Supporting information for

Infrared Photodissociation Spectroscopy of Mass-Selected $[TaO_3(CO_2)_n]^+$ (n = 2–5) Complexes in the Gas Phase

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Contents:

of theory (bond lengths in Ångströms and bond angles in degrees).

Table S1. Binding energies of successive CO_2 ligands calculated for the singlet and triplet complex isomers at the PBE0-D3(BJ)/def2-TZVP level of theory (in kcal/mol).

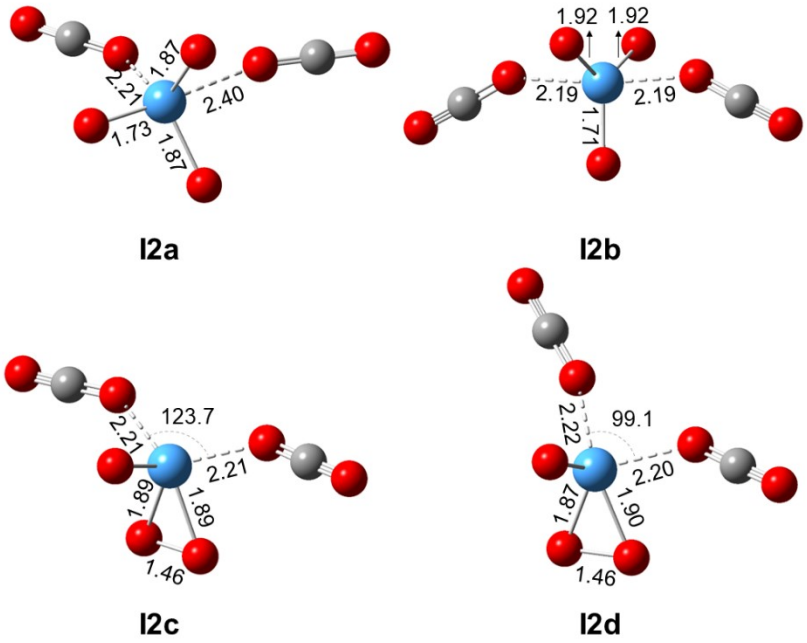

Figure S1. Optimized geometries of the $[TaO_3(CO_2)_2]^+$ complex isomers in the singlet and triplet states calculated at the PBE0-D3(BJ)/def2-TZVP level of theory (bond lengths in Ångströms and bond angles in degrees).

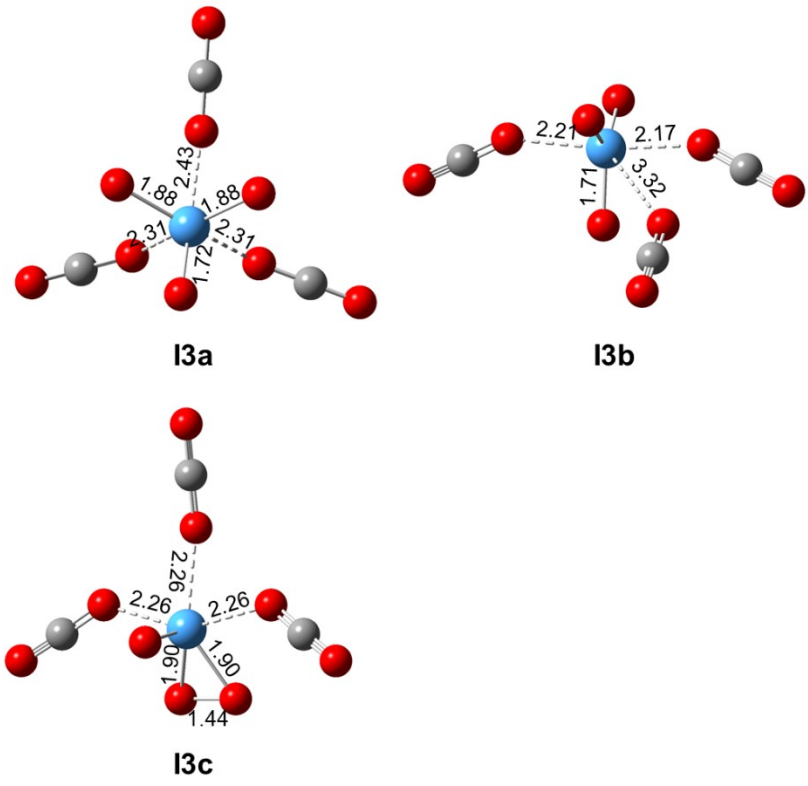

Figure S2. Optimized geometries of the $[TaO_3(CO_2)_3]^+$ complex isomers in the singlet and triplet states calculated at the PBE0-D3(BJ)/def2-TZVP level of theory (bond lengths in Ångströms and bond angles in degrees).

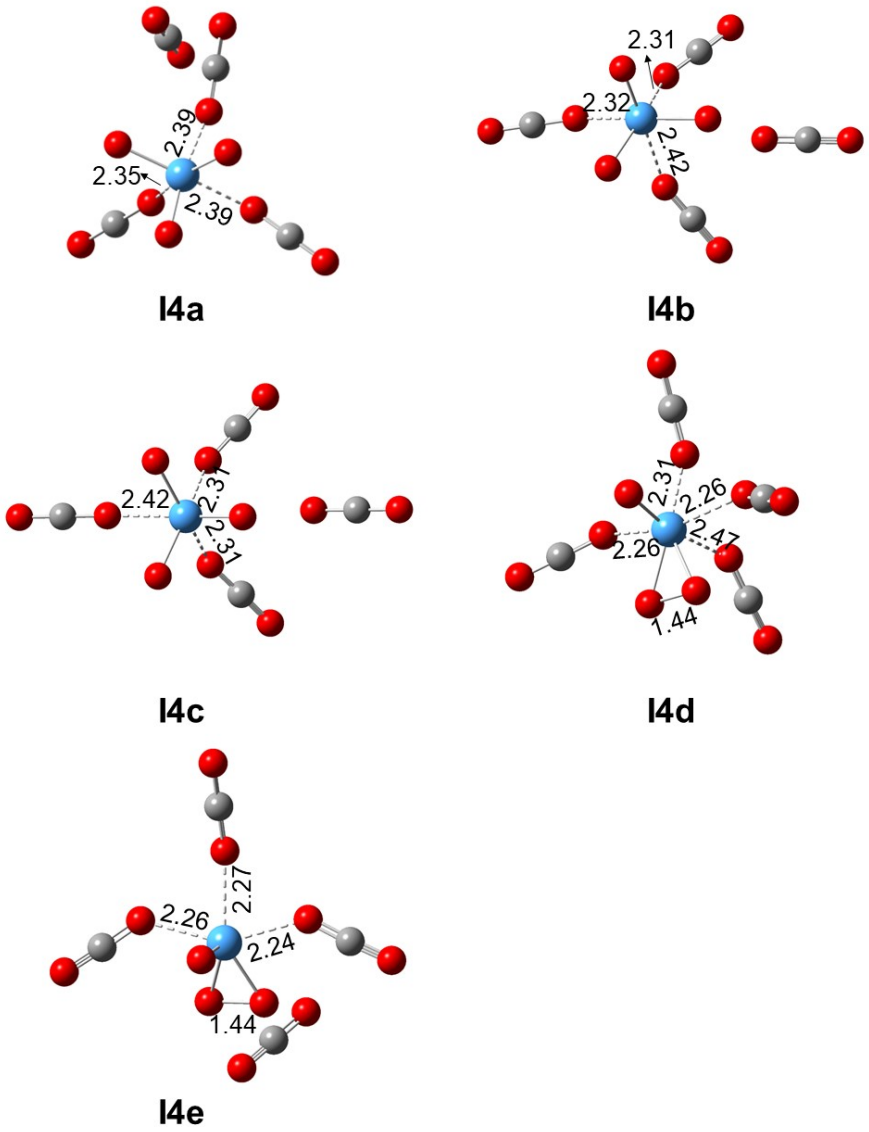

Figure S3. Optimized geometries of the $[TaO_3(CO_2)_4]^+$ complex isomers in the singlet and triplet states calculated at the PBE0-D3(BJ)/def2-TZVP level of theory (bond lengths in Ångströms and bond angles in degrees).

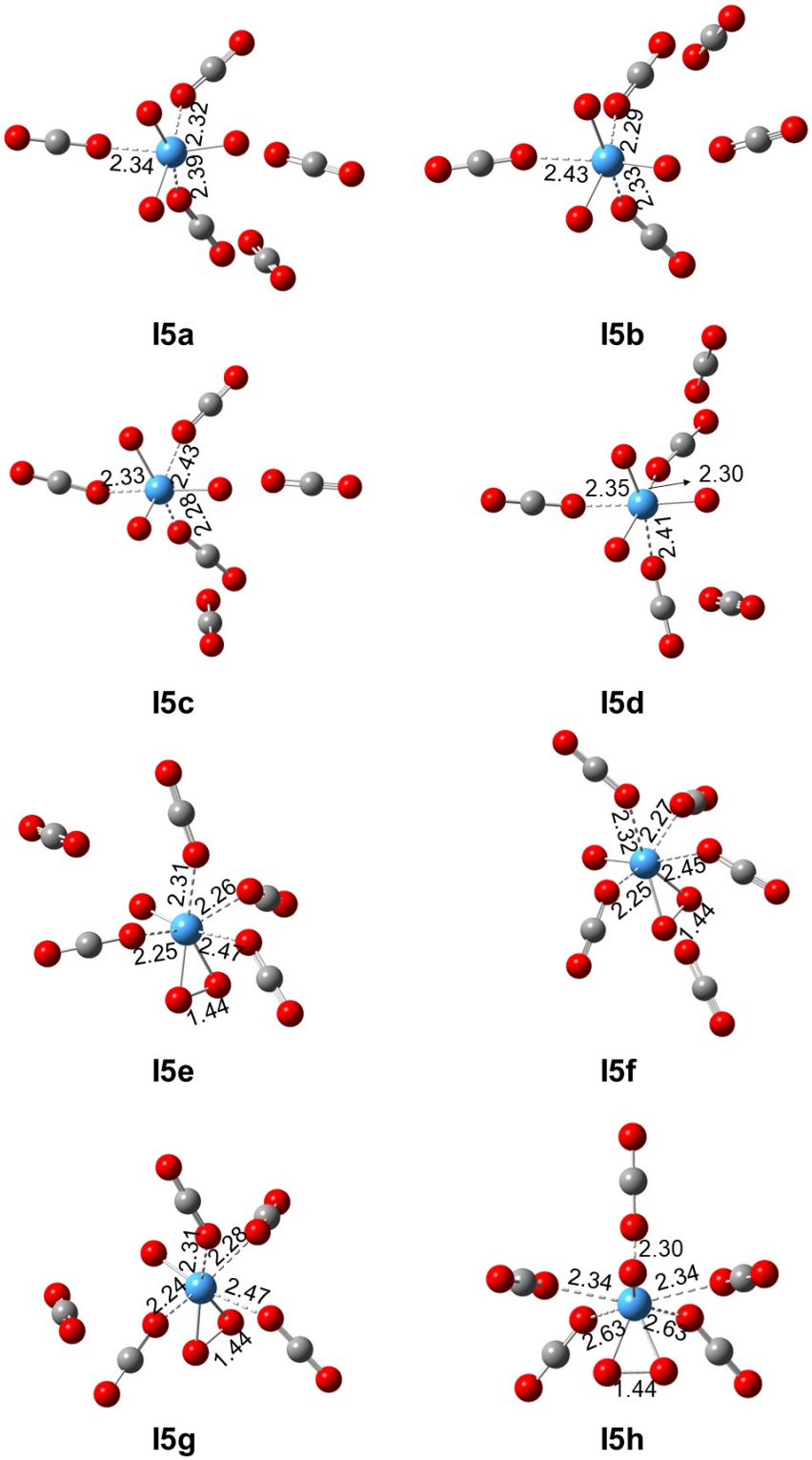

Figure S4. Optimized geometries of the $[TaO_3(CO_2)_5]^+$ complex isomers in the singlet and triplet states calculated at the PBE0-D3(BJ)/def2-TZVP level of theory (bond lengths in Ångströms and bond angles in degrees).

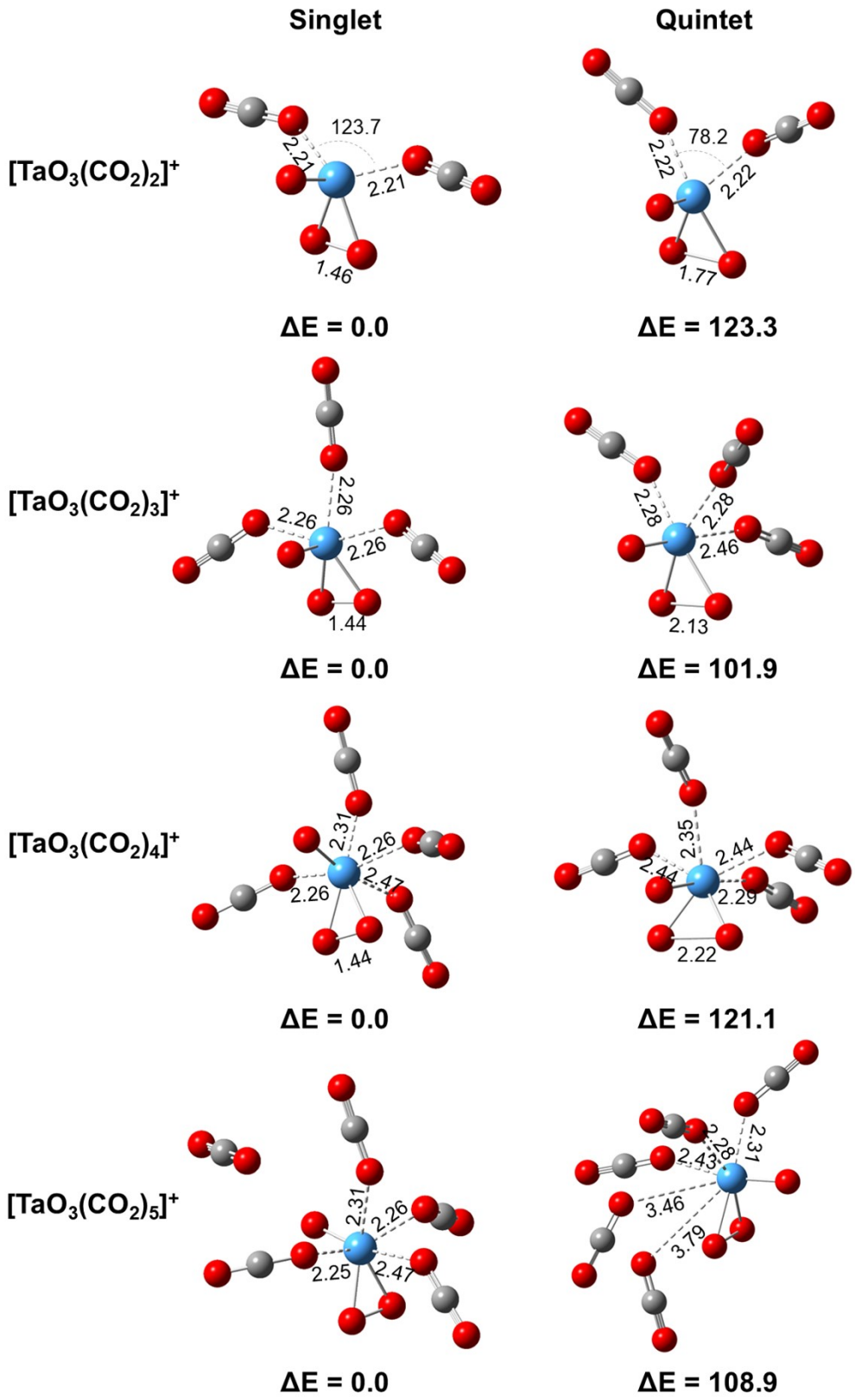

Figure S5. Relative energies (in kcal/mol) of the $[TaO_3(CO_2)_n]^+$ (n=2-5) complexes in the singlet and quintet states calculated at the PBE0-D3(BJ)/def2-TZVP level of theory (bond lengths in Ångströms and bond angles in degrees).

Table S1. Binding energies of successive CO_2 ligands calculated for the singlet and triplet complex isomers at the PBE0-D3(BJ)/def2-TZVP level of theory (in kcal/mol).

	Binding energy (kcal/mol)	
	singlet	triplet
$TaO_3(CO_2)^+-CO_2$	29.5	17.8
$TaO_3(CO_2)_2^+-CO_2$	20.2	15.1
$TaO_3(CO_2)_3^+-CO_2$	12.8	5.8
$TaO_3(CO_2)_4^+-CO_2$	5.6	5.7