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# Correction: Core-excited and shape resonances of uracil†

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 Correction for 'Core-excited and shape resonances of uracil' by Mark A. Fennimore *et al.*, *Phys. Chem. Chem. Phys.*, 2016, **18**, 30536–30545.

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The complex energies of the resonances reported in Tables 1, 2, and 4 of our original work were based on locating branch points rather than stationary points. The correct values representing stationary points are listed in the updated Tables 1, 2 and 4 shown below. The changes in the values of the positions of the resonances  $E_r$  are very small. On average the absolute values of the positions differ by 0.02 eV compared to the previous values (we calculated the average using the values from Table 1). The changes of the widths  $\Gamma$  are somewhat larger (on average 0.05 eV). This change is still smaller than the uncertainty we expect in the calculated widths. In addition to these changes, we cannot converge the stationary points using the (3,3,3,3) GPA, so these values are missing from the updated Table 1. This has no effect since the (3,3,3,3) values are very similar to those for the other GPAs, and they were only reported for extra checking.

**Table 1** Complex energies of the first three  $A''$  shape resonances associated with analytic continuation using the EOM-EA-CCSD/aug-ccpVDZ+1s,1p,1d stabilization graph. Results for each avoided crossing (X  $i$ ) are shown

|     | GPA     | $1\pi^*$<br>$E_r(\Gamma)$ [eV] | $2\pi^*$<br>$E_r(\Gamma)$ [eV] | $3\pi^*$<br>$E_r(\Gamma)$ [eV] |
|-----|---------|--------------------------------|--------------------------------|--------------------------------|
| X 1 | (3,3,3) | 0.644 (0.035)                  | 2.216 (0.075)                  | 5.288 (0.488)                  |
|     | (4,4,4) | 0.615 (0.020)                  | 2.216 (0.075)                  | 5.311 (0.486)                  |
|     | (5,5,5) | 0.608 (0.020)                  | 2.214 (0.079)                  | 5.301 (0.473)                  |
| X 2 | (3,3,3) |                                | 2.317 (0.050)                  | 4.453 (0.306)                  |
|     | (4,4,4) |                                | 2.317 (0.050)                  | 4.449 (0.304)                  |
|     | (5,5,5) |                                | 2.315 (0.049)                  | 4.450 (0.308)                  |
| X 3 | (3,3,3) |                                | 2.254 (0.178)                  | 5.033 (0.236)                  |
|     | (4,4,4) |                                | 2.236 (0.180)                  | 5.034 (0.238)                  |
|     | (5,5,5) |                                | 2.314 (0.094)                  | 5.185 (0.235)                  |

**Table 2** Energies  $E_r$  and widths  $\Gamma$  (in parenthesis) of resonances of uracil obtained in this work at the EOM-EA-CCSD level using different basis sets. When several avoided crossings are used to obtain the resonances, the average value and standard deviation are reported here. Complete list of values can be found in ESI

|                      | $1\pi^*$    | $2\pi^*$                            | $3\pi^*$                            | $\pi^1(\pi^*)^2$ | $n^1(\pi^*)^2$ |
|----------------------|-------------|-------------------------------------|-------------------------------------|------------------|----------------|
| 6-31+G(d)            | 0.94 (0.00) | $2.61 \pm 0.00$ ( $0.11 \pm 0.01$ ) | $5.61 \pm 0.24$ ( $0.19 \pm 0.18$ ) | 5.66 (0.09)      | 6.54 (0.04)    |
| 6-311+G(d)           | 1.00 (0.00) | $2.50 \pm 0.01$ ( $0.10 \pm 0.01$ ) | $5.46 \pm 0.20$ ( $0.20 \pm 0.18$ ) | 5.56 (0.10)      | 6.30 (0.04)    |
| aug-cc-pVDZ          | 0.76 (0.02) | $2.37 \pm 0.03$ ( $0.08 \pm 0.04$ ) | $5.10 \pm 0.28$ ( $0.22 \pm 0.16$ ) | 5.32 (0.09)      |                |
| aug-cc-pVDZ+1s,1p,1d | 0.61 (0.02) | $2.28 \pm 0.06$ ( $0.07 \pm 0.02$ ) | $4.98 \pm 0.46$ ( $0.34 \pm 0.12$ ) | 5.25 (0.17)      |                |

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**Table 4** Energies  $E_r$  and widths  $\Gamma$  (in parenthesis) of resonances of uracil obtained at the CASSCF/6-31+G(d) and XMCQDPT2/6-31+G(d) levels, and comparisons with EOM-EA-CCSD/aug-cc-pVDZ +1s,1p,1d and experimental results. The real component of the complex energies ( $E_r$ ) is shifted down, so that the first resonance state corresponds to the experimentally determined  $\pi^*$  state of 0.22 eV

|                    | $1\pi^*$    | $2\pi^*$    | $3\pi^*$    | $\pi^1(\pi^*)^2$ |
|--------------------|-------------|-------------|-------------|------------------|
| EOM-EA-CCSD        | 0.22 (0.02) | 1.87 (0.07) | 4.57 (0.34) | 4.84 (0.17)      |
| CASSCF             | 0.22 (0.00) | 1.80 (0.00) | 4.80 (0.00) | 5.54 (0.14)      |
| XMCQDPT2           | 0.22 (0.00) | 1.06 (0.00) | 3.98 (0.00) | 4.63 (0.00)      |
| Exp. <sup>42</sup> | 0.22        | 1.58        | 3.83        |                  |

Overall, the new values of the resonances have no effect on the conclusions and the overall discussion presented in the original paper.

Since the values in the main manuscript were obtained from extended tables presented in the ESI, we have also updated the tables in ESI.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

