

Supplementary Materials for
**A variational reformulation of molecular properties in
electronic-structure theory**

Poul Jørgensen *et al.*

Corresponding author: Poul Jørgensen, pou@chem.au.dk; Kurt V. Mikkelsen, kmi@chem.ku.dk;
Trygve Helgaker, helgaker@uio.no

Sci. Adv. **10**, eadn3454 (2024)
DOI: 10.1126/sciadv.adn3454

The PDF file includes:

Table S1

Dataset

Table S1

Coordinates for H₂O in Ångström

	X	Y	Z
O	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.756950000140	0.585882000133
H	0.000000000000	-0.756950000140	0.585882000133

Other Supplementary Materials for this manuscript include the following:

Link to the molecular dataset used in the paper

https://lcpq.github.io/QUESTDB_website/dataset/