Supplementary Materials: Core-valence double ionization of carbon suboxide

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Table S1. Comparison of single ionization energies of C_3O_2
Energies calculated with OSRHF and Koopmans energies for UPS (eV). Comparison to our experimental values, peak energies from Gelius et al.[1] and adiabatic ionization energies from Rabalais et al.[2].
[*]adiabatic ionization energies

Spec.	State	OSRHF	Koop.	RASPT2	Exp. (this work)	Gelius et al.	Rabalais et al.[*]
UPS	$2\pi_u$	10.52	11.15	10.86	10.9 ± 0.5	10.8 ± 0.2[1]	10.61[2]
	$1\pi_g$	16.74	17.40	15.21	14.9 ± 0.5	15.0 ± 0.2[1]	14.55[2]
	$1\pi_u$	17.67	18.26	16.07	15.9 ± 0.5	16.0 ± 0.2[1]	15.75[2]
	$5\sigma_u$	19.60	20.43	16.84	17.2 ± 0.5	17.3 ± 0.1[1]	16.98[2]
	$6\sigma_g$	19.97	20.76	17.07		17.5 ± 0.1[1]	17.26[2]
	$4\sigma_u$	25.02	25.69	22.09	21.7 ± 0.5	21.9 ± 0.2[1]	
	$5\sigma_g$	29.48	30.32	26.16	25.3 ± 0.5	25.6 ± 0.1[1]	
	$3\sigma_u$	39.71	40.73			35.5 ± 0.1[1]	
	$4\sigma_g$	39.75	40.76			35.5 ± 0.1[1]	
XPS	C_C 1s	291.61	306.53	291.48	291.5 ± 1	291.4 ± 0.1[1]	
	C_O 1s	296.88	311.28	295.43	294.9 ± 1	294.9 ± 0.1[1]	
	O 1s	539.90	562.38	539.69	539.7 ± 1	539.7 ± 0.1[1]	

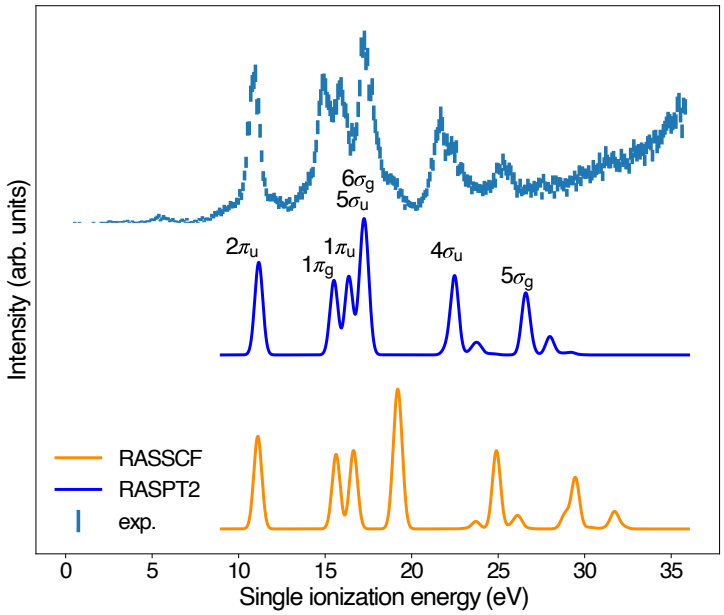

Figure S1. Comparison of the experimental single ionization electron spectrum taken at 40.81 eV (top) and the computed spectra from RASPT2 (middle) and RASSCF (bottom).

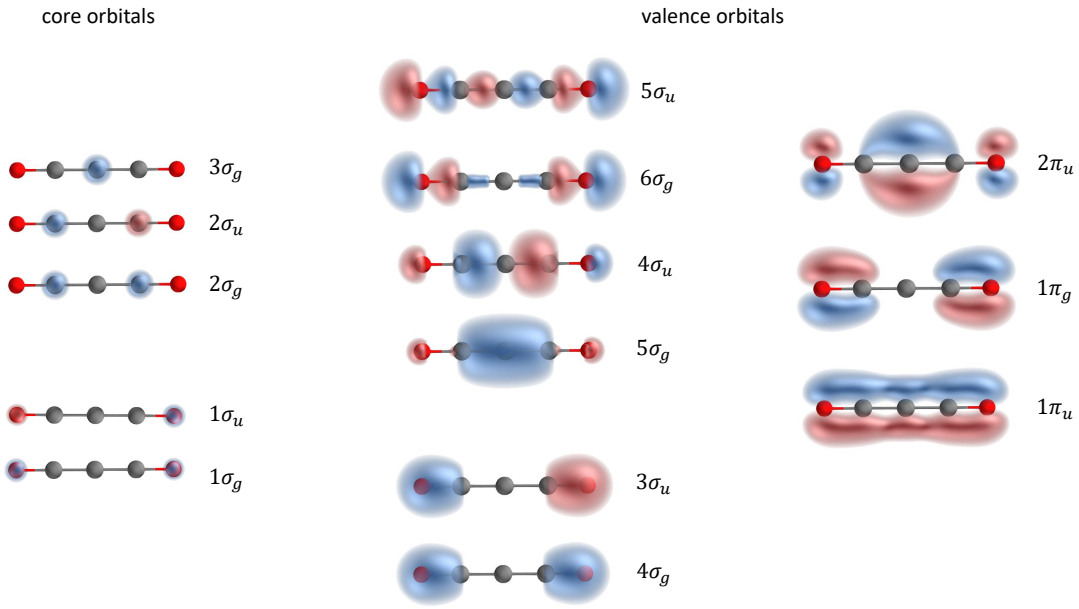

Figure S2. Molecular orbitals of carbon suboxide.

References

1. Gelius, U., Allan, C., Allison, D., Siegbahn, H. & Siegbahn, K. The electronic structure of carbon suboxide from ESCA and AB initio calculations. *Chem. Phys. Lett.* **11**, 224–228, DOI: https://doi.org/10.1016/0009-2614(71)80364-0 (1971).
2. Rabalais, J. W. *et al.* The high-resolution electron spectrum of carbon suboxide. *Electron Spectrosc.* (1972).