

**Table 7-ESI** *EEs* (eV) and oscillator strengths *f* for the F 1s excitation spectrum of **II** from SR ZORA TD-DFT calculations. Only excitations lying at *EE* lower than 683 eV and having  $f \geq 10 \times 10^{-3}$  and contributions  $\geq 20\%$  are reported.

|   | <i>imo</i>                 | <i>imol</i>     | <i>EE</i> | $\Delta EE$ | Sym             | $f \times 10^3$ | <i>fmo</i>                                            | <i>fmo character</i>    |
|---|----------------------------|-----------------|-----------|-------------|-----------------|-----------------|-------------------------------------------------------|-------------------------|
| 1 | $2b_{1u} + 2a_u + 2b_{2g}$ | F <sup>49</sup> | 681.25    | -           | B <sub>2u</sub> | 13.668          | $22b_{3g}^{(31)} + 22b_{2g}^{(31)} + 21a_u^{(22)}$    | $\pi_{  }^* (e_{2u}^1)$ |
| 2 | $2a_u + 2b_{1u} + 2b_{3g}$ | F <sup>49</sup> | 681.25    | -           | B <sub>3u</sub> | 13.668          | $22b_{3g}^{(31)} + 22b_{2g}^{(29)} + 21a_u^{(22)}$    | $\pi_{  }^* (e_{2u}^1)$ |
| 3 | $1b_{1u} + 1a_u + 1b_{2g}$ | F <sup>57</sup> | 681.35    | 0.10        | B <sub>2u</sub> | 13.296          | $22b_{3g}^{(31)} + 22b_{2g}^{(29)} + 21a_u^{(22)}$    | $\pi_{  }^* (e_{2u}^1)$ |
| 4 | $1a_u + 1b_{1u} + 1b_{3g}$ | F <sup>57</sup> | 681.35    | 0.10        | B <sub>3u</sub> | 12.439          | $22b_{3g}^{(31)} + 22b_{2g}^{(29)} + 21a_u^{(22)}$    | $\pi_{  }^* (e_{2u}^1)$ |
| 5 | $2a_u + 2b_{3g} + 2b_{2g}$ | F <sup>49</sup> | 681.53    | 0.18        | B <sub>1u</sub> | 14.651          | $39b_{1g}^{(38)} + 42b_{2u}^{(23)} + 42b_{3u}^{(23)}$ | $\sigma^*$              |
| 6 | $1a_u + 1b_{2g} + 1b_{3g}$ | F <sup>57</sup> | 681.69    | 0.44        | B <sub>1u</sub> | 29.504          | $39b_{1g}^{(33)} + 42b_{3u}^{(24)} + 42b_{2u}^{(24)}$ | $\sigma^*$              |
| 7 | $1b_{3u} + 1b_{1g} + 1a_g$ | F <sup>65</sup> | 681.82    | 0.57        | B <sub>2u</sub> | 11.459          | $39b_{1g}^{(31)} + 42b_{3u}^{(25)} + 42b_{2u}^{(24)}$ | $\sigma^*$              |
| 8 | $1b_{2u} + 1a_g + 1b_{1g}$ | F <sup>65</sup> | 681.82    | 0.57        | B <sub>3u</sub> | 12.497          | $39b_{1g}^{(31)} + 42b_{3u}^{(25)} + 42b_{2u}^{(24)}$ | $\sigma^*$              |