



Supporting Information

Comparative Theoretical Investigation on Energetic Substituted Furazanyl Ethers

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Table S1. The total energies (E_0), zero point energies (ZPE), thermal corrections (H_T), and heats of formation (HOFs) for the reference compounds

Compd.	E_0 [a.u.]	ZPE [a.u.]	H_T [kJ·mol ⁻¹]	HOF (Exp.) [kJ·mol ⁻¹]	HOF (Cal.) [kJ·mol ⁻¹]	Relative errors [%]
CH ₄	-40.5337	0.0446	10.01	-74.60	-73.27	1.78
CH ₃ CH ₃	-79.8563	0.0744	11.63	-84.00	-78.44	6.62
CH ₃ NO ₂	-245.0817	0.0497	13.85	-81.00	-86.87	-7.25
CH ₃ NF ₂	-294.2983	0.0468	13.61	-115.23	-119.29	-3.52
CH ₃ NH ₂	-95.8884	0.0638	11.44	-23.50	-20.59	12.38
CH ₃ N ₃	-204.1497	0.0501	14.23	296.50	299.74	1.09
CH ₃ CN	-132.7933	0.0452	11.93	74.04	76.31	3.06
CH ₃ OCH ₃	-155.0719	0.0793	13.85	-184.10	-178.45	3.07
CH ₃ SCH ₃	-478.0658	0.0754	15.37	-37.50	-35.13	6.32
CH ₃ ONO ₂	-320.2827	0.0542	15.53	-124.40	-126.50	-1.69
CH ₃ NHNO ₂	-300.4345	0.0672	16.04		-7.94	
CH ₃ NHNH ₂	-151.2206	0.0811	13.72	94.50	95.16	0.70
CH ₃ N ₂ CH ₃	-189.3112	0.0833	16.29		155.41	
CH ₃ N(O)NCH ₃	-264.5414	0.0900	17.41		55.40	
CH ₃ N(O)N NO ₂	-429.7283	0.0639	19.99		186.12	
CH ₂ (NO ₂) ₂	-449.6167	0.0528	19.30	-58.90	-53.22	9.64
CHF(NO ₂) ₂	-548.8703	0.0446	18.74	-235.00	-231.22	1.61
Furazan	-262.1121	0.0456	11.58	196.27	199.48	1.64
Furoxan	-337.2942	0.0493	13.98		212.36	

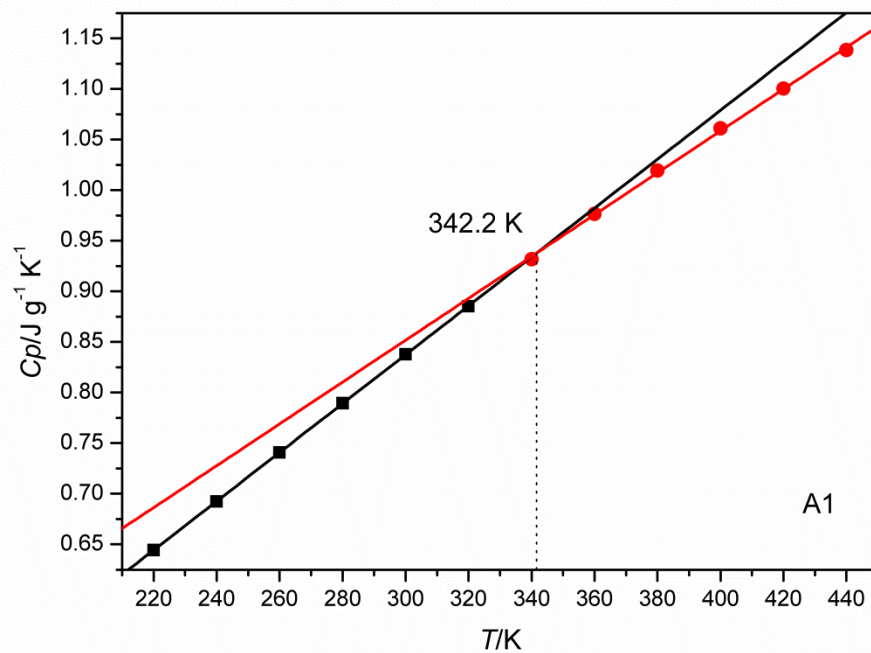


Figure S1. The specific heat capacity vs. temperature relationship for A1

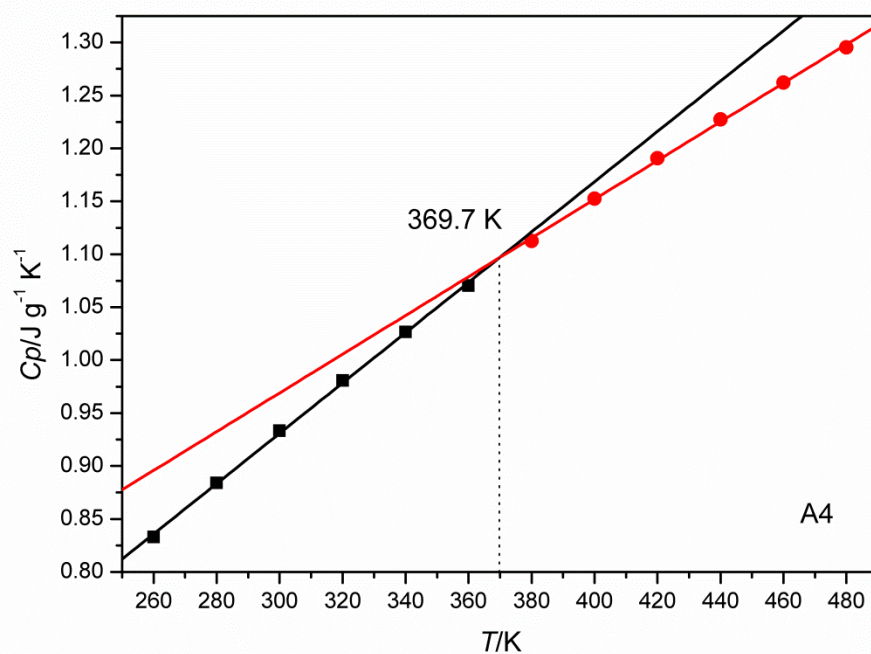


Figure S2. The specific heat capacity vs. temperature relationship for A4

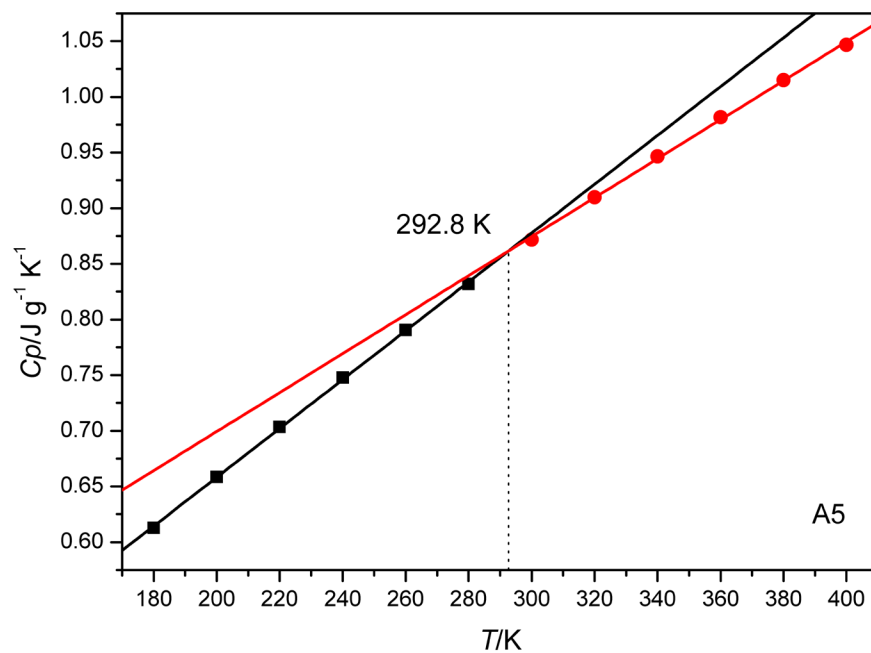


Figure S3. The specific heat capacity vs. temperature relationship for A5

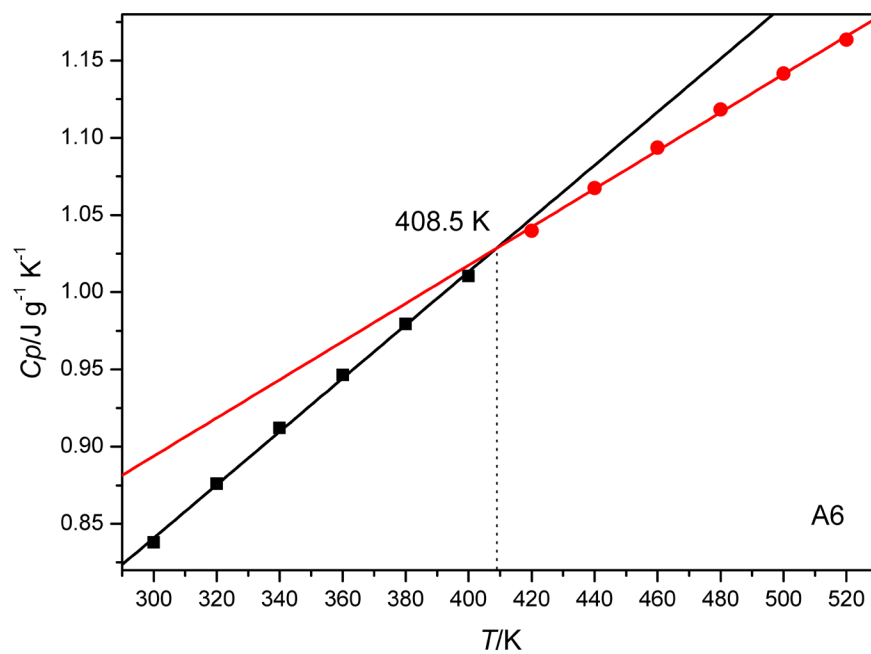


Figure S4. The specific heat capacity vs. temperature relationship for A6

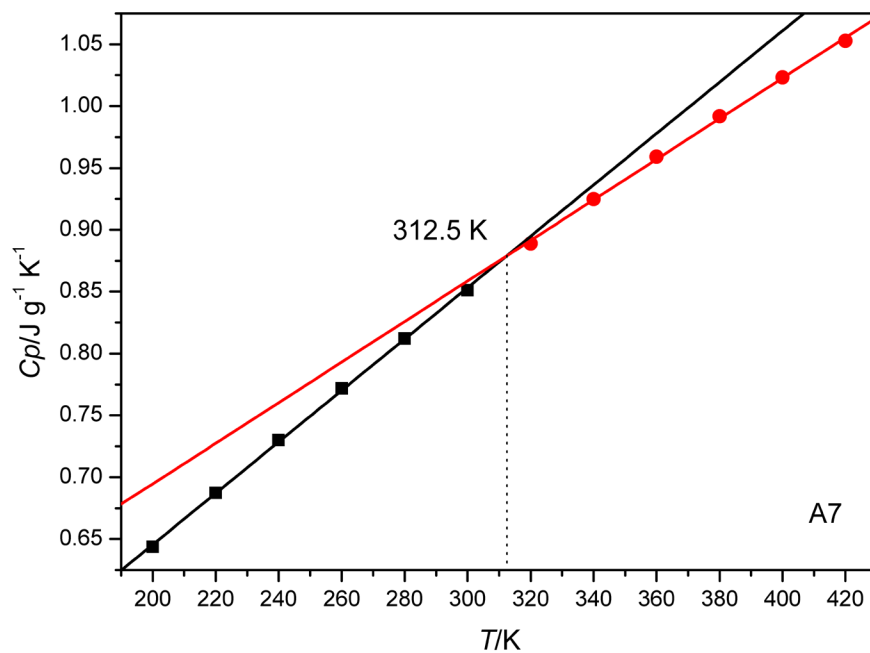


Figure S5. The specific heat capacity vs. temperature relationship for A7

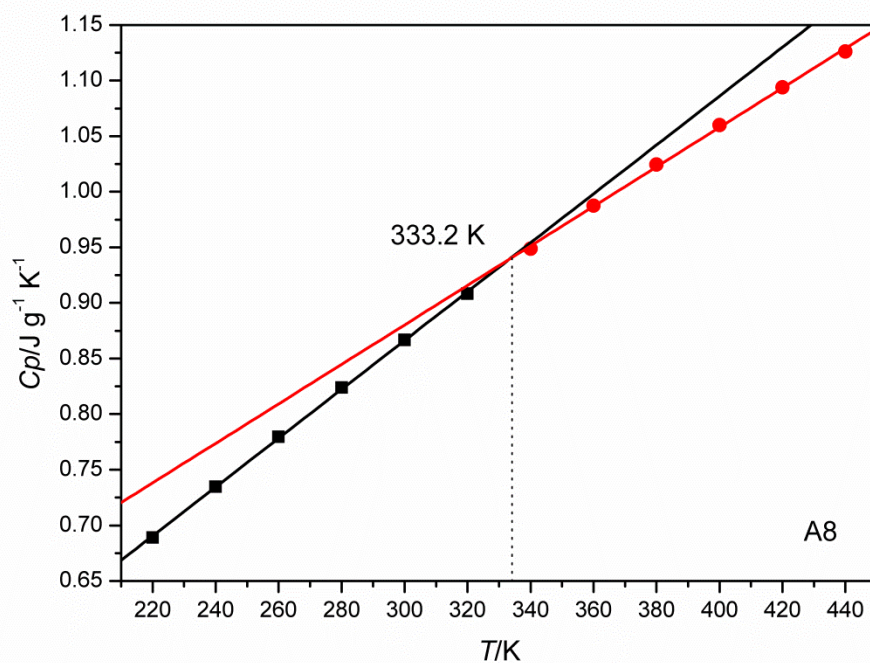


Figure S6. The specific heat capacity vs. temperature relationship for A8

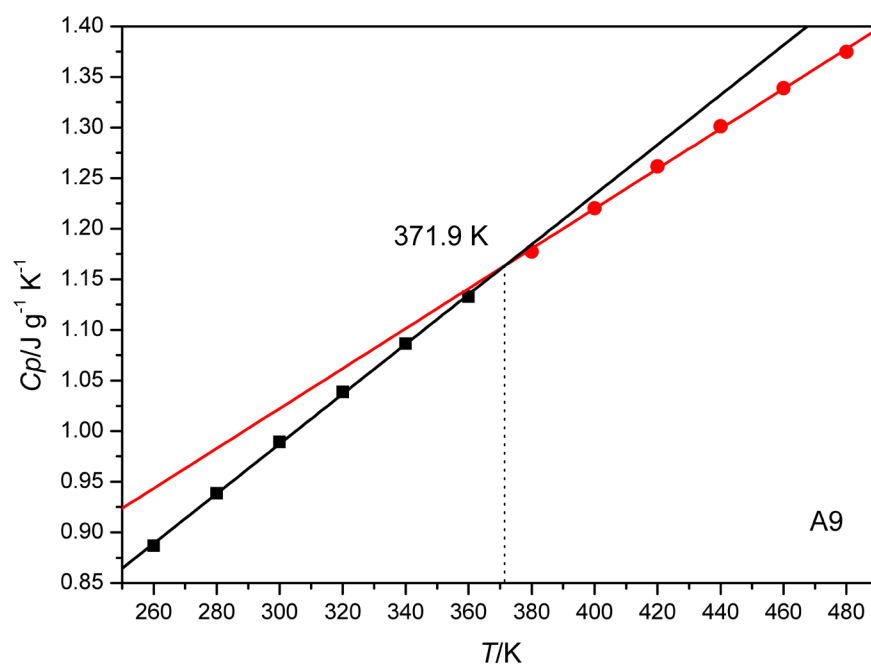


Figure S7. The specific heat capacity vs. temperature relationship for A9

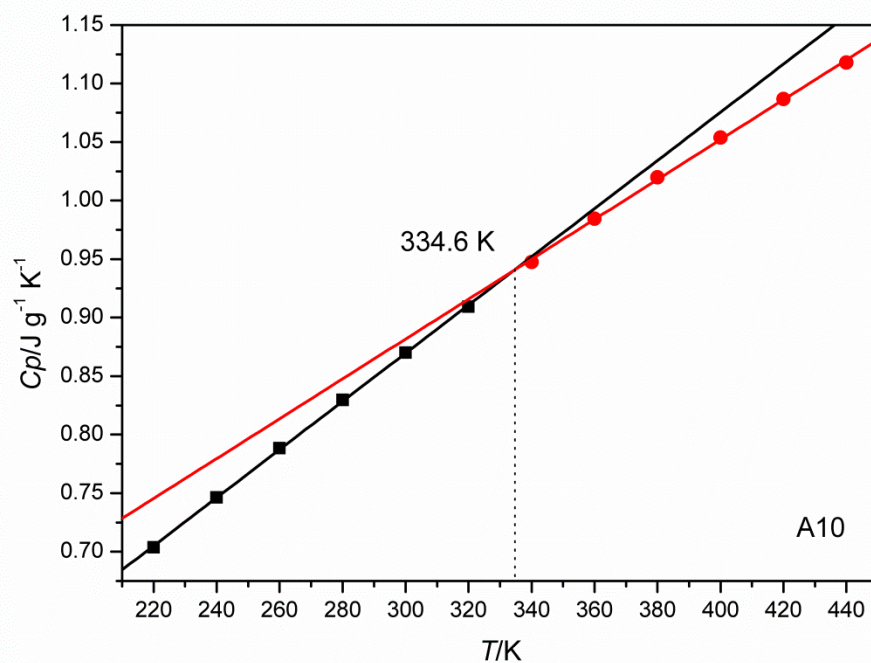


Figure S8. The specific heat capacity vs. temperature relationship for A10

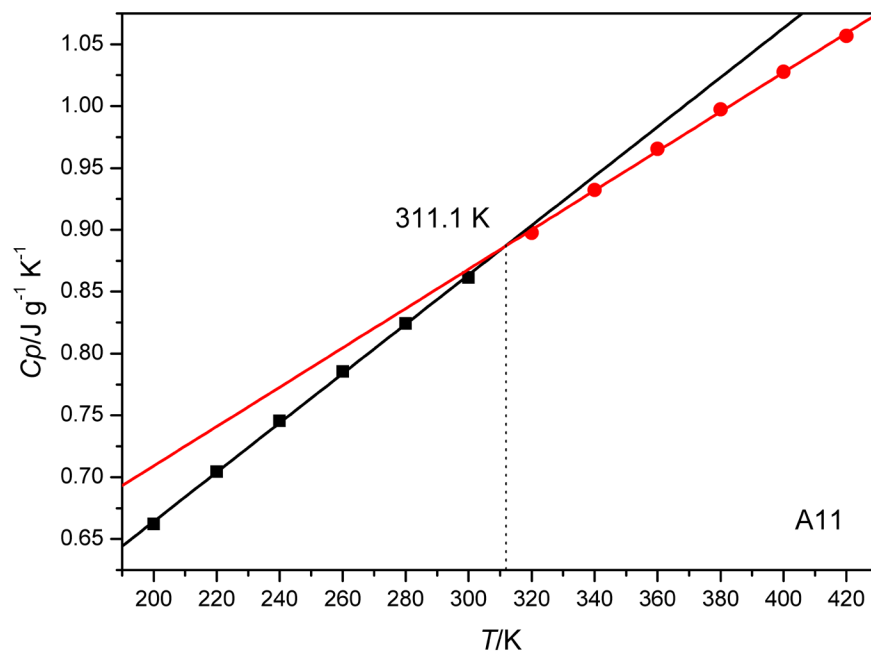


Figure S9. The specific heat capacity vs. temperature relationship for A11

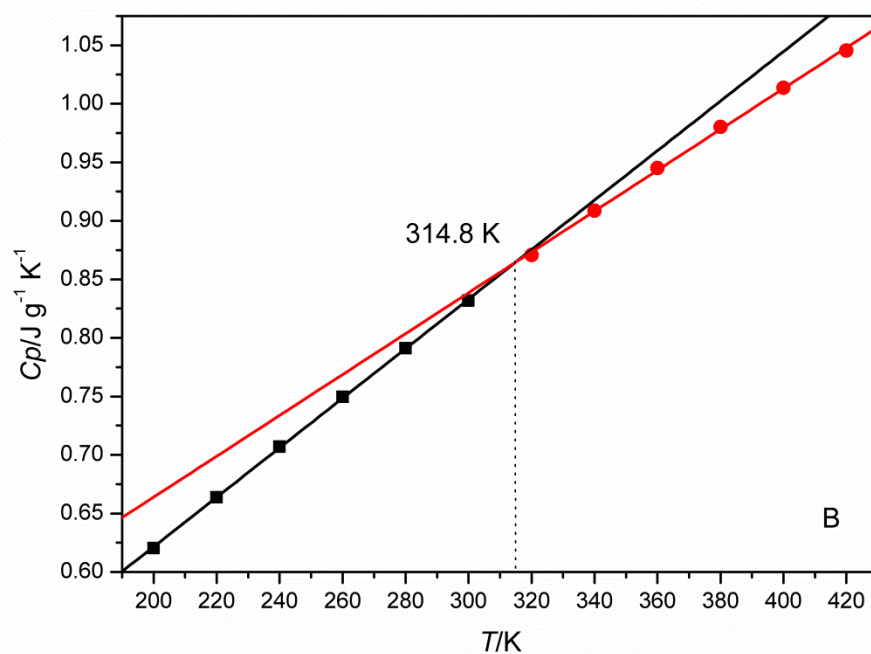


Figure S10. The specific heat capacity vs. temperature relationship for B

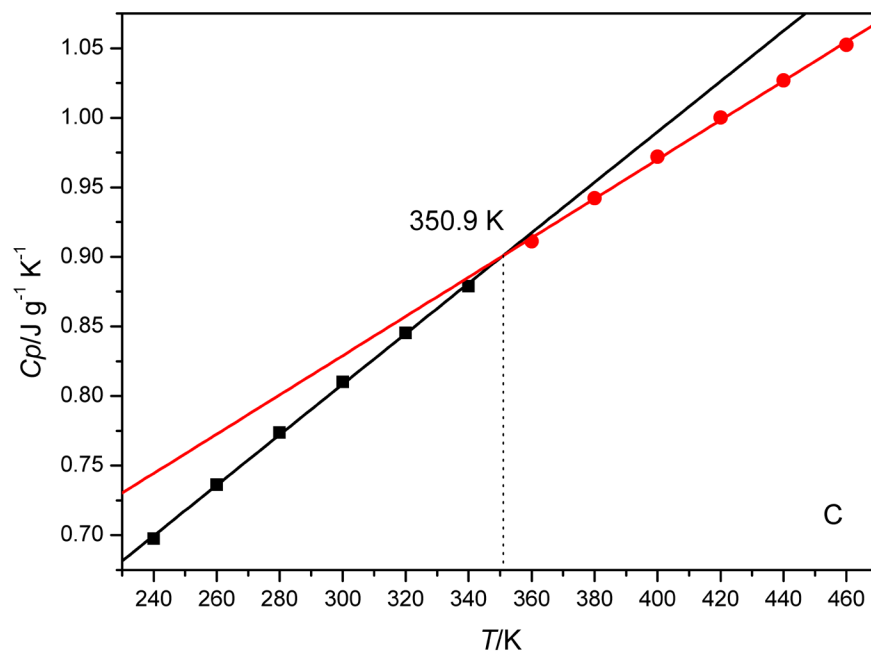


Figure S11. The specific heat capacity vs. temperature relationship for C

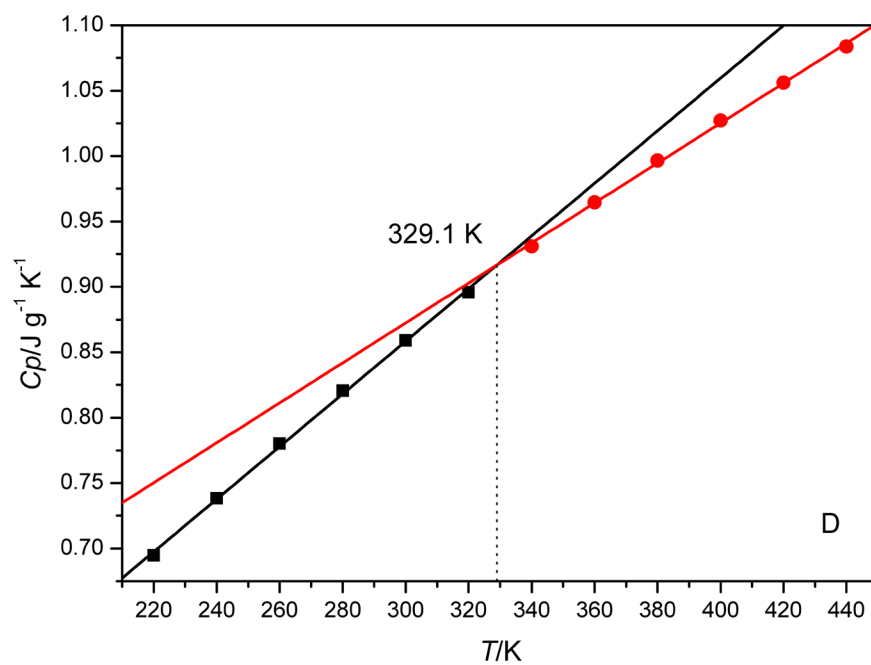


Figure S12. The specific heat capacity vs. temperature relationship for D

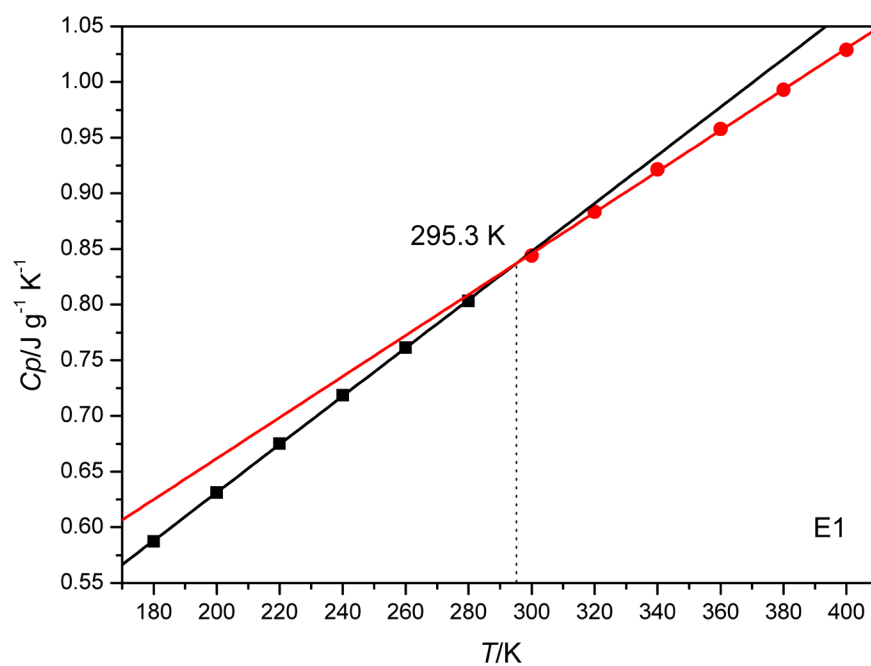


Figure S13. The specific heat capacity vs. temperature relationship for E1

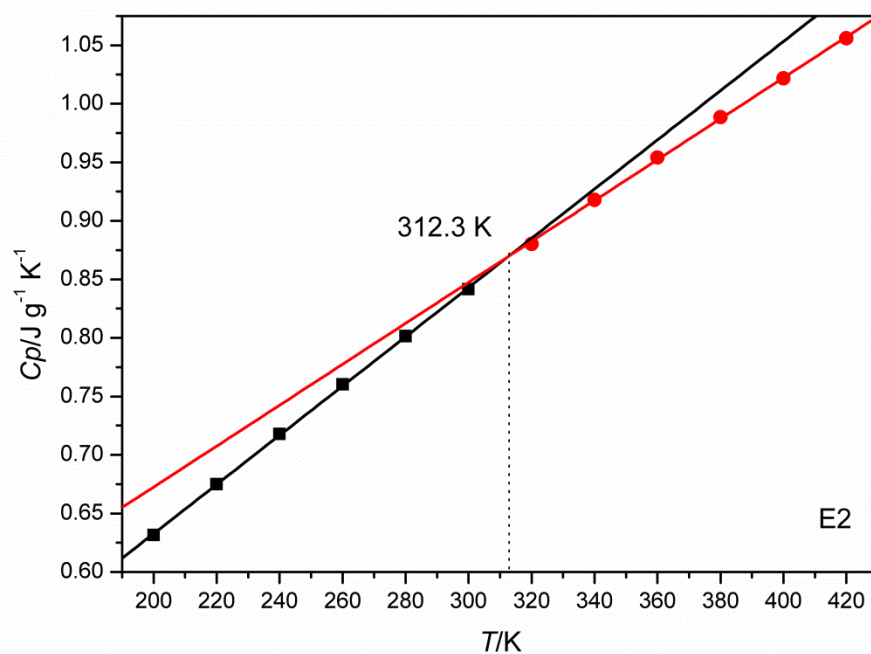


Figure S14. The specific heat capacity vs. temperature relationship for E2

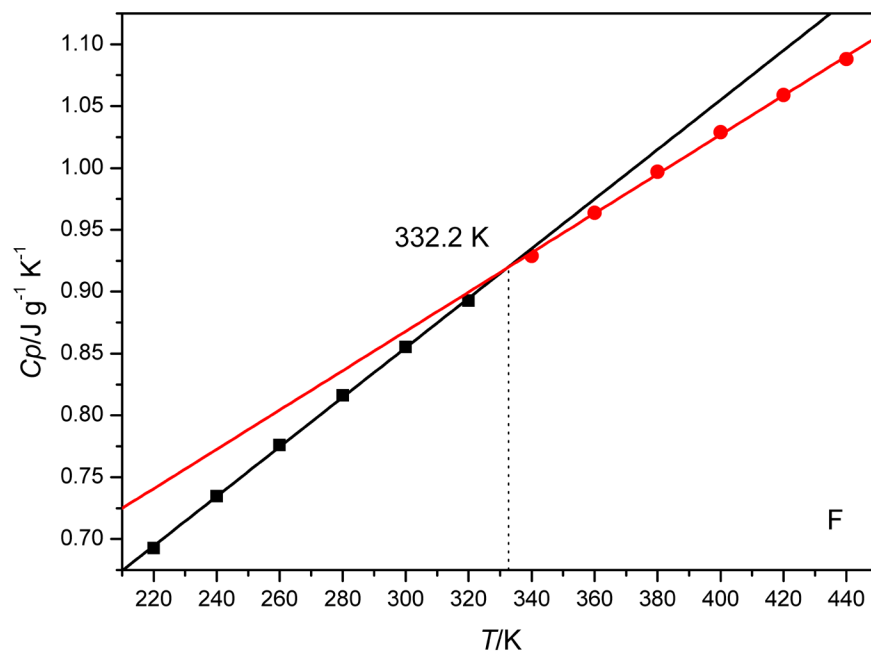


Figure S15. The specific heat capacity vs. temperature relationship for F

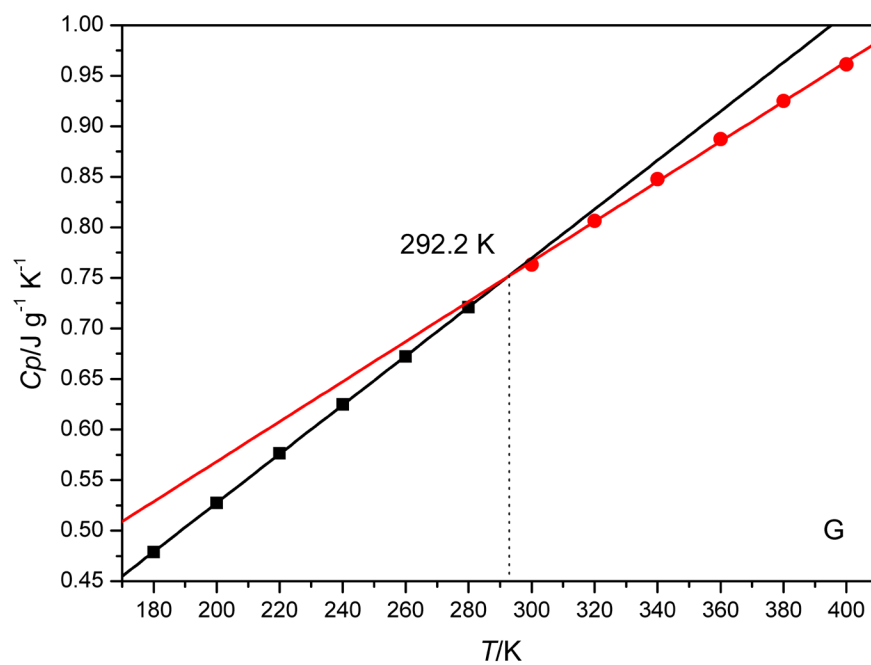


Figure S16. The specific heat capacity vs. temperature relationship for G

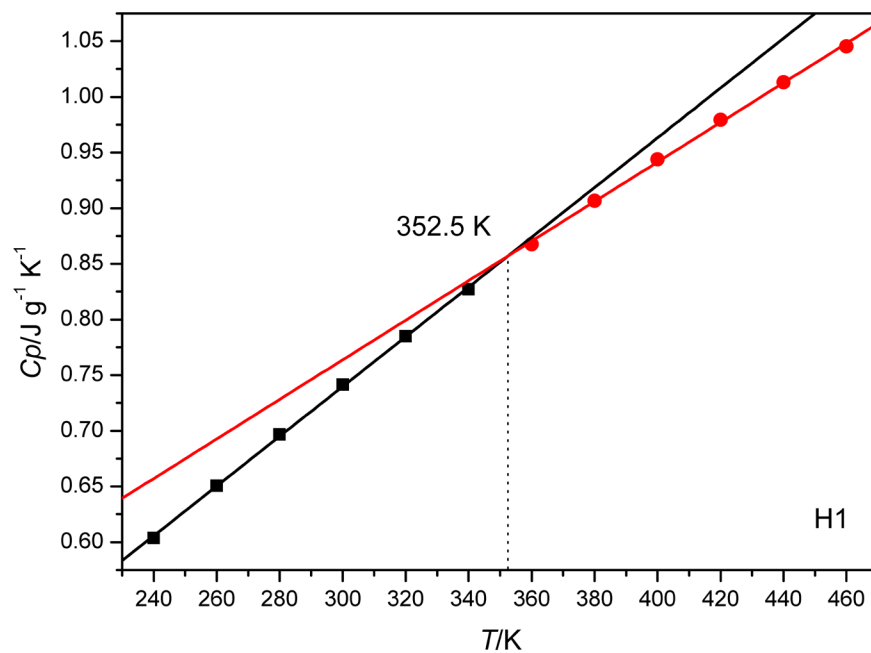


Figure S17. The specific heat capacity vs. temperature relationship for H1

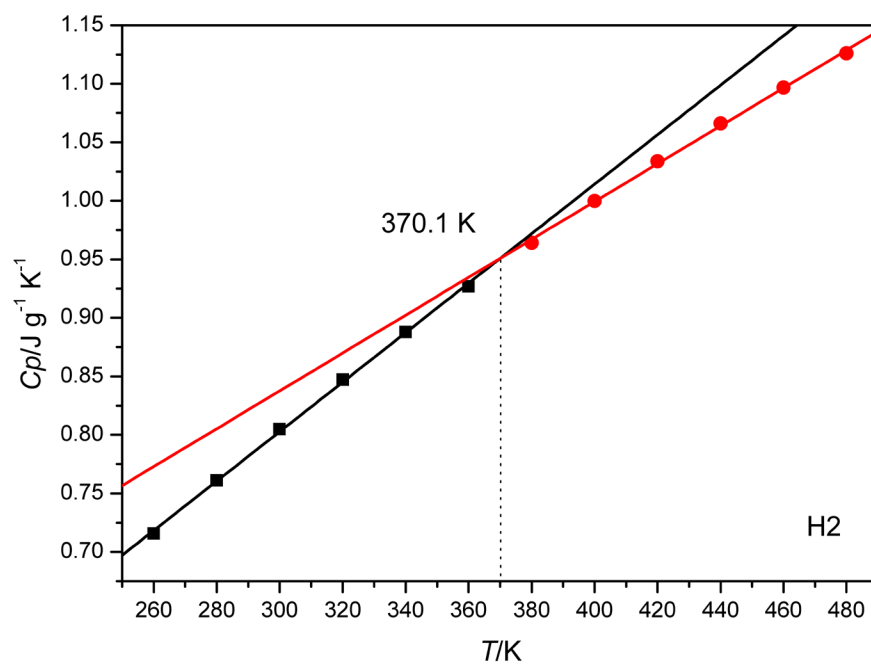


Figure S18. The specific heat capacity vs. temperature relationship for H2

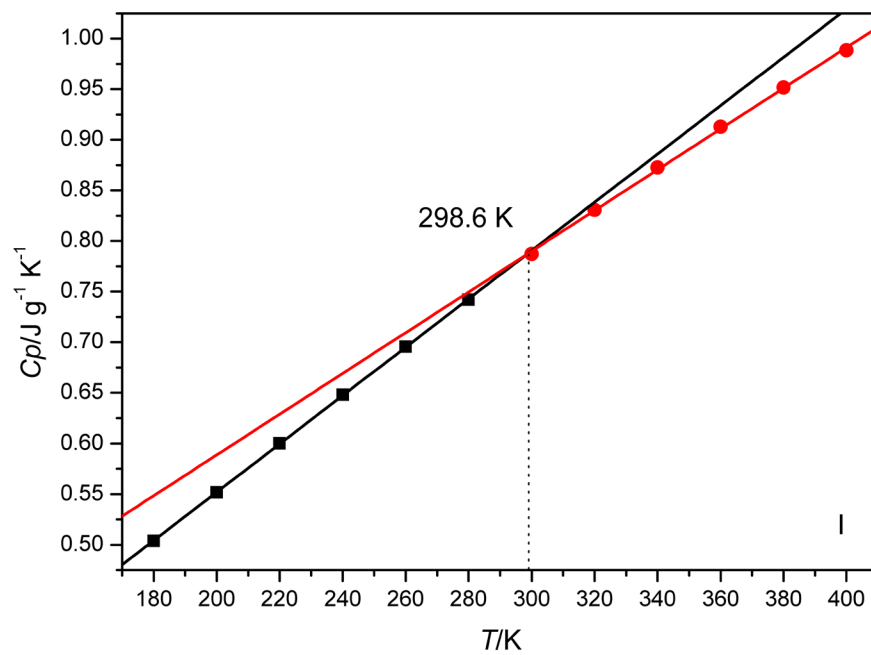


Figure S19. The specific heat capacity vs. temperature relationship for I