

## Pursuing accuracy in intermolecular potentials and spectra

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We obtained a new, highly accurate ab initio ground-state intermolecular potential-energy surface (IPES) for the CO-N<sub>2</sub> complex [1]. Thousands of intermolecular geometries were selected using a Gaussian-quadrature approach. The corresponding interaction energies were calculated with the CCSD(T) method and Dunning's aug-cc-pVQZ basis set extended with a set of 3s3p2d1f1g midbond functions and were fitted to an analytical function.

The symmetry-adapted Lanczos algorithm was used to compute rovibrational energies (up to J = 20) for the new IPES. The RMSE with respect to experiment was found to be on the order of 0.038 cm<sup>-1</sup> which confirms the high accuracy of the potential. This level of agreement is among the best reported in the literature for weakly bound systems and considerably improves on those of previously published potentials.

In the second part of the talk, I will show results on the reparametrization of semiempirical potentials to improve the description of non-covalent interactions within the MOPAC program.

For this, we use as benchmark ab initio CCSD(T) interaction energies.

To end, I will present preliminary results on vibrational circular dichroism spectra of phenylacetylenes.

### References

1. H. Cybulski, C. Henriksen, R. Dawes, X.-G. Wang, N. Bora, G. Avila, T. Carrington Jr., B. Fernández, *Phys. Chem. Chem. Phys.* **20** (2018), 12624. M.