

Supporting Information: Many-body theory predictions of positron binding energies in five-membered heterocycles involving N, O, S and NH substituents.

1 Convergence of positron binding energies

All the positron binding energies in this work are converged with respect to the number of positron and electron states used to construct the self-energy diagrams. The graphs below show examples of this convergence for four of the heterocycles, all completed with the basis employed to obtain the result in Table 1.

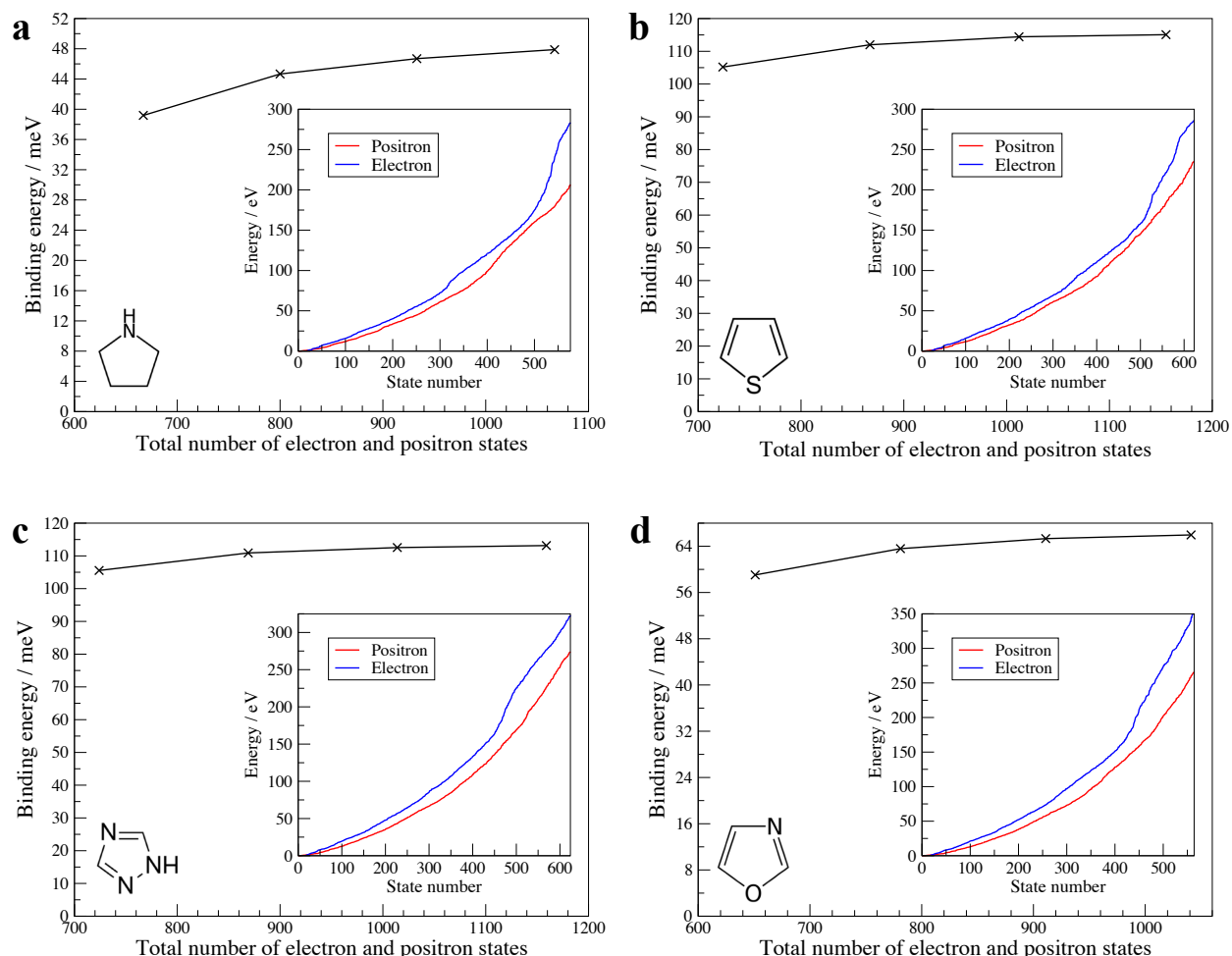


Figure S1: Convergence of $GW + \tilde{\Gamma} + \tilde{\Lambda}$ positron binding energies with respect to the number of states used to construct the self-energy for (a) pyrrolidine, (b) thiophene (c) triazole and (d) oxazole. The ratio of positron to electron states was 1.17 in each case. Inset graphs show the energies of the electron and positron states.

2 Basis sets

Table S1 contains details of the positron and electron bases used to obtain the positron binding energies in Table 1, including the types of basis sets and the total number of ghost centers used for each molecule.

Table S1: Basis sets used for the binding calculations in Table 1. Basis types are denoted in shorthand in the table where TZ = aug-cc-pVTZ; QZ = aug-cc-pVQZ; ET = even-tempered, $10s9p8d7f3g$ with $\beta = 2.2$, $\zeta_0 = 10^{-3}$ for s and p functions, $\zeta_0 = 10^{-2}$ for d and f functions, and $\zeta_0 = 10^{-1}$ for g functions. G1 are ghost centers placed around the molecule and G2 is the single ghost center placed at the center of the molecule’s ring. Where TZ or QZ bases are used on either type of ghost center, these are hydrogen aug-cc-pVTZ or aug-cc-pVQZ bases. See the INPUTs.zip in the Supplemental Information for input files with xyz geometry data for the atoms and ghost placement.

Molecule		C	H	N	O	S	G1	G2	No. ghosts
Furan	e^-	TZ	TZ	–	QZ	–	QZ (H)	QZ (H)	10
	e^+	TZ	TZ	–	QZ	–	QZ (H)	ET	
Tetrahydrofuran	e^-	TZ	TZ	–	QZ	–	QZ (H)	QZ (H)	6
	e^+	TZ	TZ	–	QZ	–	QZ (H)	ET	
Thiophene	e^-	TZ	TZ	–	–	QZ	QZ (H)	QZ (H)	8
	e^+	TZ	TZ	–	–	QZ	QZ (H)	ET	
Tetrahydrothiophene	e^-	TZ	TZ	–	–	QZ	QZ (H)	TZ	6
	e^+	TZ	TZ	–	–	QZ	QZ (H)	ET	
Pyrrole	e^-	TZ	TZ	QZ	–	–	QZ (H)	QZ (H)	6
	e^+	TZ	TZ	QZ	–	–	QZ (H)	ET	
Pyrrolidine	e^-	TZ	TZ	QZ	–	–	QZ (H)	QZ (H)	4
	e^+	TZ	TZ	QZ	–	–	QZ (H)	ET	
Imidazole	e^-	TZ	TZ	QZ	–	–	QZ (H)	QZ (H)	6
	e^+	TZ	TZ	QZ	–	–	QZ (H)	ET	
Pyrazole	e^-	TZ	TZ	QZ	–	–	QZ (H)	QZ (H)	6
	e^+	TZ	TZ	QZ	–	–	QZ (H)	ET	
Triazole	e^-	TZ	TZ	QZ	–	–	QZ (H)	QZ (H)	7
	e^+	TZ	TZ	QZ	–	–	QZ (H)	ET	
Oxazole	e^-	TZ	TZ	QZ	QZ	–	QZ (H)	QZ (H)	6
	e^+	TZ	TZ	QZ	QZ	–	QZ (H)	ET	
Isoxazole	e^-	TZ	TZ	QZ	QZ	–	QZ (H)	QZ (H)	5
	e^+	TZ	TZ	QZ	QZ	–	QZ (H)	ET	
Thiazole	e^-	TZ	TZ	QZ	–	QZ	QZ (H)	QZ (H)	6
	e^+	TZ	TZ	QZ	–	QZ	QZ (H)	ET	
Isothiazole	e^-	TZ	TZ	QZ	–	QZ	QZ (H)	QZ (H)	7
	e^+	TZ	TZ	QZ	–	QZ	QZ (H)	ET	
1,3-Oxathiole	e^-	TZ	TZ	–	TZ	QZ	QZ (H)	QZ (H)	8
	e^+	TZ	TZ	–	TZ	QZ	QZ (H)	ET	
1,2-Oxathiole	e^-	TZ	TZ	–	TZ	QZ	QZ (H)	QZ (H)	8
	e^+	TZ	TZ	–	TZ	QZ	QZ (H)	ET	