{2u}^{(73)}$	$\pi_{\parallel}^* (b_{2g})$	D
40	$7b_{1g}$	C^2	286.92	5.78	b_{3u}	11.334	$35b_{2u}^{(93)}$	σ^*	D
41	$4b_{3u}$	C^5	286.94	5.80	b_{1u}	23.754	$16b_{2g}^{(90)}$	$\sigma^* + \pi_{\perp}^*$	D
42	$3b_{2u} + 3b_{3u}$	C^6	286.99	5.85	b_{1u}	15.450	$16b_{3g}^{(56)} + 16b_{2g}^{(26)}$	$\sigma^* + \pi_{\perp}^*$	D
43	$9b_{3u}$	C^{45}	287.00	5.86	b_{2u}	15.750	$32b_{1g}^{(87)}$	σ^*	D
44	$9b_{2u}$	C^{47}	287.00	5.86	b_{3u}	14.953	$32b_{1g}^{(87)}$	σ^*	D
45	$8b_{3u}$	C^2	287.14	6.00	b_{2u}	11.433	$32b_{1g}^{(97)}$	σ^*	D
46	$3b_{3u}$	C^6	287.24	6.10	b_{1u}	76.781	$16b_{2g}^{(70)}$	$\sigma^* + \pi_{\perp}^*$	D
47	$2b_{2u}$	C^1	287.49	6.35	b_{1u}	20.889	$16b_{3g}^{(69)}$	$\sigma^* + \pi_{\perp}^*$	D
48	$4b_{3u}$	C^5	287.55	6.41	b_{1u}	20.885	$17b_{2g}^{(79)}$	$\pi_{\perp}^*$	D
49	$2b_{3u}$	C^1	287.68	6.54	b_{1u}	47.257	$16b_{2g}^{(82)}$	$\sigma^* + \pi_{\perp}^*$	D
50	$3b_{1g}$	C^1	287.68	6.54	b_{1u}	14.884	$16a_u^{(94)}$	σ^*	D