Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
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**Supporting Information**

Theoretical study of electronically excited radical cations of naphthalene and anthracene as archetypical models for astrophysical observations. II. Dynamical consequences

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**Table S1**

TABLE S1: *Ab initio* calculated geometry parameters of the electronic ground state of $An^+$ optimized at the UMP2/cc-pVDZ level of theory.

| Parameter | Value |
|---|---|
| Bond lenght ($\AA$) | |
| $C_1$ - $C_2$ | 1.3958 |
| $C_1$ - $C_6$ | 1.4185 |
| $C_2$ - $C_3$ | 1.4235 |
| $C_3$ - $C_4$ | 1.4375 |
| $C_3$ - $C_7$ | 1.4165 |
| $C_1$ - $H_{17}$ | 1.0944 |
| $C_2$ - $H_{18}$ | 1.0956 |
| $C_7$ - $H_{16}$ | 1.0976 |
| Bond Angle (deg) | |
| $C_1$ - $C_2$ - $C_3$ | 120.148 |
| $C_2$ - $C_3$ - $C_4$ | 119.380 |
| $C_2$ - $C_3$ - $C_7$ | 121.437 |
| $C_2$ - $C_1$ - $C_6$ | 120.472 |
| $C_5$ - $C_6$ - $C_1$ | 120.472 |
| $C_3$ - $C_7$ - $C_{10}$ | 121.634 |
| $C_7$ - $C_{10}$ - $C_9$ | 119.183 |
| $C_7$ - $C_3$ - $C_4$ | 119.183 |
| $H_{17}$ - $C_2$ - $C_3$ | 119.831 |
| $H_{17}$ - $C_2$ - $C_3$ | 119.697 |
| $H_{18}$ - $C_2$ - $C_3$ | 119.284 |
| $H_{18}$ - $C_2$ - $C_3$ | 120.568 |
| $H_{16}$ - $C_7$ - $C_3$ | 119.183 |