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Hosting of diamantane alcohols in water and hydrogen-bonded organic solvents: the (non-)classical hydrophobic effect

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Keywords: cyclodextrins, diamondoids, host-guest chemistry, hydrophobic effect, thermodynamics

Contents

Microcalorimetric titrations in water: Cyclodextrins

1-DAOH with **β-CD** in H_2O

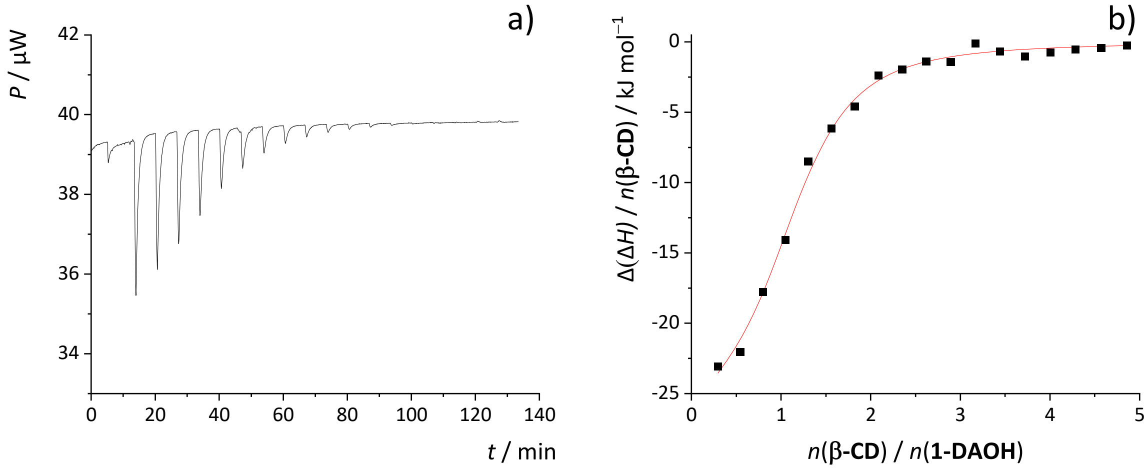


Figure S1. Microcalorimetric titration of **1-DAOH** ($c_0 = 3\cdot10^{-5}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 7\cdot10^{-3}$ mol dm^{-3}) in H_2O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

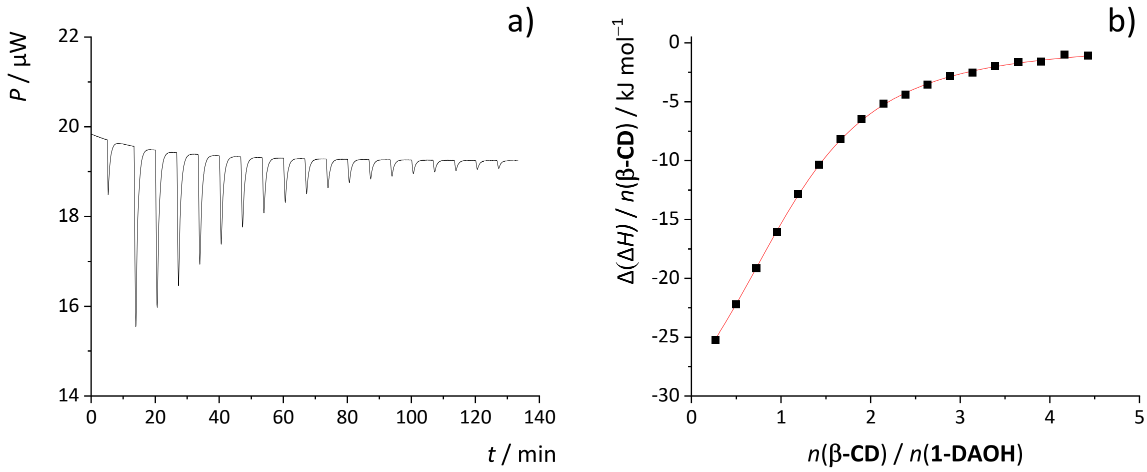


Figure S2. Microcalorimetric titration of **1-DAOH** ($c_0 = 3\cdot10^{-5}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 6\cdot10^{-3}$ mol dm^{-3}) in at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

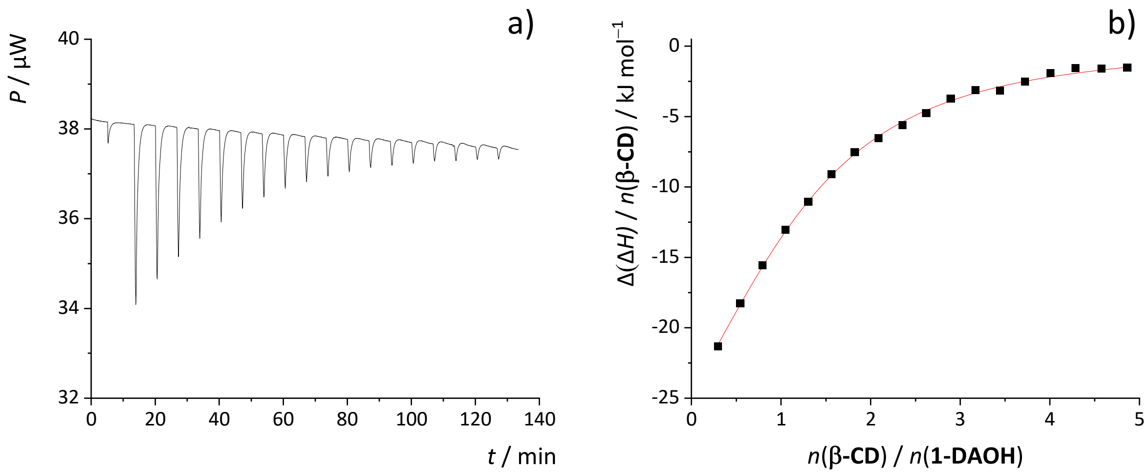


Figure S3. Microcalorimetric titration of **1-DAOH** ($c_0 = 3\cdot10^{-5}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 7\cdot10^{-3}$ mol dm^{-3}) in at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

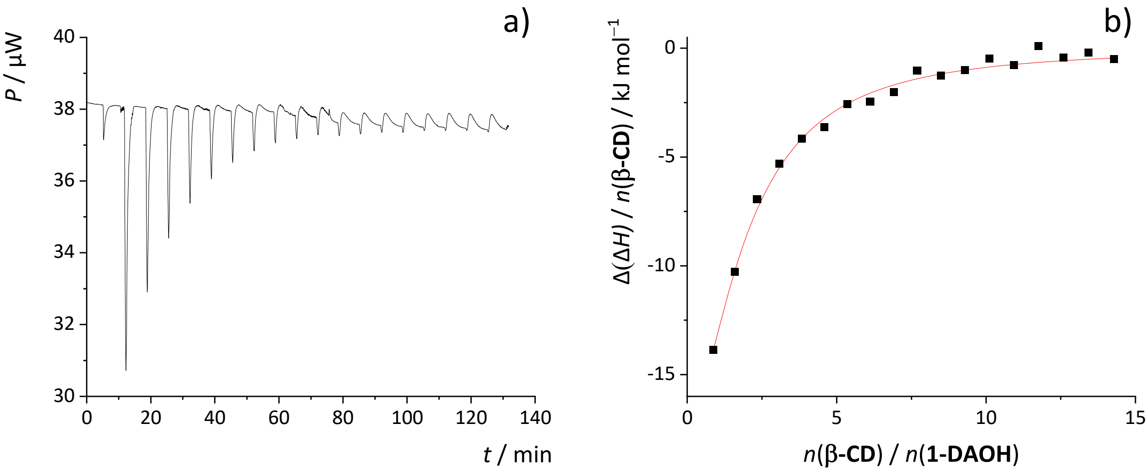


Figure S4. Microcalorimetric titration of **1-DAOH** ($c_0 = 3{\cdot}10^{-5}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 2{\cdot}10^{-3}$ mol dm^{-3}) in H_2O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

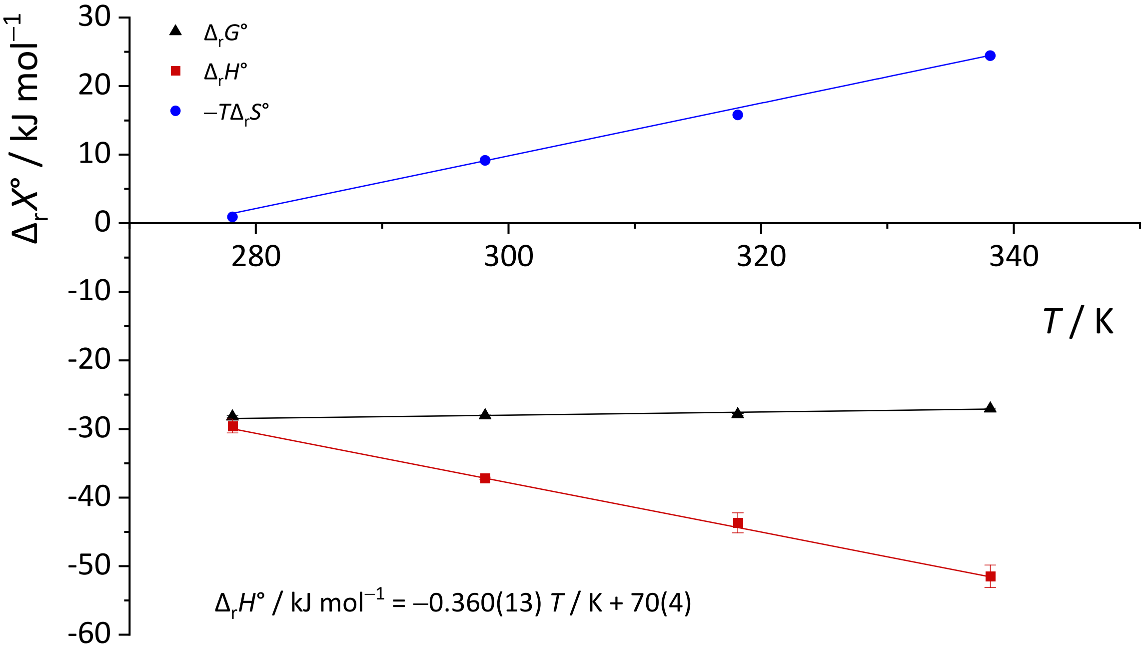


Figure S5. The temperature dependence of standard complexation parameters of **1-DAOH** with **β-CD** in H_2O.

4-DAOH with **β-CD** in H_2O

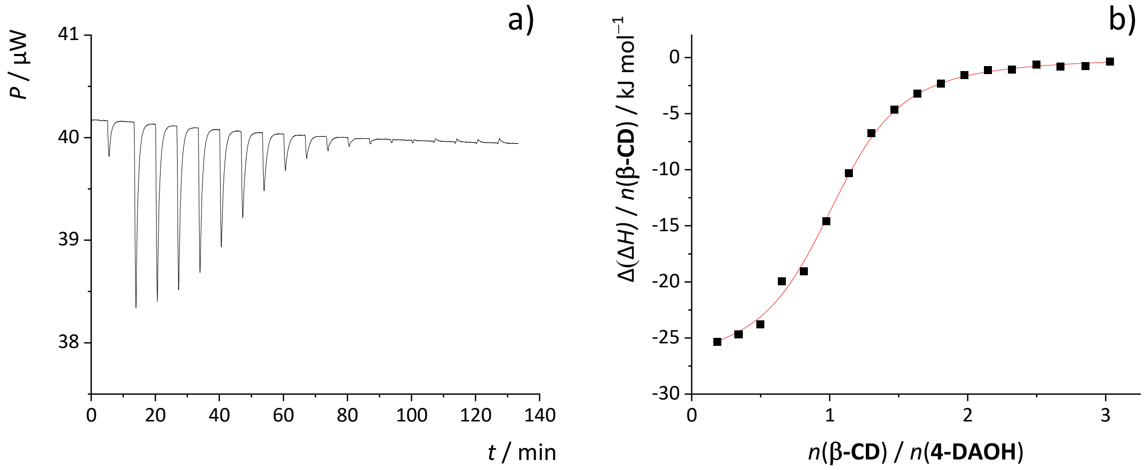


Figure S6. Microcalorimetric titration of **4-DAOH** ($c_0 = 2{\cdot}10^{-5}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 3{\cdot}10^{-4}$ mol dm^{-3}) in H_2O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

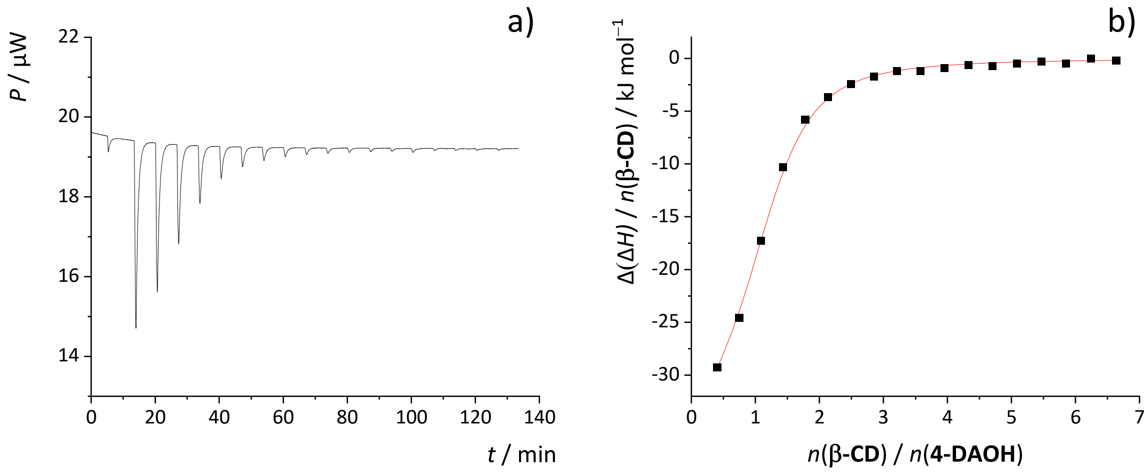


Figure S7. Microcalorimetric titration of **4-DAOH** ($c_0 = 2{\cdot}10^{-5}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 6{\cdot}10^{-4}$ mol dm^{-3}) in H_2O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

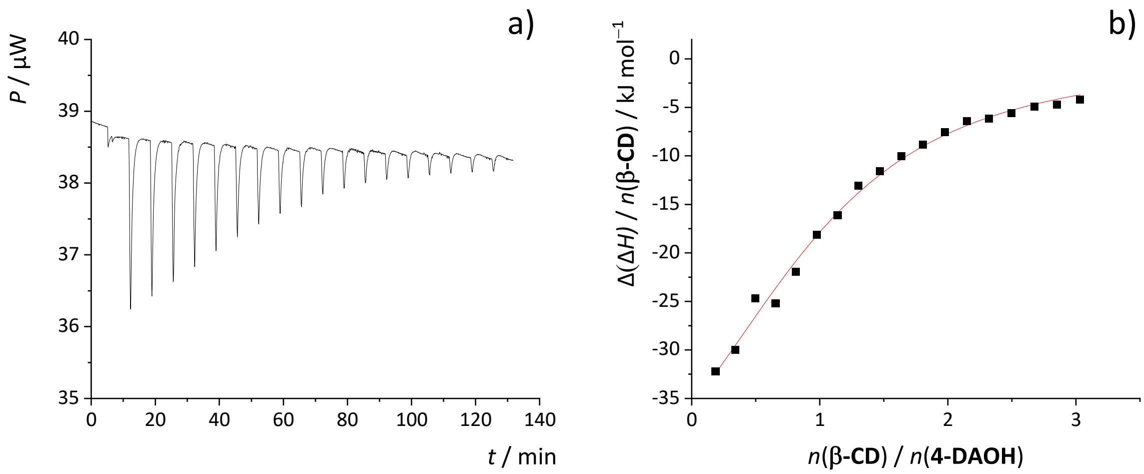


Figure S8. Microcalorimetric titration of **4-DAOH** ($c_0 = 2{\cdot}10^{-5}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 3{\cdot}10^{-4}$ mol dm^{-3}) in H_2O at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

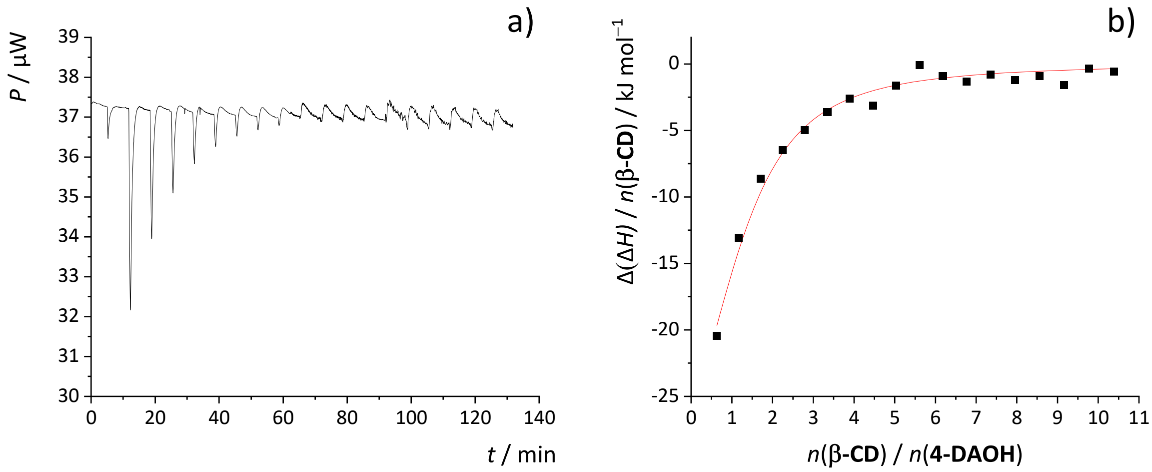


Figure S9. Microcalorimetric titration **4-DAOH** ($c_0 = 2\cdot10^{-5}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 1\cdot10^{-3}$ mol dm^{-3}) in H_2O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

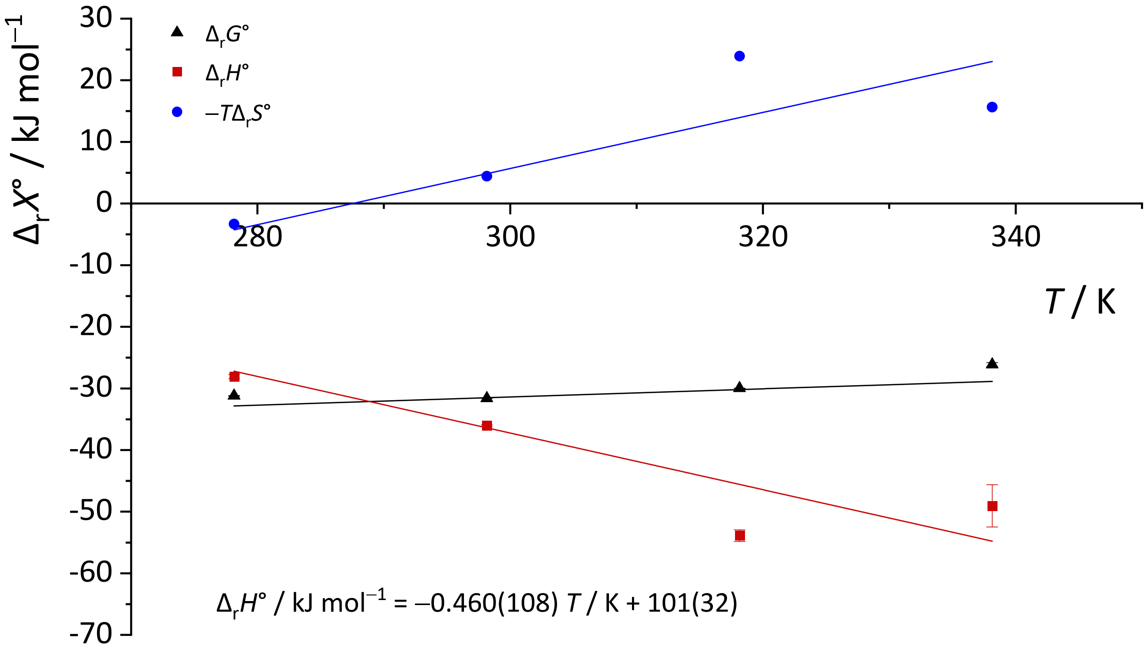


Figure S10. The temperature dependence of standard complexation parameters of **4-DAOH** with **β-CD** in H_2O.

4,9-DA(OH)$_2$ with **β-CD** in H_2O

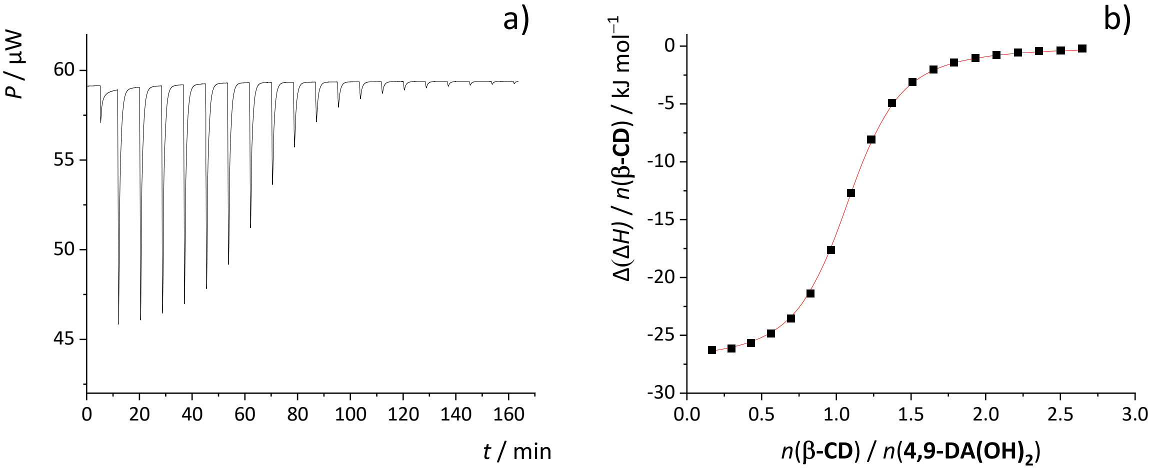


Figure S11. Microcalorimetric titration of **4,9-DA(OH)$_2$** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 3\cdot10^{-3}$ mol dm^{-3}) in H_2O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

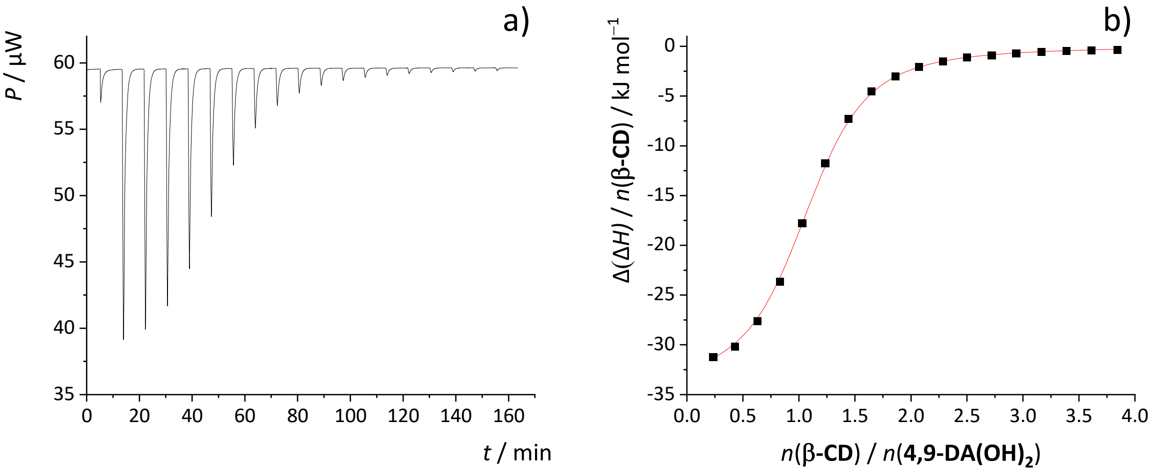


Figure S12. Microcalorimetric titration of **4,9-DA(OH)$_2$** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 3\cdot10^{-3}$ mol dm^{-3}) in H_2O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

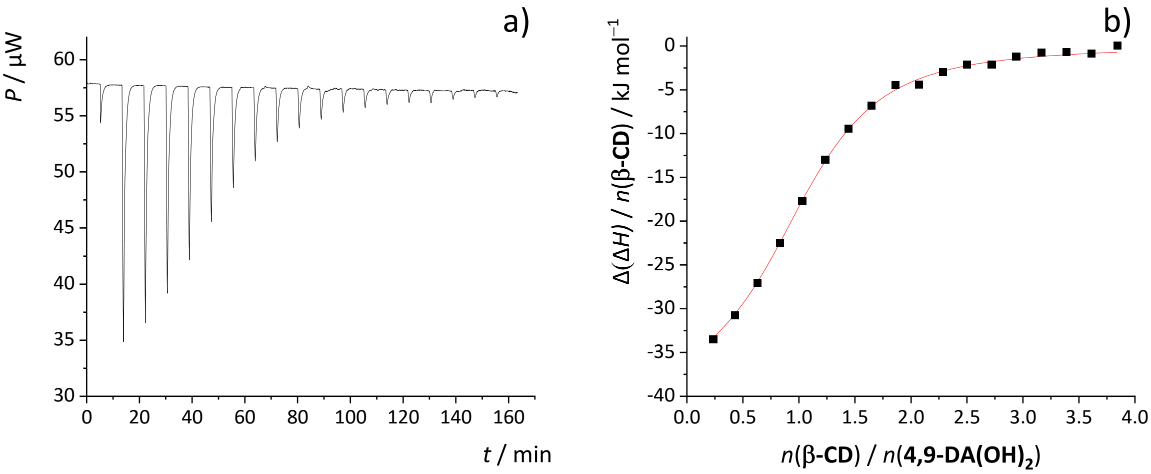


Figure S13. Microcalorimetric titration of **4,9-DA(OH)$_2$** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 3\cdot10^{-3}$ mol dm^{-3}) in H_2O at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

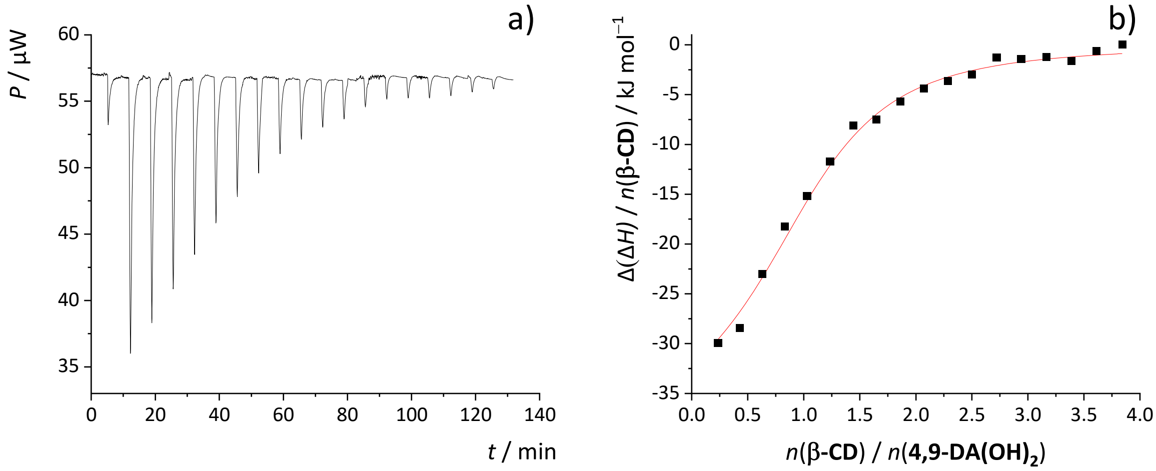


Figure S14. Microcalorimetric titration of **4,9-DA(OH)$_2$** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 3\cdot10^{-3}$ mol dm^{-3}) in H_2O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

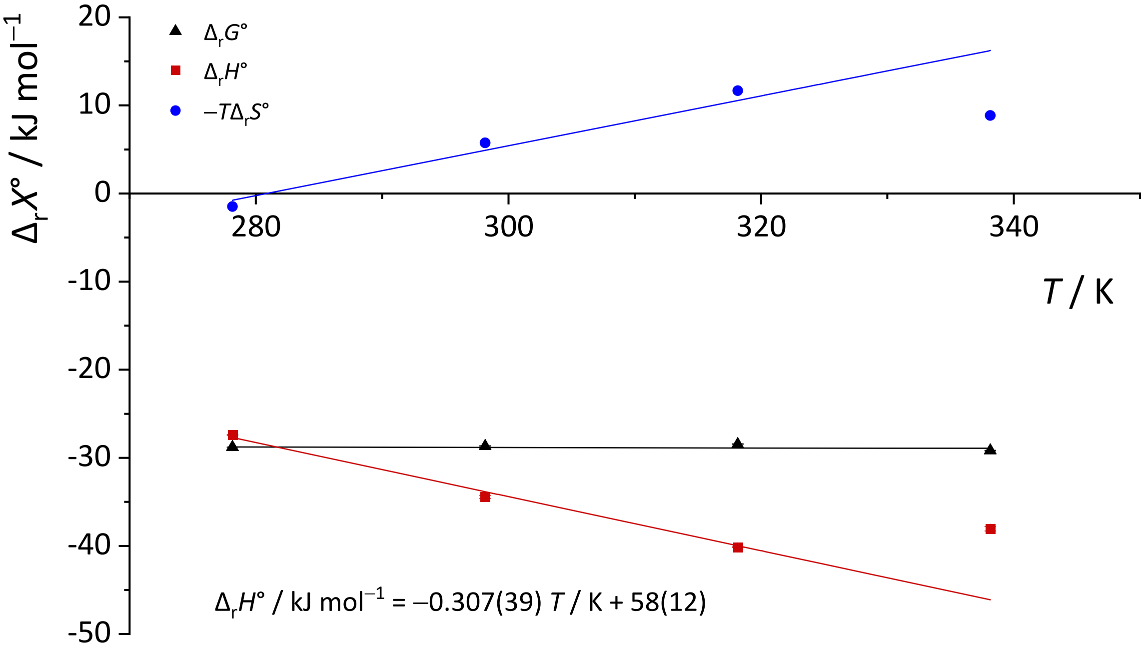


Figure S15. The temperature dependence of standard complexation parameters of **4,9-DA(OH)$_2$** with **β-CD** in H_2O.

Table S1. Thermodynamic parameters for complexation of **1-AdOH** and diamantane alcohols with **β-CD** in H_2O.[a]

GUEST · β-CD	T / K	log K	$\Delta_r G°$ / kJ mol^{-1}	$\Delta_r H°$ / kJ mol^{-1}	$-T\Delta_r S°$ / kJ mol^{-1}	$\Delta_r C_p°$ / J K^{-1} mol^{-1}
1-AdOH[b]	278	4.90(1)	−26.08(1)	−14.88(5)	−11.23(5)	−391(36)
	298	4.66(1)	−26.38(3)	−21.86(6)	−4.53(5)	
	308	4.49(1)	−26.46(3)	−27.68(7)	1.20(9)	
	338	4.06(1)	−26.26(4)	−36.5(2)	10.2(3)	
1-DAOH	278	5.30(4)	−28.2(2)	−30(1)	1(1)	−360(13)
	298	4.91(1)	−28.02(6)	−37.2(2)	9.2(2)	
	318	4.58(2)	−27.9(1)	−44(1)	16(2)	
	338	4.18(1)	−27.03(7)	−52(2)	24(2)	
4-DAOH	278	5.86(1)	−31.21(6)	−28.1(3)	−3.3(3)	−460(108)
	298	5.54(1)	−31.61(1)	−36.0(1)	4.4(2)	
	318	4.92(1)	−29.97(2)	−53.9(9)	24(1)	
	338	4.74(6)	−26.1(3)	−49(3)	16(3)	
4,9-DA(OH)$_2$	278	5.41(1)	−28.79(1)	−27.41(7)	−1.5(1)	−307(39)
	298	5.02(1)	−28.67(4)	−34.5(2)	5.8(2)	
	318	4.67(1)	−28.45(6)	−40.13(3)	11.68(8)	
	338	4.51(1)	−29.17(5)	−38.0(3)	8.9(3)	

[a] Uncertainties of the last digit(s) are given in parentheses as standard errors of the mean (N = 3−5), or standard deviations obtained by weighted linear regression analysis (for $\Delta_r C_p°$ values); [b] Reference: K. Leko, M. Hanževački, Z. Brkljača, K. Pičuljan, R. Ribić, J. Požar, *Chem. Eur. J.* **2020**, *26*, 5208–5219.

Even though larger thermal noise was in some cases associated with experiments carried out at 278 and 338 K, or that complexation enthalpy was occasionally close to zero, the obtained linear $\Delta_r H°(T)$ dependencies and the standard errors of the mean obtained by repetitive titration experiments indicate the reliability of determined thermodynamic complexation parameters.

1-AdOH with **γ-CD** in H_2O

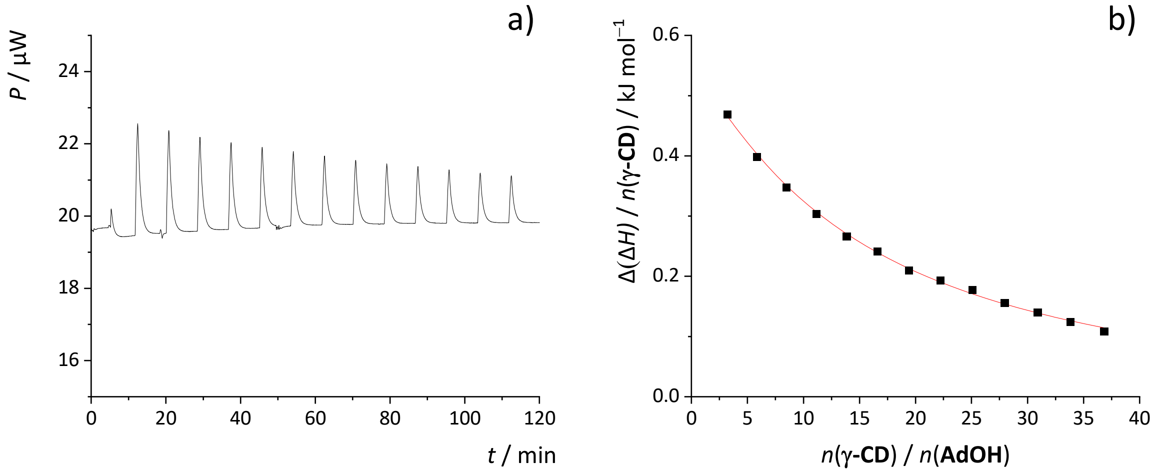


Figure S16. Microcalorimetric titration of **1-AdOH** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, V_0 = 1.45 mL) with **γ-CD** ($c = 2\cdot10^{-2}$ mol dm^{-3}) in H_2O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

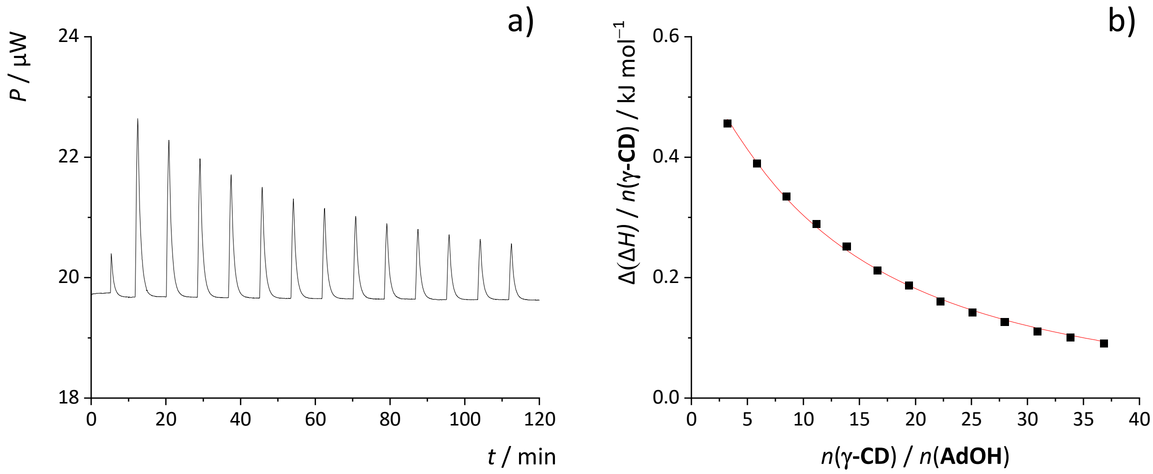


Figure S17. Microcalorimetric titration of **1-AdOH** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, V_0 = 1.45 mL) with **γ-CD** ($c = 2\cdot10^{-2}$ mol dm^{-3}) in H_2O at 288 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

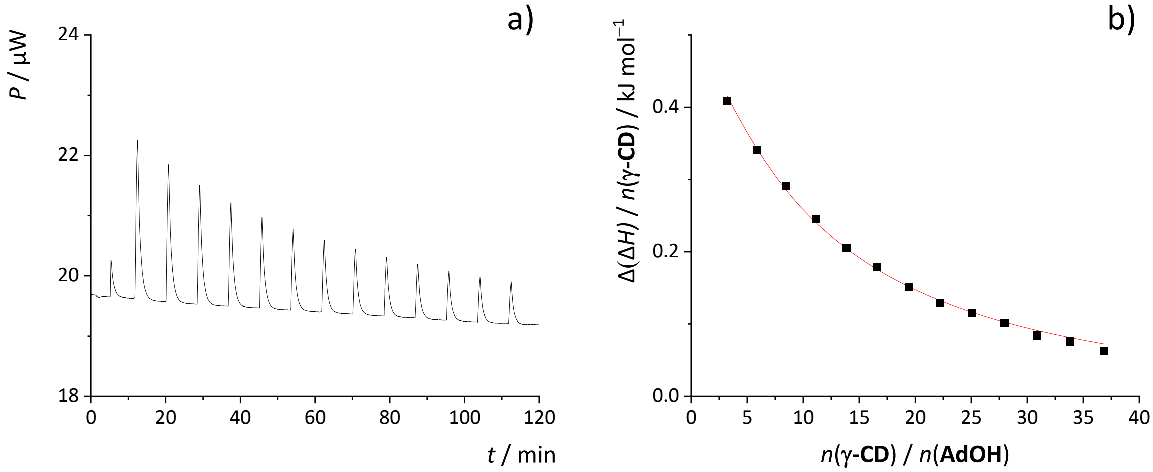


Figure S18. Microcalorimetric titration of **1-AdOH** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, V_0 = 1.45 mL) with **γ-CD** ($c = 2\cdot10^{-2}$ mol dm^{-3}) in H_2O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

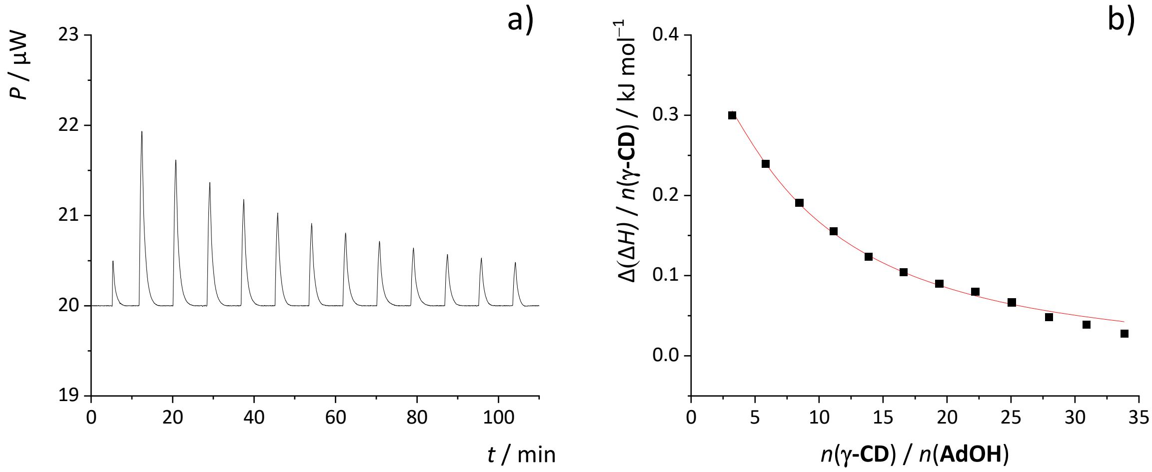


Figure S19. Microcalorimetric titration of **1-AdOH** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, V_0 = 1.45 mL) with **γ-CD** ($c = 2\cdot10^{-2}$ mol dm^{-3}) in H_2O at 308 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

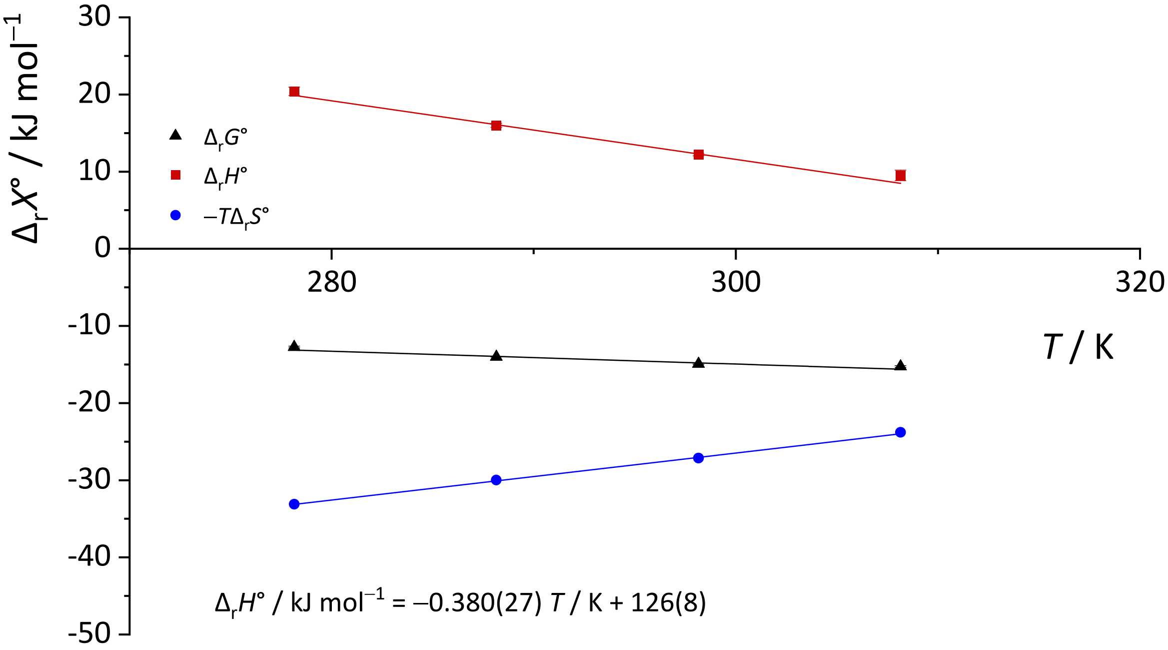


Figure S20. The temperature dependence of standard complexation parameters of **1-AdOH** with **γ-CD** in H_2O.

1-DAOH with **γ-CD** in H_2O

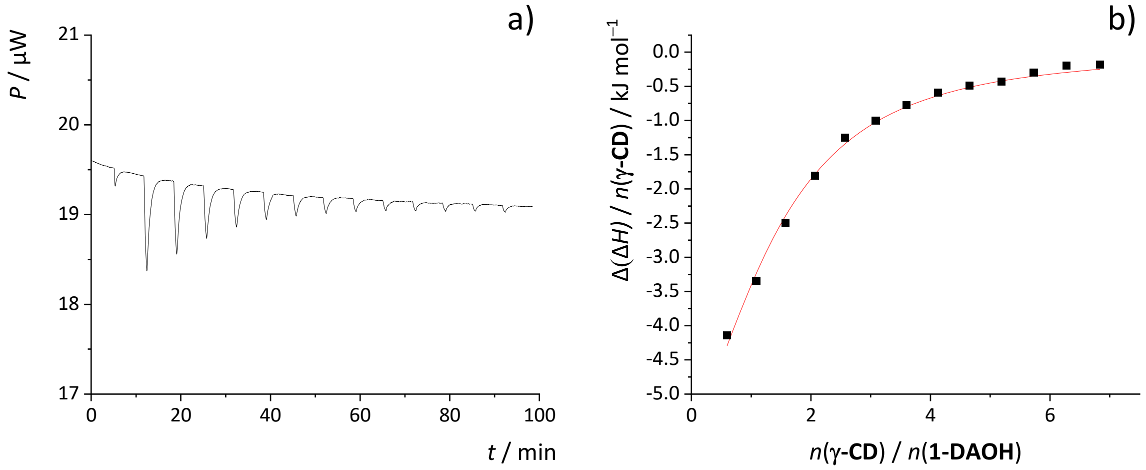


Figure S21. Microcalorimetric titration of **1-DAOH** ($c_0 = 1\cdot10^{-5}$ mol dm^{-3}, V_0 = 1.45 mL) with **γ-CD** ($c = 1\cdot10^{-3}$ mol dm^{-3}) in H_2O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

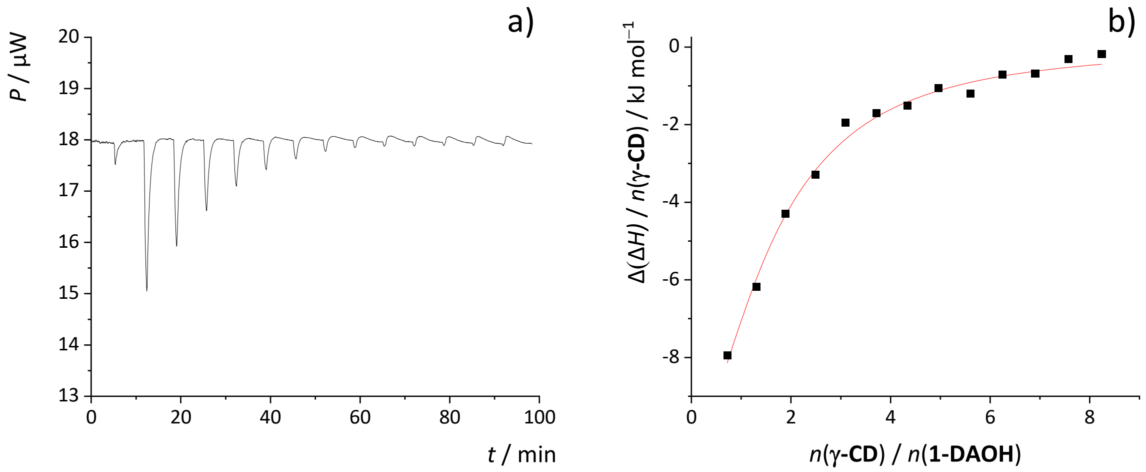


Figure S22. Microcalorimetric titration of **1-DAOH** ($c_0 = 1\cdot10^{-5}$ mol dm^{-3}, V_0 = 1.45 mL) with **γ-CD** ($c = 1\cdot10^{-3}$ mol dm^{-3}) in H_2O at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

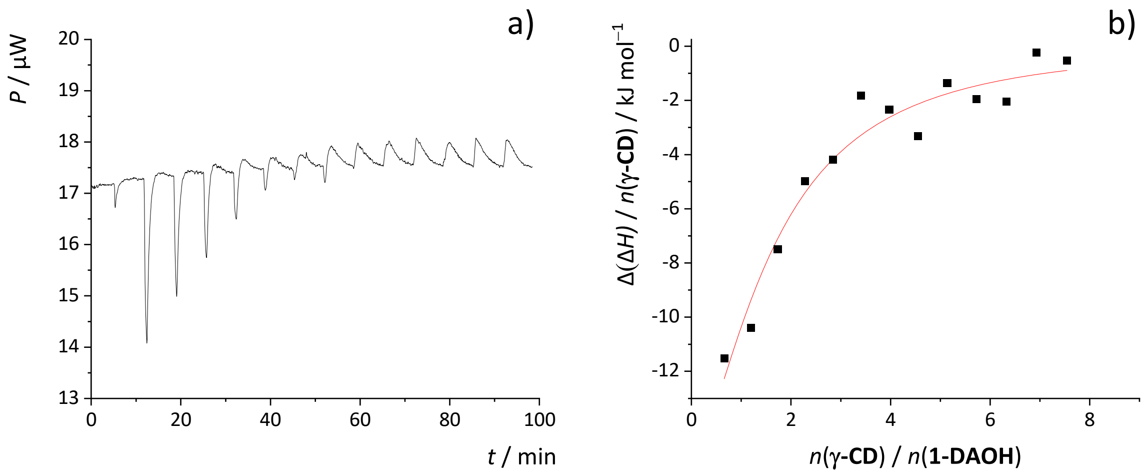


Figure S23. Microcalorimetric titration of **1-DAOH** ($c_0 = 1\cdot10^{-5}$ mol dm^{-3}, V_0 = 1.45 mL) with **γ-CD** ($c = 1\cdot10^{-3}$ mol dm^{-3}) in H_2O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

4-DAOH with **γ-CD** in H_2O

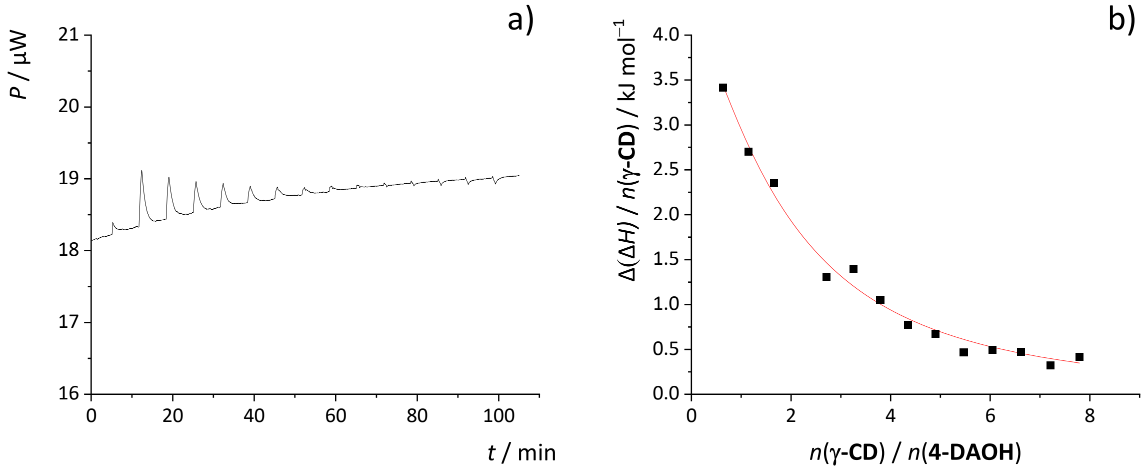


Figure S24. Microcalorimetric titration of **4-DAOH** ($c_0 = 1\cdot10^{-5}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **γ-CD** ($c = 1\cdot10^{-3}$ mol dm^{-3}) in H_2O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

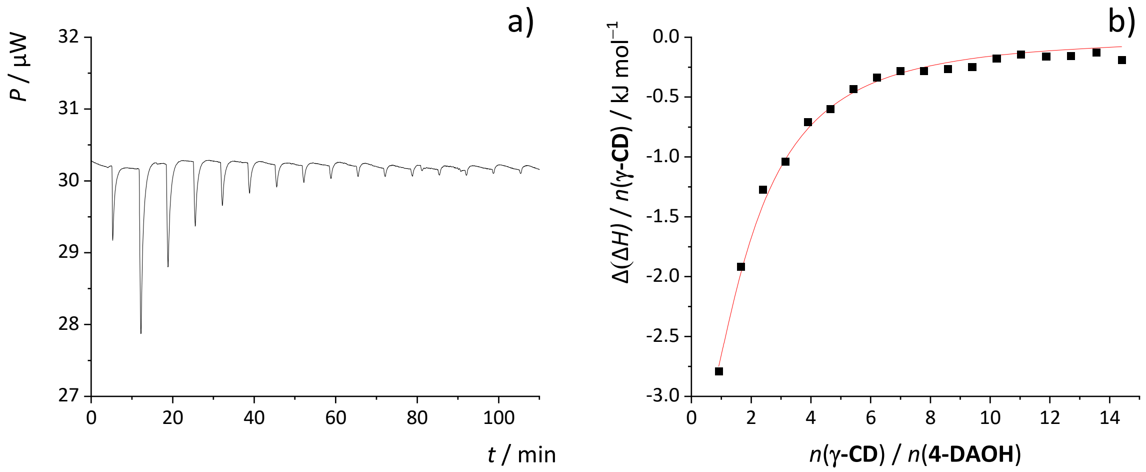


Figure S25. Microcalorimetric titration of **4-DAOH** ($c_0 = 4\cdot10^{-5}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **γ-CD** ($c = 3\cdot10^{-3}$ mol dm^{-3}) in H_2O at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

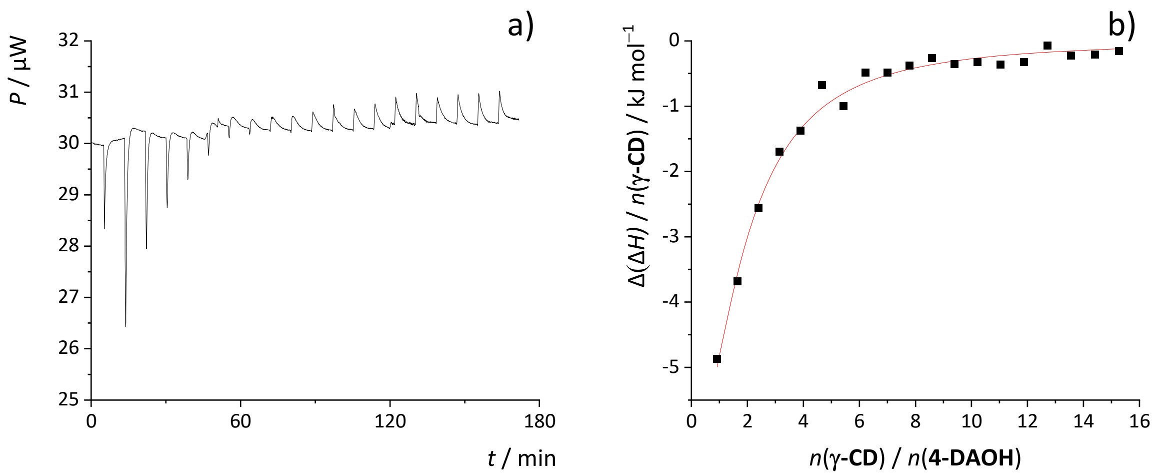


Figure S26. Microcalorimetric titration of **4-DAOH** ($c_0 = 4\cdot10^{-5}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **γ-CD** ($c = 3\cdot10^{-3}$ mol dm^{-3}) in H_2O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

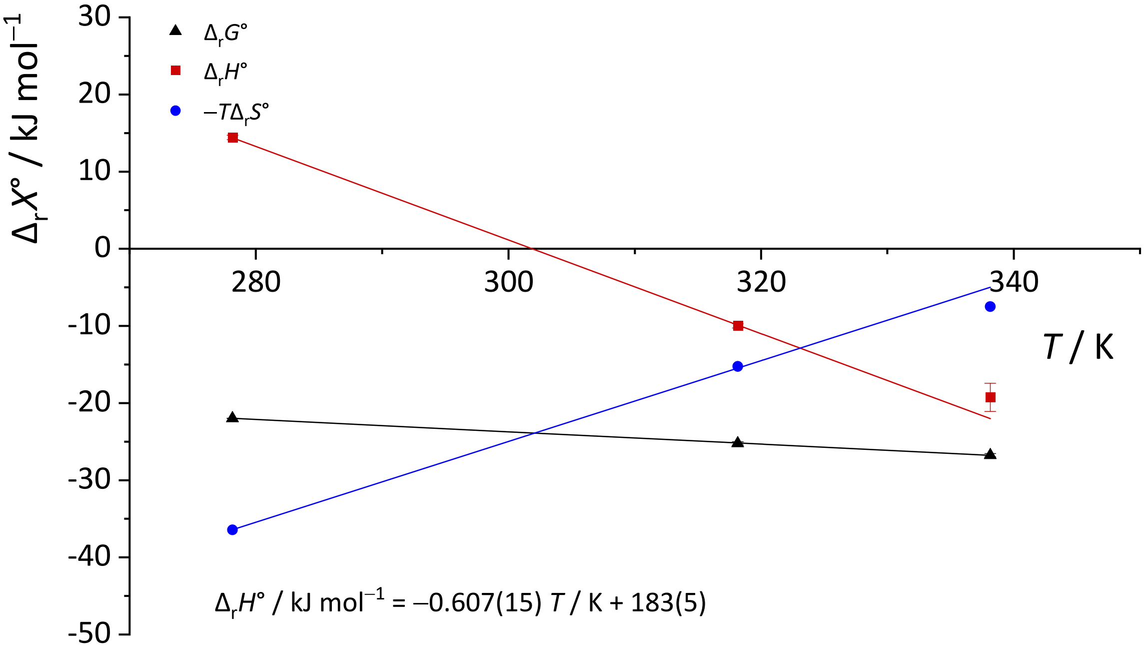


Figure S27. The temperature dependence of standard complexation parameters of **4-DAOH** with **γ-CD** in H_2O.

4,9-DA(OH)$_2$ with γ-CD in H_2O

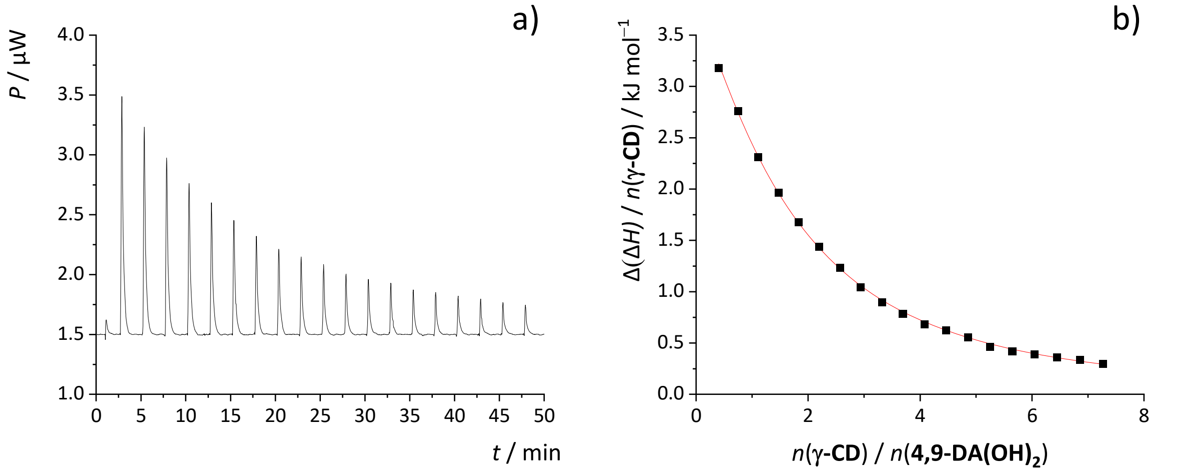


Figure S28. Microcalorimetric titration of **4,9-DA(OH)$_2$** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **γ-CD** ($c = 5\cdot10^{-3}$ mol dm^{-3}) in H_2O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

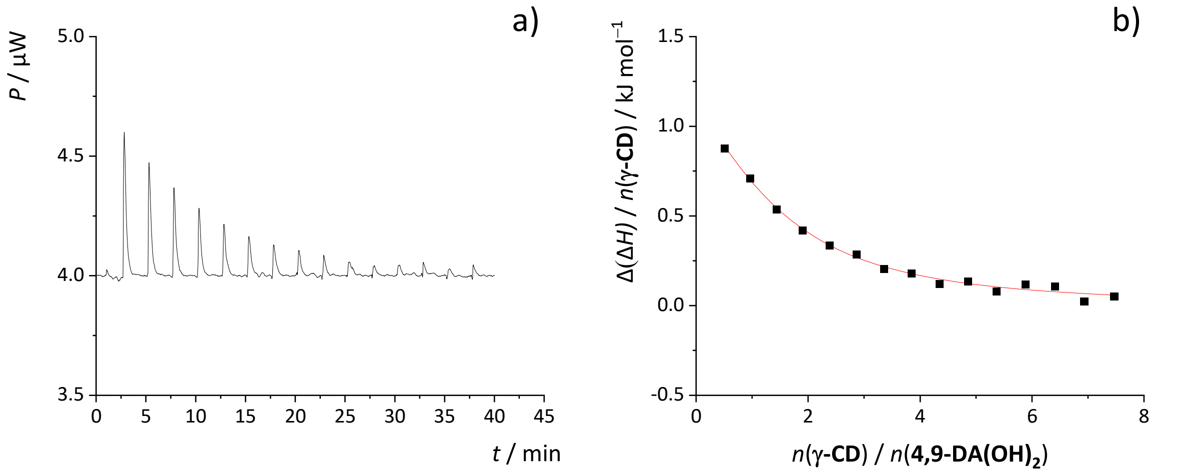


Figure S29. Microcalorimetric titration of **4,9-DA(OH)$_2$** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **γ-CD** ($c = 5\cdot10^{-3}$ mol dm^{-3}) in H_2O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

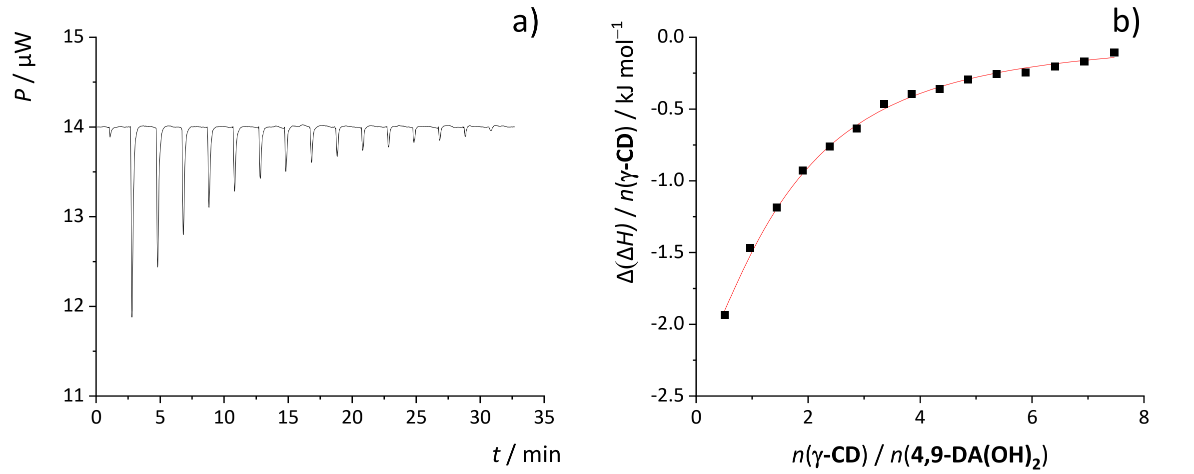


Figure S30. Microcalorimetric titration of **4,9-DA(OH)$_2$** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **γ-CD** ($c = 5\cdot10^{-3}$ mol dm^{-3}) in H_2O at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

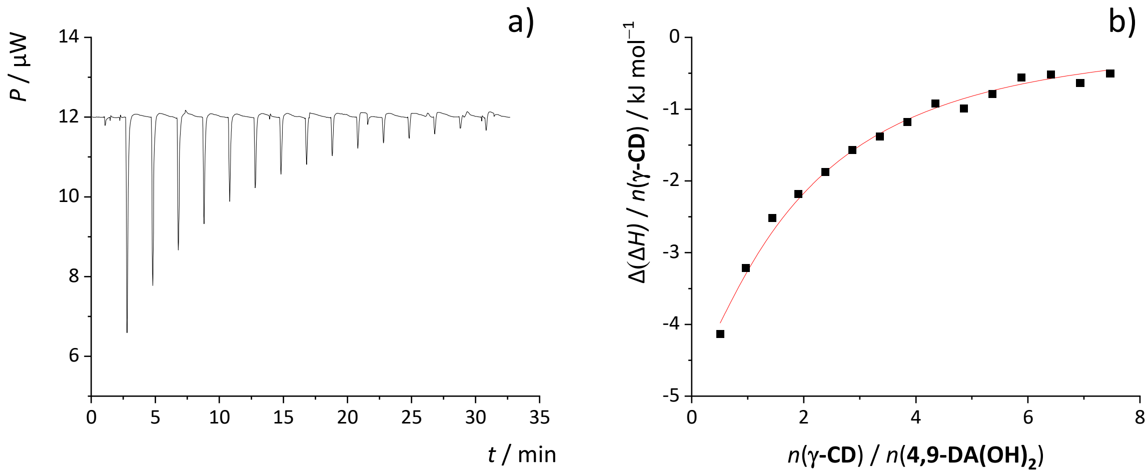


Figure S31. Microcalorimetric titration of **4,9-DA(OH)₂** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **γ-CD** ($c = 5\cdot10^{-3}$ mol dm^{-3}) in H_2O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

Table S2. Thermodynamic parameters for complexation of **1-AdOH** and diamantane alcohols with **γ-CD** in H_2O.[a]

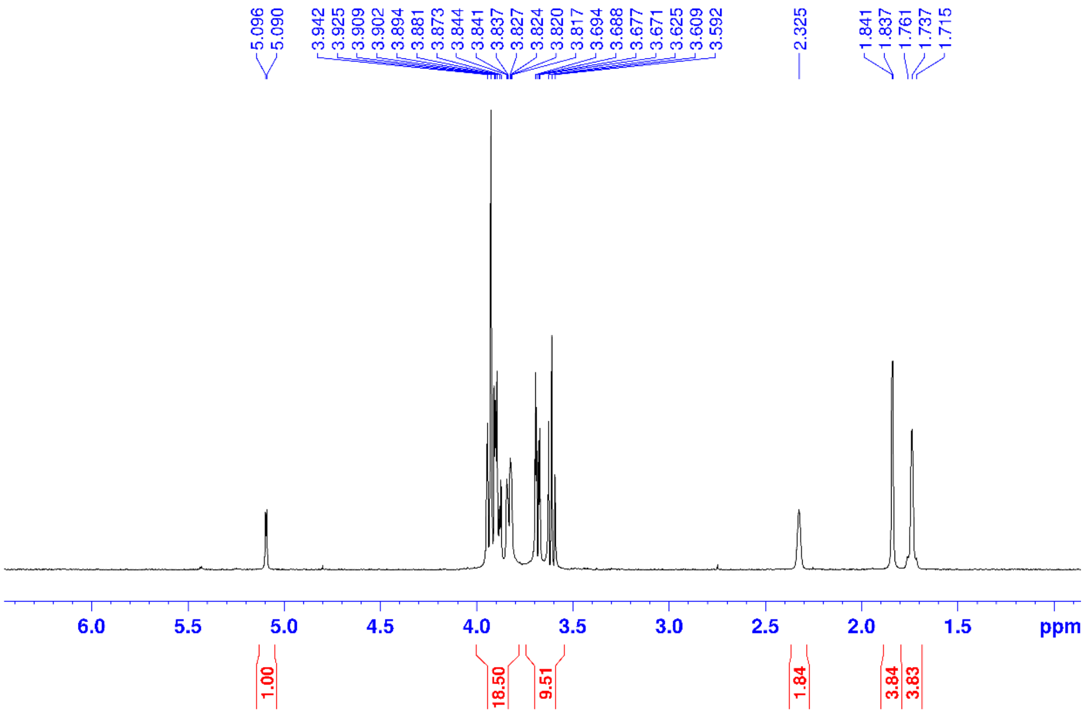
GUEST · γ-CD	T / K	log K	$\Delta_r G°$ / kJ mol^{-1}	$\Delta_r H°$ / kJ mol^{-1}	$-T\Delta_r S°$ / kJ mol^{-1}	$\Delta_r C_p°$ / J K^{-1} mol^{-1}
1-AdOH	278	2.39(2)	−12.7(1)	20.4(5)	−33.1(4)	−380(27)
	288	2.54(1)	−14.00(3)	16.0(3)	−30.0(4)	
	298	2.62(1)	−19.9(1)	12.2(2)	−27.1(1)	
	308	2.59(2)	−15.3(1)	9.5(7)	−23.8(2)	
1-DAOH	278			≈ 0		−715(37)
	298	4.48(1)	−25.57(5)	−10.8(2)	−14.7(2)	
	318	4.36(1)	−26.56(5)	−24.6(2)	−2.0(3)	
	338	4.25(5)	−27.5(2)	−40.7(6)	13.1(8)	
4-DAOH	278	4.13(1)	−21.98(2)	14.4(3)	−36.4(3)	−607(15)
	298	4.14[b]	−23.6[b]	2.25[b]	−25.9[b]	
	318	4.14(3)	−25.2(2)	−10.0(3)	−15.3(5)	
	338	4.13(3)	−26.7(2)	−19(2)	−8(2)	
4,9-DA(OH)$_2$	278	3.54(1)	−18.83(1)	11.27(3)	−30.13(3)	−440(11)
	298	3.64(3)	−20.8(2)	2.76(7)	−23.5(1)	
	318	3.53(4)	−21.5(2)	−6.8(3)	−14.8(5)	
	338	3.47(2)	−22.5(1)	−16.1(3)	−6.4(4)	

[a] Uncertainties of the last digit(s) are given in parentheses as standard errors of the mean (N = 3−5), or standard deviations obtained by weighted linear regression analysis (for $\Delta_r C_p°$ values); [b] obtained by interpolation based on herein determined temperature dependence of thermodynamic complexation parameters.

Even though larger thermal noise was in some cases associated with experiments carried out at 278 and 338 K, or that complexation enthalpy was occasionally close to zero, the obtained linear $\Delta_r H°(T)$ dependencies and the standard errors of the mean obtained by repetitive titration experiments indicate the reliability of determined thermodynamic complexation parameters.

2D NMR Spectra of investigated host-guest systems

a)



b)

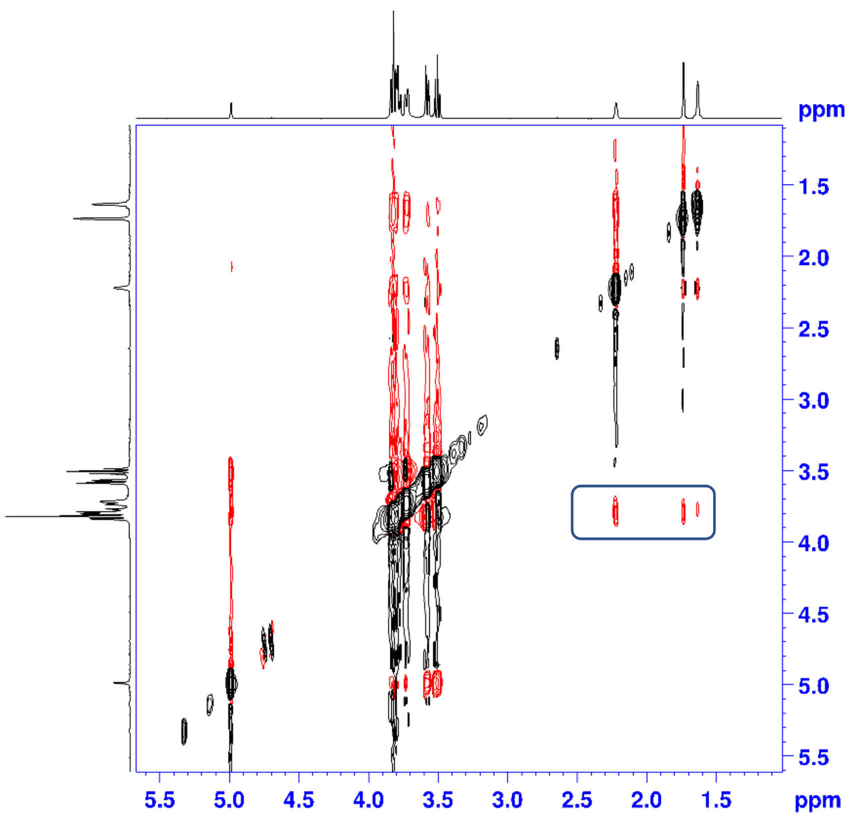
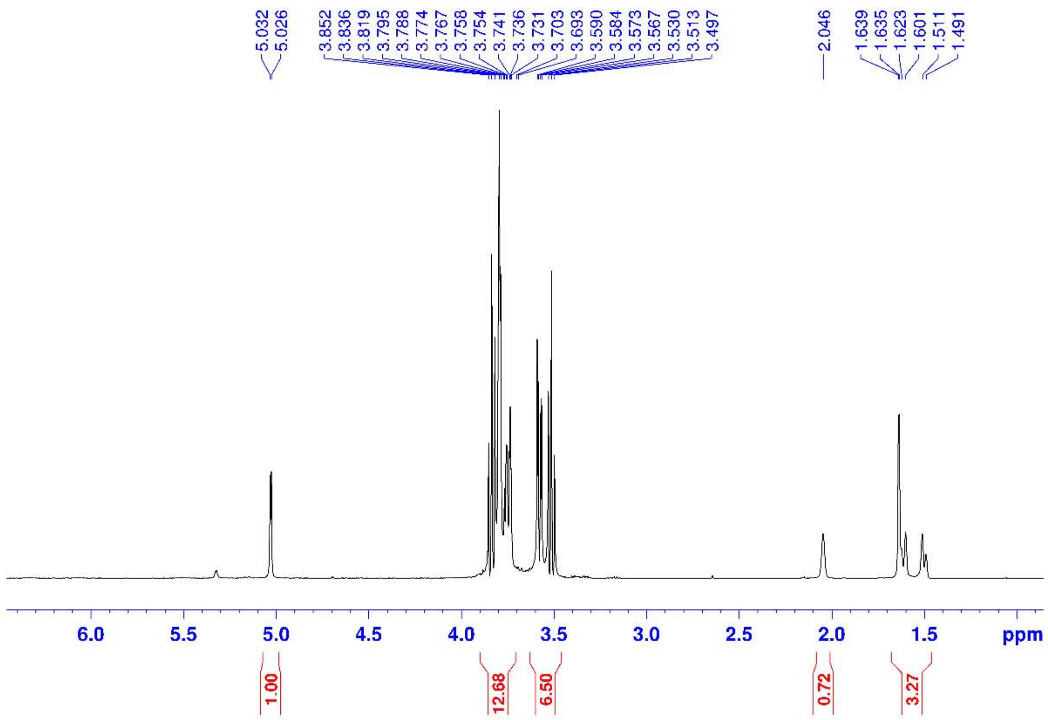


Figure S32. a) 600 MHz ^{1}H NMR spectrum with water suppression of **1-AdOH·β-CD** in D_2O. b) Contour plot of the ROESY ^{1}H NMR spectrum of the reaction mixture containing **1-AdOH** ($c = 5\cdot10^{-3}$ mol dm^{-3}) and **β-CD** ($c = 2\cdot10^{-3}$ mol dm^{-3}) at 298 K in D_2O.

a)



b)

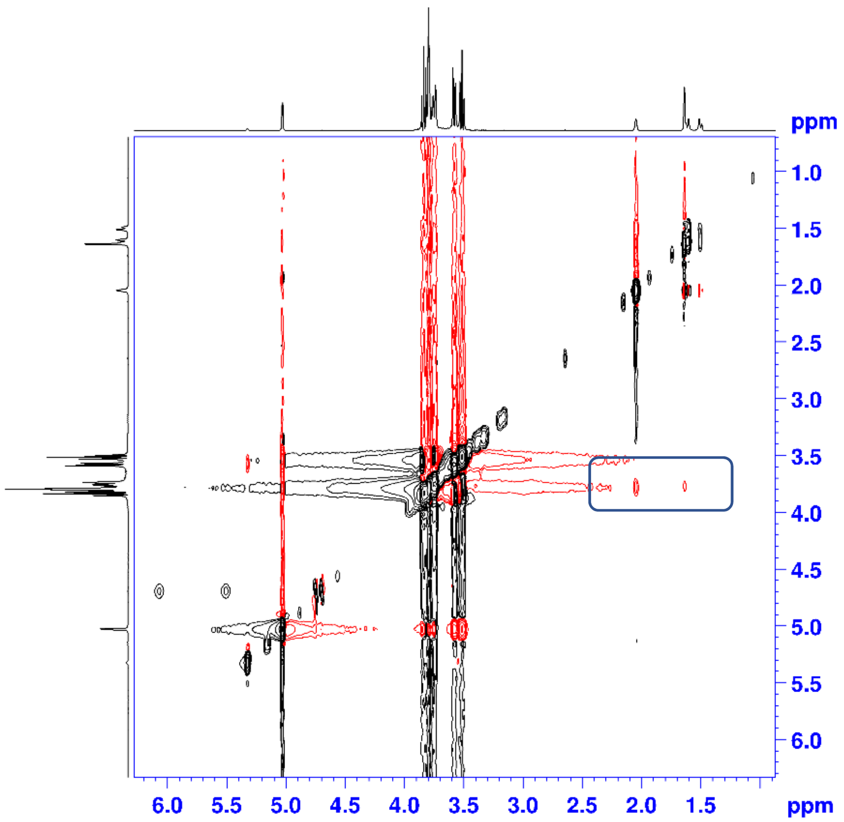
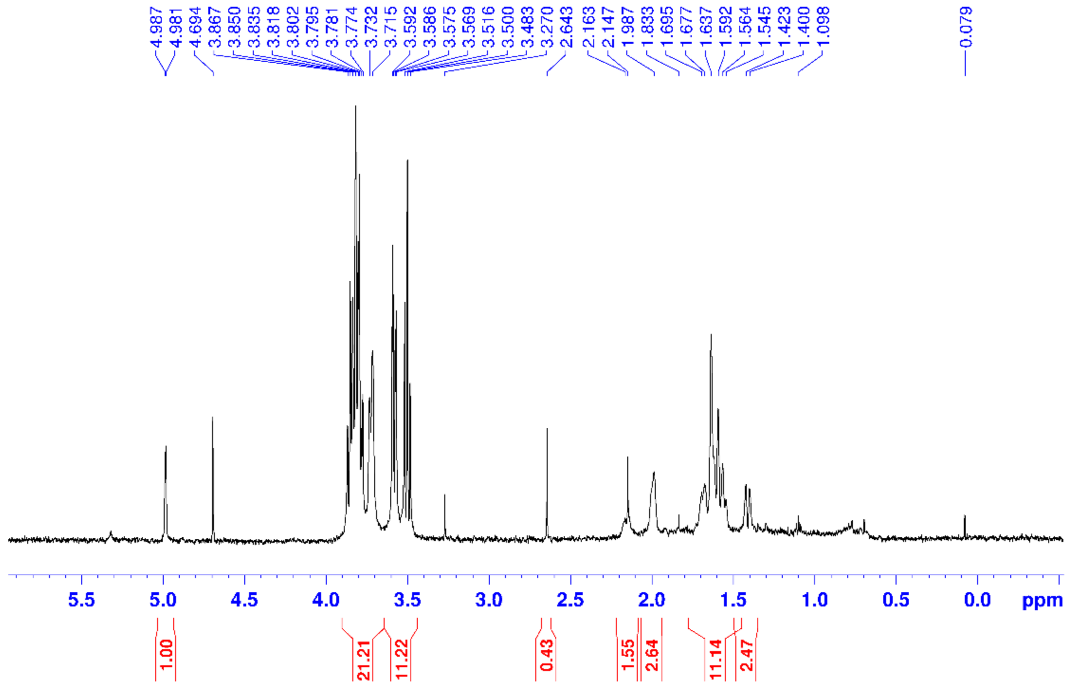


Figure S33. a) 600 MHz ¹H NMR spectrum with water suppression of **1-AdOH·γ-CD** in D_2O. Contour plot of the ROESY ¹H NMR spectrum of the reaction mixture containing **1-AdOH** ($c = 3\cdot10^{-3}$ mol dm^{-3}) and **γ-CD** ($c = 4\cdot10^{-3}$ mol dm^{-3}) at 298 K in D_2O.

a)



b)

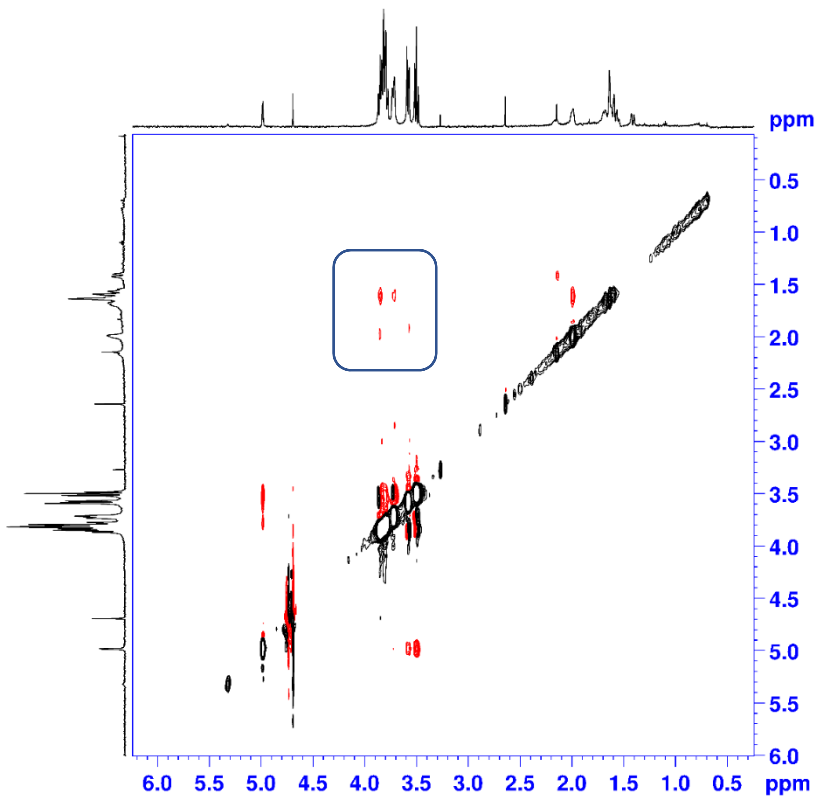
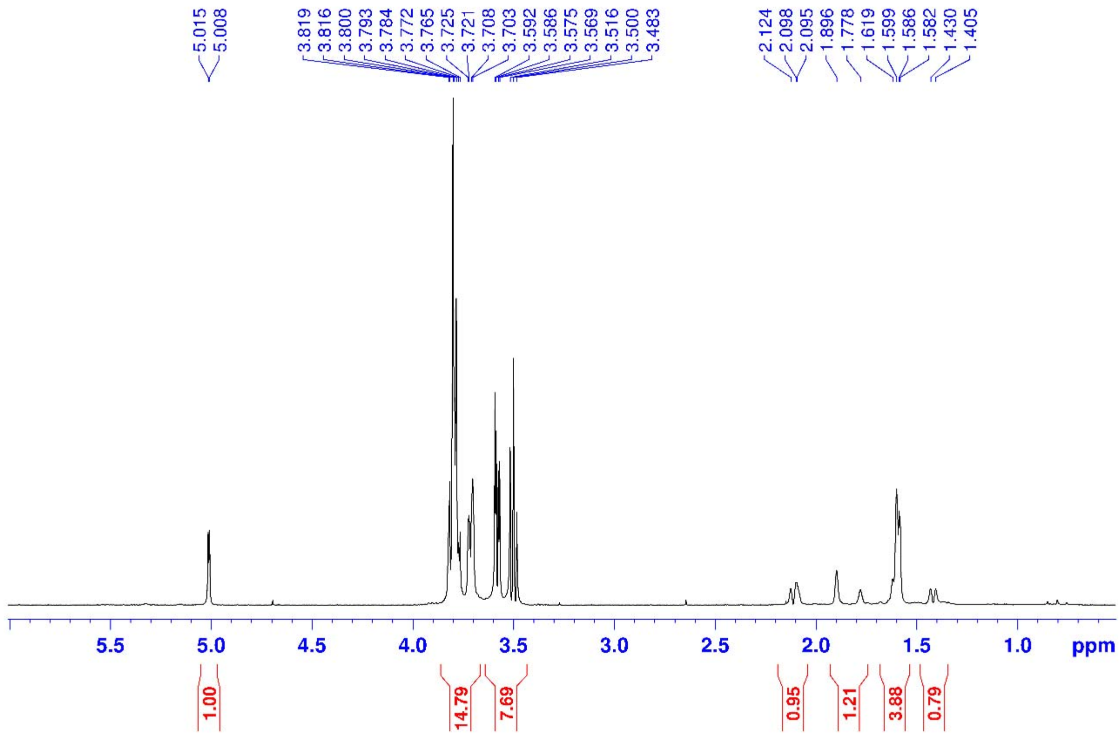


Figure S34. a) 600 MHz [1]H NMR spectrum with water suppression of **1-DAOH ·β-CD** in D_2O. b) Contour plot of the ROESY [1]H NMR spectrum of the reaction mixture containing **1-DAOH** ($c = 1.6 \cdot 10^{-3}$ mol dm^{-3}) and **β-CD** ($c = 1.9 \cdot 10^{-3}$ mol dm^{-3}) at 298 K in D_2O.

a)



b)

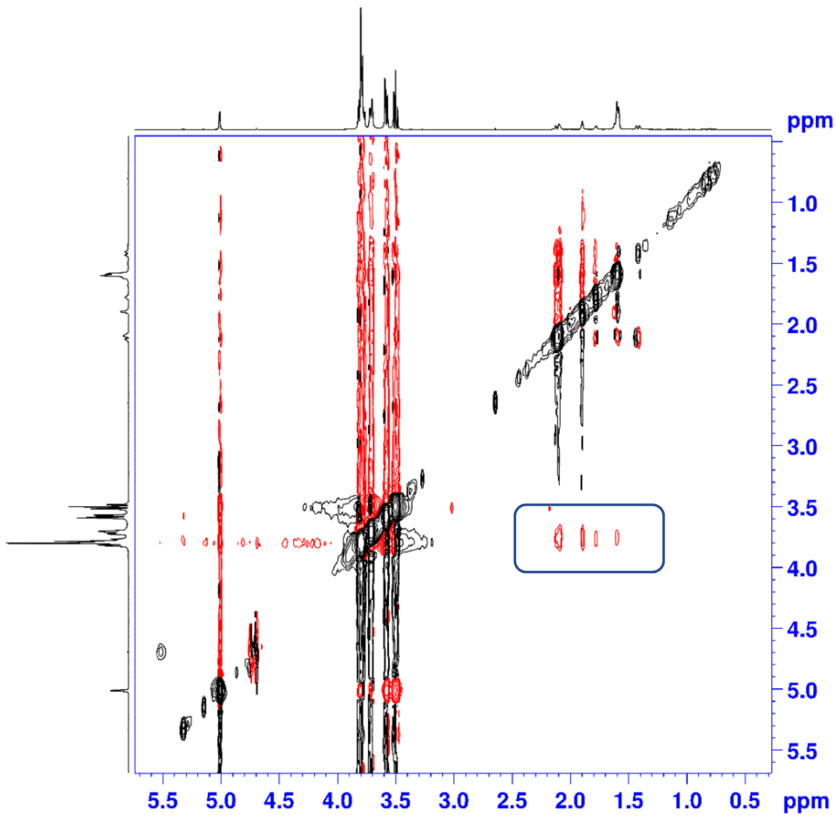
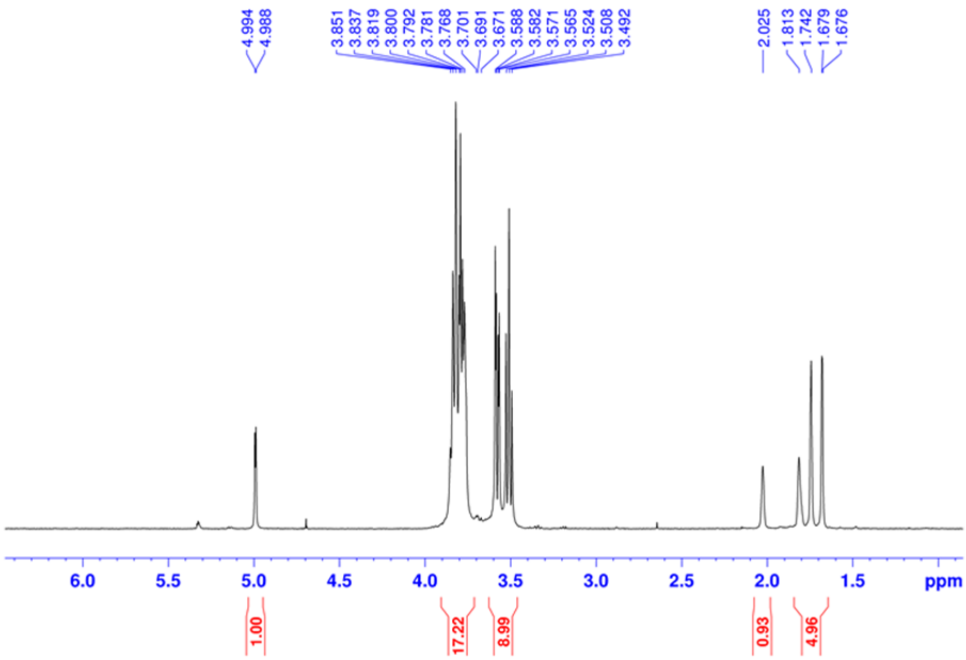


Figure S35. a) 600 MHz [1]H NMR spectrum with water suppression of **1-DAOH·γ-CD** in D_2O. b) Contour plot of the ROESY [1]H NMR spectrum of the reaction mixture containing **1-DAOH** ($c = 1.9 \cdot 10^{-3}$ mol dm^{-3}) and **γ-CD** ($c = 2 \cdot 10^{-3}$ mol dm^{-3}) at 298 K in D_2O.

a)



b)

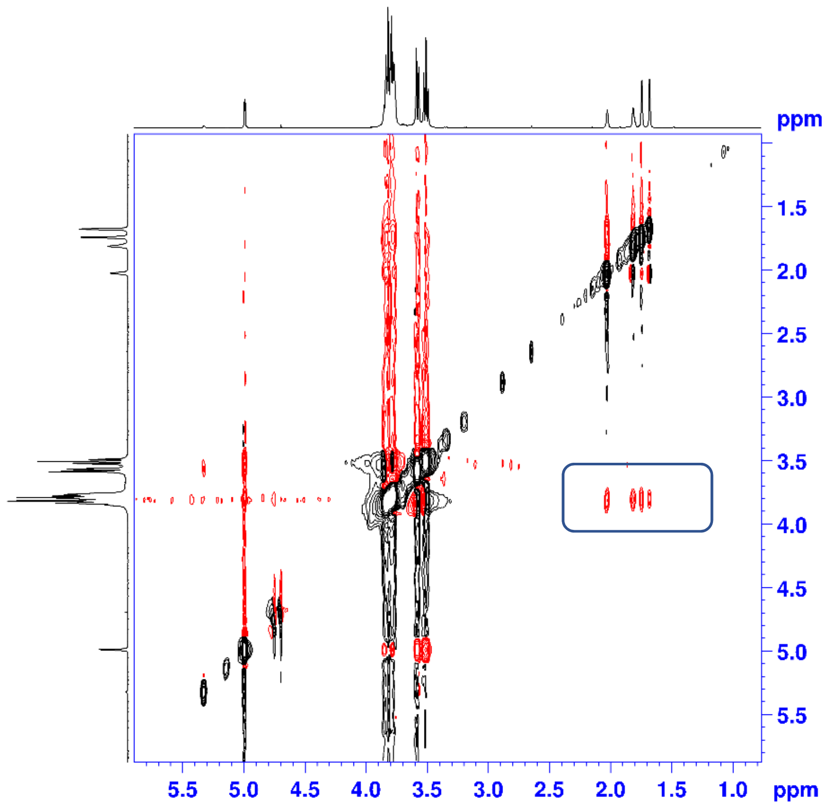
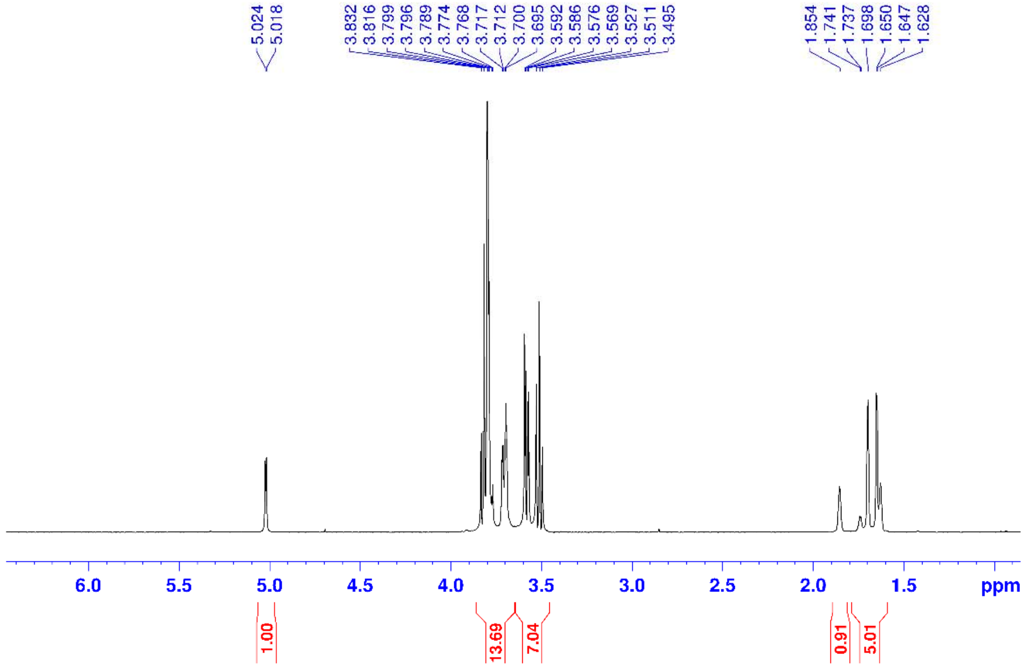


Figure S36. a) 600 MHz [1]H NMR spectrum with water suppression of **4-DAOH·β-CD** in D_2O. b) Contour plot of the ROESY [1]H NMR spectrum of the reaction mixture containing **4-DAOH** ($c = 9\cdot10^{-4}$ mol dm^{-3}) and **β-CD** ($c = 1\cdot10^{-3}$ mol dm^{-3}) at 298 K in D_2O.

a)



b)

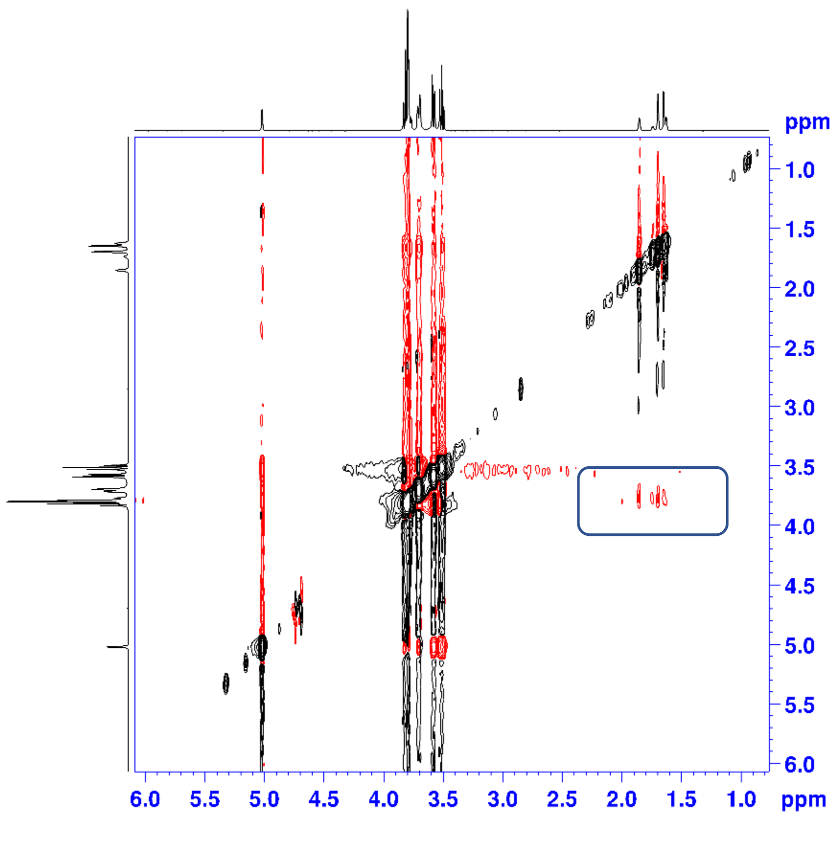


Figure S37. A) 600 MHz ^{1}H NMR spectrum with water suppression of **4-DAOH ·γ-CD** in D_2O. B) Contour plot of the ROESY ^{1}H NMR spectrum of the reaction mixture containing **4-DAOH** (c =$1\cdot10^{-3}$ mol dm^{-3}) and **γ-CD** (c =$1.4\cdot10^{-3}$ mol dm^{-3}) at 298 K in D_2O.

a)

b)

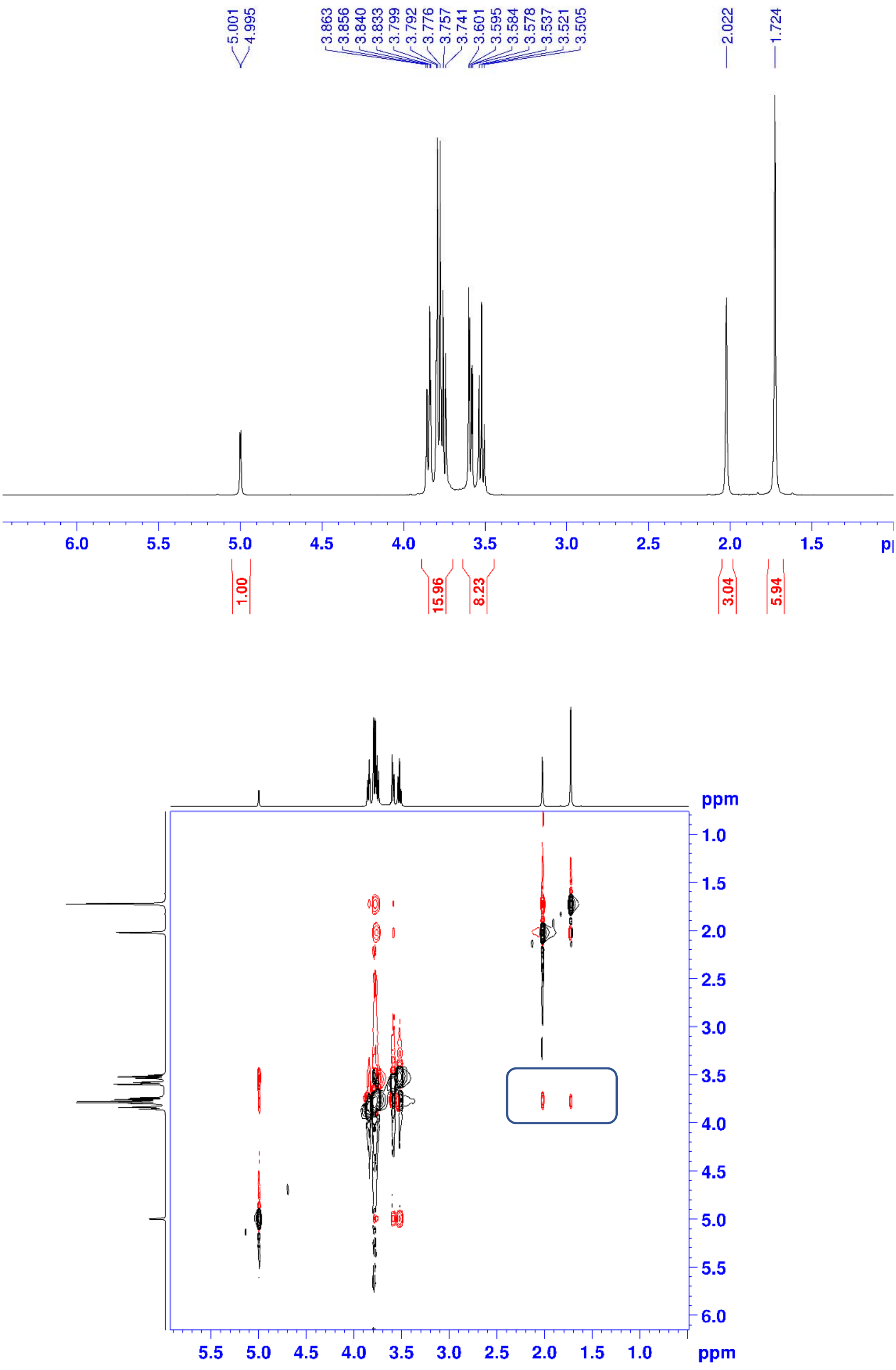


Figure S38. a) 600 MHz ^{1}H NMR spectrum with water suppression of **4,9-DA(OH)$_2$·β-CD** in D_2O. b) Contour plot of the ROESY ^{1}H NMR spectrum of the reaction mixture containing **4,9-DA(OH)$_2$** ($c = 4\cdot10^{-3}$ mol dm^{-3}) and **β-CD** ($c = 5\cdot10^{-3}$ mol dm^{-3}) at 298 K in D_2O.

a)

b)

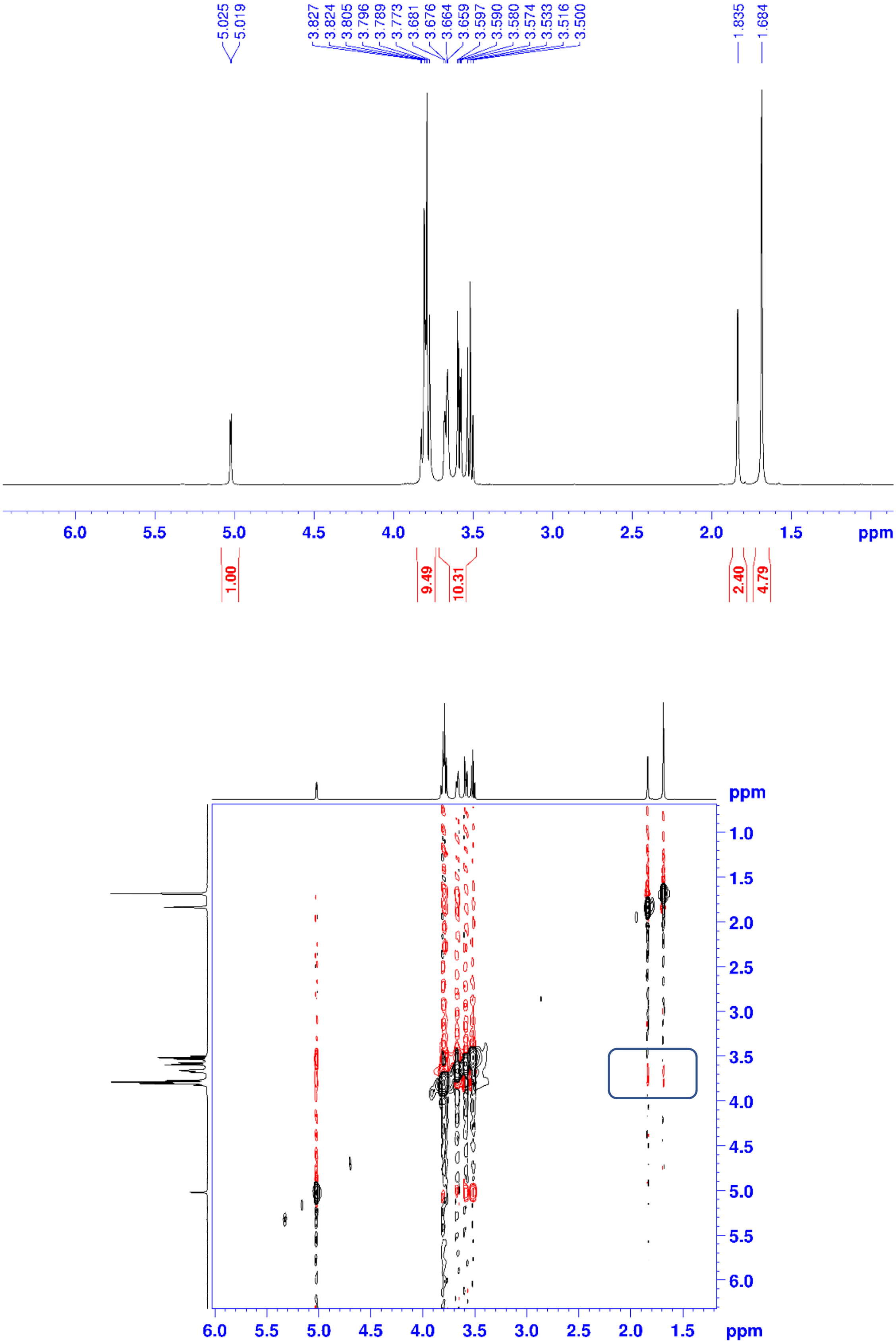


Figure S39. a) 600 MHz ^{1}H NMR spectrum with water suppression of **4,9-DA(OH)$_2$·γ-CD** in D_2O. b) Contour plot of the ROESY ^{1}H NMR spectrum of the reaction mixture containing **4-DAOH** ($c = 3 \cdot 10^{-3}$ mol dm^{-3}) and **γ-CD** ($c = 5 \cdot 10^{-3}$ mol dm^{-3}) at 298 K in D_2O

Minimized geometries obtained by CREST computations

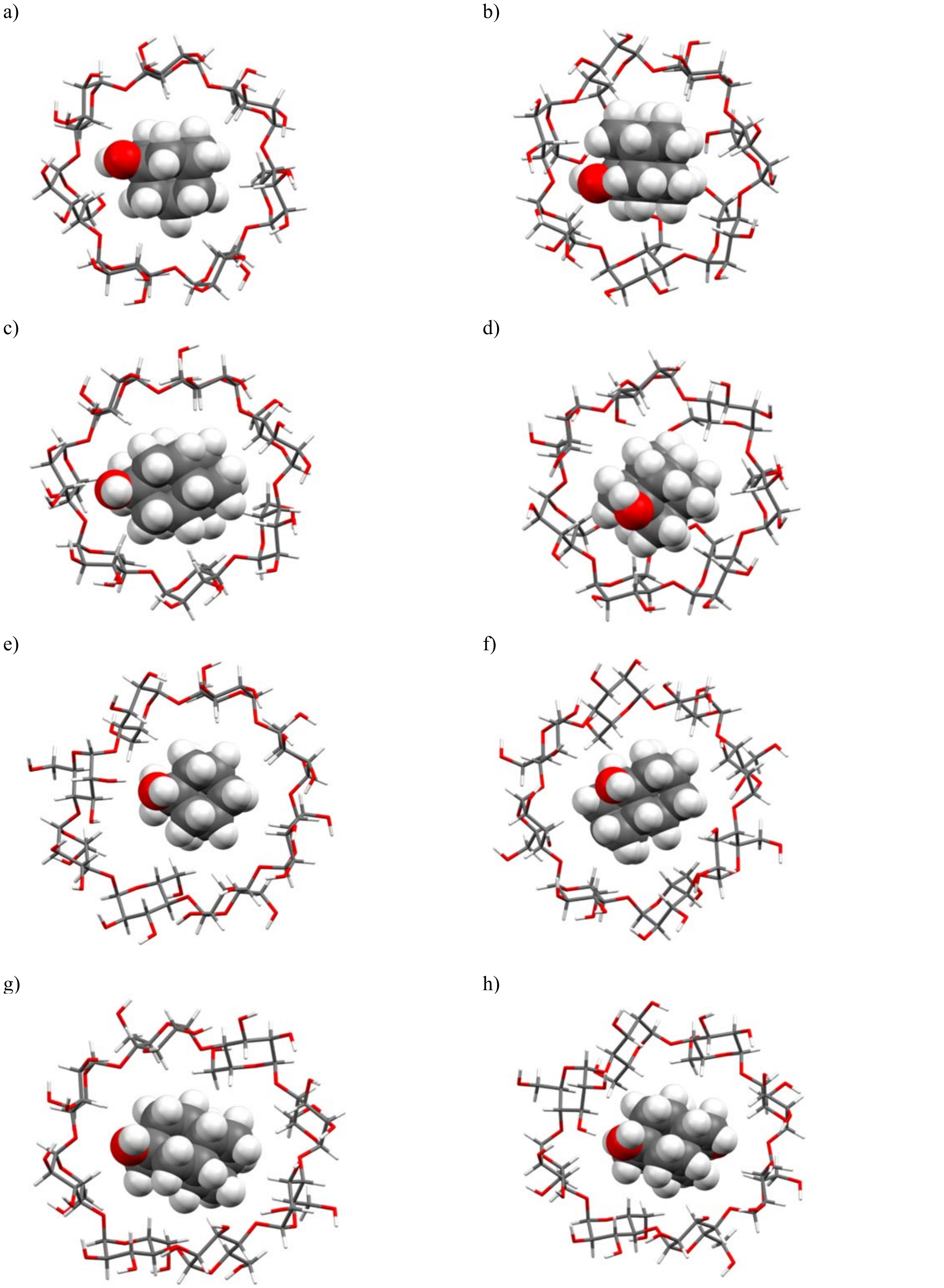


Figure S40. Representations of the minimized geometries of the studied **CD** complexes with diamondoid alcohols (top view): a) **1-AdOH·β-CD**; b) **1-DAOH·β-CD;** c) **4-DAOH·β-CD**; and d) **4,9-DA(OH)$_2$·β-CD**, e) **1-AdOH·γ-CD**; f) **1-DAOH·γ-CD;** g) **4-DAOH·γ-CD**; and h) **4,9-DA(OH)$_2$·γ-CD**.

Microcalorimetric titrations in water: Cucurbiturils

1-DAOH with **CB[7]** in H_2O

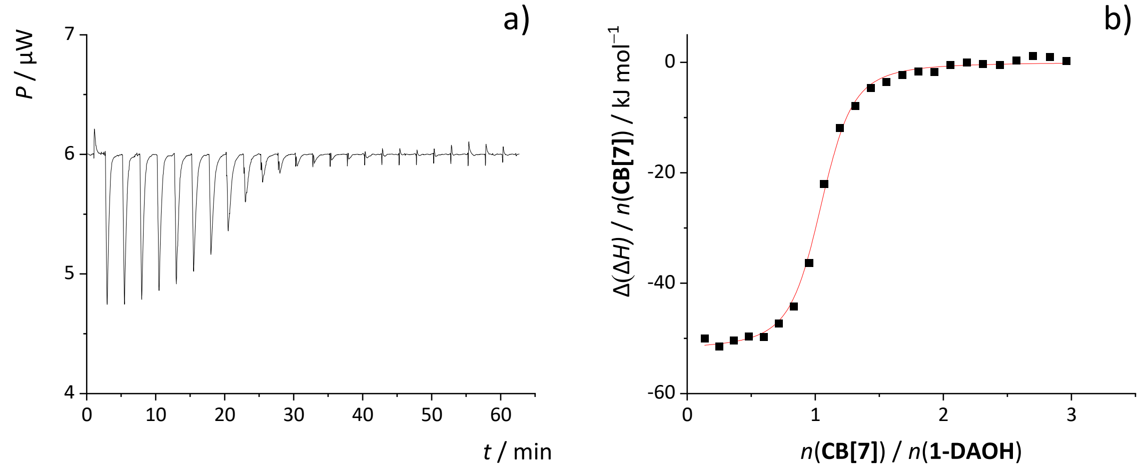


Figure S41. Microcalorimetric titration of **1-DAOH** ($c_0 = 3\cdot10^{-5}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **CB[7]** ($c = 4\cdot10^{-4}$ mol dm^{-3}) in H_2O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

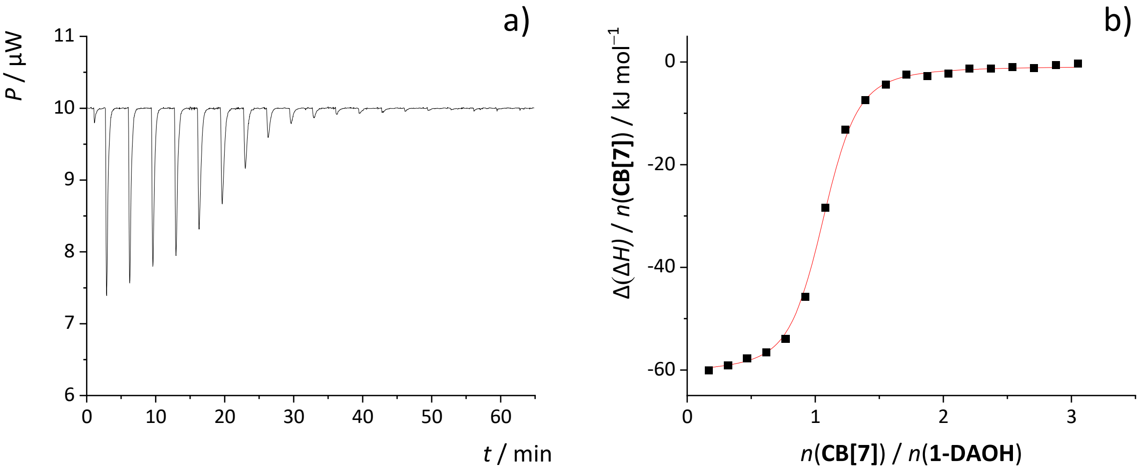


Figure S42. Microcalorimetric titration of **1-DAOH** ($c_0 = 3\cdot10^{-5}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **CB[7]** ($c = 4\cdot10^{-4}$ mol dm^{-3}) in H_2O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

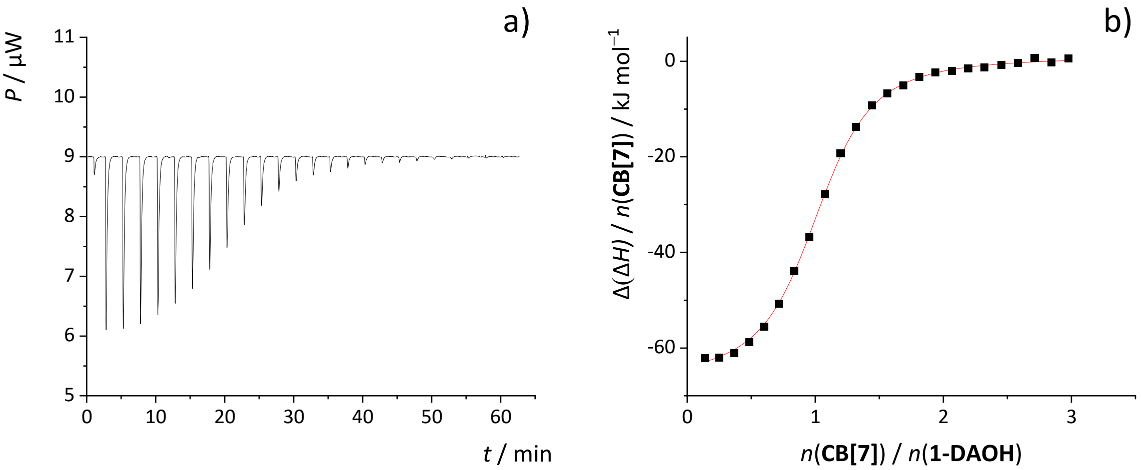


Figure S43. Microcalorimetric titration of **1-DAOH** ($c_0 = 3\cdot10^{-5}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **CB[7]** ($c = 4\cdot10^{-4}$ mol dm^{-3}) in H_2O at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

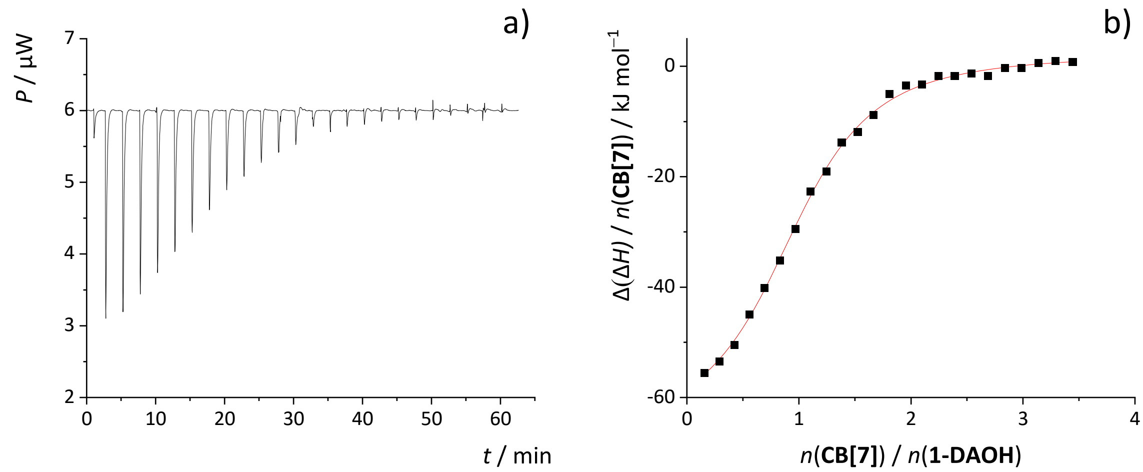


Figure S44. Microcalorimetric titration of **1-DAOH** ($c_0 = 3\cdot10^{-5}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **CB[7]** ($c = 4\cdot10^{-4}$ mol dm^{-3}) in H_2O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

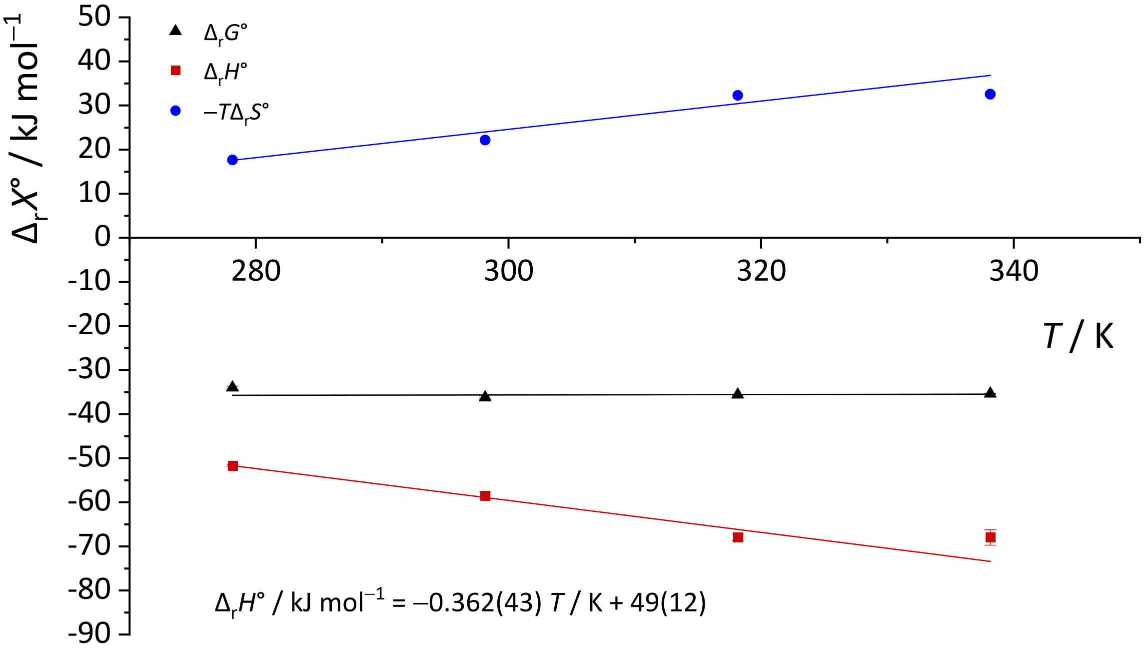


Figure S45. The temperature dependence of standard complexation parameters of **1-DAOH** with **CB[7]** in H_2O.

4-DAOH with **CB[7]** in H_2O

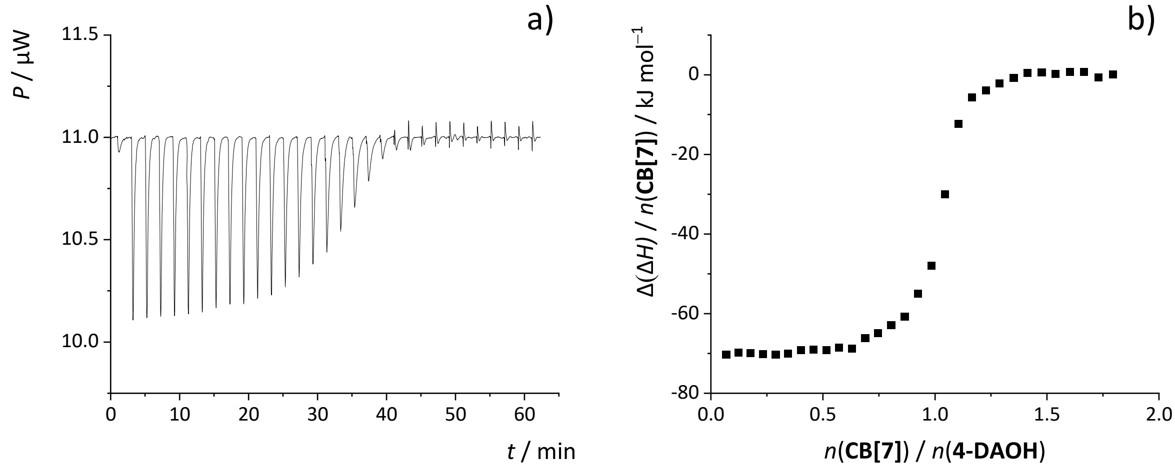


Figure S46. Microcalorimetric titration of **4-DAOH** ($c_0 = 2\cdot10^{-5}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **CB[7]** ($c = 2\cdot10^{-4}$ mol dm^{-3}) in H_2O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio.

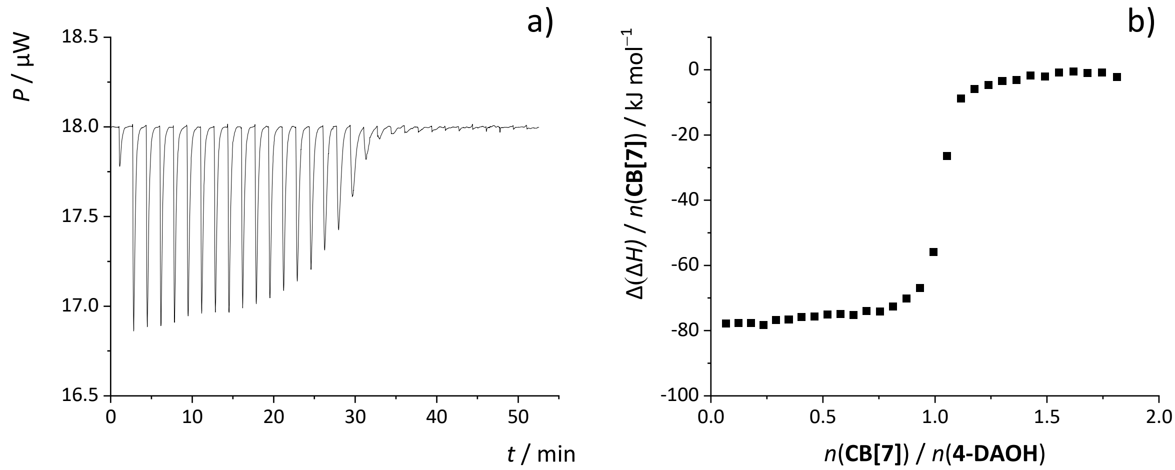


Figure S47. Microcalorimetric titration of **4-DAOH** ($c_0 = 2\cdot10^{-5}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **CB[7]** ($c = 2\cdot10^{-4}$ mol dm^{-3}) in H_2O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio.

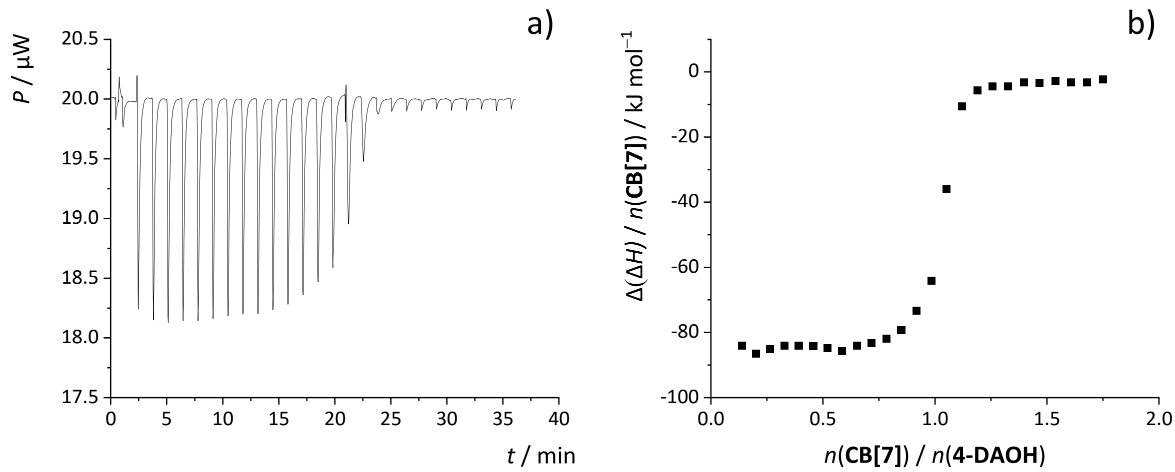


Figure S48. Microcalorimetric titration of **4-DAOH** ($c_0 = 2\cdot10^{-5}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **CB[7]** ($c = 2\cdot10^{-4}$ mol dm^{-3}) in H_2O at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio.

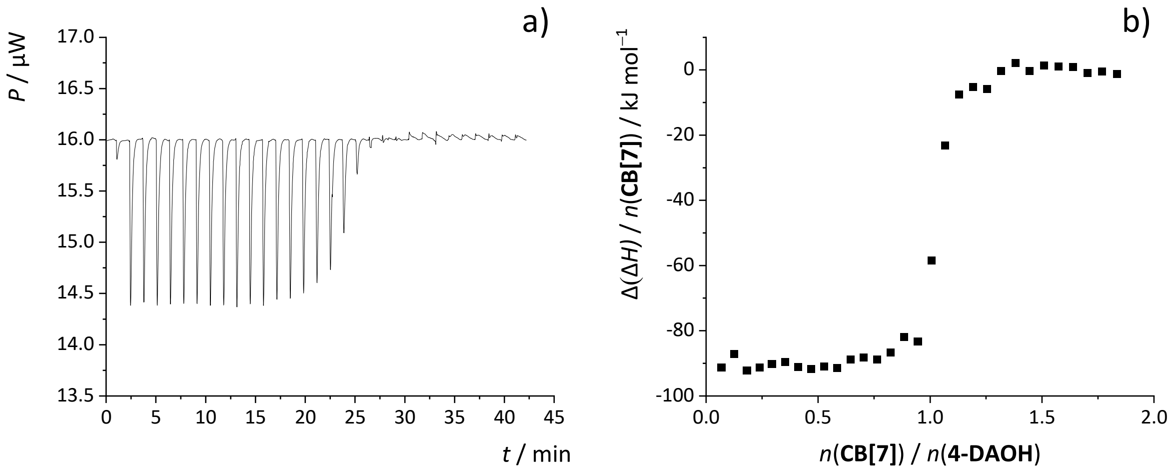


Figure S49. Microcalorimetric titration of **4-DAOH** ($c_0 = 2\cdot10^{-5}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **CB[7]** ($c = 2\cdot10^{-4}$ mol dm^{-3}) in H_2O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio.

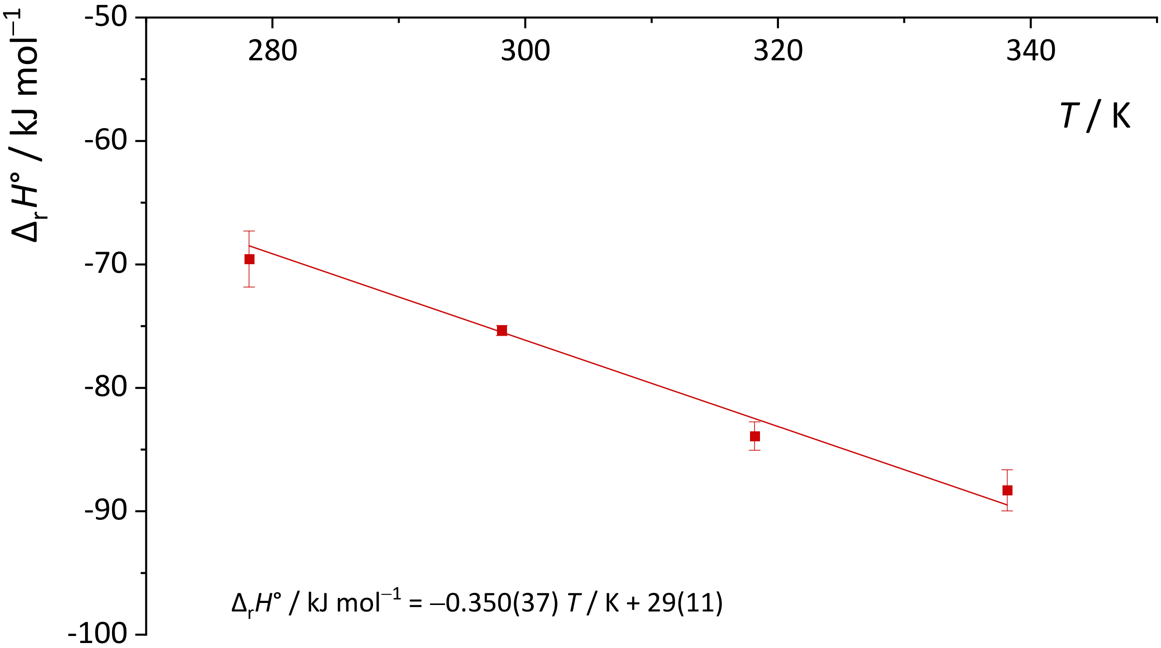


Figure S50. The temperature dependence of standard reaction enthalpy for complexation of **4-DAOH** with **CB[7]** in H_2O.

4,9-DA(OH)$_2$ with **CB[7]** in H_2O

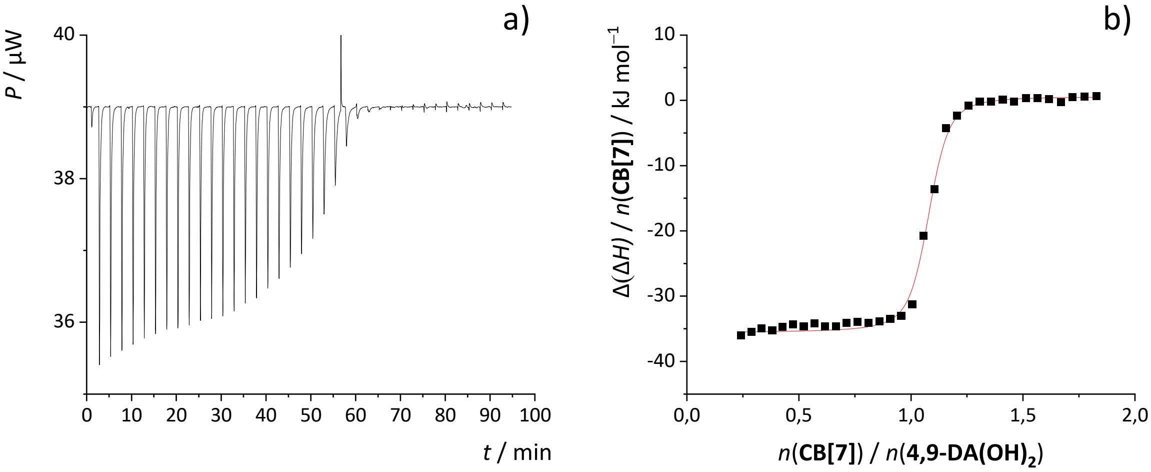


Figure S51. Microcalorimetric titration of **4,9-DA(OH)$_2$** (c_0 = 1·10^{-4} mol dm^{-3}, V_0 = 0.205 mL) with **CB[7]** (c = 1·10^{-3} mol dm^{-3}) in H_2O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

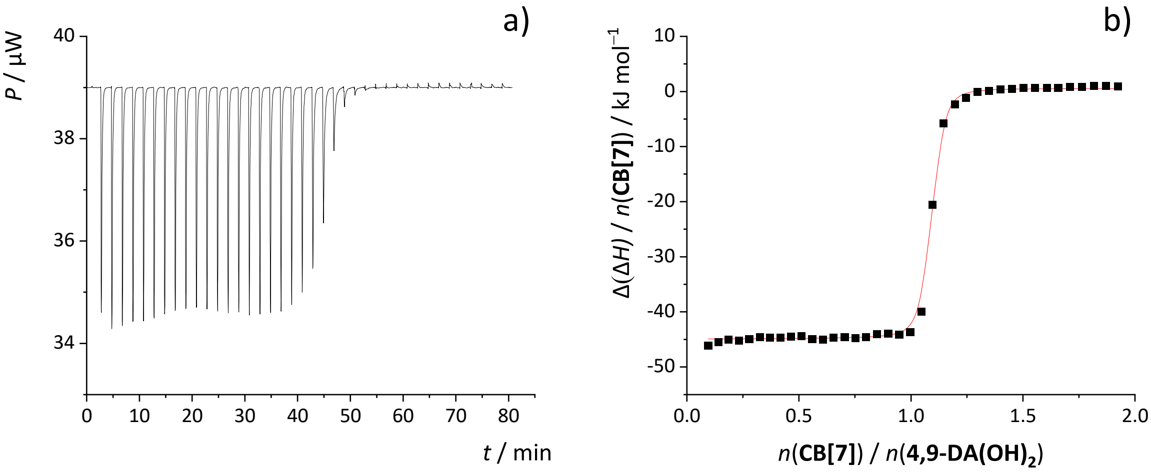


Figure S52. Microcalorimetric titration of **4,9-DA(OH)$_2$** (c_0 = 1·10^{-4} mol dm^{-3}, V_0 = 0.205 mL) with **CB[7]** (c = 1·10^{-3} mol dm^{-3}) in H_2O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

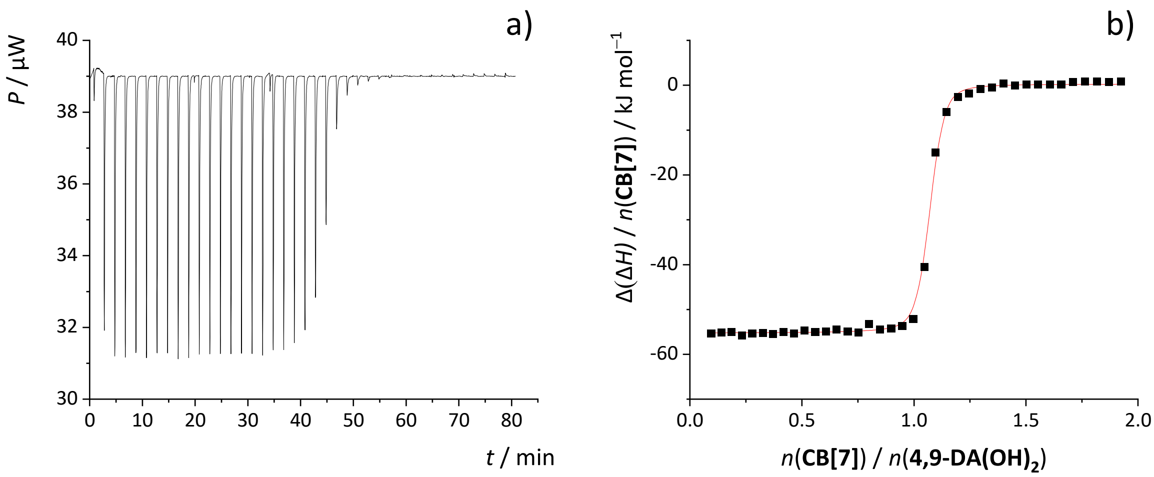


Figure S53. Microcalorimetric titration of **4,9-DA(OH)₂** ($c_0 = 1 \cdot 10^{-4}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **CB[7]** ($c = 1 \cdot 10^{-3}$ mol dm^{-3}) in H_2O at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

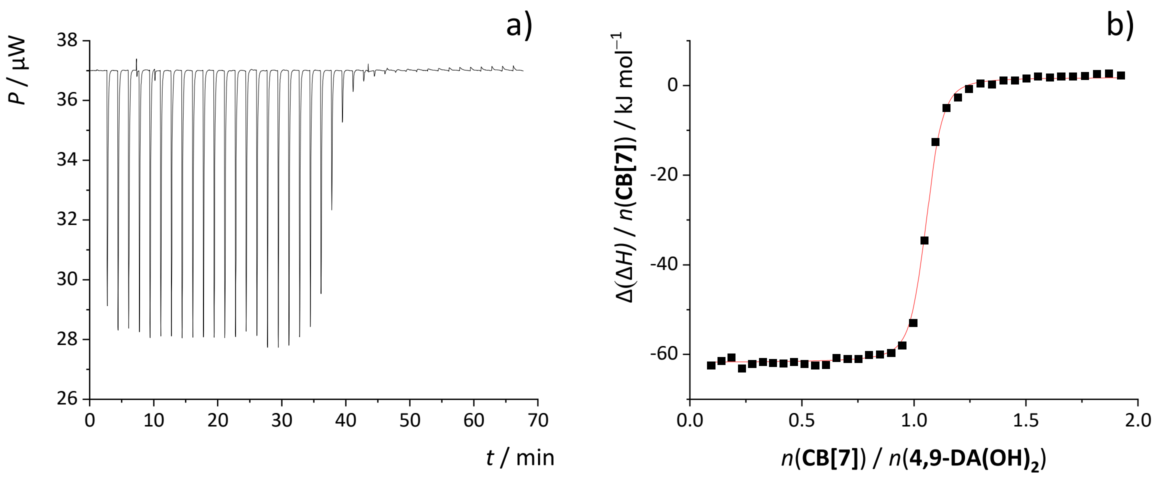


Figure S54. Microcalorimetric titration of **4,9-DA(OH)₂** ($c_0 = 1 \cdot 10^{-4}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **CB[7]** ($c = 1 \cdot 10^{-3}$ mol dm^{-3}) in H_2O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

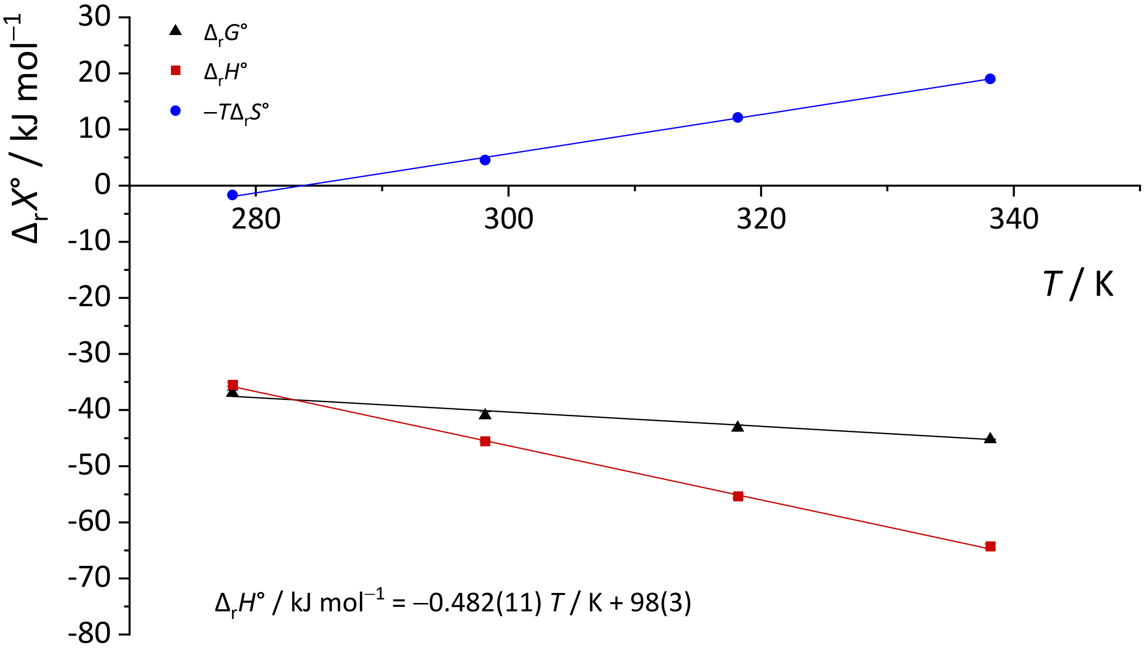


Figure S55. The temperature dependence of standard complexation parameters of **4,9-DA(OH)$_2$** with **CB[7]** in H_2O.

Table S3. Thermodynamic parameters for complexation of **1-AdOH** and diamantane alcohols with **CB[7]** in H_2O.[a]

GUEST · CB[7]	T / K	log K	$\Delta_r G°$ / kJ mol^{-1}	$\Delta_r H°$ / kJ mol^{-1}	$-T\Delta_r S°$ / kJ mol^{-1}	$\Delta_r C_p°$ / J K^{-1} mol^{-1}
1-AdOH	278			−65.4(4)		−482(11)
	298	10.4[b]	−59.4[b]	−76.70(1) −79.5[b]	20.1[b]	
	318			−83.0(4)		
	338			−90.1(4)		
1-DAOH	278	6.39(7)	−34.0(4)	−51.7(2)	17.6(3)	−361(43)
	298	6.35(6)	−36.2(3)	−58.5(8)	22.2(8)	
	318	5.85(1)	−35.62(5)	−67.9(8)	32.3(8)	
	338	5.46(1)	−35.36(8)	−68(2)	33(2)	
4-DAOH	278			−70(2)		−350(37)
	298	6.8[b]	−40.2[b]	−75.4(4) −50.2[b]	11.7[b]	
	318			−84(1)		
	338			−88(2)		
4,9-DA(OH)$_2$	278	6.9(1)	−37.0(5)	−35.4(4)	−1.7(9)	−482(11)
	298	7.2(1) 7.1[b]	−41.0(6) −40.2[b]	−45.6(1) −52.7[b]	4.5(8) 12.6[b]	
	318	7.09(9)	−43.2(5)	−55.4(3)	12.2(6)	
	338	6.99(2)	−45.2(1)	−64.0(5)	19.0(5)	

[a] Uncertainties of the last digit(s) are given in parentheses as standard errors of the mean (N = 3−5), or standard deviations obtained by weighted linear regression analysis (for $\Delta_r C_p°$ values); [b] Reference: L. M. Grimm, S. Spicher, B. Tkachenko, P. R. Schreiner, S. Grimme, F. Biedermann, *Chem. Eur. J.*, 2022, **28**, e202200529.

Even though larger thermal noise was in some cases associated with experiments carried out at 278 and 338 K, or that complexation enthalpy was occasionally close to zero, the obtained linear $\Delta_r H°(T)$ dependencies and the standard errors of the mean obtained by repetitive titration experiments indicate the reliability of determined thermodynamic complexation parameters.

1-AdOH with **CB[8]** in H_2O

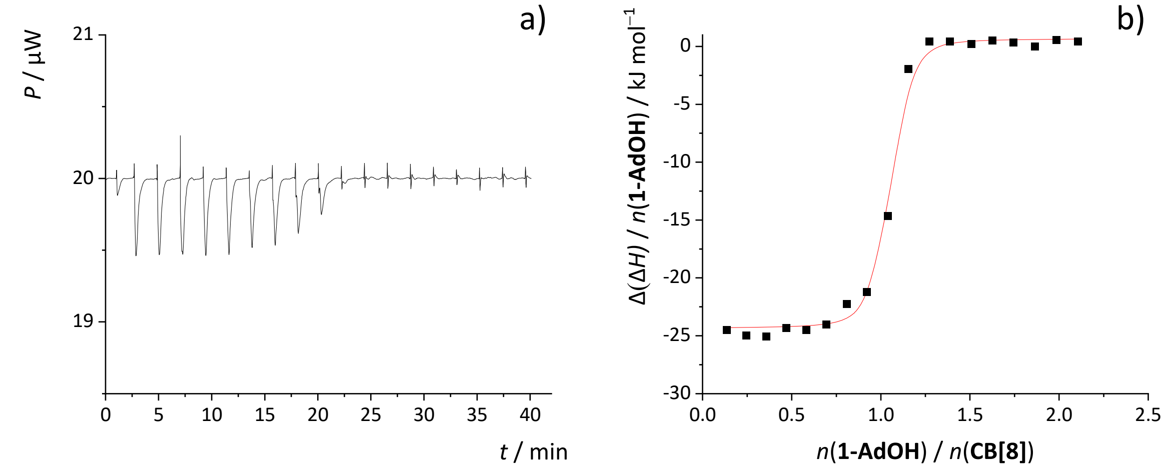


Figure S56. Microcalorimetric titration of **CB[8]** ($c_0 = 2\cdot10^{-5}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **1-AdOH** ($c = 4\cdot10^{-4}$ mol dm^{-3}) in H_2O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on guest to host molar ratio. ■ experimental; – calculated.

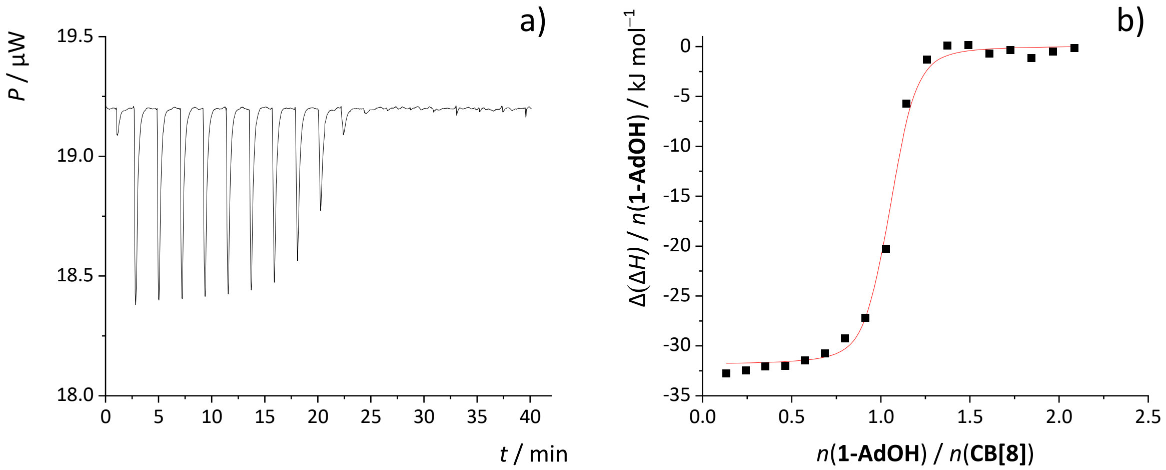


Figure S57. Microcalorimetric titration of **CB[8]** ($c_0 = 2\cdot10^{-5}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **1-AdOH** ($c = 4\cdot10^{-4}$ mol dm^{-3}) in H_2O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on guest to host molar ratio. ■ experimental; – calculated.

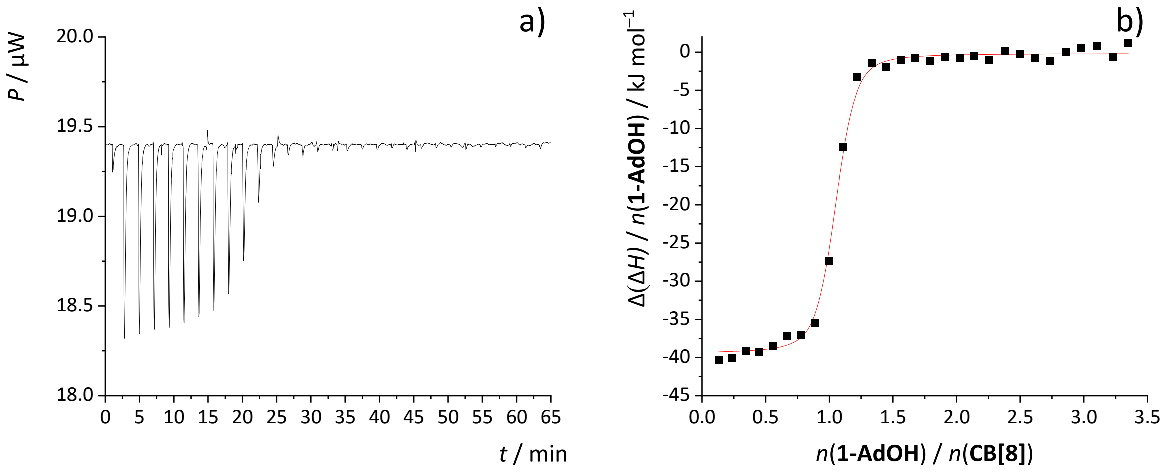


Figure S58. Microcalorimetric titration of **CB[8]** ($c_0 = 2 \cdot 10^{-5}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **1-AdOH** ($c = 4 \cdot 10^{-4}$ mol dm^{-3}) in H_2O at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on guest to host molar ratio. ■ experimental; – calculated.

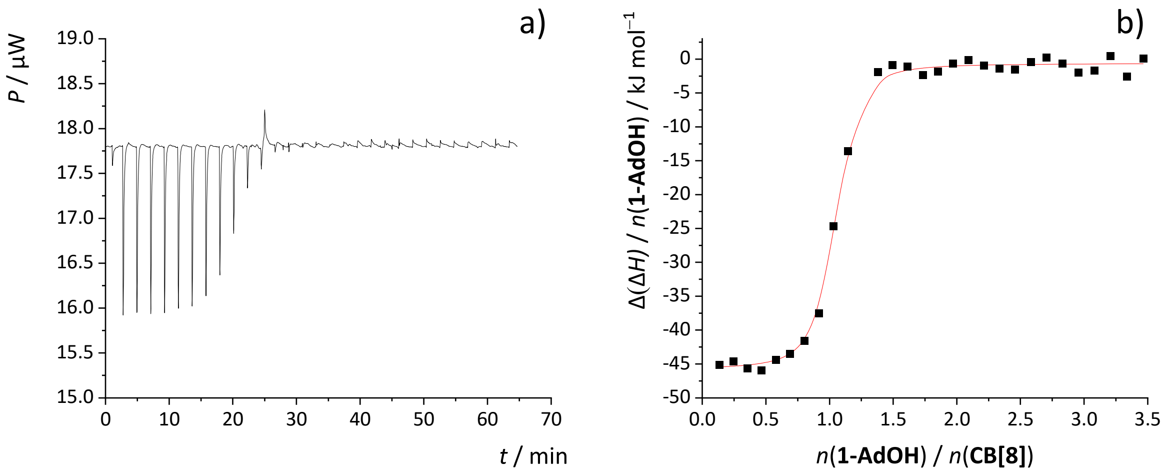


Figure S59. Microcalorimetric titration of **CB[8]** ($c_0 = 2 \cdot 10^{-5}$ mol dm^{-3}, $V_0 = 0.205$ mL) with **1-AdOH** ($c = 4 \cdot 10^{-4}$ mol dm^{-3}) in H_2O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on guest to host molar ratio. ■ experimental; – calculated.

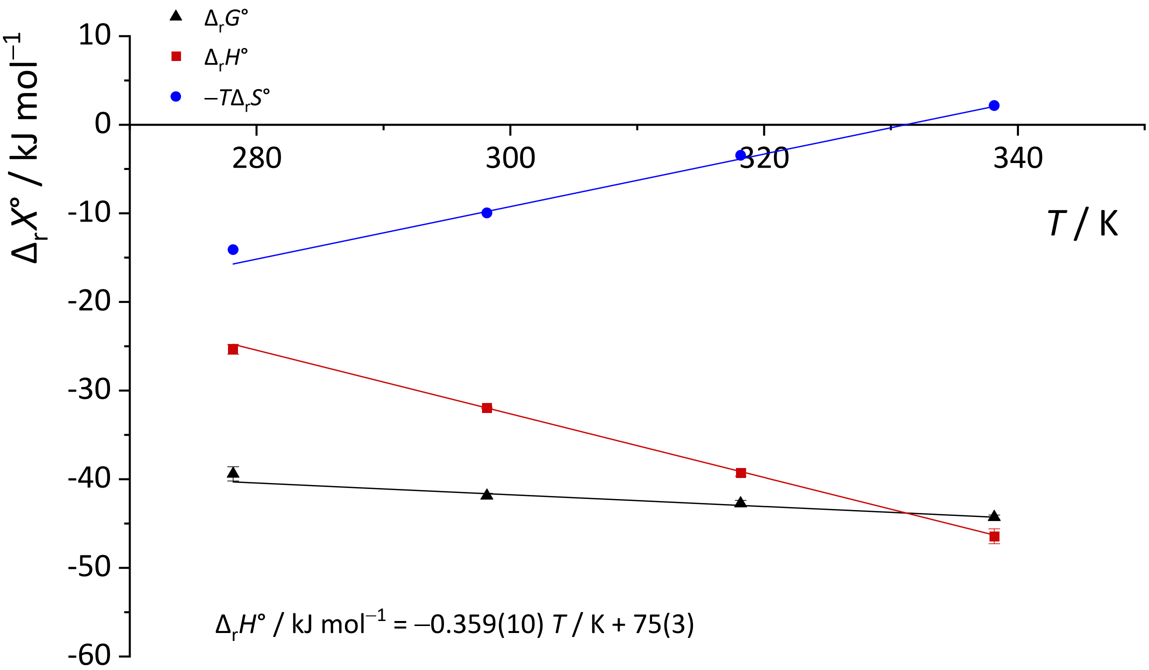


Figure S60. The temperature dependence of standard complexation parameters of **1-AdOH** with **CB[8]** in H_2O.

4,9-DA(OH)$_2$ with **CB[8]** in H_2O

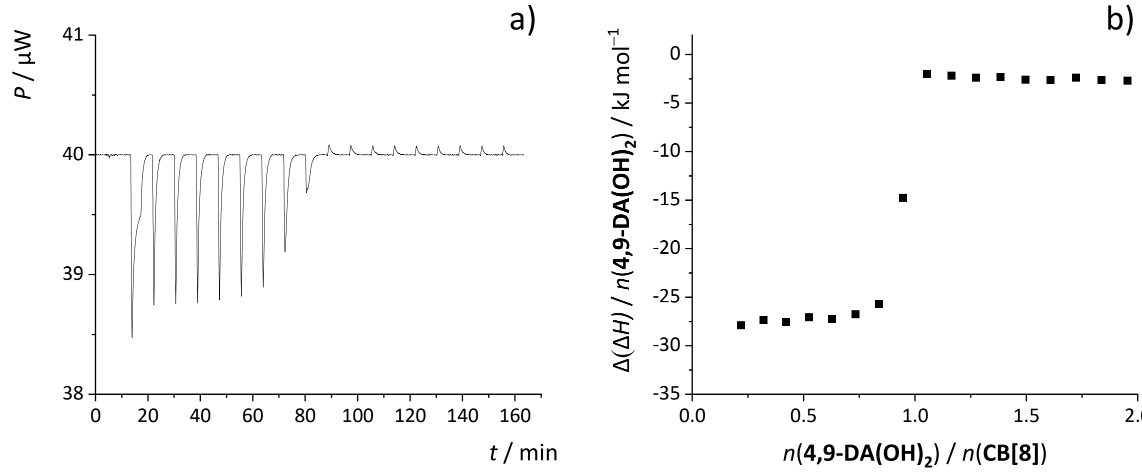


Figure S61. Microcalorimetric titration of **CB[8]** ($c_0 = 2\cdot10^{-5}$ mol dm^{-3}, V_0 = 1.45 mL) with **4,9-DA(OH)$_2$** ($c = 2\cdot10^{-4}$ mol dm^{-3}) in H_2O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on guest to host molar ratio.

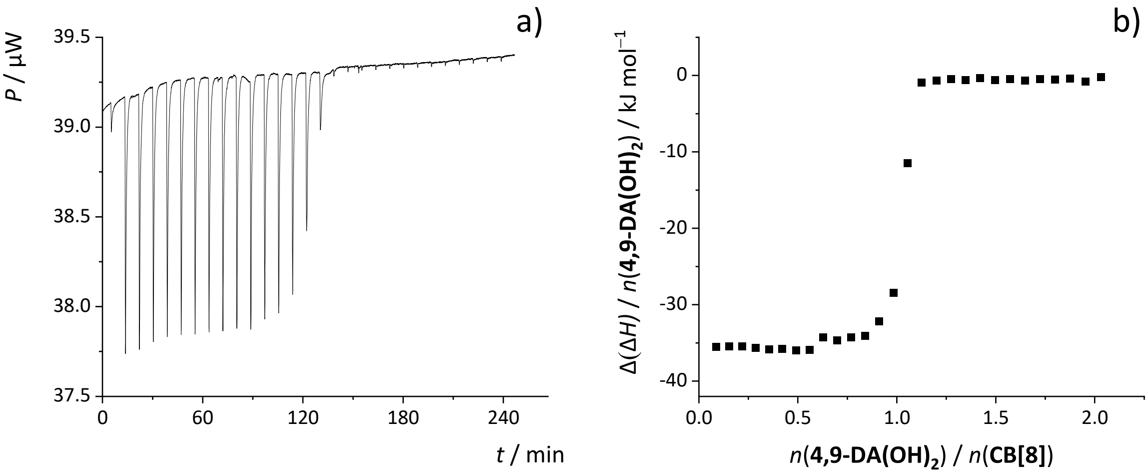


Figure S62. Microcalorimetric titration of **CB[8]** ($c_0 = 2\cdot10^{-5}$ mol dm^{-3}, V_0 = 1.45 mL) with **4,9-DA(OH)$_2$** ($c = 2\cdot10^{-4}$ mol dm^{-3}) in H_2O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on guest to host molar ratio.

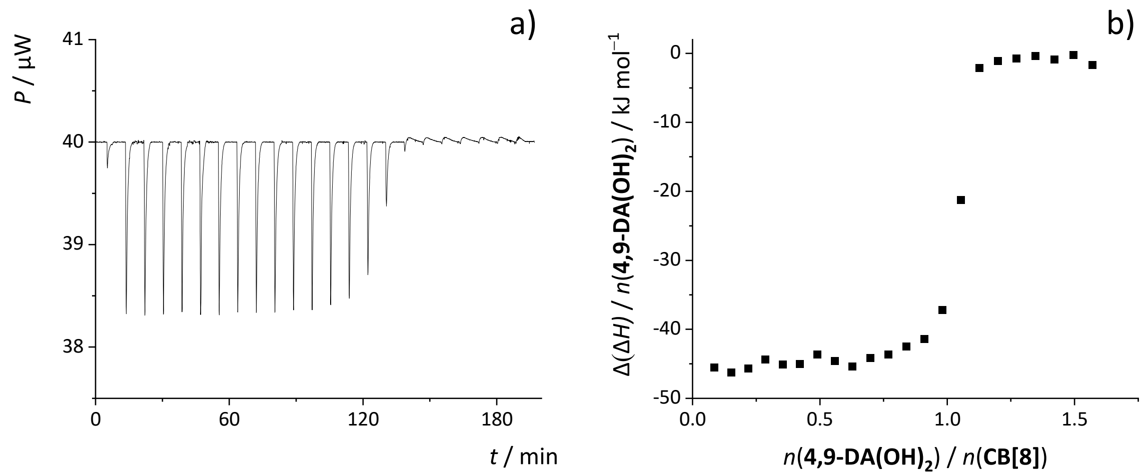


Figure S63. Microcalorimetric titration of **CB[8]** ($c_0 = 2\cdot10^{-5}$ mol dm^{-3}, V_0 = 1.45 mL) with **4,9-DA(OH)$_2$** ($c = 2\cdot10^{-4}$ mol dm^{-3}) in H_2O at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on guest to host molar ratio.

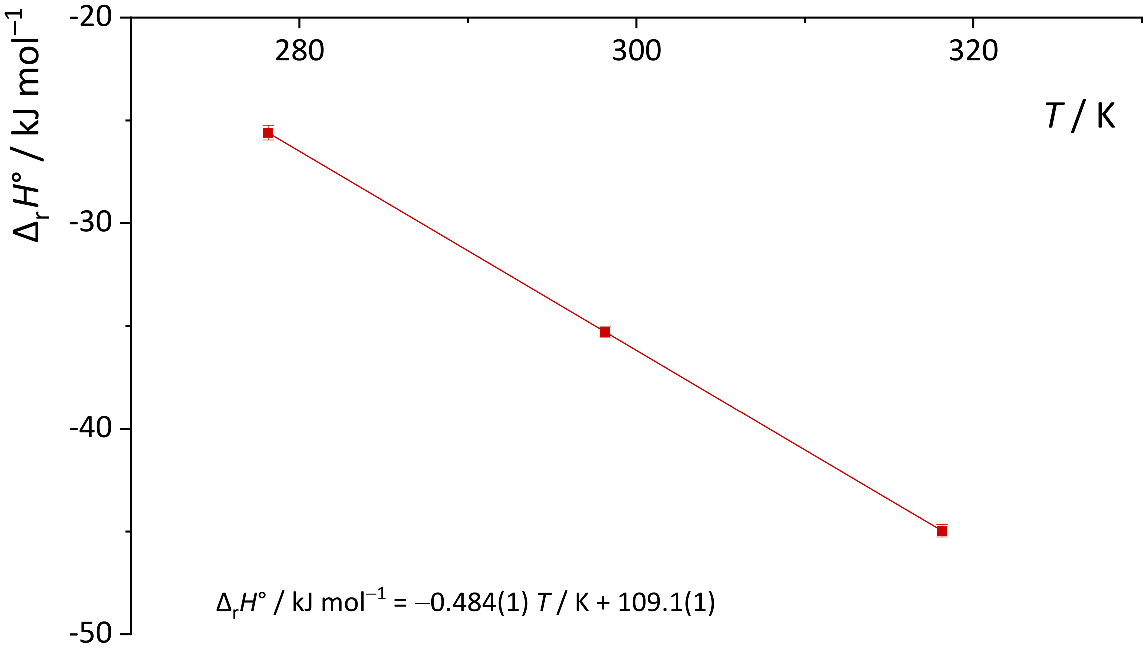


Figure S64. The temperature dependence of standard complexation parameters of **4,9-DA(OH)$_2$** with **CB[8]** in H_2O.

Table S4. Thermodynamic parameters for complexation of **1-AdOH** and diamantane alcohols with **CB[8]** in H_2O.[a]

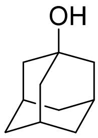
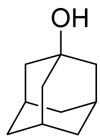
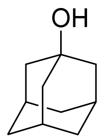
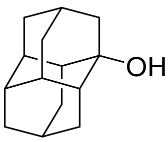
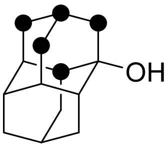
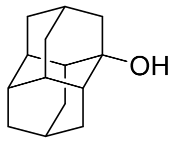
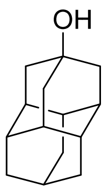
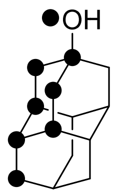
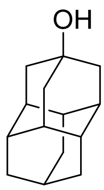
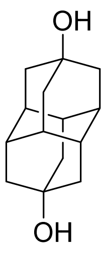
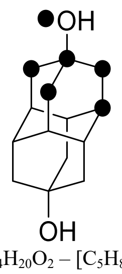
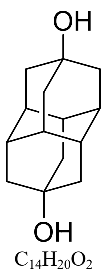
GUEST · **CB[8]**	T / K	log $K°$	$\Delta_rG°$ / kJ mol^{-1}	$\Delta_rH°$ / kJ mol^{-1}	$-T\Delta_rS°$ / kJ mol^{-1}	$\Delta_rC_p°$ / J K^{-1} mol^{-1}
1-AdOH	278	7.4(1)	−39.4(8)	−25.3(6)	−14(1)	−359(10)
	298	7.34(5) 6.8[b]	−41.9(3) −38.9[b]	−31.93(3) −33.9[b]	−10.0(3) −5.0[b]	
	318	7.02(6)	−42.7(4)	−39.3(4)	−3.5(7)	
	338	6.84(4)	−44.3(2)	−46.4(8)	2(1)	
4-DAOH	298	6.6[b]	−38.1[b]	−32.6[b]	−5.0[b]	
4,9-DA(OH)$_2$	278	7.9(1)	−42(1)	−25.6(4)	−17(1)	−484(1)
	298	7.78(4) 7.2[b]	−44.4(2) −41.4[b]	−35.3(2) −32.2[b]	−9.1(2) −9.6[b]	
	318	7.6(1)	−46.2(6)	−45.0(3)	−1.2(6)	

[a] Uncertainties of the last digit(s) are given in parentheses as standard errors of the mean (N = 3−5), or standard deviations obtained by weighted linear regression analysis (for $\Delta_rC_p°$ values); [b] Reference: L. M. Grimm, S. Spicher, B. Tkachenko, P. R. Schreiner, S. Grimme, F. Biedermann, *Chem. Eur. J.*, 2022, **28**, e202200529.

Even though larger thermal noise was in some cases associated with experiments carried out at 278 and 338 K, or that complexation enthalpy was occasionally close to zero, the obtained linear $\Delta_rH°(T)$ dependencies and the standard errors of the mean obtained by repetitive titration experiments indicate the reliability of determined thermodynamic complexation parameters

Packing coefficients

Table S5. Guest volumes and packing coefficients (PCs) of the studied **CD** complexes with diamondoid alcohols. Guest atoms/groups not located in the inner **CD** cavity and therefore not included in PC calculations are marked with black dots.[a,b]

Guest	**β-CD**•guest	**γ-CD**•guest
1-AdOH  volume = 153 Å^3	 $C_{10}H_{16}O$ volume buried in cavity = 153 Å^3 packing coefficient = 58%	 $C_{10}H_{16}O$ volume buried in cavity = 153 Å^3 packing coefficient = 36%
1-DAOH  volume = 198 Å^3	 $C_{14}H_{20}O$ – [C_5H_8] volume buried in cavity = 153 Å^3 packing coefficient = 58%	 $C_{14}H_{20}O$ volume buried in cavity = 198 Å^3 packing coefficient = 46%
4-DAOH  volume = 198 Å^3	 $C_{14}H_{20}O$ – [$C_7H_{10}O$] volume buried in cavity = 112 Å^3 packing coefficient = 43%	 $C_{14}H_{20}O$ volume buried in cavity = 198 Å^3 packing coefficient = 46%
4,9-DA(OH)$_2$  volume = 206 Å^3	 $C_{14}H_{20}O_2$ – [C_5H_8O] volume buried in cavity = 143 Å^3 packing coefficient = 55%	 $C_{14}H_{20}O_2$ volume buried in cavity = 206 Å^3 packing coefficient = 48%

[a] Complex geometries obtained from CREST/GFN2-xTB computations with included ALPB(water) solvation. [b] **CD** cavity volumes taken as *V*(**β-CD**)=262 Å^3, *V*(**γ-CD**)=427 Å^3, according to reference J. Szejtli, *Chem. Rev.* **1998**, *98*, 1743–1753.

Microcalorimetric titrations in formamide (FMD)

1-DAOH with **β-CD** in FMD

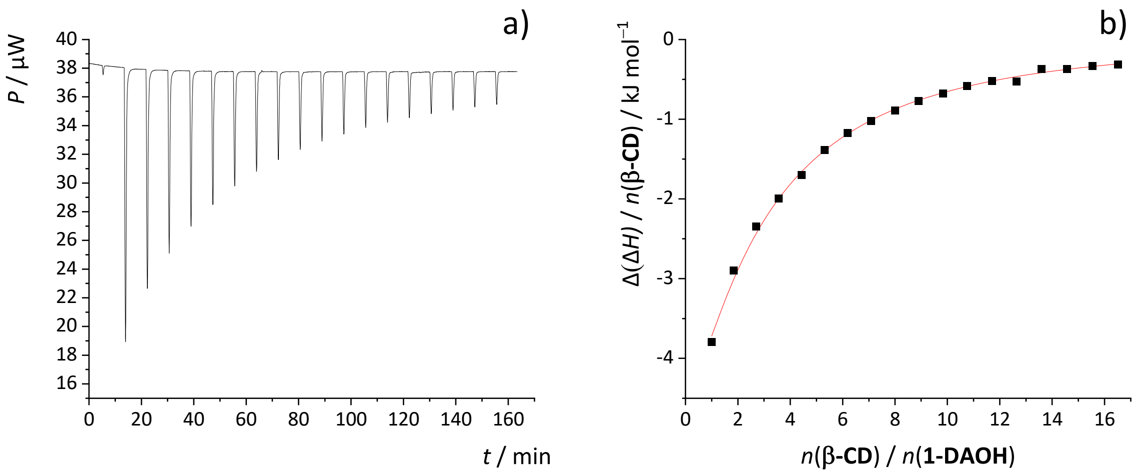


Figure S65. Microcalorimetric titration of **1-DAOH** ($c_0 = 2\cdot10^{-5}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 1\cdot10^{-2}$ mol dm^{-3}) in FMD at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

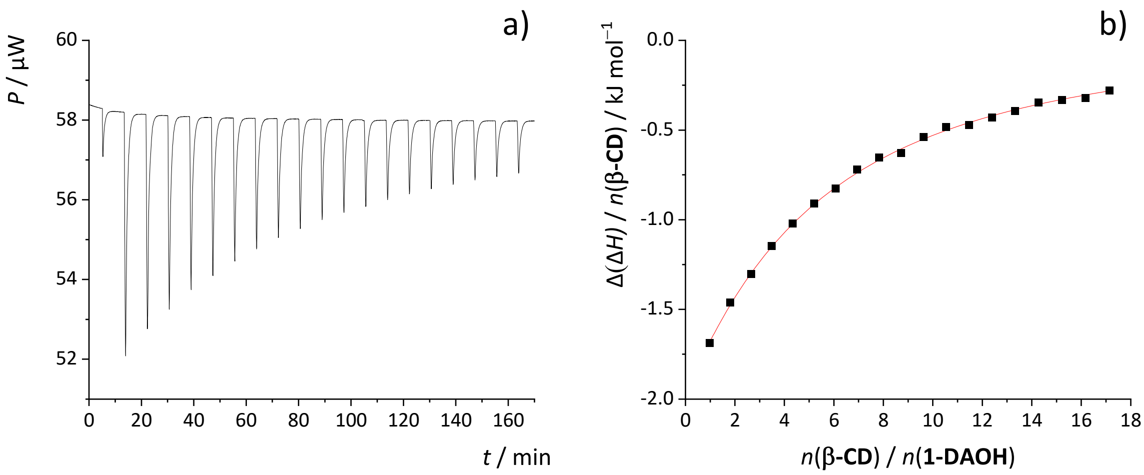


Figure S66. Microcalorimetric titration of **1-DAOH** ($c_0 = 2\cdot10^{-5}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 1\cdot10^{-2}$ mol dm^{-3}) in FMD at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

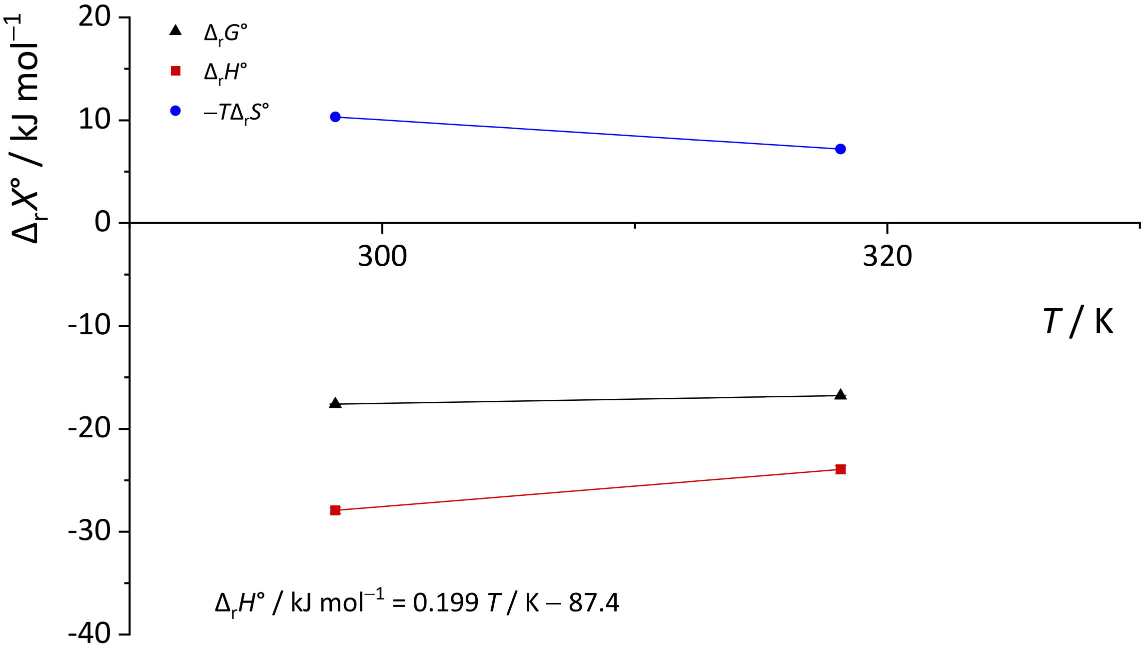


Figure S67. The temperature dependence of standard complexation parameters of **1-DAOH** with **β-CD** in FMD.

4-DAOH with **β-CD** in FMD

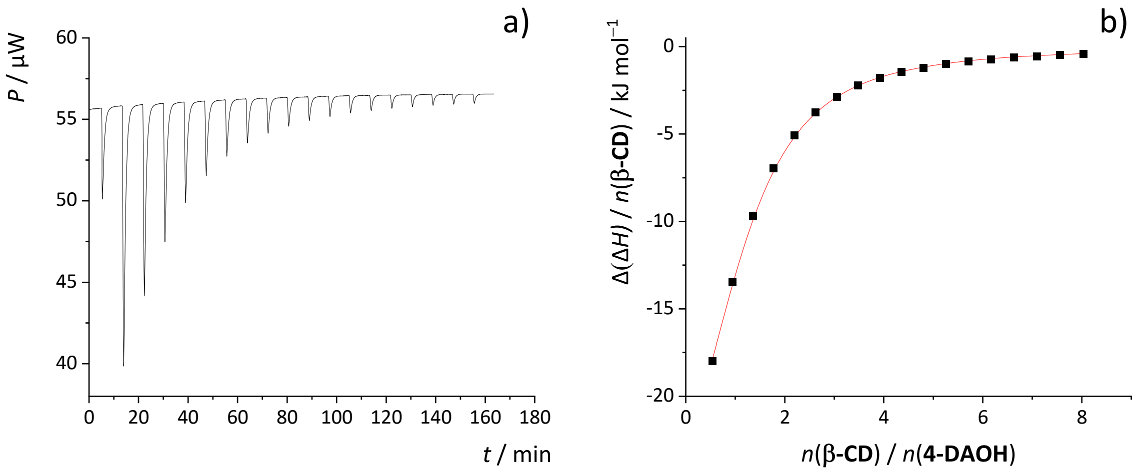


Figure S68. Microcalorimetric titration of **4-DAOH** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 6\cdot10^{-3}$ mol dm^{-3}) in FMD at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

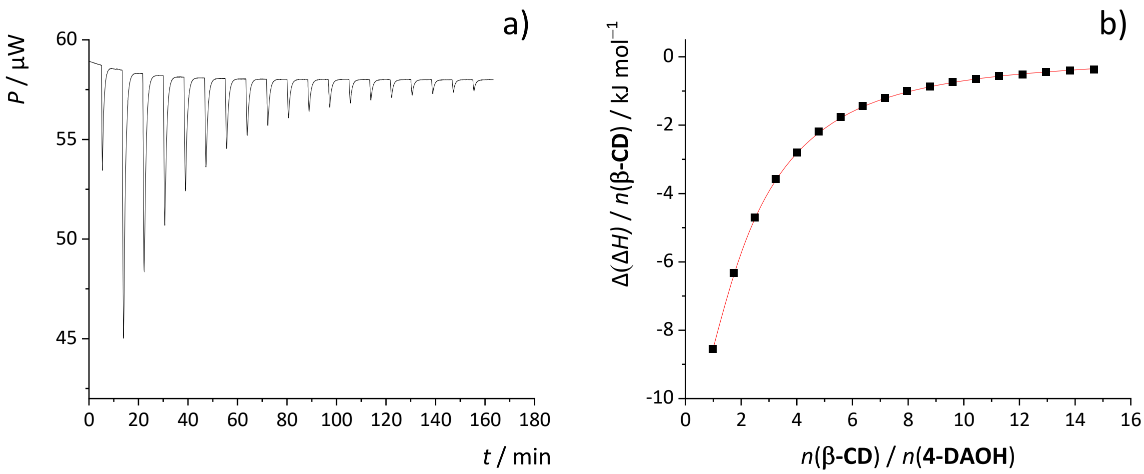


Figure S69. Microcalorimetric titration of **4-DAOH** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 6\cdot10^{-3}$ mol dm^{-3}) in FMD at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

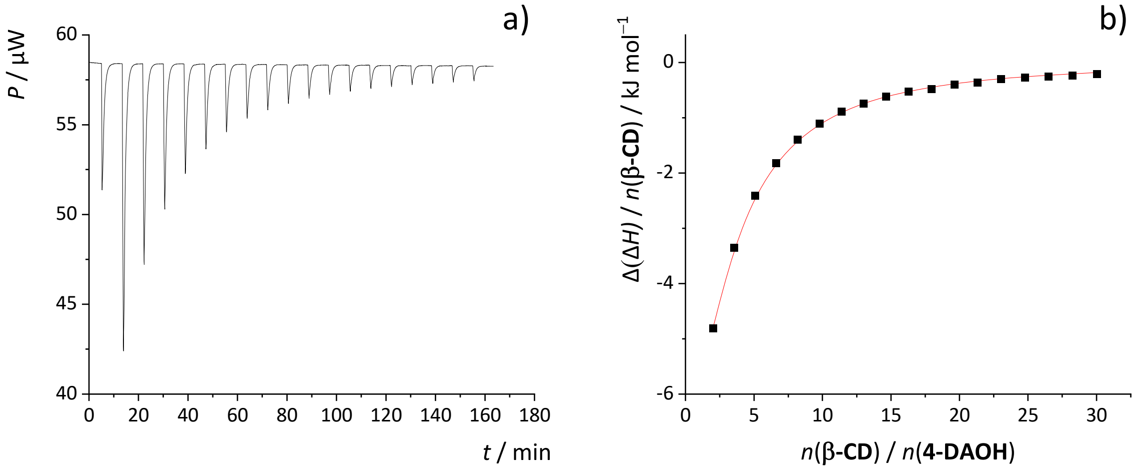


Figure S70. Microcalorimetric titration of **4-DAOH** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 2\cdot10^{-2}$ mol dm^{-3}) in FMD at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

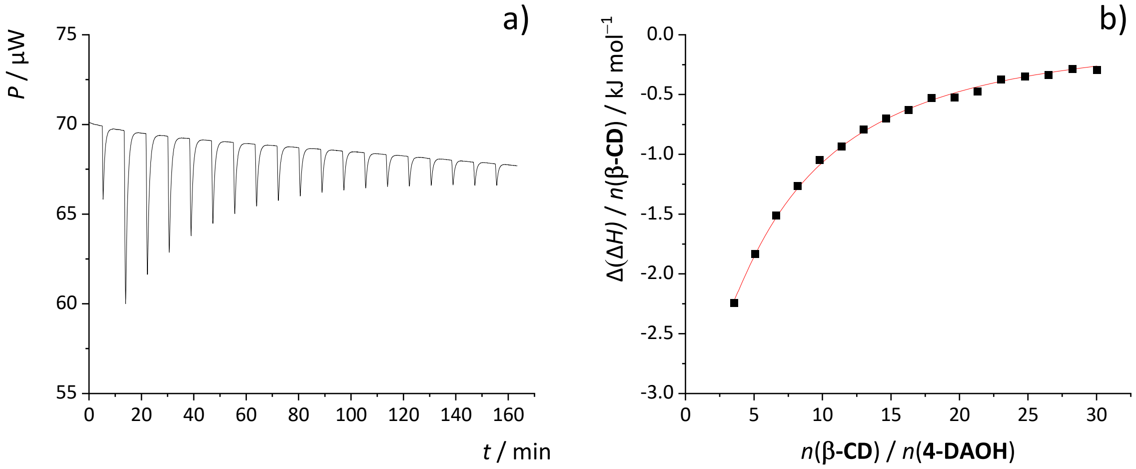


Figure S71. Microcalorimetric titration of **4-DAOH** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, $V_0 = 1.45$ mL) with **β-CD** ($c = 2\cdot10^{-2}$ mol dm^{-3}) in FMD at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

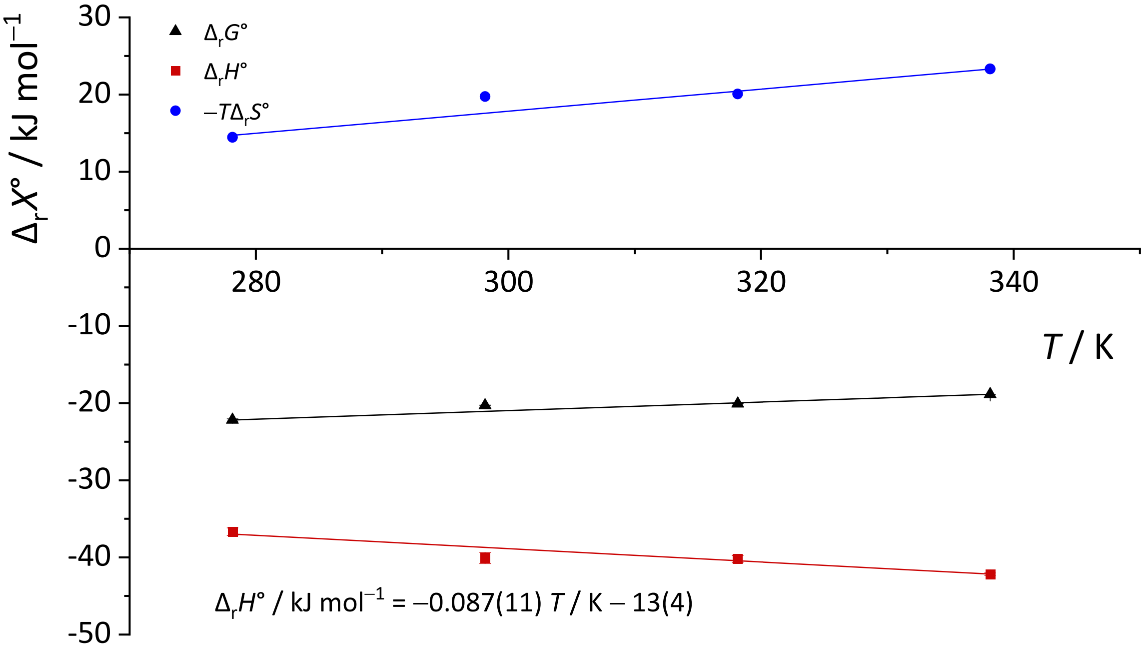


Figure S72. The temperature dependence of standard complexation parameters of **4-DAOH** with **β-CD** in FMD.

4,9-DA(OH)$_2$ with **β-CD** in FMD

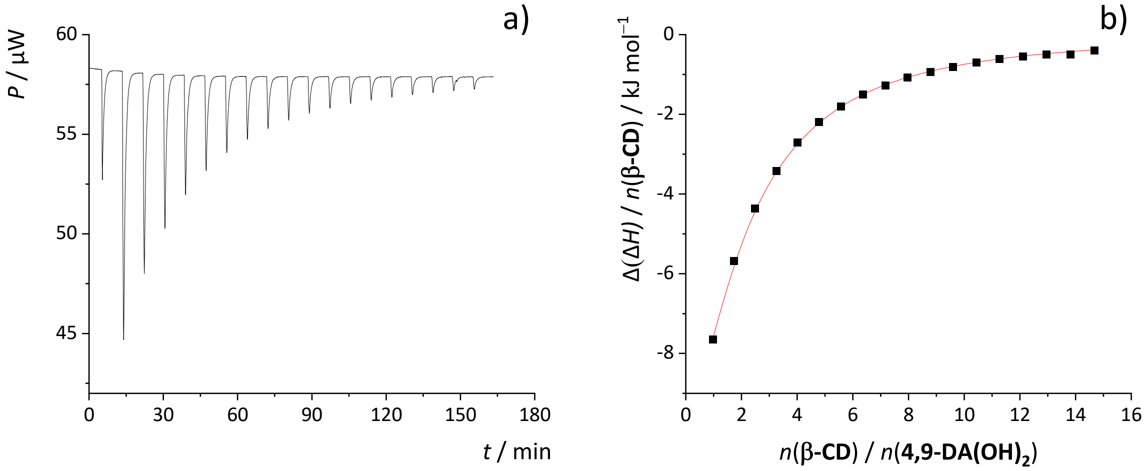


Figure S73. Microcalorimetric titration of **4,9-DA(OH)$_2$** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, V_0 = 1.45 mL) with **β-CD** ($c = 8\cdot10^{-3}$ mol dm^{-3}) in FMD at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

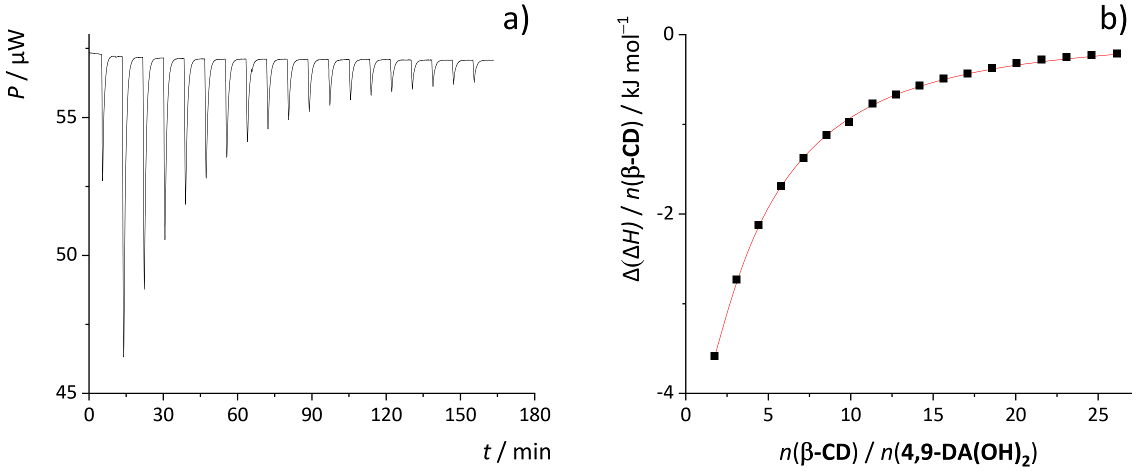


Figure S74. Microcalorimetric titration of **4,9-DA(OH)$_2$** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, V_0 = 1.45 mL) with **β-CD** ($c = 1\cdot10^{-2}$ mol dm^{-3}) in FMD at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

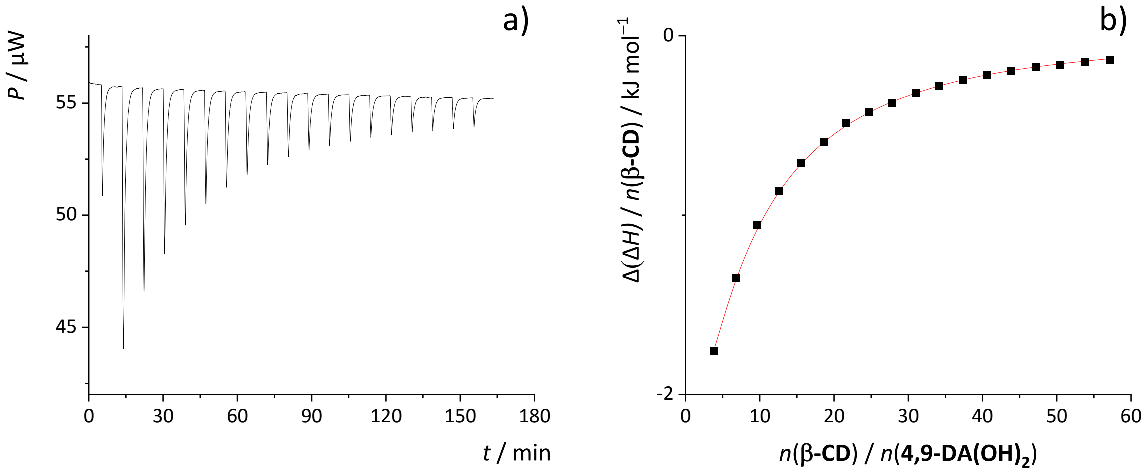


Figure S75. Microcalorimetric titration of **44,9-DA(OH)$_2$** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, V_0 = 1.45 mL) with **β-CD** ($c = 3\cdot10^{-2}$ mol dm^{-3}) in FMD at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; – calculated.

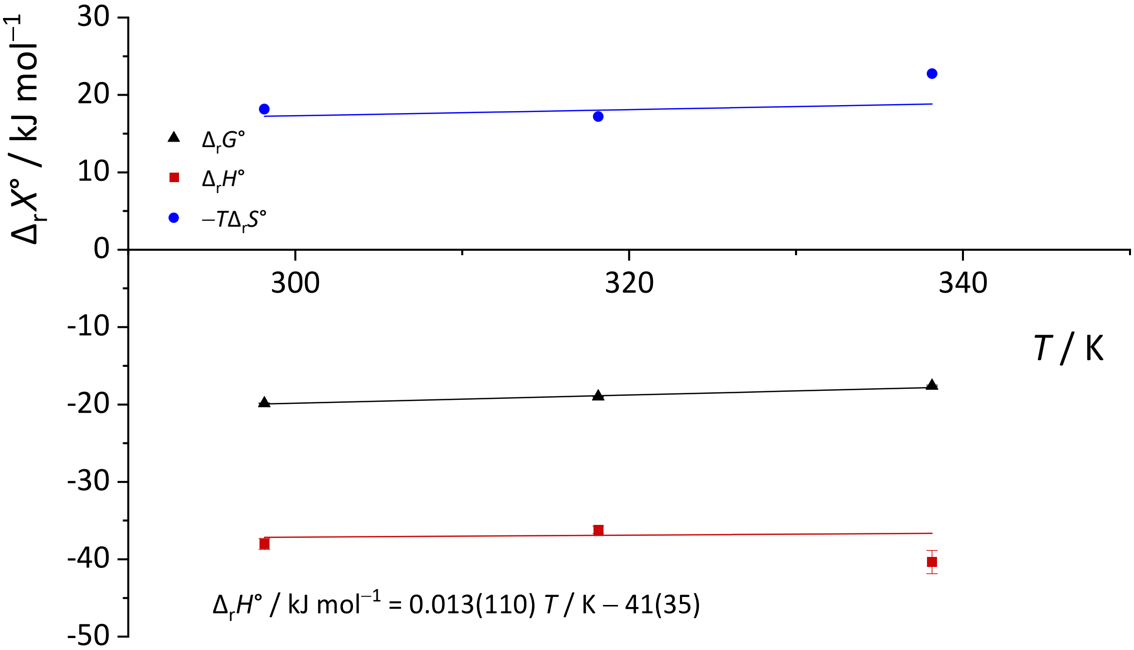


Figure S76. The temperature dependence of standard complexation parameters of **4,9-DA(OH)$_2$** with **β-CD** in FMD.

Table S6. Thermodynamic parameters for complexation of **AdOH** and diamantane alcohols with **β-CD** in FMD.[a]

GUEST · **β-CD**	T / K	log K°	$\Delta_r G$° / kJ mol^{-1}	$\Delta_r H$° / kJ mol^{-1}	$-T\Delta_r S$° / kJ mol^{-1}	$\Delta_r C_p$° / J K^{-1} mol^{-1}
1-AdOH	278	3.71(1)	−19.76(4)	−33.7(3)	14.0(4)	−173(25)
	298	3.32(1)	−18.94(8)	−35.6(5)	16.6(6)	
	338	2.64(1)	−17.08(2)	−40.5(2)	23.4(2)	
1-DAOH	298	3.08(1)	−17.60(4)	−27.9(3)	10.3(3)	199
	318	2.75(1)	−16.77(2)	−23.9(4)	7.2(4)	
4-DAOH	278	4.17(3)	−22.2(2)	−36.7(5)	14.5(4)	−87(11)
	298	3.56(1)	−20.3(1)	−40.1(7)	19.7(8)	
	318	3.30(1)	−20.08(2)	−40.2(4)	20.1(4)	
	338	2.91(1)	−18.84(1)	−42.2(4)	23.3(2)	
4,9-DA(OH)$_2$	298	3.48(1)	−19.86(6)	−38.0(7)	18.2(8)	≈ 0
	318	3.12(1)	−18.98(1)	−36.2(5)	17.20(2)	
	338	2.72(2)	−17.6(1)	−40(2)	23(2)	

[a] Uncertainties of the last digit(s) are given in parentheses as standard errors of the mean (N = 3−5), or standard deviations obtained by weighted linear regression analysis (for $\Delta_r C_p$° values).
Even though larger thermal noise was in some cases associated with experiments carried out at 278 and 338 K, or that complexation enthalpy was occasionally close to zero, the obtained linear $\Delta_r H$°(T) dependencies and the standard errors of the mean obtained by repetitive titration experiments indicate the reliability of determined thermodynamic complexation parameters

Microcalorimetric titrations in ethylene glycol (EG)

1-DAOH with **β-CD** in EG

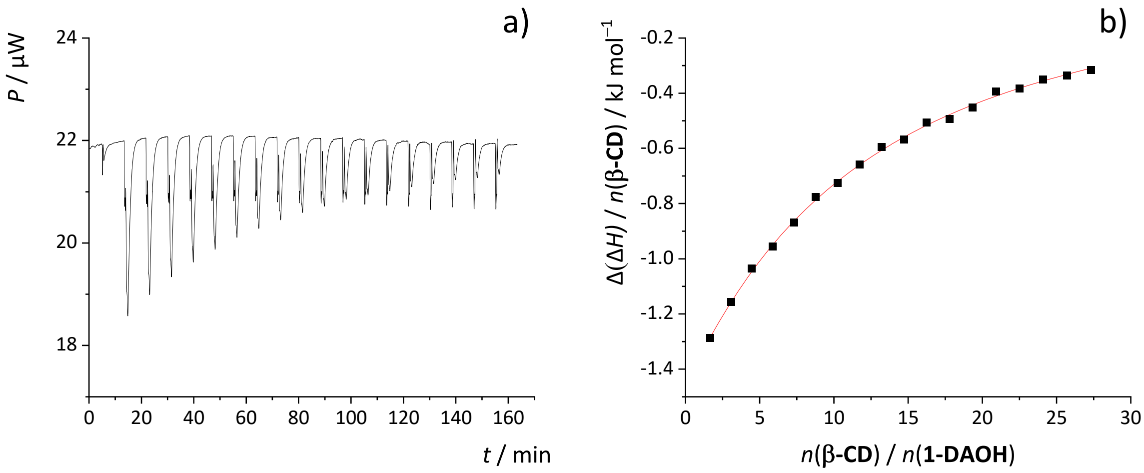


Figure S77. Microcalorimetric titration of **1-DAOH** ($c_0 = 1·10^{-4}$ mol dm^{-3}, V_0 = 1.45 mL) with **β-CD** ($c = 2·10^{-2}$ mol dm^{-3}) in EG at 288 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated. The peculiar $P(t)$ dependence is a consequence of slow heat compensation in ethylene glycol.

4-DAOH with **β-CD** in EG

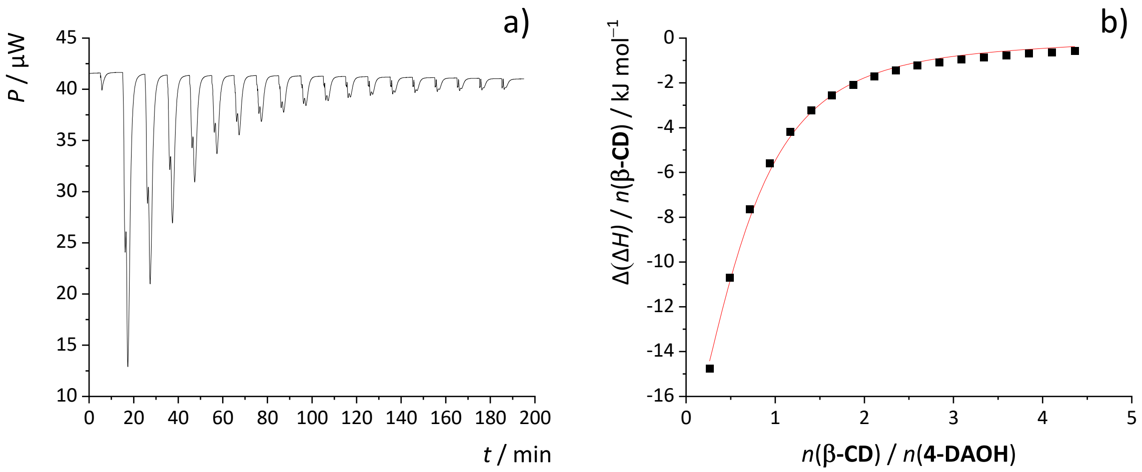


Figure S78. Microcalorimetric titration of **4-DAOH** ($c_0 = 4\cdot10^{-4}$ mol dm^{-3}, V_0 = 1.45 mL) with **β-CD** ($c = 2\cdot10^{-2}$ mol dm^{-3}) in EG at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated. The peculiar $P(t)$ dependence is a consequence of slow heat compensation in ethylene glycol.

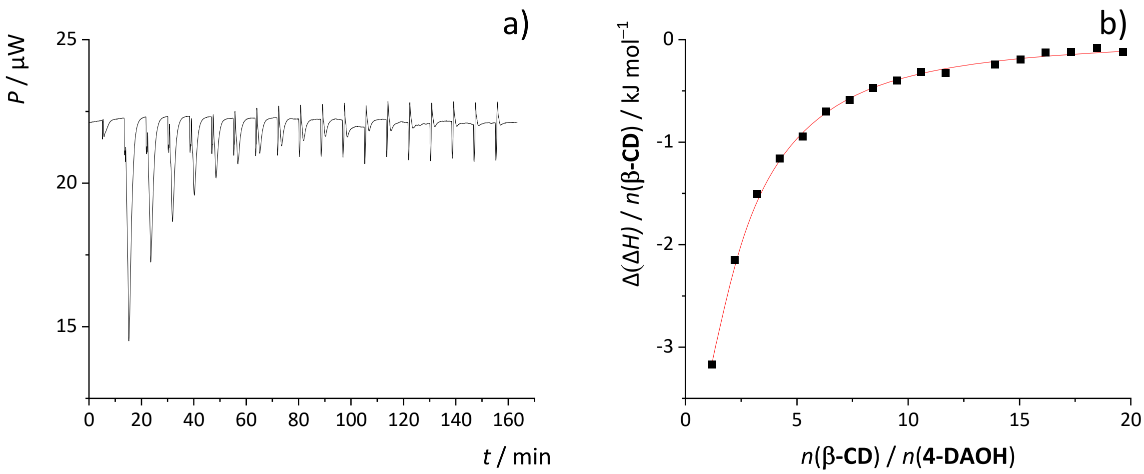


Figure S79. Microcalorimetric titration of **4-DAOH** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, V_0 = 1.45 mL) with **β-CD** ($c = 2\cdot10^{-2}$ mol dm^{-3}) in EG at 288 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated. The peculiar $P(t)$ dependence is a consequence of slow heat compensation in ethylene glycol.

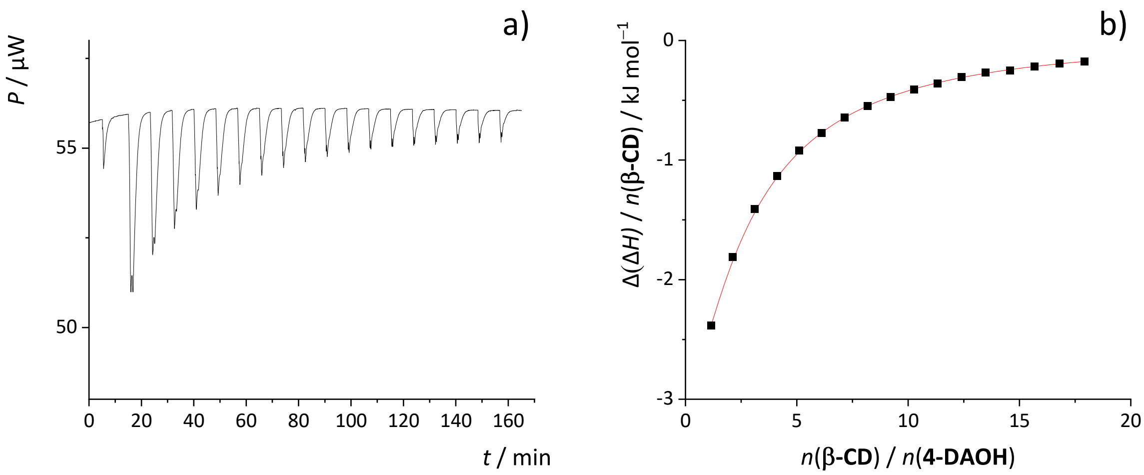


Figure S80. Microcalorimetric titration of **4-DAOH** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, V_0 = 1.45 mL) with **β-CD** ($c = 2\cdot10^{-2}$ mol dm^{-3}) in EG at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated. The peculiar $P(t)$ dependence is a consequence of slow heat compensation in ethylene glycol.

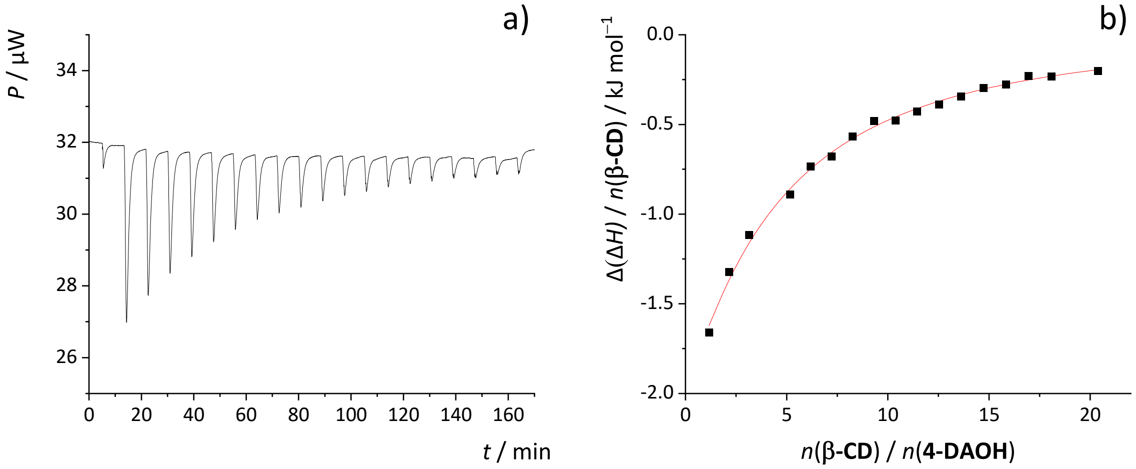


Figure S81. Microcalorimetric titration of **4-DAOH** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, V_0 = 1.45 mL) with **β-CD** ($c = 2\cdot10^{-2}$ mol dm^{-3}) in EG at 308 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

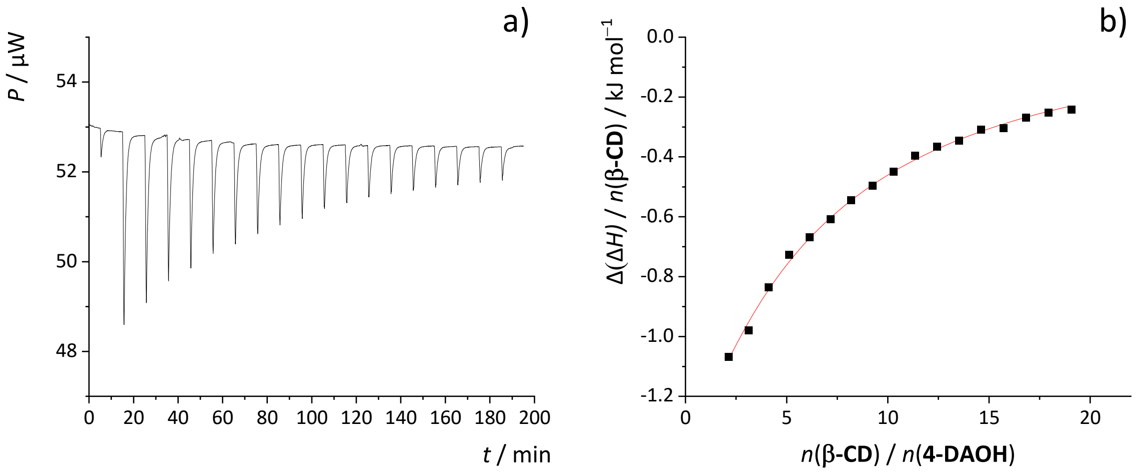


Figure S82. Microcalorimetric titration of **4-DAOH** ($c_0 = 1\cdot10^{-4}$ mol dm^{-3}, V_0 = 1.45 mL) with **β-CD** ($c = 2\cdot10^{-2}$ mol dm^{-3}) in EG at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

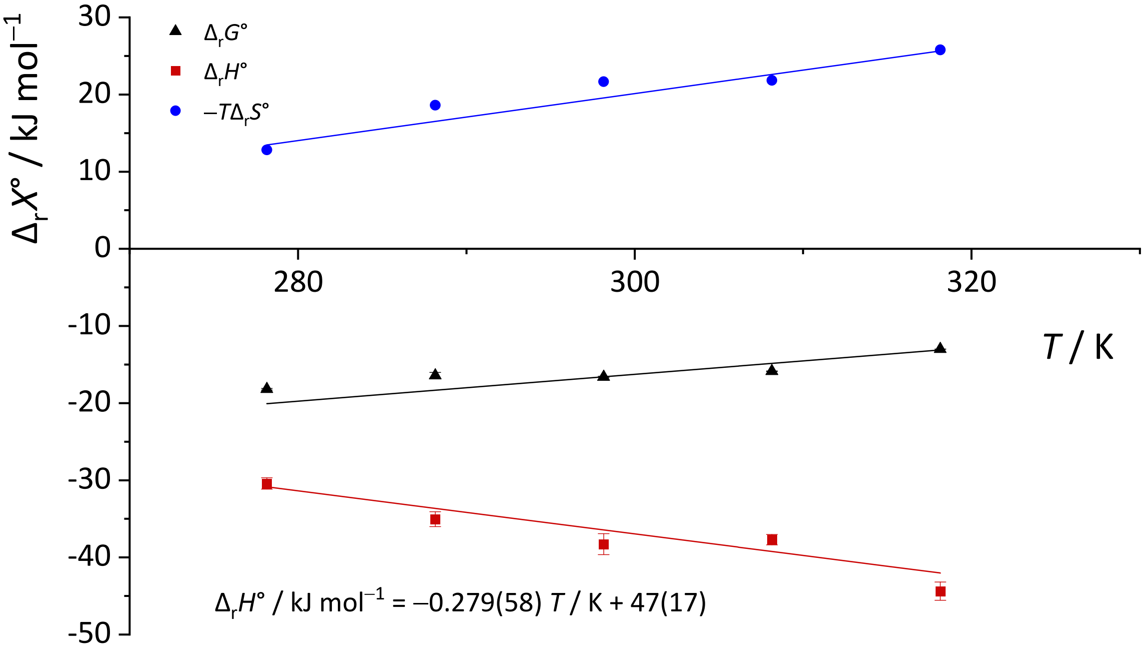


Figure S83. The temperature dependence of standard complexation parameters of **4-DAOH** with **β-CD** in EG.

4,9-DA(OH)$_2$ with **β-CD** in EG

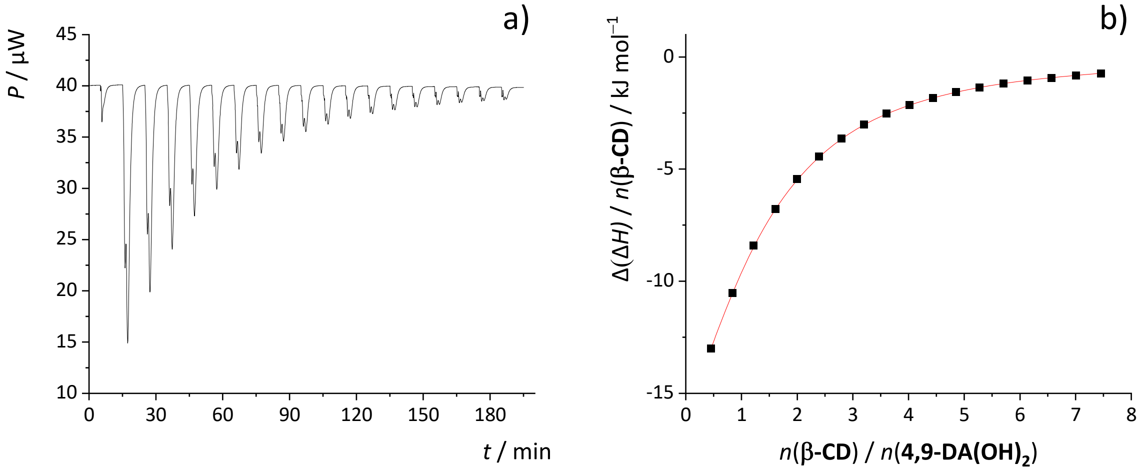


Figure S84. Microcalorimetric titration of **4,9-DA(OH)$_2$** ($c_0 = 5\cdot10^{-4}$ mol dm^{-3}, V_0 = 1.45 mL) with **β-CD** ($c = 2\cdot10^{-2}$ mol dm^{-3}) in EG at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated. The peculiar $P(t)$ dependence is a consequence of slow heat compensation in ethylene glycol.

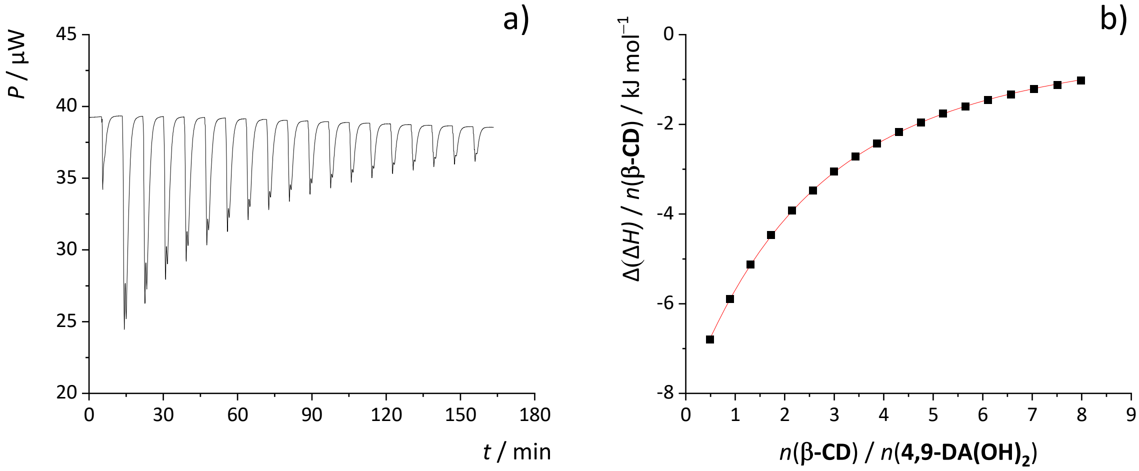


Figure S85. Microcalorimetric titration of **4,9-DA(OH)$_2$** ($c_0 = 5\cdot10^{-4}$ mol dm^{-3}, V_0 = 1.45 mL) with **β-CD** ($c = 2\cdot10^{-2}$ mol dm^{-3}) in EG at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated. The peculiar $P(t)$ dependence is a consequence of slow heat compensation in ethylene glycol.

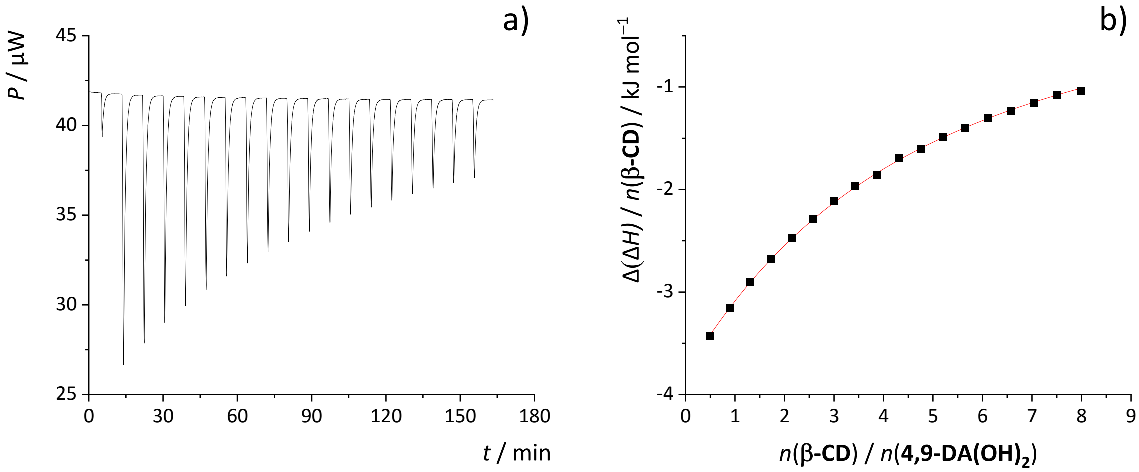


Figure S86. Microcalorimetric titration of **4,9-DA(OH)$_2$** ($c_0 = 3\cdot10^{-4}$ mol dm^{-3}, V_0 = 1.45 mL) with **β-CD** ($c = 2\cdot10^{-2}$ mol dm^{-3}) in EG at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. ■ experimental; − calculated.

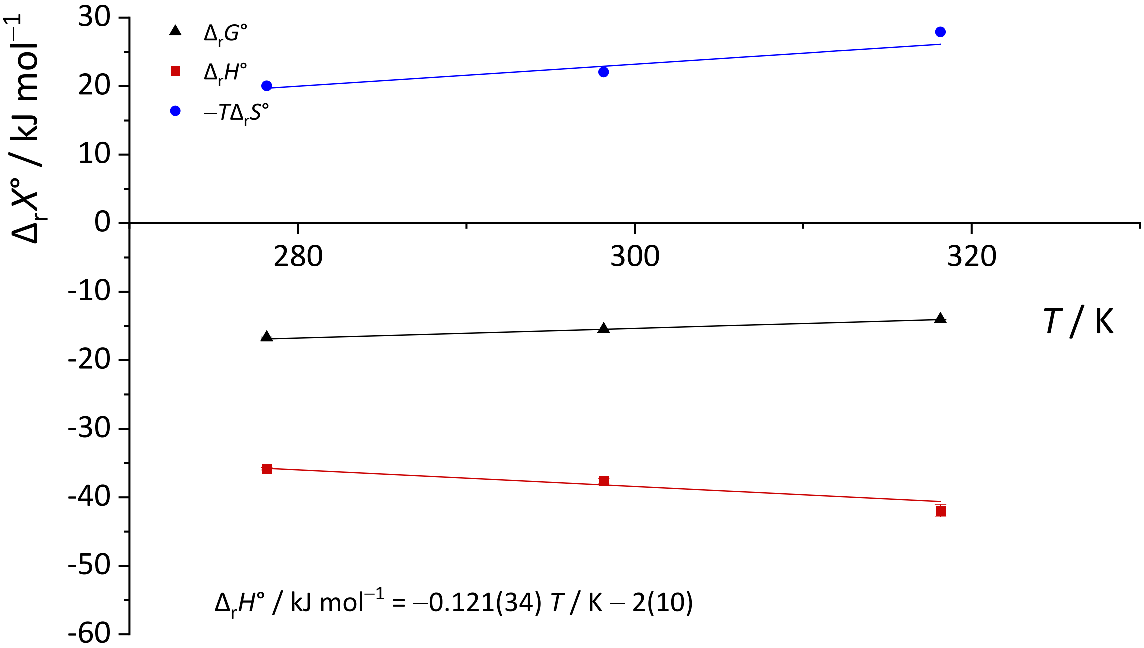


Figure S87. The temperature dependence of standard complexation parameters of **4,9-DA(OH)$_2$** with **β-CD** in EG.

Table S7. Thermodynamic parameters for complexation of diamantane alcohols with **β-CD** in EG.[a]

GUEST · **β-CD**	T / K	log $K°$	$\Delta_r G°$ / kJ mol^{-1}	$\Delta_r H°$ / kJ mol^{-1}	$-T\Delta_r S°$ / kJ mol^{-1}	$\Delta_r C_p°$ / J K^{-1} mol^{-1}
1-DAOH	288	2.41(1)	−13.28(6)	−38(1)	25(1)	
4-DAOH	278	3.42(1)	−18.2(1)	−30.4(7)	12.8(6)	−279(58)
	288	2.98(7)	−16.4(4)	−35(1)	19(1)	
	298	2.91(2)	−16.6(1)	−38(1)	22(1)	
	308	2.69(1)	−15.86(4)	−37.7(7)	21.8(7)	
	318	2.44(1)	−13.00(1)	−44(1)	26(1)	
4,9-DA(OH)$_2$	278	3.13(2)	−16.7(9)	−35.8(2)	20.0(4)	−121(34)
	298	2.72(1)	−15.51(2)	−37.6(4)	22.1(4)	
	318	2.31(1)	−14.04(3)	−42.0(9)	27.9(9)	

[a] Uncertainties of the last digit(s) are given in parentheses as standard errors of the mean (N = 3−5), or standard deviations obtained by weighted linear regression analysis (for $\Delta_r C_p°$ values).
Even though larger thermal noise was in some cases associated with experiments carried out at 278 and 338 K, or that complexation enthalpy was occasionally close to zero, the obtained linear $\Delta_r H°(T)$ dependencies and the standard errors of the mean obtained by repetitive titration experiments indicate the reliability of determined thermodynamic complexation parameters

Geometries of studied CD complexes

Table S8. Geometries of the studied **CD** complexes with diamondoid alcohols in Cartesian coordinates in Å obtained from CREST/GFN2-xTB computations with included ALPB(water) solvation.

1-AdOH·β-CD			
6	1.656278710	0.014408140	1.622611659
1	1.863378441	−0.414938465	2.605083301
1	2.578367949	0.464913345	1.247373231
6	0.562252904	1.075978323	1.742151846
1	0.885365952	1.858549015	2.436738234
6	−0.721717738	0.437704627	2.268788087
1	−1.514722313	1.182784872	2.359323640
1	−0.564271320	−0.001544021	3.255103719
6	−1.182516404	−0.658865314	1.305487602
8	−2.372508124	−1.222439753	1.845018522
6	−1.437855033	−0.046749273	−0.074610587
1	−1.768246723	−0.830653836	−0.763856906
1	−2.237403134	0.695671615	0.005933128
6	−0.082778990	−1.721784254	1.194444649
1	0.089352786	−2.149315166	2.185047111
1	−0.409478851	−2.530993560	0.536067268
6	1.197405435	−1.081716438	0.660988151
1	1.973637469	−1.850743077	0.577938812
6	0.934185903	−0.471009307	−0.715792535
1	1.852937693	−0.021750440	−1.101507514
1	0.620088718	−1.247020747	−1.418888804
6	−0.154198173	0.597010093	−0.598367819
1	−0.346351740	1.034021583	−1.584996767
6	0.296072031	1.691202767	0.369004478
1	1.206427230	2.170387860	0.000334155
6	2.475024363	5.583264414	−0.323580719
1	3.389313866	6.128460144	−0.590369105
8	2.757933614	4.238944654	−0.030529088
6	1.815592520	6.218018595	0.913550770
1	1.590490208	7.269228947	0.697999659
8	2.643729847	6.211401571	2.040779267
1	3.195808617	5.405596211	2.057945268
6	0.501533461	5.467670237	1.172844918
1	0.728090708	4.407741202	1.356366025
8	−0.201701787	6.005019627	2.266765863
1	0.440378128	6.220773376	2.962701238
6	−0.386134102	5.580261805	−0.070213096
1	−0.671025614	6.631934051	−0.203814421
6	0.359708182	5.100227469	−1.326621500
1	0.464095503	4.009844634	−1.272698298
8	1.645129883	5.706347132	−1.443988983
6	−0.407603860	5.489437236	−2.599850315
1	−1.423944439	5.096074301	−2.541503402
1	0.103625173	5.056432242	−3.467059952
8	−0.526308863	6.880730584	−2.733981687
1	0.363375790	7.253199532	−2.823852723
6	5.836207929	1.486080569	−0.374583845
1	6.824736615	1.106509749	−0.662466932
8	5.008881479	0.441864994	0.073013688
6	5.972982130	2.515122149	0.762684475
1	6.658732890	3.309250832	0.445434618
8	6.519672564	1.962153342	1.925592088
1	6.166836649	1.063879754	2.077957742
6	4.590139665	3.128623688	1.025746482
1	3.897358325	2.333165354	1.339238995
8	4.648175995	4.127440180	2.013994226
1	5.243488544	3.823087206	2.718607004
6	4.068879179	3.753999982	−0.272010521
1	4.730906673	4.579955334	−0.561074732
6	4.057536488	2.706227462	−1.397349872
1	3.295208781	1.950703395	−1.165167920
8	5.330270680	2.081770646	−1.535903640
6	3.752702676	3.359790260	−2.753585130
1	2.817259055	3.917339245	−2.681476804

1	3.652806315	2.574360063	−3.511470510
8	4.739792819	4.285840340	−3.119750820
1	5.580095032	3.813207082	−3.214794206
6	4.923713201	−3.695743393	0.073941267
1	5.286877388	−4.720657685	−0.074783749
8	3.548939911	−3.685981307	0.359804432
6	5.654328176	−3.036810020	1.258200044
1	6.735227424	−3.076484705	1.080783681
8	5.423857354	−3.705520974	2.466008190
1	4.503974424	−4.029746097	2.505820597
6	5.214096074	−1.566977785	1.335454330
1	4.132194104	−1.528377630	1.524498842
8	5.902225255	−0.870764763	2.345925531
1	5.957056758	−1.444504733	3.127213170
6	5.507835262	−0.884345222	−0.003613838
1	6.594199261	−0.868515825	−0.159616809
6	4.849212085	−1.656241918	−1.158535388
1	3.760050725	−1.554018310	−1.073557591
8	5.210635023	−3.035014127	−1.125866146
6	5.319530935	−1.124293925	−2.520536214
1	5.097123266	−0.057867522	−2.587166094
1	4.782195829	−1.658690638	−3.312093652
8	6.707208914	−1.253035751	−2.682248045
1	6.928196336	−2.196099235	−2.674194970
6	0.229800855	−6.135269502	0.068593404
1	−0.345400037	−7.050763060	−0.122082095
8	−0.623401733	−5.039034451	0.264006595
6	1.083400012	−6.305885398	1.336110831
1	1.726679362	−7.186285225	1.217152567
8	0.306282090	−6.524439287	2.479665115
1	−0.557466428	−6.079256957	2.396026098
6	1.971506017	−5.061278556	1.485874294
1	1.328613086	−4.177332556	1.602076901
8	2.842705578	−5.170971919	2.584635373
1	2.346880236	−5.549715379	3.328408248
6	2.817249781	−4.892772133	0.219122522
1	3.505559714	−5.743420894	0.134218997
6	1.915492199	−4.847998306	−1.024701107
1	1.333287069	−3.917664257	−0.998368898
8	1.036724372	−5.971835522	−1.064260772
6	2.739644756	−4.909800651	−2.318965776
1	3.471244757	−4.100404331	−2.318659386
1	2.063465571	−4.788445453	−3.173304897
8	3.468122333	−6.104447926	−2.419035342
1	2.841384129	−6.841753561	−2.460364269
6	−4.546773316	−3.895072569	−0.455369559
1	−5.570535963	−4.000678587	−0.834833998
8	−4.314014359	−2.578244420	−0.013918243
6	−4.323913550	−4.859947684	0.724645534
1	−4.578759303	−5.875345710	0.397826100
8	−5.154458370	−4.575949748	1.813558842
1	−5.235650077	−3.611346061	1.946626659
6	−2.839418562	−4.830245374	1.120486244
1	−2.577081604	−3.825543014	1.481471993
8	−2.549624981	−5.780057798	2.118413141
1	−3.252957969	−5.741971682	2.786571626
6	−1.986039042	−5.164788735	−0.108793840
1	−2.201246622	−6.198047798	−0.409749397
6	−2.327638935	−4.218552211	−1.272032374
1	−2.008233632	−3.201593484	−1.005094442
8	−3.726654801	−4.222101382	−1.541887694
6	−1.621811732	−4.647916138	−2.566641233
1	−2.163856054	−5.503837600	−2.982429394
1	−0.600066089	−4.949553319	−2.332035810
8	−1.515875711	−3.606614194	−3.500698578
1	−2.386094535	−3.430458584	−3.883702231
6	−6.002988935	1.171229402	−0.243342905
1	−6.728021054	1.966528198	−0.457422914
8	−4.747747167	1.709074012	0.090866601
6	−6.491905858	0.307232499	0.934545699
1	−7.478331829	−0.103611625	0.691325658

8	−6.654009598	1.050644399	2.109068061
1	−5.908190450	1.670204798	2.223421161
6	−5.493844119	−0.844580889	1.124991495
1	−4.521406943	−0.418978809	1.407959069
8	−5.925667673	−1.755578584	2.109203172
1	−6.207382179	−1.251345958	2.888299228
6	−5.352754656	−1.620801469	−0.187902046
1	−6.301823082	−2.133825448	−0.389226005
6	−5.031663229	−0.684059861	−1.363760927
1	−4.007928050	−0.310055563	−1.245558207
8	−5.937057789	0.414721703	−1.418522458
6	−5.166432848	−1.419264599	−2.704992958
1	−4.501714351	−2.284689222	−2.704590340
1	−4.879678067	−0.734986132	−3.511153071
8	−6.463394177	−1.914540274	−2.906613747
1	−7.072252631	−1.162857607	−2.954130379
6	−2.800868102	5.374100326	−0.052702125
1	−2.707054380	6.454861659	−0.219590283
8	−1.543123148	4.788384395	0.156870606
6	−3.666922762	5.103081291	1.190515436
1	−4.636482950	5.600051467	1.065621339
8	−3.103904711	5.616219500	2.363872556
1	−2.129298534	5.562203212	2.331794314
6	−3.901273939	3.588020275	1.292393259
1	−2.930402226	3.079637742	1.398376749
8	−4.731757704	3.264010667	2.378653862
1	−4.487078376	3.832265864	3.127522124
6	−4.573002150	3.112469246	0.000630364
1	−5.548262957	3.607064918	−0.093126656
6	−3.704536971	3.490694801	−1.211296510
1	−2.770420035	2.914463722	−1.171233416
8	−3.414484910	4.886197942	−1.212971313
6	−4.438758836	3.208801103	−2.530748304
1	−4.734689873	2.158859177	−2.562031982
1	−3.760305511	3.422356192	−3.364486357
8	−5.618992101	3.958480443	−2.641813198
1	−5.382497325	4.897810550	−2.655011375
1	−0.479714656	2.457583331	0.446557730
1	−2.814263386	−1.745524553	1.158748785

1-DAOH·β-CD			
6	-0.418700000	-1.145100000	-2.035700000
1	-0.692800000	-1.923500000	-2.757600000
6	-0.132400000	-1.789300000	-0.682500000
6	-1.570400000	-0.142700000	-1.913300000
1	-2.467800000	-0.659600000	-1.550100000
6	-1.860300000	0.486500000	-3.275300000
1	-2.688100000	1.194100000	-3.190900000
1	-2.151700000	-0.289400000	-3.986500000
6	-0.613200000	1.210500000	-3.778300000
1	-0.819600000	1.664700000	-4.753300000
6	-0.221800000	2.299100000	-2.782300000
1	0.672400000	2.816000000	-3.136700000
1	-1.026400000	3.032000000	-2.691400000
6	0.540100000	0.218700000	-3.910800000
1	0.286200000	-0.562100000	-4.630900000
1	1.437300000	0.731800000	-4.259800000
6	0.823500000	-0.413400000	-2.549100000
1	1.659600000	-1.116100000	-2.643800000
6	1.221800000	0.668500000	-1.533800000
6	1.493100000	0.028300000	-0.167400000
8	2.402700000	1.295500000	-2.022500000
6	0.061000000	1.671600000	-1.417900000
1	0.339800000	2.465000000	-0.711100000
6	-1.177700000	0.935200000	-0.898900000
6	-0.894500000	0.297600000	0.461100000
6	-3.701100000	-4.920300000	0.136400000
1	-3.806200000	-5.978900000	0.410300000
8	-2.378200000	-4.620200000	-0.195900000
6	-4.586100000	-4.624600000	-1.087300000
1	-5.605700000	-4.973400000	-0.865000000
8	-4.051300000	-5.323900000	-2.178200000
1	-4.547200000	-5.064000000	-2.971200000

6	-4.645500000	-3.115100000	-1.340200000
1	-3.650100000	-2.763900000	-1.651600000
8	-5.588300000	-2.896400000	-2.359800000
1	-5.774000000	-1.943100000	-2.434300000
6	-5.032300000	-2.387900000	-0.041800000
1	-6.050800000	-2.686300000	0.241000000
6	-4.067300000	-2.789900000	1.085800000
1	-3.048300000	-2.509300000	0.786000000
8	-4.132400000	-4.204200000	1.260900000
6	-4.377300000	-2.135000000	2.444700000
1	-4.673200000	-2.933700000	3.135200000
1	-5.204400000	-1.429800000	2.341300000
8	-3.300600000	-1.393600000	2.950200000
1	-2.553600000	-1.995400000	3.131600000
6	1.447500000	-6.002700000	0.560000000
1	2.218100000	-6.694500000	0.925900000
8	2.018600000	-4.800900000	0.130600000
6	0.718000000	-6.639800000	-0.634300000
1	0.357400000	-7.632800000	-0.327700000
8	1.639100000	-6.749700000	-1.685600000
1	1.160300000	-7.058900000	-2.471200000
6	-0.494600000	-5.785700000	-1.014100000
1	-0.144300000	-4.820100000	-1.407000000
8	-1.215600000	-6.486800000	-1.996700000
1	-2.073500000	-6.049700000	-2.141100000
6	-1.358200000	-5.510400000	0.228300000
1	-1.795000000	-6.456600000	0.575200000
6	-0.493500000	-4.912300000	1.352000000
1	-0.073500000	-3.963900000	0.995300000
8	0.576600000	-5.813700000	1.641400000
6	-1.253000000	-4.652000000	2.665500000
1	-0.870600000	-5.353600000	3.415700000
1	-2.321100000	-4.827200000	2.525600000
8	-1.139600000	-3.323400000	3.108000000
1	-0.206000000	-3.120600000	3.304400000
6	5.396400000	-2.491500000	0.815100000
1	6.385400000	-2.269200000	1.235000000
8	4.855900000	-1.357600000	0.191800000
6	5.524900000	-3.617500000	-0.227600000
1	6.044800000	-4.466300000	0.240300000
8	6.264900000	-3.122100000	-1.311700000
1	6.276200000	-3.808100000	-1.998600000
6	4.130400000	-4.080400000	-0.654700000
1	3.615700000	-3.248800000	-1.159800000
8	4.289100000	-5.168700000	-1.529500000
1	3.425800000	-5.592900000	-1.680100000
6	3.319600000	-4.469600000	0.588900000
1	3.793100000	-5.341200000	1.060400000
6	3.290400000	-3.303600000	1.593500000
1	2.745600000	-2.467200000	1.135400000
8	4.621300000	-2.894700000	1.908300000
6	2.612000000	-3.693200000	2.920300000
1	3.400700000	-3.872100000	3.657200000
1	2.037300000	-4.610400000	2.783300000
8	1.690000000	-2.733700000	3.374500000
1	2.159200000	-1.967700000	3.731200000
6	5.424400000	2.717200000	0.030300000
1	5.951700000	3.678200000	0.103500000
8	4.055900000	2.926300000	-0.185900000
6	6.004200000	1.922600000	-1.150900000
1	7.097800000	1.885900000	-1.026400000
8	5.668100000	2.611400000	-2.325600000
1	5.914500000	2.054300000	-3.080100000
6	5.487200000	0.480400000	-1.153400000
1	4.430400000	0.473700000	-1.454500000
8	6.263300000	-0.229800000	-2.093500000
1	6.160200000	-1.185100000	-1.937700000
6	5.603600000	-0.148900000	0.241400000
1	6.661600000	-0.366000000	0.442300000
6	5.072100000	0.781200000	1.343300000
1	3.984400000	0.871500000	1.247300000
8	5.672100000	2.072900000	1.244800000
6	5.412000000	0.252500000	2.742400000
1	4.995200000	-0.749000000	2.857300000
1	4.960400000	0.921700000	3.483000000

8	6.797600000	0.133200000	2.942800000
1	7.189900000	1.016100000	2.877700000
6	1.230800000	5.900700000	0.407000000
1	0.853300000	6.878500000	0.734800000
8	0.183500000	5.063700000	0.017200000
6	2.165800000	6.094000000	-0.799000000
1	2.936300000	6.828400000	-0.520800000
8	1.388200000	6.569000000	-1.863100000
1	1.953700000	6.617600000	-2.650300000
6	2.863900000	4.770600000	-1.132700000
1	2.110100000	4.058100000	-1.496900000
8	3.817900000	5.033900000	-2.131300000
1	4.334600000	4.227600000	-2.308700000
6	3.519500000	4.201000000	0.138200000
1	4.320100000	4.882600000	0.453600000
6	2.484100000	4.096700000	1.268800000
1	1.684100000	3.416400000	0.944100000
8	1.928000000	5.387000000	1.510800000
6	3.062300000	3.575400000	2.598300000
1	2.915400000	4.358100000	3.351600000
1	4.131700000	3.381700000	2.492700000
8	2.489300000	2.361000000	3.001000000
1	1.545800000	2.502200000	3.203700000
6	-3.845000000	4.447800000	0.757800000
1	-4.830400000	4.653700000	1.193800000
8	-3.839600000	3.205700000	0.105400000
6	-3.497400000	5.542300000	-0.268100000
1	-3.606100000	6.522700000	0.217500000
8	-4.390700000	5.419000000	-1.343300000
1	-4.129800000	6.062400000	-2.021800000
6	-2.043600000	5.379700000	-0.717000000
1	-1.941600000	4.424600000	-1.253200000
8	-1.730700000	6.458400000	-1.562300000
1	-0.778800000	6.445800000	-1.762900000
6	-1.120200000	5.338000000	0.508800000
1	-1.144700000	6.315800000	1.007700000
6	-1.590400000	4.251200000	1.492300000
1	-1.486000000	3.276300000	0.998000000
8	-2.957900000	4.463400000	1.838700000
6	-0.787300000	4.252600000	2.806300000
1	-1.411100000	4.714800000	3.577100000
1	0.120700000	4.844800000	2.682300000
8	-0.358000000	2.969400000	3.192100000
1	-1.104000000	2.464000000	3.542900000
6	-6.116200000	-0.231400000	-0.032500000
1	-7.005500000	-0.869400000	0.064700000
8	-4.982100000	-0.997400000	-0.315700000
6	-6.329800000	0.763300000	-1.185000000
1	-7.267700000	1.308400000	-1.001400000
8	-6.412600000	0.026200000	-2.374800000
1	-6.456700000	0.654300000	-3.113100000
6	-5.178800000	1.773400000	-1.206400000
1	-4.249800000	1.238500000	-1.453100000
8	-5.463300000	2.736900000	-2.191900000
1	-5.026700000	3.576500000	-1.961500000
6	-5.013100000	2.409600000	0.177800000
1	-5.886500000	3.041500000	0.388900000
6	-4.902400000	1.332000000	1.268700000
1	-3.967800000	0.775100000	1.130900000
8	-6.011900000	0.436800000	1.192100000
6	-4.933600000	1.935700000	2.678100000
1	-4.121900000	2.657400000	2.777800000
1	-4.793200000	1.125700000	3.402300000
8	-6.124300000	2.639700000	2.925700000
1	-6.860600000	2.012100000	2.886200000
1	-2.000800000	1.653900000	-0.795900000
6	0.248400000	-0.706600000	0.324900000
1	0.451300000	-1.164300000	1.298700000
1	1.772500000	0.809100000	0.547400000
1	2.341600000	-0.656100000	-0.262100000
1	0.685000000	-2.510200000	-0.779700000
1	-1.019600000	-2.327800000	-0.340200000
1	-1.790800000	-0.204100000	0.833800000
1	-0.617100000	1.067400000	1.184900000
1	2.753400000	1.889000000	-1.340800000

4-DAOH·β-CD			
6	-0.335800000	0.815000000	-2.835300000
1	-0.389600000	0.944600000	-3.922300000
6	-0.875300000	2.066800000	-2.151300000
6	1.120200000	0.578300000	-2.426500000
1	1.725900000	1.440800000	-2.726400000
6	1.658300000	-0.671400000	-3.119400000
1	2.700400000	-0.841500000	-2.843200000
1	1.613300000	-0.543000000	-4.204000000
6	0.824900000	-1.888800000	-2.705700000
8	1.340600000	-3.085000000	-3.271800000
6	0.896200000	-2.050700000	-1.186100000
1	0.314900000	-2.928100000	-0.893300000
1	1.935200000	-2.226500000	-0.896700000
6	-0.631200000	-1.655400000	-3.123800000
1	-0.689000000	-1.533800000	-4.208500000
1	-1.230800000	-2.525400000	-2.850300000
6	-1.167000000	-0.405100000	-2.430900000
1	-2.208900000	-0.246600000	-2.731900000
6	-1.102200000	-0.568900000	-0.910000000
6	-1.641400000	0.682500000	-0.220500000
1	-1.705700000	-1.436800000	-0.613200000
6	0.356000000	-0.800900000	-0.503100000
1	0.412200000	-0.936600000	0.584400000
6	1.188200000	0.420200000	-0.905300000
6	0.642700000	1.668800000	-0.215000000
6	-5.252800000	-2.781100000	0.173800000
1	-5.769700000	-3.733600000	0.349300000
8	-3.896300000	-3.001000000	-0.123000000
6	-5.896000000	-2.046400000	-1.016600000
1	-6.972100000	-1.945600000	-0.830500000
8	-5.763400000	-2.752500000	-2.217600000
1	-4.913100000	-3.229400000	-2.241500000
6	-5.277600000	-0.643700000	-1.115700000
1	-4.196700000	-0.748000000	-1.292100000
8	-5.860100000	0.113000000	-2.148100000
1	-6.049200000	-0.482100000	-2.891800000
6	-5.502500000	0.088800000	0.212200000
1	-6.582000000	0.202800000	0.375700000
6	-4.907000000	-0.734300000	1.366700000
1	-3.815200000	-0.756600000	1.257200000
8	-5.424500000	-2.063400000	1.362000000
6	-5.289500000	-0.143100000	2.732000000
1	-4.960800000	0.896000000	2.781800000
1	-4.792300000	-0.722300000	3.518500000
8	-6.679000000	-0.130700000	2.924100000
1	-6.993600000	-1.046900000	2.926100000
6	-1.089500000	-6.044300000	0.272500000
1	-0.721400000	-7.045700000	0.530700000
8	-0.028200000	-5.184000000	-0.037900000
6	-2.006700000	-6.113200000	-0.960300000
1	-2.818900000	-6.824300000	-0.766700000
8	-1.334600000	-6.566500000	-2.101300000
1	-0.393600000	-6.312700000	-2.066000000
6	-2.610000000	-4.717200000	-1.181100000
1	-1.789000000	-4.003900000	-1.349800000
8	-3.494000000	-4.694300000	-2.273700000
1	-3.150000000	-5.295200000	-2.954700000
6	-3.374800000	-4.305600000	0.081500000
1	-4.196900000	-5.014800000	0.243300000
6	-2.434900000	-4.350500000	1.297700000
1	-1.680500000	-3.559300000	1.188200000
8	-1.798200000	-5.621600000	1.404800000
6	-3.209800000	-4.163800000	2.611200000
1	-3.779800000	-3.234900000	2.566800000
1	-2.493400000	-4.115500000	3.439400000
8	-4.141500000	-5.191600000	2.816100000
1	-3.659300000	-6.028500000	2.890900000
6	4.017900000	-4.667200000	0.483300000
1	5.048400000	-4.859500000	0.810000000
8	3.886300000	-3.357400000	-0.006100000
6	3.630800000	-5.649300000	-0.639100000
1	3.798600000	-6.672900000	-0.285200000
8	4.437800000	-5.486500000	-1.772100000

1	4.550700000	-4.538100000	-1.964000000
6	2.142300000	-5.470800000	-0.972400000
1	1.996900000	-4.483700000	-1.428400000
8	1.683500000	-6.469900000	-1.857800000
1	2.326900000	-6.552400000	-2.578500000
6	1.294500000	-5.580200000	0.300800000
1	1.300500000	-6.626700000	0.632800000
6	1.835400000	-4.693500000	1.433000000
1	1.628700000	-3.645400000	1.182300000
8	3.234700000	-4.878600000	1.623500000
6	1.181400000	-5.055700000	2.775600000
1	0.096500000	-4.997400000	2.678000000
1	1.520100000	-4.343400000	3.537100000
8	1.473800000	-6.372100000	3.160600000
1	2.433700000	-6.451800000	3.264000000
6	5.918000000	0.267600000	0.257900000
1	6.770900000	0.915200000	0.499700000
8	4.794300000	1.037200000	-0.089400000
6	6.271600000	-0.643200000	-0.932000000
1	7.203400000	-1.175500000	-0.707100000
8	6.500200000	0.081200000	-2.107800000
1	5.899500000	0.848600000	-2.158300000
6	5.148100000	-1.674400000	-1.116300000
1	4.212500000	-1.140400000	-1.344300000
8	5.441400000	-2.586900000	-2.143400000
1	5.897100000	-2.108500000	-2.855100000
6	4.961700000	-2.453700000	0.189800000
1	5.883000000	-3.010300000	0.405900000
6	4.685200000	-1.475100000	1.344100000
1	3.707300000	-1.002500000	1.179300000
8	5.702900000	-0.479600000	1.420700000
6	4.704000000	-2.184900000	2.706500000
1	3.972300000	-2.993700000	2.706300000
1	4.445200000	-1.456800000	3.484100000
8	5.949100000	-2.774500000	2.969900000
1	6.615200000	-2.072400000	3.014000000
6	3.512200000	4.977600000	0.309000000
1	3.615800000	6.043400000	0.552100000
8	2.171600000	4.654300000	0.051600000
6	4.330800000	4.641300000	-0.950600000
1	5.367300000	4.965500000	-0.797500000
8	3.862300000	5.313600000	-2.086100000
1	2.898200000	5.449300000	-2.029400000
6	4.320400000	3.117600000	-1.156300000
1	3.286400000	2.782000000	-1.320700000
8	5.122900000	2.735600000	-2.246300000
1	5.009100000	3.391300000	-2.953300000
6	4.867600000	2.442000000	0.105100000
1	5.914400000	2.744800000	0.238400000
6	4.061900000	2.885800000	1.337200000
1	3.046200000	2.478300000	1.258600000
8	4.013700000	4.308300000	1.431100000
6	4.722100000	2.407200000	2.639300000
1	4.829500000	1.321900000	2.613200000
1	4.082500000	2.691300000	3.482900000
8	6.014000000	2.931600000	2.793700000
1	5.944500000	3.895500000	2.861500000
6	-1.663000000	6.041800000	0.745300000
1	-2.461600000	6.706400000	1.098900000
8	-2.185400000	4.809300000	0.322200000
6	-0.923100000	6.678000000	-0.446000000
1	-0.535700000	7.658400000	-0.145600000
8	-1.762400000	6.900800000	-1.543200000
1	-2.404800000	6.171400000	-1.635600000
6	0.253800000	5.762500000	-0.813400000
1	-0.143800000	4.778300000	-1.099200000
8	1.024500000	6.290400000	-1.865900000
1	0.422300000	6.707900000	-2.503100000
6	1.163600000	5.591000000	0.407400000
1	1.620100000	6.559300000	0.649900000
6	0.355800000	5.096900000	1.619600000
1	0.064500000	4.054600000	1.440300000
8	-0.805400000	5.895200000	1.842100000
6	1.182100000	5.197300000	2.911100000
1	2.118800000	4.652600000	2.783800000

1	0.608600000	4.753500000	3.732900000
8	1.531200000	6.523500000	3.205600000
1	0.716400000	7.026400000	3.352600000
6	-5.600700000	2.488500000	0.572300000
1	-6.632800000	2.220100000	0.831800000
8	-4.893400000	1.365800000	0.108500000
6	-5.589500000	3.548600000	-0.544800000
1	-6.189800000	4.409300000	-0.229100000
8	-6.164200000	3.076300000	-1.730900000
1	-5.913000000	2.145600000	-1.882200000
6	-4.138700000	4.001000000	-0.765600000
1	-3.545600000	3.134200000	-1.091000000
8	-4.051000000	5.027600000	-1.723400000
1	-4.682800000	4.836000000	-2.435300000
6	-3.556800000	4.522500000	0.552600000
1	-4.090400000	5.436300000	0.843300000
6	-3.713200000	3.469100000	1.662200000
1	-3.042900000	2.628900000	1.442100000
8	-5.057100000	3.002200000	1.755000000
6	-3.375100000	4.065400000	3.037100000
1	-2.365600000	4.479700000	3.011300000
1	-3.424600000	3.270100000	3.789500000
8	-4.231400000	5.124500000	3.372700000
1	-5.133200000	4.777200000	3.439400000
1	2.232700000	0.268100000	-0.603600000
1	1.332300000	-3.010300000	-4.236000000
6	-0.807500000	1.892000000	-0.635900000
1	-1.198400000	2.791200000	-0.149900000
1	-1.590300000	0.553200000	0.864800000
1	-2.687800000	0.840500000	-0.486900000
1	-1.907500000	2.241000000	-2.461700000
1	-0.282800000	2.933300000	-2.452700000
1	1.241700000	2.543000000	-0.476600000
1	0.697900000	1.539600000	0.870100000

4,9-DA(OH)$_2$·β-CD			
6	0.739100000	-1.383800000	-0.803000000
1	1.349000000	-2.289200000	-0.694300000
6	0.094800000	-1.046200000	0.541000000
6	-0.344500000	-1.623300000	-1.858900000
1	-0.974500000	-2.462300000	-1.539900000
6	0.287500000	-1.961500000	-3.205900000
1	-0.481100000	-2.138600000	-3.960300000
1	0.895100000	-2.865500000	-3.134000000
6	1.179400000	-0.806900000	-3.666300000
8	1.735700000	-1.187400000	-4.917200000
6	0.336900000	0.467100000	-3.795500000
1	0.971100000	1.295900000	-4.119500000
1	-0.433100000	0.312700000	-4.554500000
6	2.270800000	-0.576100000	-2.617100000
1	2.873200000	-1.483100000	-2.531700000
1	2.929900000	0.233800000	-2.938100000
6	1.635300000	-0.234200000	-1.270300000
1	2.432200000	-0.068000000	-0.535300000
6	0.781500000	1.031000000	-1.389800000
6	0.140300000	1.369300000	-0.045500000
1	1.417700000	1.870800000	-1.693500000
6	-0.301300000	0.797300000	-2.447700000
1	-0.907100000	1.705200000	-2.549100000
6	-1.197200000	-0.357200000	-1.988100000
6	-1.846200000	-0.016500000	-0.649600000
6	-2.449800000	-5.500900000	0.328800000
1	-2.301300000	-6.538600000	0.656900000
8	-1.241700000	-4.935800000	-0.088200000
6	-3.436400000	-5.487100000	-0.854600000
1	-4.319700000	-6.075700000	-0.564500000
8	-2.787500000	-6.074900000	-1.949200000
1	-3.373500000	-6.003500000	-2.719500000
6	-3.908100000	-4.060000000	-1.159800000
1	-3.066500000	-3.480900000	-1.569100000
8	-4.943500000	-4.156500000	-2.105300000
1	-5.358200000	-3.283100000	-2.225100000
6	-4.376300000	-3.377700000	0.136700000
1	-5.254100000	-3.909500000	0.525900000
6	-3.246300000	-3.457200000	1.175200000

1	-2.348500000	-3.001900000	0.736500000
8	-2.979200000	-4.832000000	1.441100000
6	-3.553500000	-2.749300000	2.505800000
1	-3.676900000	-3.518000000	3.275200000
1	-4.481400000	-2.181800000	2.419500000
8	-2.554700000	-1.827200000	2.861800000
1	-1.750300000	-2.322500000	3.121100000
6	2.822100000	-5.347300000	0.631900000
1	3.734500000	-5.843900000	0.989000000
8	3.096500000	-4.042900000	0.212800000
6	2.253100000	-6.132100000	-0.562100000
1	2.151500000	-7.185300000	-0.260900000
8	3.160600000	-6.004300000	-1.622500000
1	2.778900000	-6.441300000	-2.400100000
6	0.860000000	-5.605500000	-0.921900000
1	0.953400000	-4.585200000	-1.322500000
8	0.320900000	-6.466900000	-1.893200000
1	-0.624400000	-6.269200000	-2.010200000
6	-0.031200000	-5.548300000	0.330600000
1	-0.221900000	-6.572700000	0.678100000
6	0.678200000	-4.760500000	1.447100000
1	0.849400000	-3.737700000	1.088900000
8	1.938900000	-5.375400000	1.718900000
6	-0.091000000	-4.703700000	2.779800000
1	0.453300000	-5.323400000	3.501500000
1	-1.097900000	-5.105100000	2.654600000
8	-0.261600000	-3.396000000	3.262400000
1	0.605100000	-2.982700000	3.439000000
6	5.756400000	-0.950900000	0.913400000
1	6.640200000	-0.454400000	1.332600000
8	4.921600000	-0.021000000	0.270100000
6	6.202300000	-2.017800000	-0.103800000
1	6.926400000	-2.684200000	0.386300000
8	6.795300000	-1.355800000	-1.190400000
1	7.009300000	-2.022400000	-1.863000000
6	4.991700000	-2.845600000	-0.538800000
1	4.289200000	-2.189700000	-1.073100000
8	5.452800000	-3.872100000	-1.382200000
1	4.725800000	-4.491800000	-1.565100000
6	4.274400000	-3.411000000	0.694600000
1	4.930800000	-4.144100000	1.182000000
6	3.939800000	-2.283800000	1.688600000
1	3.197300000	-1.625800000	1.217900000
8	5.110600000	-1.532400000	2.006900000
6	3.385700000	-2.827200000	3.018100000
1	4.205800000	-2.833000000	3.742400000
1	3.029500000	-3.848500000	2.875300000
8	2.280900000	-2.100800000	3.495200000
1	2.568400000	-1.253300000	3.860700000
6	4.606400000	4.071000000	-0.122200000
1	4.907600000	5.127600000	-0.116900000
8	3.229300000	3.940200000	-0.309400000
6	5.305200000	3.340700000	-1.280800000
1	6.391400000	3.479500000	-1.178700000
8	4.846400000	3.903100000	-2.481100000
1	5.210500000	3.379200000	-3.212500000
6	4.987500000	1.843800000	-1.186300000
1	3.904100000	1.711600000	-1.320600000
8	5.682400000	1.174900000	-2.210700000
1	5.974500000	0.301300000	-1.891200000
6	5.362300000	1.327000000	0.205400000
1	6.453000000	1.375000000	0.324700000
6	4.702000000	2.185300000	1.298600000
1	3.613700000	2.058300000	1.250300000
8	5.027900000	3.561800000	1.111200000
6	5.193300000	1.805900000	2.700300000
1	4.990500000	0.748800000	2.877000000
1	4.643200000	2.409400000	3.430200000
8	6.582200000	1.972800000	2.837900000
1	6.784200000	2.914200000	2.737100000
6	-0.283200000	6.045400000	0.201300000
1	-0.928700000	6.898800000	0.447900000
8	-1.045300000	4.894400000	-0.033700000
6	0.521800000	6.370500000	-1.069700000
1	1.062400000	7.313500000	-0.899300000

8	-0.375500000	6.505600000	-2.138500000
1	0.142800000	6.572700000	-2.956900000
6	1.546200000	5.262000000	-1.314700000
1	1.011500000	4.322800000	-1.520800000
8	2.331100000	5.638000000	-2.419700000
1	3.091400000	5.034300000	-2.497500000
6	2.398500000	5.060600000	-0.052200000
1	3.005400000	5.960500000	0.115500000
6	1.491100000	4.818600000	1.165700000
1	0.930000000	3.892600000	0.993600000
8	0.567100000	5.898500000	1.302700000
6	2.254700000	4.691300000	2.496200000
1	1.901100000	5.495800000	3.153200000
1	3.328300000	4.809200000	2.334700000
8	2.095400000	3.436600000	3.101200000
1	1.141900000	3.274300000	3.225800000
6	-4.916700000	3.538500000	0.631400000
1	-5.933000000	3.575400000	1.043300000
8	-4.666200000	2.299500000	0.029800000
6	-4.751900000	4.629700000	-0.440800000
1	-5.052600000	5.593500000	-0.005300000
8	-5.577900000	4.294500000	-1.524400000
1	-5.421400000	4.946000000	-2.227000000
6	-3.281600000	4.730000000	-0.858200000
1	-2.988800000	3.798600000	-1.365800000
8	-3.175600000	5.825200000	-1.732300000
1	-2.237400000	5.992700000	-1.941300000
6	-2.399500000	4.895500000	0.391400000
1	-2.648300000	5.850200000	0.873500000
6	-2.683600000	3.755500000	1.384400000
1	-2.446600000	2.795400000	0.906900000
8	-4.069500000	3.770100000	1.723000000
6	-1.890800000	3.856900000	2.699100000
1	-2.568500000	3.547300000	3.505100000
1	-1.577500000	4.888500000	2.877900000
8	-0.720800000	3.086700000	2.705900000
1	-0.940300000	2.162200000	2.464400000
6	-5.996400000	-1.588000000	0.131200000
1	-6.676300000	-2.435600000	0.292800000
8	-4.709500000	-2.037000000	-0.183600000
6	-6.515600000	-0.738400000	-1.039100000
1	-7.557600000	-0.456900000	-0.827300000
8	-6.442200000	-1.521300000	-2.200400000
1	-6.657300000	-0.953100000	-2.957200000
6	-5.682300000	0.540100000	-1.151100000
1	-4.657600000	0.268000000	-1.443200000
8	-6.273900000	1.353000000	-2.135500000
1	-5.958200000	2.267300000	-2.028700000
6	-5.618900000	1.260600000	0.202000000
1	-6.606700000	1.684300000	0.429200000
6	-5.209300000	0.306000000	1.334200000
1	-4.157000000	0.031400000	1.199300000
8	-6.025500000	-0.867400000	1.329400000
6	-5.394600000	0.946500000	2.716100000
1	-4.798200000	1.857900000	2.773900000
1	-5.046200000	0.239600000	3.477300000
8	-6.728600000	1.321300000	2.949500000
1	-7.272000000	0.519600000	2.953500000
1	-1.981800000	-0.525300000	-2.734600000
1	2.343400000	-0.498200000	-5.218000000
6	-0.760100000	0.215700000	0.406400000
1	-0.449100000	2.284700000	-0.133900000
1	0.912600000	1.536800000	0.708600000
1	0.859900000	-0.882100000	1.302700000
1	-0.534700000	-1.874500000	0.873100000
1	-2.505300000	-0.829300000	-0.333100000
1	-2.454100000	0.888500000	-0.738900000
8	-1.349700000	0.576700000	1.653000000
1	-1.760400000	-0.208600000	2.059000000

1-AdOH·γ-CD			
6	−6.100500000	−1.413700000	−0.825300000
6	−6.594900000	−2.352400000	0.287700000
6	−5.397400000	−2.847200000	1.116900000
6	−4.333700000	−3.463200000	0.193800000

6	−3.989200000	−2.459100000	−0.918300000
6	−3.020200000	−3.027600000	−1.962400000
8	−7.552000000	−1.737500000	1.105900000
8	−5.832600000	−3.800100000	2.057300000
8	−3.132700000	−3.743900000	0.903900000
8	−5.154300000	−2.057500000	−1.629800000
8	−3.468000000	−4.227500000	−2.529400000
6	−5.782200000	3.833300000	−0.690200000
6	−6.647000000	3.225800000	0.430500000
6	−6.121600000	1.815400000	0.737800000
6	−6.117100000	0.988800000	−0.550500000
6	−5.316700000	1.708300000	−1.648300000
6	−5.448600000	0.998500000	−3.003300000
8	−6.670500000	4.027600000	1.577400000
8	−6.927900000	1.151500000	1.680100000
8	−5.547200000	−0.267400000	−0.227500000
8	−5.806800000	3.033400000	−1.838500000
8	−6.786400000	0.882800000	−3.411200000
6	−1.421400000	6.783600000	−0.247800000
6	−2.461500000	6.928300000	0.879700000
6	−3.209400000	5.594600000	1.012300000
6	−3.848600000	5.249700000	−0.335700000
6	−2.779000000	5.223200000	−1.440000000
6	−3.417300000	5.103400000	−2.832000000
8	−1.886800000	7.320400000	2.093400000
8	−4.225400000	5.659000000	1.983300000
8	−4.477300000	3.986300000	−0.194500000
8	−2.031900000	6.437300000	−1.457600000
8	−4.255500000	6.191700000	−3.117300000
6	3.654900000	5.450100000	0.283300000
6	2.973300000	6.033600000	1.537800000
6	1.483300000	5.669800000	1.491100000
6	0.887500000	6.201800000	0.184800000
6	1.667600000	5.638300000	−1.014800000
6	1.215000000	6.291400000	−2.328900000
8	3.572900000	5.593500000	2.723500000
8	0.775700000	6.229800000	2.570400000
8	−0.476100000	5.817900000	0.140800000
8	3.058600000	5.922400000	−0.888600000
8	1.410500000	7.680800000	−2.316300000
6	6.329200000	0.925800000	0.134500000
6	5.924900000	1.400900000	1.541600000
6	4.621400000	2.199500000	1.446500000
6	4.813700000	3.341500000	0.444900000
6	5.258900000	2.770800000	−0.911900000
6	5.588600000	3.881100000	−1.918600000
8	5.729500000	0.335600000	2.431900000
8	4.252900000	2.751800000	2.686500000
8	3.588000000	4.043100000	0.346300000
8	6.448600000	2.005400000	−0.749800000
8	6.588600000	4.743600000	−1.441600000
6	5.551000000	−3.990100000	−1.443700000
6	6.643500000	−3.555900000	−0.446400000
6	6.193600000	−2.242000000	0.203900000
6	5.943500000	−1.196600000	−0.890900000
6	4.941100000	−1.747600000	−1.916800000
6	4.817100000	−0.812200000	−3.127600000
8	6.917700000	−4.530900000	0.519700000
8	7.165800000	−1.769600000	1.113600000
8	5.392300000	−0.015000000	−0.327900000
8	5.362800000	−3.010400000	−2.424700000
8	6.031800000	−0.659500000	−3.809800000
6	1.432200000	−7.007300000	−0.168200000
6	2.565100000	−7.030300000	0.885000000
6	3.348900000	−5.719700000	0.765000000
6	3.833000000	−5.520800000	−0.673700000
6	2.684300000	−5.699600000	−1.681600000
6	3.211600000	−5.756200000	−3.122100000
8	2.112000000	−7.235700000	2.193300000
8	4.478100000	−5.704000000	1.606800000
8	4.354600000	−4.203800000	−0.736600000

8	1.981300000	−6.920000000	−1.448800000
8	4.175500000	−6.761800000	−3.298400000
6	−3.136100000	−4.977800000	1.580900000
6	−1.972800000	−4.981000000	2.589000000
6	−0.647700000	−4.936800000	1.821700000
6	−0.582300000	−6.093100000	0.820200000
6	−1.835400000	−6.086100000	−0.073400000
6	−1.897900000	−7.330800000	−0.966500000
8	−2.044500000	−3.950800000	3.528000000
8	0.446700000	−5.023000000	2.706300000
8	0.575000000	−5.903500000	0.021100000
8	−3.027600000	−6.069700000	0.705700000
8	−1.839300000	−8.525600000	−0.230800000
1	−6.926600000	−1.150700000	−1.497100000
1	−7.088300000	−3.217900000	−0.168200000
1	−4.943600000	−1.987600000	1.635500000
1	−4.720200000	−4.391300000	−0.245700000
1	−3.533800000	−1.578100000	−0.448500000
1	−2.868600000	−2.262600000	−2.733600000
1	−2.064100000	−3.241100000	−1.481500000
1	−7.252600000	−0.842400000	1.356200000
1	−7.162800000	1.783800000	2.378200000
1	−6.197900000	4.797800000	−1.008400000
1	−7.683300000	3.149900000	0.081900000
1	−5.089900000	1.889900000	1.112500000
1	−7.152700000	0.857000000	−0.889000000
1	−4.261200000	1.742200000	−1.350500000
1	−4.860300000	1.550700000	−3.744800000
1	−5.059400000	−0.017700000	−2.917600000
1	−5.790200000	4.418600000	1.737200000
1	−7.137800000	1.772800000	−3.561600000
1	−0.937900000	7.749200000	−0.443200000
1	−3.175600000	7.714300000	0.608900000
1	−2.488300000	4.806300000	1.274500000
1	−4.595800000	6.015400000	−0.581000000
1	−2.109000000	4.373000000	−1.258300000
1	−2.619800000	5.019200000	−3.579100000
1	−4.045000000	4.211600000	−2.867200000
1	−3.893800000	6.177100000	2.734700000
1	−3.716000000	6.996200000	−3.126900000
1	4.696500000	5.789800000	0.227400000
1	3.080200000	7.124000000	1.527900000
1	1.385400000	4.574600000	1.507500000
1	0.970100000	7.296200000	0.177900000
1	1.512600000	4.552600000	−1.060900000
1	1.760400000	5.827800000	−3.158500000
1	0.143800000	6.130000000	−2.462400000
1	3.700600000	4.624700000	2.699000000
1	1.332200000	6.167500000	3.363800000
1	2.360600000	7.853200000	−2.239800000
1	7.332300000	0.484500000	0.173800000
1	6.721800000	2.066100000	1.914100000
1	3.829000000	1.529600000	1.082700000
1	5.599100000	4.009000000	0.822100000
1	4.455300000	2.136600000	−1.308100000
1	4.700600000	4.494000000	−2.083400000
1	5.891200000	3.413700000	−2.862200000
1	6.319300000	−0.402200000	2.189200000
1	4.424100000	2.090700000	3.375200000
1	7.409200000	4.236800000	−1.353200000
1	5.862200000	−4.892800000	−1.983400000
1	7.579800000	−3.393200000	−0.991500000
1	5.246600000	−2.418200000	0.736500000
1	6.885600000	−0.962300000	−1.403500000
1	3.965100000	−1.850600000	−1.427100000
1	4.528700000	0.179400000	−2.776300000
1	4.041100000	−1.204300000	−3.794600000
1	6.085800000	−4.859200000	0.915100000
1	7.569900000	−2.547400000	1.535800000
1	0.871700000	−7.950900000	−0.139800000
1	3.221600000	−7.876900000	0.655000000

1	2.677600000	−4.886200000	1.024300000
1	4.619600000	−6.255300000	−0.887800000
1	1.994000000	−4.854200000	−1.577400000
1	3.700700000	−4.809400000	−3.359800000
1	2.361700000	−5.905500000	−3.796200000
1	1.536500000	−6.488200000	2.458500000
1	4.231300000	−6.098700000	2.458900000
1	3.747200000	−7.620600000	−3.169900000
1	−4.087800000	−5.125300000	2.104500000
1	−2.031600000	−5.915500000	3.158900000
1	−0.595500000	−3.990000000	1.263600000
1	−0.527800000	−7.045500000	1.360000000
1	−1.797300000	−5.200600000	−0.716700000
1	−2.813700000	−7.276400000	−1.564400000
1	−1.034900000	−7.328700000	−1.634700000
1	−1.971600000	−3.088300000	3.073800000
1	0.214400000	−4.535100000	3.514800000
1	−2.635100000	−8.584000000	0.317700000
1	−4.292700000	−4.051000000	−3.005600000
1	6.303200000	−1.527300000	−4.143900000
1	−1.052500000	6.835500000	2.248200000
1	−6.650400000	−3.466900000	2.463000000
6	−1.414200000	0.906800000	−0.732000000
1	−2.258500000	0.312900000	−1.091500000
1	−1.161600000	1.634500000	−1.506400000
6	−0.214500000	−0.003300000	−0.465700000
1	0.057700000	−0.529100000	−1.386700000
6	−0.570400000	−1.030100000	0.609000000
1	0.288500000	−1.673800000	0.813300000
1	−1.397500000	−1.666800000	0.289100000
6	−0.968100000	−0.309200000	1.898000000
8	−1.300800000	−1.310100000	2.856700000
6	0.216100000	0.537500000	2.379300000
1	−0.048200000	1.051700000	3.306400000
1	1.064200000	−0.119000000	2.583400000
6	−2.169300000	0.604500000	1.626100000
1	−3.018900000	0.001100000	1.294700000
1	−2.458600000	1.114000000	2.548900000
6	−1.798400000	1.632500000	0.557500000
1	−2.657600000	2.287400000	0.370300000
6	−0.617200000	2.471900000	1.046000000
1	−0.363900000	3.229700000	0.301300000
1	−0.888900000	2.994700000	1.966000000
6	0.583300000	1.561500000	1.304900000
1	1.432500000	2.161200000	1.650600000
6	0.968100000	0.840300000	0.013500000
1	1.240800000	1.572700000	−0.749600000
1	1.837200000	0.200300000	0.184900000
1	−1.479400000	−0.880100000	3.704700000

1-DAOH·γ-CD			
6	-6.784668952	0.303032581	0.080414039
6	-6.985736530	1.526063994	-0.836772216
6	-5.734598191	2.409996130	-0.743643189
6	-5.492394296	2.776551511	0.722387807
6	-5.375959288	1.497557812	1.569750876
6	-5.284850192	1.832442840	3.064388088
8	-7.249361956	1.153155212	-2.160677794
8	-5.884294107	3.594237991	-1.491236615
8	-4.301929992	3.542687449	0.791112031
8	-6.540075262	0.689491092	1.401948576
8	-6.394415076	2.568288404	3.510751243
6	-4.912263726	-4.411252553	-1.301655703
6	-5.355315273	-3.528634281	-2.483968848
6	-5.167855048	-2.059544750	-2.079448330
6	-5.960665498	-1.791600321	-0.797769961
6	-5.531079672	-2.769542622	0.307657142
6	-6.431736628	-2.655118925	1.545372577
8	-4.663334756	-3.831956754	-3.662362634
8	-5.629912540	-1.181369643	-3.076950995
8	-5.713162235	-0.447142033	-0.434359723
8	-5.644589938	-4.117834786	-0.146333920

8	-7.782725832	-2.883812002	1.238802185
6	-0.132631968	-6.449294078	-0.374402872
6	-0.453682905	-6.157904012	-1.850781231
6	-1.465546760	-5.010878895	-1.939459869
6	-2.688749772	-5.341398574	-1.078500733
6	-2.261942060	-5.690787908	0.355957498
6	-3.442666650	-6.208678207	1.188959967
8	0.686196539	-5.805244795	-2.587101737
8	-1.914389237	-4.823458550	-3.260300386
8	-3.536384718	-4.207595797	-1.106233700
8	-1.297682901	-6.738606660	0.346316671
8	-3.998001661	-7.374921398	0.639730397
6	4.295835772	-4.620213796	1.700845819
6	4.235260214	-5.832061699	0.745842367
6	2.936950265	-5.729530850	-0.060520711
6	1.741013022	-5.680926201	0.899337750
6	1.940684760	-4.584530381	1.955352196
6	0.896398591	-4.701054884	3.073954168
8	5.347914597	-5.949418839	-0.093407510
8	2.798756897	-6.825711937	-0.941110620
8	0.553959888	-5.360326556	0.187834357
8	3.215930086	-4.663480006	2.583871485
8	0.992160999	-5.914014133	3.768448195
6	6.840546447	-0.372400738	-0.125248810
6	6.821246739	-1.603369294	-1.050559311
6	5.532624422	-2.391003286	-0.770747468
6	5.495391110	-2.770336438	0.712411301
6	5.638117818	-1.504712502	1.578241592
6	5.773454622	-1.863078908	3.064540603
8	6.929123178	-1.266748490	-2.404194530
8	5.472168270	-3.558756766	-1.555024688
8	4.255554582	-3.404116761	0.984896355
8	6.800495035	-0.762097139	1.218224199
8	6.833163132	-2.750807958	3.306945997
6	4.933232622	4.429236855	-1.247984111
6	5.371242487	3.568735606	-2.448376682
6	5.175618944	2.092127488	-2.076024532
6	5.985047840	1.791416250	-0.811413453
6	5.566445074	2.745336113	0.319602257
6	6.496845088	2.603975817	1.533421597
8	4.683141986	3.897502932	-3.621916869
8	5.608270018	1.235644547	-3.104148679
8	5.741775686	0.441040135	-0.455875727
8	5.661624864	4.105017930	-0.098899281
8	7.827797526	2.908356237	1.210247494
6	0.176427839	6.534941782	-0.362285244
6	0.514646482	6.247123496	-1.835849161
6	1.483981673	5.062985498	-1.888189307
6	2.718367005	5.383286446	-1.040150747
6	2.293788147	5.753044507	0.390713381
6	3.481513200	6.266184793	1.216902086
8	-0.617213024	5.924521201	-2.597258973
8	1.910297950	4.785753694	-3.198657512
8	3.552915700	4.238347792	-1.058273819
8	1.337956519	6.808551766	0.371155793
8	4.060785738	7.409957165	0.645642277
6	-4.319312652	4.714929046	1.570860840
6	-4.214543506	5.947697746	0.651117049
6	-2.897234976	5.843257205	-0.126820254
6	-1.727753759	5.749914660	0.862154758
6	-1.975835738	4.610871052	1.862108549
6	-0.941094534	4.631038104	2.995101255
8	-5.304336669	6.087830073	-0.214431493
8	-2.725625340	6.957208613	-0.978892380
8	-0.521772257	5.441053947	0.178176703
8	-3.254647683	4.704923728	2.477602582
8	-1.003110062	5.808667946	3.751151388
1	-7.703900408	-0.294891302	0.120945191
1	-7.858112064	2.095317823	-0.497568257
1	-4.869571327	1.839537277	-1.112177889
1	-6.342258181	3.367876220	1.085824191
1	-4.483737360	0.934106438	1.258518490
1	-5.181734732	0.898403736	3.627044763
1	-4.406665215	2.456814402	3.238460658
1	-6.628552842	0.453101517	-2.440716857

1	-5.354510784	-1.532225296	-3.939432736
1	-5.128142692	-5.466447026	-1.513194953
1	-6.416152406	-3.709494131	-2.691931877
1	-4.101094662	-1.876821920	-1.880508783
1	-7.029045194	-1.935205662	-1.007625752
1	-4.492269070	-2.551049257	0.584074857
1	-6.078032889	-3.365523944	2.300890124
1	-6.367387304	-1.641165686	1.943522743
1	-3.723002266	-4.010493937	-3.466647274
1	-7.874383632	-3.799057866	0.935504628
1	0.472189129	-7.362007736	-0.306916545
1	-0.916202403	-7.064311124	-2.276956648
1	-0.997787886	-4.088512794	-1.565767566
1	-3.202400130	-6.207076380	-1.517528895
1	-1.837320133	-4.791620533	0.820892531
1	-3.094410761	-6.387784298	2.212688124
1	-4.236753719	-5.460438082	1.197735051
1	-1.137934620	-4.785825540	-3.839523976
1	-3.319296216	-8.065959328	0.651041690
1	5.195185711	-4.674361443	2.327958821
1	4.219436023	-6.742239821	1.356193097
1	2.955112386	-4.793346592	-0.640160444
1	1.630891238	-6.652070321	1.399921713
1	1.831923811	-3.616453206	1.454228396
1	1.017836977	-3.850635418	3.754598889
1	-0.098930651	-4.671879178	2.627614462
1	5.426512259	-5.146275912	-0.650434681
1	3.691020560	-7.075698949	-1.238142686
1	1.863810841	-5.954109754	4.189212319
1	7.784506804	0.175319642	-0.236558698
1	7.685778102	-2.236300097	-0.820206857
1	4.665349050	-1.751469526	-0.991943757
1	6.326786423	-3.450727328	0.930907990
1	4.746874022	-0.883484853	1.434815496
1	4.861091882	-2.367518871	3.388738985
1	5.898514279	-0.937783600	3.637047658
1	6.378000737	-0.485777529	-2.607062996
1	5.820830035	-3.346171234	-2.437205730
1	7.665436667	-2.296283747	3.110882776
1	5.160402935	5.486307654	-1.435736662
1	6.432968424	3.748505905	-2.651728360
1	4.110470372	1.914938179	-1.864140948
1	7.050865533	1.938353729	-1.027329068
1	4.533133897	2.514869506	0.608214021
1	6.489212631	1.566698651	1.873383535
1	6.131221053	3.254023016	2.336153863
1	3.741432156	4.069614388	-3.427821138
1	5.355214521	1.630067875	-3.954868555
1	-0.422827626	7.450364205	-0.292105522
1	1.013154027	7.138211281	-2.251463002
1	0.973222917	4.186902475	-1.461690807
1	3.241382129	6.237987556	-1.488425167
1	1.861234286	4.863571277	0.866959907
1	4.261269444	5.503111564	1.242219596
1	3.134036775	6.470780076	2.235737335
1	-1.388528108	6.413988539	-2.255222374
1	1.133718478	4.802988012	-3.779831684
1	3.402896833	8.120619889	0.658083513
1	-5.226234316	4.769385552	2.185357456
1	-4.201417162	6.848901900	1.274476567
1	-2.916077066	4.920767798	-0.727581261
1	-1.622126685	6.698269387	1.405031034
1	-1.905159861	3.665494505	1.310996064
1	-1.098263214	3.750340993	3.628730645
1	0.058067215	4.591058814	2.558377649
1	-5.469899779	5.246371632	-0.686698784
1	-3.608666943	7.221173259	-1.291291483
1	-1.878201115	5.858957540	4.163496947
1	-7.183910444	2.016313149	3.410346359
1	7.871618403	3.839436417	0.946725004
1	1.460720268	-6.279675165	-2.231994356
1	-6.322432385	3.369447747	-2.328377621
6	0.442078966	-0.709928058	1.665114220
1	0.254309367	-1.280125711	2.581700747
6	1.951587354	-0.612979408	1.433345181

6	-0.143967992	0.699119830	1.811841705
1	0.332725607	1.209310028	2.655713397
6	-1.668586501	0.604716741	2.064478409
1	-2.085439335	1.606197329	2.181306984
1	-1.850610960	0.040869853	2.980633009
6	-2.234768601	-0.088931837	0.874160943
6	-2.079438389	0.688286998	-0.385624868
1	-2.565968588	0.180871219	-1.220513309
1	-2.488713170	1.697012996	-0.291689478
6	-1.770570884	-1.498206750	0.749576956
1	-2.238828029	-2.014237475	-0.090547405
1	-1.952916711	-2.068472043	1.663219955
6	-0.242588045	-1.423758965	0.496425220
1	0.148265284	-2.441456825	0.379844841
6	0.030013915	-0.640650711	-0.794897666
6	1.547897726	-0.544795773	-1.021372953
8	-0.574663038	-1.350469109	-1.867770174
6	-0.555346002	0.775630932	-0.650731207
1	-0.378688848	1.340100876	-1.574576366
6	0.128837780	1.480615735	0.523202609
6	1.637043551	1.575583111	0.286282441
1	-0.277560679	2.494678407	0.613592135
6	2.216113445	0.169690690	0.149617386
1	3.294885905	0.232519197	-0.033439279
1	1.742032084	-0.001560050	-1.950333845
1	1.948982225	-1.555957556	-1.128828731
1	2.389801408	-1.609813008	1.354834634
1	2.418218534	-0.108109935	2.282174320
1	2.106148553	2.091788826	1.127360218
1	1.843433845	2.161085043	-0.612410546
1	-0.372355623	-0.890375042	-2.693798881

4-DAOH·γ-CD			
6	6.130300000	-1.769000000	-0.504000000
6	5.725500000	-2.270800000	-1.901200000
6	4.372500000	-2.983500000	-1.815900000
6	4.433500000	-4.075300000	-0.741500000
6	4.873200000	-3.453900000	0.593600000
6	5.048500000	-4.494000000	1.705000000
8	5.615300000	-1.229200000	-2.833500000
8	4.025400000	-3.592100000	-3.035100000
8	3.145200000	-4.657200000	-0.665300000
8	6.135200000	-2.813300000	0.429400000
8	5.113600000	-3.906600000	2.977100000
6	5.705100000	3.225800000	0.962100000
6	6.748000000	2.712300000	-0.050400000
6	6.199100000	1.424900000	-0.675700000
6	5.900700000	0.412800000	0.437000000
6	4.965500000	1.034300000	1.484300000
6	4.826300000	0.120900000	2.710200000
8	7.070600000	3.657700000	-1.030100000
8	7.122100000	0.869100000	-1.589100000
8	5.265900000	-0.734600000	-0.107600000
8	5.479300000	2.274500000	1.961600000
8	6.056300000	-0.115500000	3.337900000
6	1.982500000	6.729900000	-0.281300000
6	3.102800000	6.562000000	-1.325500000
6	3.621400000	5.119000000	-1.235500000
6	4.101000000	4.863700000	0.195500000
6	2.974600000	5.161200000	1.199100000
6	3.481900000	5.085400000	2.645900000
8	2.684400000	6.882700000	-2.620800000
8	4.704800000	4.906600000	-2.110800000
8	4.506700000	3.509400000	0.280000000
8	2.462000000	6.478100000	1.011000000
8	4.552900000	5.962200000	2.879000000
6	-3.181100000	5.857800000	-1.038500000
6	-2.370500000	6.289200000	-2.275400000
6	-0.913400000	5.837700000	-2.106500000
6	-0.363700000	6.382100000	-0.784700000
6	-1.273700000	5.970000000	0.383700000
6	-0.854500000	6.671500000	1.684000000
8	-2.925700000	5.801500000	-3.464700000
8	-0.109200000	6.326600000	-3.153200000
8	0.938800000	5.853200000	-0.614300000

8	-2.622800000	6.357900000	0.141600000
8	-0.950300000	8.066900000	1.578700000
6	-6.207200000	1.590900000	-0.533200000
6	-5.804200000	1.919200000	-1.980100000
6	-4.450300000	2.635500000	-1.969200000
6	-4.534200000	3.861000000	-1.054500000
6	-5.012600000	3.443600000	0.345800000
6	-5.266000000	4.654900000	1.253300000
8	-5.696300000	0.770500000	-2.778000000
8	-4.076300000	3.070500000	-3.253200000
8	-3.246800000	4.451500000	-1.015800000
8	-6.250800000	2.747600000	0.254600000
8	-6.216400000	5.531400000	0.706000000
6	-5.732800000	-3.135000000	1.632500000
6	-6.800900000	-2.751400000	0.590600000
6	-6.255500000	-1.578300000	-0.234500000
6	-5.917300000	-0.420500000	0.713300000
6	-4.931400000	-0.905200000	1.785500000
6	-4.698300000	0.167700000	2.858500000
8	-7.166700000	-3.824700000	-0.229100000
8	-7.194500000	-1.154300000	-1.199700000
8	-5.312700000	0.643300000	-0.006500000
8	-5.436300000	-2.049400000	2.465300000
8	-5.880600000	0.533400000	3.513800000
6	-1.913600000	-6.703700000	0.990200000
6	-3.117500000	-6.864800000	0.039400000
6	-3.746300000	-5.481400000	-0.169600000
6	-4.117100000	-4.883900000	1.190100000
6	-2.899200000	-4.872200000	2.128400000
6	-3.299700000	-4.472400000	3.555200000
8	-2.764100000	-7.459800000	-1.177000000
8	-4.913600000	-5.550300000	-0.953100000
8	-4.585000000	-3.567800000	0.947800000
8	-2.311900000	-6.168700000	2.218000000
8	-4.265700000	-5.336300000	4.094000000
6	3.046800000	-6.058000000	-0.642000000
6	2.046900000	-6.482000000	-1.734000000
6	0.665900000	-5.923800000	-1.361400000
6	0.288900000	-6.438200000	0.031000000
6	1.376700000	-6.052200000	1.047400000
6	1.112500000	-6.682800000	2.421500000
8	2.444100000	-6.070400000	-3.010600000
8	-0.321800000	-6.329700000	-2.275700000
8	-0.959900000	-5.868500000	0.375000000
8	2.652100000	-6.524700000	0.616700000
8	1.031800000	-8.082400000	2.354100000
1	7.167700000	-1.414500000	-0.534700000
1	6.487200000	-2.997500000	-2.229700000
1	3.609800000	-2.244700000	-1.531100000
1	5.171000000	-4.828200000	-1.049300000
1	4.121600000	-2.714500000	0.900900000
1	4.184400000	-5.160000000	1.721600000
1	5.954100000	-5.075700000	1.493500000
1	6.227900000	-0.508900000	-2.593200000
1	7.561000000	1.607900000	-2.044900000
1	6.084100000	4.112800000	1.484400000
1	7.680700000	2.492400000	0.481000000
1	5.258600000	1.659500000	-1.197500000
1	6.837900000	0.122600000	0.929700000
1	3.982700000	1.193800000	1.026800000
1	4.112700000	0.576400000	3.406100000
1	4.446800000	-0.850000000	2.388300000
1	6.255000000	4.025700000	-1.426600000
1	6.396000000	0.728300000	3.669900000
1	1.634800000	7.770700000	-0.258000000
1	3.920900000	7.251900000	-1.086900000
1	2.802000000	4.424800000	-1.474600000
1	4.950900000	5.526000000	0.405000000
1	2.174300000	4.426200000	1.049800000
1	2.646700000	5.300800000	3.321600000
1	3.854000000	4.077700000	2.840700000
1	4.489000000	5.323100000	-2.960900000
1	4.231500000	6.869900000	2.775900000
1	-4.187500000	6.293500000	-1.079300000
1	-2.393900000	7.382400000	-2.351500000

1	-0.863900000	4.738900000	-2.079000000
1	-0.325300000	7.477800000	-0.838400000
1	-1.213300000	4.880700000	0.506800000
1	-1.478800000	6.298400000	2.504000000
1	0.193200000	6.447200000	1.892400000
1	-3.163900000	4.859800000	-3.364100000
1	-0.605100000	6.239600000	-3.983300000
1	-1.877300000	8.296300000	1.415100000
1	-7.233100000	1.203600000	-0.519600000
1	-6.564300000	2.600300000	-2.397000000
1	-3.697200000	1.941300000	-1.571200000
1	-5.258100000	4.567200000	-1.481600000
1	-4.249400000	2.795500000	0.796600000
1	-4.342200000	5.225100000	1.363300000
1	-5.589400000	4.288200000	2.234000000
1	-6.296600000	0.081300000	-2.439700000
1	-4.282600000	2.363300000	-3.883800000
1	-7.065000000	5.066800000	0.659400000
1	-6.113700000	-3.915600000	2.302400000
1	-7.712400000	-2.436100000	1.110800000
1	-5.329900000	-1.897700000	-0.737200000
1	-6.830600000	-0.064300000	1.207000000
1	-3.981100000	-1.152700000	1.295200000
1	-4.314600000	1.068500000	2.377000000
1	-3.956200000	-0.207700000	3.573100000
1	-6.373200000	-4.314700000	-0.522400000
1	-7.654700000	-1.947400000	-1.524600000
1	-1.484100000	-7.684700000	1.228000000
1	-3.852100000	-7.531700000	0.503800000
1	-3.007200000	-4.824000000	-0.652300000
1	-4.912400000	-5.491900000	1.639600000
1	-2.163400000	-4.161100000	1.735500000
1	-3.746800000	-3.476700000	3.536400000
1	-2.399600000	-4.454000000	4.179800000
1	-1.985600000	-7.008300000	-1.559100000
1	-4.756200000	-6.174200000	-1.680200000
1	-3.873400000	-6.218000000	4.175900000
1	4.023000000	-6.524000000	-0.827400000
1	1.991100000	-7.576400000	-1.763600000
1	0.720900000	-4.824800000	-1.332000000
1	0.208700000	-7.532000000	-0.006800000
1	1.397200000	-4.959200000	1.145500000
1	1.904100000	-6.365800000	3.109600000
1	0.148600000	-6.331500000	2.794600000
1	2.841800000	-5.179000000	-2.974200000
1	0.055500000	-6.287200000	-3.169800000
1	1.901200000	-8.427700000	2.103500000
1	5.880500000	-3.316700000	3.012500000
1	-6.225200000	-0.244400000	3.977400000
1	1.787200000	6.531700000	-2.784200000
1	4.194000000	-2.958700000	-3.750000000
6	-0.500700000	0.630000000	0.956400000
1	-0.884800000	1.577900000	1.352000000
6	-0.782600000	-0.488400000	1.958900000
6	1.008400000	0.755300000	0.724000000
1	1.503800000	0.987100000	1.673900000
6	1.291500000	1.878300000	-0.270300000
1	2.365700000	2.002900000	-0.426800000
1	0.901000000	2.830200000	0.099300000
6	0.620400000	1.567400000	-1.608200000
8	0.925200000	2.639400000	-2.491600000
6	1.154300000	0.235900000	-2.145500000
1	0.683400000	0.011600000	-3.106300000
1	2.232800000	0.318000000	-2.302900000
6	-0.893100000	1.446900000	-1.387400000
1	-1.282200000	2.402400000	-1.024400000
1	-1.384000000	1.226400000	-2.338600000
6	-1.182400000	0.332400000	-0.382200000
1	-2.267100000	0.261800000	-0.228500000
6	-0.655600000	-1.003200000	-0.916000000
6	-0.949100000	-2.121200000	0.083500000
1	-1.149700000	-1.231000000	-1.867500000
6	0.854100000	-0.879300000	-1.146000000
1	1.235600000	-1.828700000	-1.540500000
6	1.539100000	-0.579100000	0.189400000

6	1.252200000	-1.704400000	1.182100000
1	2.622200000	-0.502200000	0.032200000
1	0.669500000	2.383900000	-3.388600000
6	-0.255400000	-1.812700000	1.409000000
1	-0.458700000	-2.615300000	2.127200000
1	-0.595300000	-3.079600000	-0.305500000
1	-2.029100000	-2.205200000	0.236000000
1	-1.857400000	-0.561600000	2.138200000
1	-0.296200000	-0.261100000	2.909400000
1	1.759000000	-1.505500000	2.129200000
1	1.638400000	-2.647500000	0.785000000

4,9-DA(OH)$_2$·γ-CD			
6	4.109800000	4.510600000	-1.647700000
6	4.359800000	3.367500000	-2.651800000
6	4.664500000	2.100900000	-1.843100000
6	5.842700000	2.341100000	-0.891300000
6	5.629700000	3.614200000	-0.053400000
6	6.906400000	4.014400000	0.696300000
8	3.250300000	3.114100000	-3.465800000
8	4.973900000	1.011800000	-2.674200000
8	5.890700000	1.216400000	-0.024600000
8	5.252200000	4.725000000	-0.860900000
8	8.009000000	4.177300000	-0.157600000
6	-0.045100000	6.249100000	1.016800000
6	0.687600000	7.046900000	-0.074900000
6	1.462900000	6.074900000	-0.980000000
6	2.399000000	5.205300000	-0.126400000
6	1.577400000	4.533200000	0.987000000
6	2.447900000	3.746500000	1.975100000
8	-0.184400000	7.844900000	-0.826800000
8	2.199700000	6.797300000	-1.938900000
8	2.980100000	4.156200000	-0.890300000
8	0.864000000	5.490400000	1.761300000
8	3.466700000	4.521900000	2.543900000
6	-4.999500000	4.461200000	0.910000000
6	-4.689100000	5.589500000	-0.094900000
6	-3.205700000	5.503100000	-0.480600000
6	-2.356500000	5.569300000	0.791300000
6	-2.786300000	4.463900000	1.770100000
6	-2.073200000	4.599400000	3.122500000
8	-5.518000000	5.543700000	-1.221400000
8	-2.823500000	6.562000000	-1.323900000
8	-1.002800000	5.425100000	0.399500000
8	-4.182300000	4.552400000	2.041300000
8	-2.329400000	5.838600000	3.728900000
6	-7.006500000	-0.254000000	-0.280600000
6	-7.140900000	0.815200000	-1.381000000
6	-5.953700000	1.780100000	-1.252000000
6	-5.955300000	2.373500000	0.158700000
6	-5.927200000	1.255900000	1.215500000
6	-6.141800000	1.822100000	2.625600000
8	-7.215900000	0.259700000	-2.663400000
8	-6.039000000	2.833800000	-2.181600000
8	-4.825100000	3.223100000	0.264600000
8	-6.990600000	0.329200000	0.990200000
8	-7.353300000	2.524200000	2.737900000
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