	Freeze and Thaw				
	ME		SE		
	$M[\rho^{ref} - \rho_B^{FT}]$	$E_{int}^{FDET-MP2}[\rho_B^{FT}]$	$M[\rho^{ref} - \rho_B^{FT}]$	$E_{int}^{FDET-MP2}[\rho_B^{FT}]$	E^{ref}
7Hq 2MeOH	0.013	-13.85	0.007	-15.02	-17.47
7Hq formate	0.036	-28.58	0.007	-34.06	-36.48
Uracil 5H2O	0.024	-38.39	0.014	-41.09	-38.62
PyrBnz 2HCOOH	0.016	-33.31	0.013	-35.92	-36.53

Table 1: Monomer (ME) and supermolecular (SE) expansion results at the MP2 level for ρ_B^{FT}. Energies are in Kcal/mol and integrated densities in a.u.

	Freeze and Thaw				
	ME		SE		
	$M[\rho^{ref} - \rho_B^{FT}]$	$E_{int}^{FDET-HF}[\rho_B^{FT}]$	$M[\rho^{ref} - \rho_B^{FT}]$	$E_{int}^{FDET-HF}[\rho_B^{FT}]$	$E^{ref,HF}$
7Hq 2MeOH	0.013	-16.05	0.007	-16.87	-7.97
7Hq formate	0.036	-33.61	0.007	-38.37	-32.29
Uracil 5H2O	0.024	-46.42	0.014	-48.29	-31.38
PyrBnz 2HCOOH	0.016	-41.84	0.013	-43.99	-29.84

Table 2: Monomer (ME) and supermolecular (SE) expansion results at the HF level for ρ_B^{FT}. Energies are in Kcal/mol and integrated densities in a.u.

	Isolated environment				
	ME		SE		
	$M[\rho^{ref} - \rho_B^{isol}]$	$E_{int}^{FDET-MP2}[\rho_B^{isol}]$	$M[\rho^{ref} - \rho_B^{isol}]$	$E_{int}^{FDET-MP2}[\rho_B^{isol}]$	E^{ref}
7Hq 2MeOH	0.123	-10.91	0.121	-11.20	-17.47
7Hq formate	0.205	-23.23	0.206	-23.34	-36.48
Uracil 5H2O	0.237	-32.00	0.234	-32.47	-38.62
PyrBnz 2HCOOH	0.185	-25.98	0.184	-27.17	-36.53

Table 3: Monomer (ME) and supermolecular (SE) expansion results at the MP2 level for ρ_B^{isol}. Energies are in Kcal/mol and integrated densities in a.u.

	Isolated environment				
	ME		SE		
	$M[\rho^{ref} - \rho_B^{isol}]$	$E_{int}^{FDET-HF}[\rho_B^{isol}]$	$M[\rho^{ref} - \rho_B^{isol}]$	$E_{int}^{FDET-HF}[\rho_B^{isol}]$	$E^{ref,HF}$
7Hq 2MeOH	0.123	-11.90	0.121	-12.06	-7.97
7Hq formate	0.205	-23.14	0.206	-23.17	-32.29
Uracil 5H2O	0.237	-36.53	0.234	-36.69	-31.38
PyrBnz 2HCOOH	0.185	-30.61	0.184	-31.56	-29.84

Table 4: Monomer (ME) and supermolecular (SE) expansion results at the HF level for ρ_B^{isol}. Energies are in Kcal/mol and integrated densities in a.u.