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

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Microcalorimetric titrations in water: Cyclodextrins

1-DAOH with β -CD in H₂O



Figure S1. Microcalorimetric titration of 1-DAOH ($c_0 = 3 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 7 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S2. Microcalorimetric titration of 1-DAOH ($c_0 = 3 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 6 \cdot 10^{-3} \text{ mol dm}^{-3}$) in at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S3. Microcalorimetric titration of 1-DAOH ($c_0 = 3 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 7 \cdot 10^{-3} \text{ mol dm}^{-3}$) in at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S4. Microcalorimetric titration of **1-DAOH** ($c_0 = 3 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 2 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S5. The temperature dependence of standard complexation parameters of 1-DAOH with β -CD in H₂O.



Figure S6. Microcalorimetric titration of **4-DAOH** ($c_0 = 2 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 3 \cdot 10^{-4} \text{ mol dm}^{-3}$) in H₂O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S7. Microcalorimetric titration of 4-DAOH ($c_0 = 2 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 6 \cdot 10^{-4} \text{ mol dm}^{-3}$) in H₂O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S8. Microcalorimetric titration of **4-DAOH** ($c_0 = 2 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 3 \cdot 10^{-4} \text{ mol dm}^{-3}$) in H₂O at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S9. Microcalorimetric titration 4-DAOH ($c_0 = 2 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 1 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S10. The temperature dependence of standard complexation parameters of 4-DAOH with β -CD in H₂O.



Figure S11. Microcalorimetric titration of 4,9-DA(OH)₂ ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 3 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O 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 ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 3 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S13. Microcalorimetric titration of 4,9-DA(OH)₂ ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 3 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S14. Microcalorimetric titration of 4,9-DA(OH)₂ ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 3 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O 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 H₂O.

GUEST · β-CD	T/K	log K	$\Delta_{\rm r}G^{\circ}$ / kJ mol ⁻¹	$\Delta_{\rm r} H^{\circ} / {\rm kJ} {\rm mol}^{-1}$	$-T\Delta_{\rm r}S^{\circ}$ / kJ mol ⁻¹	$\Delta_{\rm r} C_p^{\circ} / \mathrm{J} \mathrm{K}^{-1} \mathrm{mol}^{-1}$
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-ДАОН	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-ДАОН	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)	

Table S1. Thermodynamic parameters for complexation of 1-AdOH and diamantane alcohols with β -CD in H₂O.^[a]

[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 $\Delta_r C_p^{\circ}$ 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 $\Delta_r H^o(T)$ dependencies and the standard errors of the mean obtained by repetitive titration experiments indicate the reliability of determined thermodynamic complexation parameters.



Figure S16. Microcalorimetric titration of **1-AdOH** ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with γ -**CD** ($c = 2 \cdot 10^{-2} \text{ mol dm}^{-3}$) in H₂O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S17. Microcalorimetric titration of **1-AdOH** ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with γ -**CD** ($c = 2 \cdot 10^{-2} \text{ mol dm}^{-3}$) in H₂O at 288 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S18. Microcalorimetric titration of 1-AdOH ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with γ -CD ($c = 2 \cdot 10^{-2} \text{ mol dm}^{-3}$) in H₂O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S19. Microcalorimetric titration of **1-AdOH** ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with γ -**CD** ($c = 2 \cdot 10^{-2} \text{ mol dm}^{-3}$) in H₂O at 308 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S20. The temperature dependence of standard complexation parameters of 1-AdOH with γ -CD in H₂O.



Figure S21. Microcalorimetric titration of **1-DAOH** ($c_0 = 1 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with γ -CD ($c = 1 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S22. Microcalorimetric titration of **1-DAOH** ($c_0 = 1 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with γ -**CD** ($c = 1 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S23. Microcalorimetric titration of **1-DAOH** ($c_0 = 1 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with γ -CD ($c = 1 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S24. Microcalorimetric titration of **4-DAOH** ($c_0 = 1 \cdot 10^{-5}$ mol dm⁻³, $V_0 = 1.45$ mL) with γ -CD ($c = 1 \cdot 10^{-3}$ mol dm⁻³) in H₂O 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** ($c_0 = 4 \cdot 10^{-5}$ mol dm⁻³, $V_0 = 1.45$ mL) with γ -CD ($c = 3 \cdot 10^{-3}$ mol dm⁻³) in H₂O at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S26. Microcalorimetric titration of **4-DAOH** ($c_0 = 4 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with γ -CD ($c = 3 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S27. The temperature dependence of standard complexation parameters of 4-DAOH with γ -CD in H₂O.



Figure S28. Microcalorimetric titration of **4,9-DA(OH)**₂ ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with γ -CD ($c = 5 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S29. Microcalorimetric titration of 4,9-DA(OH)₂ ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with γ -CD ($c = 5 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S30. Microcalorimetric titration of 4,9-DA(OH)₂ ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with γ -CD ($c = 5 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S31. Microcalorimetric titration of 4,9-DA(OH)₂ ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with γ -CD ($c = 5 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.

GUEST · γ-CD	T/K	log K	$\Delta_{\rm r}G^{\circ}$ / kJ mol ⁻¹	$\Delta_{\rm r} H^{\circ} / {\rm kJ} {\rm mol}^{-1}$	$-T\Delta_{\rm r}S^{\circ}$ / kJ mol ⁻¹	$\Delta_{\rm r} C_p^{\circ} / \mathrm{J} \mathrm{K}^{-1} \mathrm{mol}^{-1}$
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-ДАОН	278			pprox 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-ДАОН	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)	

Table S2. Thermodynamic parameters for complexation of 1-AdOH and diamantane alcohols with γ -CD in H₂O.^[a]

[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 $\Delta_r C_\rho^{\circ}$ 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 $\Delta_r H^o(T)$ 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)



Figure S32. a) 600 MHz ¹H NMR spectrum with water suppression of **1-AdOH**· β -**CD** in D₂O. b) Contour plot of the ROESY ¹H NMR spectrum of the reaction mixture containing **1-AdOH** ($c = 5 \cdot 10^{-3} \text{ mol dm}^{-3}$) and β -**CD** ($c = 2 \cdot 10^{-3} \text{ mol dm}^{-3}$) at 298 K in D₂O.



Figure S33. a) 600 MHz ¹H NMR spectrum with water suppression of **1-AdOH** γ -**CD** in D₂O. Contour plot of the ROESY ¹H NMR spectrum of the reaction mixture containing **1-AdOH** ($c = 3 \cdot 10^{-3} \text{ mol dm}^{-3}$) and γ -**CD** ($c = 4 \cdot 10^{-3} \text{ mol dm}^{-3}$) at 298 K in D₂O.



Figure S34. a) 600 MHz ¹H NMR spectrum with water suppression of **1-DAOH** $\cdot\beta$ -CD in D₂O. b) Contour plot of the ROESY ¹H 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 D₂O.



Figure S35. a) 600 MHz ¹H NMR spectrum with water suppression of **1-DAOH** γ -**CD** in D₂O. b) Contour plot of the ROESY ¹H NMR spectrum of the reaction mixture containing **1-DAOH** ($c = 1.9 \cdot 10^{-3} \text{ mol dm}^{-3}$) and γ -**CD** ($c = 2 \cdot 10^{-3} \text{ mol dm}^{-3}$) at 298 K in D₂O.



Figure S36. a) 600 MHz ¹H NMR spectrum with water suppression of **4-DAOH**· β -**CD** in D₂O. b) Contour plot of the ROESY ¹H NMR spectrum of the reaction mixture containing **4-DAOH** ($c = 9 \cdot 10^{-4} \text{ mol dm}^{-3}$) and β -**CD** ($c = 1 \cdot 10^{-3} \text{ mol dm}^{-3}$) at 298 K in D₂O.



Figure S37. A) 600 MHz ¹H NMR spectrum with water suppression of **4-DAOH** $\cdot\gamma$ -**CD** in D₂O. B) Contour plot of the ROESY ¹H NMR spectrum of the reaction mixture containing **4-DAOH** ($c = 1 \cdot 10^{-3}$ mol dm⁻³) and γ -**CD** ($c = 1.4 \cdot 10^{-3}$ mol dm⁻³) at 298 K in D₂O.



Figure S38. a) 600 MHz ¹H NMR spectrum with water suppression of **4,9-DA(OH)**₂· β -**CD** in D₂O. b) Contour plot of the ROESY ¹H NMR spectrum of the reaction mixture containing **4,9-DA(OH)**₂ ($c = 4 \cdot 10^{-3} \text{ mol dm}^{-3}$) and β -**CD** ($c = 5 \cdot 10^{-3} \text{ mol dm}^{-3}$) at 298 K in D₂O.



Figure S39. a) 600 MHz ¹H NMR spectrum with water suppression of **4,9-DA(OH)**₂· γ -**CD** in D₂O. b) Contour plot of the ROESY ¹H NMR spectrum of the reaction mixture containing **4-DAOH** ($c = 3 \cdot 10^{-3} \text{ mol dm}^{-3}$) and γ -**CD** ($c = 5 \cdot 10^{-3} \text{ mol dm}^{-3}$) at 298 K in D₂O

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 ($c_0 = 3 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with CB[7] ($c = 4 \cdot 10^{-4} \text{ mol dm}^{-3}$) in H₂O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S42. Microcalorimetric titration of **1-DAOH** ($c_0 = 3 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with **CB[7]** ($c = 4 \cdot 10^{-4} \text{ mol dm}^{-3}$) in H₂O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S43. Microcalorimetric titration of **1-DAOH** ($c_0 = 3 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with **CB[7]** ($c = 4 \cdot 10^{-4} \text{ mol dm}^{-3}$) in H₂O at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S44. Microcalorimetric titration of **1-DAOH** ($c_0 = 3 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with **CB[7]** ($c = 4 \cdot 10^{-4} \text{ mol dm}^{-3}$) in H₂O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S45. The temperature dependence of standard complexation parameters of 1-DAOH with CB[7] in H₂O.



Figure S46. Microcalorimetric titration of **4-DAOH** ($c_0 = 2 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with **CB[7]** ($c = 2 \cdot 10^{-4} \text{ mol dm}^{-3}$) in H₂O 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** ($c_0 = 2 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with **CB[7]** ($c = 2 \cdot 10^{-4} \text{ mol dm}^{-3}$) in H₂O 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** ($c_0 = 2 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with **CB[7]** ($c = 2 \cdot 10^{-4} \text{ mol dm}^{-3}$) in H₂O 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** ($c_0 = 2 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with **CB[7]** ($c = 2 \cdot 10^{-4} \text{ mol dm}^{-3}$) in H₂O 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 H2O.



Figure S51. Microcalorimetric titration of **4,9-DA(OH)**₂ ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with **CB[7]** ($c = 1 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S52. Microcalorimetric titration of 4,9-DA(OH)₂ ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with CB[7] ($c = 1 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S53. Microcalorimetric titration of **4,9-DA(OH)**₂ ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with **CB[7]** ($c = 1 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O 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 ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with **CB[7]** ($c = 1 \cdot 10^{-3} \text{ mol dm}^{-3}$) in H₂O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S55. The temperature dependence of standard complexation parameters of 4,9-DA(OH)₂ with CB[7] in H₂O.

GUEST · CB[7]	T/\mathbf{K}	log K	$\Delta_{\rm r}G^{\circ}$ / kJ mol ⁻¹	$\Delta_{\rm r} H^{\rm o} / {\rm kJ mol}^{-1}$	$-T\Delta_{\rm r}S^{\circ}$ / kJ mol ⁻¹	$\Delta_{\rm r} C_p^{\circ} / \mathrm{J} \mathrm{K}^{-1} \mathrm{mol}^{-1}$
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-ДАОН	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)	

Table S3. Thermodynamic parameters for complexation of 1-AdOH and diamantane alcohols with CB[7] in H₂O.^[a]

[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 $\Delta_r C_p^{\circ}$ 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 $\Delta_r H^{\circ}(T)$ dependencies and the standard errors of the mean obtained by repetitive titration experiments indicate the reliability of determined thermodynamic complexation parameters.


Figure S56. Microcalorimetric titration of **CB[8]** ($c_0 = 2 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with **1-AdOH** ($c = 4 \cdot 10^{-4} \text{ mol dm}^{-3}$) in H₂O at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on guest to host molar ratio. \blacksquare experimental; – calculated.



Figure S57. Microcalorimetric titration of **CB[8]** ($c_0 = 2 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with **1-AdOH** ($c = 4 \cdot 10^{-4} \text{ mol dm}^{-3}$) in H₂O at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on guest to host molar ratio. \blacksquare experimental; – calculated.



Figure S58. Microcalorimetric titration of **CB[8]** ($c_0 = 2 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with **1-AdOH** ($c = 4 \cdot 10^{-4} \text{ mol dm}^{-3}$) in H₂O at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on guest to host molar ratio. \blacksquare experimental; – calculated.



Figure S59. Microcalorimetric titration of CB[8] ($c_0 = 2 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 0.205 \text{ mL}$) with 1-AdOH ($c = 4 \cdot 10^{-4} \text{ mol dm}^{-3}$) in H₂O at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on guest to host molar ratio. \blacksquare experimental; – calculated.



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



Figure S61. Microcalorimetric titration of **CB[8]** ($c_0 = 2 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with **4,9-DA(OH)**₂ ($c = 2 \cdot 10^{-4} \text{ mol dm}^{-3}$) in H₂O 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]** $(c_0 = 2 \cdot 10^{-5} \text{ mol dm}^{-3}, V_0 = 1.45 \text{ mL})$ with **4,9-DA(OH)**₂ $(c = 2 \cdot 10^{-4} \text{ mol dm}^{-3})$ in H₂O 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]** ($c_0 = 2 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with **4,9-DA(OH)**₂ ($c = 2 \cdot 10^{-4} \text{ mol dm}^{-3}$) in H₂O 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 H2O.

GUEST · CB[8]	T/K	$\log K^{\circ}$	$\Delta_{\rm r}G^{\circ}$ / kJ mol ⁻¹	$\Delta_{\rm r} H^{\circ} / {\rm kJ} {\rm mol}^{-1}$	$-T\Delta_{\rm r}S^{\circ}$ / kJ mol ⁻¹	$\Delta_{\rm r} C_p^{\circ} / \mathrm{J} \mathrm{K}^{-1} \mathrm{mol}^{-1}$
	278	7.4(1)	-39.4(8)	-25.3(6)	-14(1)	
1-AdOH	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]	-359(10)
	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]	
	278	7.9(1)	-42(1)	-25.6(4)	-17(1)	
4,9-DA(OH) ₂	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]	-484(1)
	318	7.6(1)	-46.2(6)	-45.0(3)	-1.2(6)	

Table S4. Thermodynamic parameters for complexation of 1-AdOH and diamantane alcohols with CB[8] in H2O.^[a]

[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 $\Delta_r C_p^{\circ}$ 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 $\Delta_t H^o(T)$ 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}



^a Complex geometries obtained from CREST/GFN2-xTB computations with included ALPB(water) solvation. ^b CD cavity volumes taken as $V(\beta$ -CD)=262 Å³, $V(\gamma$ -CD)=427 Å³, according to reference J. Szejtli, *Chem. Rev.* **1998**, *98*, 1743–1753.

Microcalorimetric titrations in formamide (FMD)

1-DAOH with $\beta\text{-}CD$ in FMD



Figure S65. Microcalorimetric titration of 1-DAOH ($c_0 = 2 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 1 \cdot 10^{-2} \text{ mol dm}^{-3}$) in FMD at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S66. Microcalorimetric titration of 1-DAOH ($c_0 = 2 \cdot 10^{-5} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 1 \cdot 10^{-2} \text{ mol dm}^{-3}$) in FMD at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



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



Figure S68. Microcalorimetric titration of 4-DAOH ($c_0 = 1 \cdot 10^{-4} \mod \text{dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 6 \cdot 10^{-3} \mod \text{dm}^{-3}$) in FMD at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S69. Microcalorimetric titration of **4-DAOH** ($c_0 = 1 \cdot 10^{-4} \mod \text{dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 6 \cdot 10^{-3} \mod \text{dm}^{-3}$) in FMD at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S70. Microcalorimetric titration of 4-DAOH ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 2 \cdot 10^{-2} \text{ mol dm}^{-3}$) in FMD at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S71. Microcalorimetric titration of 4-DAOH ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 2 \cdot 10^{-2} \text{ mol dm}^{-3}$) in FMD at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



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



Figure S73. Microcalorimetric titration of 4,9-DA(OH)₂ ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 8 \cdot 10^{-3} \text{ mol dm}^{-3}$) in FMD at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S74. Microcalorimetric titration of 4,9-DA(OH)₂ ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 1 \cdot 10^{-2} \text{ mol dm}^{-3}$) in FMD at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S75. Microcalorimetric titration of 44,9-DA(OH)₂ ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 3 \cdot 10^{-2} \text{ mol dm}^{-3}$) in FMD at 338 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S76. The temperature dependence of standard complexation parameters of 4,9-DA(OH)₂ with β -CD in FMD.

GUEST $\cdot \beta$ -CD	T/K	log K°	$\Delta_{\rm r}G^{\circ}$ / kJ mol ⁻¹	$\Delta_{\rm r} H^{\circ} / {\rm kJ \ mol}^{-1}$	$-T\Delta_{\rm r}S^{\circ}$ / kJ mol ⁻¹	$\Delta_{\rm r} C_p^{\circ} / \mathrm{J} \mathrm{K}^{-1} \mathrm{mol}^{-1}$
	278	3.71(1)	-19.76(4)	-33.7(3)	14.0(4)	
1-AdOH	298	3.32(1)	-18.94(8)	-35.6(5)	16.6(6)	-173(25)
	338	2.64(1)	-17.08(2)	-40.5(2)	23.4(2)	
1 0404	298	3.08(1)	-17.60(4)	-27.9(3)	10.3(3)	100
I-DAOII	318	2.75(1)	-16.77(2)	-23.9(4)	7.2(4)	199
	278	4.17(3)	-22.2(2)	-36.7(5)	14.5(4)	
4 DAOH	298	3.56(1)	-20.3(1)	-40.1(7)	19.7(8)	-87(11)
4-DAOII	318	3.30(1)	-20.08(2)	-40.2(4)	20.1(4)	0/(11)
	338	2.91(1)	-18.84(1)	-42.2(4)	23.3(2)	
	298	3.48(1)	-19.86(6)	-38.0(7)	18.2(8)	
4,9-DA(OH) ₂	318	3.12(1)	-18.98(1)	-36.2(5)	17.20(2)	≈ 0
	338	2.72(2)	-17.6(1)	-40(2)	23(2)	

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

[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 $\Delta_r C_p^{\circ}$ 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 $\Delta_r H^{\circ}(T)$ 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** ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 2 \cdot 10^{-2} \text{ mol dm}^{-3}$) in EG at 288 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated. The peculiar P(t) dependence is a consequence of slow heat compensation in ethylene glycol.



Figure S78. Microcalorimetric titration of **4-DAOH** ($c_0 = 4 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 2 \cdot 10^{-2} \text{ mol dm}^{-3}$) in EG at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated. The peculiar P(t) dependence is a consequence of slow heat compensation in ethylene glycol.



Figure S79. Microcalorimetric titration of **4-DAOH** ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 2 \cdot 10^{-2} \text{ mol dm}^{-3}$) in EG at 288 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated. The peculiar P(t) dependence is a consequence of slow heat compensation in ethylene glycol.



Figure S80. Microcalorimetric titration of 4-DAOH ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 2 \cdot 10^{-2} \text{ mol dm}^{-3}$) in EG at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated. The peculiar P(t) dependence is a consequence of slow heat compensation in ethylene glycol.



Figure S81. Microcalorimetric titration of 4-DAOH ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 2 \cdot 10^{-2} \text{ mol dm}^{-3}$) in EG at 308 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S82. Microcalorimetric titration of 4-DAOH ($c_0 = 1 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 2 \cdot 10^{-2} \text{ mol dm}^{-3}$) in EG at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



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



Figure S84. Microcalorimetric titration of **4,9-DA(OH)**₂ ($c_0 = 5 \cdot 10^{-4} \mod \text{dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 2 \cdot 10^{-2} \mod \text{dm}^{-3}$) in EG at 278 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare 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 ($c_0 = 5 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 2 \cdot 10^{-2} \text{ mol dm}^{-3}$) in EG at 298 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare 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 ($c_0 = 3 \cdot 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 1.45 \text{ mL}$) with β -CD ($c = 2 \cdot 10^{-2} \text{ mol dm}^{-3}$) in EG at 318 K. a) Thermogram. b) The dependence of normalized successive enthalpy changes on host to guest molar ratio. \blacksquare experimental; – calculated.



Figure S87. The temperature dependence of standard complexation parameters of 4,9-DA(OH)₂ with β -CD in EG.

GUEST · β-CD	T/K	log K°	$\Delta_{\rm r} G^{\circ} / {\rm kJ} {\rm mol}^{-1}$	$\Delta_{\rm r} H^{\circ} / {\rm kJ} {\rm mol}^{-1}$	$-T\Delta_{\rm r}S^{\circ}$ / kJ mol ⁻¹	$\Delta_{\rm r} C_p^{\circ} / \mathrm{J} \mathrm{K}^{-1} \mathrm{mol}^{-1}$
1-ДАОН	288	2.41(1)	-13.28(6)	-38(1)	25(1)	
	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)	
4-DAOH	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)	
	278	3.13(2)	-16.7(9)	-35.8(2)	20.0(4)	-121(34)
4,9-DA(OH) ₂	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)	

Table S7. Thermodynamic parameters for complexation of diamantane alcohols with $\beta\text{-CD}$ in EG. $^{[a]}$

[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 $\Delta_r C_p^{\circ}$ 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 $\Delta_r H^{\circ}(T)$ 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/GFN2xTB computations with included ALPB(water) solvation.

1-A	dOH·B-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
I	-0.5642/1320	-0.001544021	3.255103/19
6	-1.182516404	-0.658865314	1.30548/602
8	-2.3/2508124	-1.222439/53	1.845018522
1	-1.437833033 -1.768246723	-0.040749273 -0.830653836	-0.074010387
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
I	1.206427230	2.170387860	0.000334155
6	2.475024363	5.583264414	-0.323580/19
0	2 757022614	0.128400144	-0.390309103
6	1 815502520	4.238944034	-0.030329088
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
0	-0.40/603860	5.006074201	-2.599850315
1	-1.423944439	5.056432242	-2.341303402
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	4.048175995	4.12/440180	2.013994226
1	5.245488544	3.82308/206	2./1800/004
0	4.0008/91/9	5.155999982 1 570055221	-0.2/2010321
6	4 057536488	706227462	-1 397349872
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$\begin{array}{c} 1 \\ 8 \\ 1 \\ 1 \\ 1 \\ \end{array}$	-3.760305511 -5.618992101 -5.382497325 -0.479714656 -2.814263386 AOH-β-CD -0.418700000 -0.692800000 -0.132400000 -1.570400000 -1.570400000 -2.467800000 -2.688100000 -2.688100000 -0.613200000 -0.819600000 -0.221800000 0.672400000 0.540100000 0.286200000 1.493100000 0.823500000 1.493100000 2.402700000 0.61000000 0.339800000 -1.177700000 -0.894500000 -3.701100000 -3.806200000 -3.701100000 -3.806200000 -3.701100000 -3.806200000 -3.70100000 -3.806200000 -3.700000 -3.806200000 -3.200000 -3.8062000000 -3.806200000 -3.806200000 -3.8062000000 -3.8062000000 -3.806200000000000000000000000000000000000	3.422356192 3.958480443 4.897810550 2.457583331 -1.745524553 -1.745524553 -1.745524553 -1.789300000 -0.142700000 -0.486500000 1.94100000 -0.289400000 1.210500000 1.210500000 1.210500000 1.264700000 2.299100000 2.816000000 3.032000000 0.218700000 -0.413400000 -0.413400000 -0.413400000 1.295500000 1.295500000 1.295500000 1.295500000 0.297600000 -4.920300000 -5.978900000 -5.978900000	-3.364486357 -2.641813198 -2.655011375 0.446557730 1.158748785 -2.035700000 -2.757600000 -2.757600000 -3.275300000 -3.275300000 -3.275300000 -3.275300000 -3.78300000 -2.782300000 -2.782300000 -2.691400000 -2.691400000 -2.691400000 -2.549100000 -2.549100000 -2.643800000 -2.643800000 -1.6733800000 -1.67400000 -2.62500000 -1.417900000 -0.167400000 -0.167400000 -0.167400000 -1.417900000 -1.417900000 -0.136400000 0.136400000 0.136400000 0.166002000
$\begin{array}{c}1\\8\\1\\1\\1\end{array}\\ \begin{array}{c}1\\6\\1\\6\\1\\1\\6\\1\\1\\6\\1\\1\\6\\6\\8\\6\\1\\6\\6\\6\\1\\8\\6\end{array}\end{array}$	-3.760305511 -5.618992101 -5.382497325 -0.479714656 -2.814263386 AOH-β-CD -0.418700000 -0.692800000 -0.132400000 -1.570400000 -1.570400000 -2.467800000 -2.688100000 -2.688100000 -0.613200000 -0.613200000 -0.819600000 0.62400000 0.540100000 0.540100000 0.823500000 1.437300000 0.823500000 1.437300000 0.823500000 1.437300000 0.61000000 0.339800000 -1.177700000 -0.894500000 -3.701100000 -3.806200000 -3.78200000 -3.78200000 -3.78200000	3.422356192 3.958480443 4.897810550 2.457583331 -1.745524553 -1.745524553 -1.745524553 -1.74570000 -1.923500000 -0.142700000 -0.486500000 1.94100000 -0.289400000 1.210500000 1.210500000 1.210500000 2.299100000 2.816000000 3.032000000 0.218700000 -0.562100000 0.218700000 -0.413400000 -0.413400000 1.295500000 1.295500000 1.295500000 0.297600000 -4.920300000 -5.978900000 -4.62020000 4.620200000	-3.364486357 -2.641813198 -2.655011375 0.446557730 1.158748785 -2.035700000 -2.757600000 -2.757600000 -3.275300000 -3.275300000 -3.190900000 -3.986500000 -3.78300000 -2.782300000 -2.782300000 -2.691400000 -2.691400000 -2.691400000 -2.549100000 -2.549100000 -2.549100000 -2.643800000 -1.533800000 -0.167400000 -2.022500000 -1.417900000 -0.36400000 0.136400000 0.136400000 0.195900000 1.097200000
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$\begin{array}{c}1\\8\\1\\1\\1\end{array}\\ \begin{array}{c}1\\6\\1\\6\\1\\1\\6\\1\\1\\6\\1\\1\\6\\1\\6\\6\\1\\8\\8\\6\\1\\8\\8\\6\\1\\8\\8\\6\\1\\8\\8\\6\\1\\8\\8\\6\\1\\8\\8\\6\\1\\8\\8\\6\\1\\8\\8\\6\\1\\8\\8\\8\\8$	-3.760305511 -5.618992101 -5.382497325 -0.479714656 -2.814263386 AOH·β-CD -0.418700000 -0.692800000 -0.692800000 -1.570400000 -1.570400000 -2.467800000 -2.688100000 -2.688100000 -0.613200000 -0.613200000 -0.613200000 -0.221800000 0.672400000 0.540100000 0.286200000 1.437300000 0.823500000 1.437300000 0.823500000 1.437300000 0.84500000 -3.701100000 -3.806200000 -3.78200000 -3.78200000 -4.586100000 -5.605700000 -4.051300000	3.422356192 3.958480443 4.897810550 2.457583331 -1.745524553 -1.745524553 -1.745524553 -1.74570000 -1.923500000 -0.142700000 -0.486500000 1.194100000 -0.289400000 1.210500000 1.210500000 1.210500000 2.299100000 2.816000000 3.032000000 0.218700000 -0.562100000 0.218700000 -0.413400000 -0.413400000 -0.413400000 1.295500000 0.28500000 0.297600000 -4.920300000 -5.978900000 -4.62000000 -4.973400000 -5.323900000	-3.364486357 -2.641813198 -2.655011375 0.446557730 1.158748785 -2.035700000 -2.757600000 -2.757600000 -3.75300000 -3.275300000 -3.275300000 -3.275300000 -3.78300000 -3.78300000 -2.782300000 -2.691400000 -2.691400000 -2.691400000 -2.549100000 -2.549100000 -2.643800000 -1.533800000 -1.533800000 -1.67400000 -2.022500000 -1.417900000 -0.167400000 -0.167400000 -0.167400000 -3.136400000 0.136400000 0.136400000 -1.087300000 -0.865000000 -2.178200000 -2.178200000

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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
I	5.883000000	-3.010300000	0.405900000
1	4.083200000	-1.4/3100000	1.344100000
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	-2.0/2400000	3.014000000
1	3.512200000	6.043400000	0.509000000
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
0	4.320400000	3.11/600000	-1.156300000
1	5.280400000	2.782000000	-1.320700000
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	4.013/00000	4.308300000	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
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	5.59100000	-2.303100000
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
0	-0.032800000	1.265800000	0.831800000
0	-4.893400000	1.505800000	0.108300000
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	4.000400000	5 426200000	0.842200000
1	-4.090400000	2.460100000	1.((2200000
0	-3./13200000	3.409100000	1.002200000
1	-3.042900000	2.628900000	1.442100000
8	-5.05/100000	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 89200000	-0.635900000
1	1 109/00000	2 701200000	0.055500000
1	-1.170400000	2.791200000	-0.149900000
1	-1.590300000	0.553200000	0.864800000
1	-2.68/800000	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
1 6	1.349000000 0.094800000	-2.289200000	-0.694300000 0.541000000
1 6 6	1.349000000 0.094800000 -0.344500000	-2.289200000 -1.046200000 -1.623300000	-0.694300000 0.541000000 -1.858900000
1 6 6	1.34900000 0.094800000 -0.344500000 -0.974500000	-2.289200000 -1.046200000 -1.623300000 -2.462300000	-0.694300000 0.541000000 -1.858900000 -1.539900000
1 6 6 1	$\begin{array}{c} 1.349000000\\ 0.094800000\\ -0.344500000\\ -0.974500000\\ 0.287500000\end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -1.961500000	-0.694300000 0.541000000 -1.858900000 -1.539900000 -3.205900000
1 6 1 6	1.34900000 0.094800000 -0.344500000 -0.974500000 0.287500000	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -1.961500000 2.138600000	-0.694300000 0.541000000 -1.858900000 -1.539900000 -3.205900000 2.960200000
1 6 1 6 1	1.34900000 0.094800000 -0.344500000 -0.974500000 0.287500000 -0.481100000 0.895100000	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -1.961500000 -2.138600000 2.865500000	-0.694300000 0.541000000 -1.858900000 -3.205900000 -3.960300000 2.124000000
1 6 1 6 1 1	1.34900000 0.09480000 -0.34450000 0.28750000 -0.48110000 0.895100000	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -1.961500000 -2.138600000 -2.865500000	-0.694300000 0.541000000 -1.858900000 -3.205900000 -3.960300000 -3.134000000
$ \begin{array}{c} 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 2 \end{array} $	1.34900000 0.094800000 -0.344500000 0.287500000 -0.481100000 0.895100000 1.179400000	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -1.961500000 -2.138600000 -2.865500000 -0.806900000	-0.694300000 0.541000000 -1.858900000 -3.205900000 -3.960300000 -3.134000000 -3.666300000
1 6 1 6 1 1 6 8	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.97450000\\ 0.28750000\\ -0.48110000\\ 0.89510000\\ 1.17940000\\ 1.73570000\\ \end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -1.961500000 -2.138600000 -2.865500000 -0.806900000 -1.187400000	-0.69430000 0.54100000 -1.85890000 -3.20590000 -3.96030000 -3.13400000 -3.66630000 -4.91720000
$ \begin{array}{c} 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \end{array} $	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.97450000\\ 0.28750000\\ -0.48110000\\ 0.89510000\\ 1.17940000\\ 1.73570000\\ 0.33690000\\ \end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -1.961500000 -2.138600000 -2.865500000 -0.806900000 -1.187400000 0.467100000	-0.69430000 0.54100000 -1.85890000 -3.20590000 -3.20590000 -3.13400000 -3.13400000 -3.66630000 -4.91720000 -3.79550000
$ \begin{array}{c} 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \end{array} $	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.974500000\\ -0.87500000\\ -0.481100000\\ 0.895100000\\ 1.179400000\\ 1.735700000\\ 0.336900000\\ 0.971100000\end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.138600000 -2.865500000 -0.806900000 -1.187400000 0.467100000 1.295900000	-0.69430000 0.54100000 -1.858900000 -3.20590000 -3.20590000 -3.13400000 -3.66300000 -4.91720000 -3.79550000 -4.11950000
$ \begin{array}{c} 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 1 \end{array} $	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.97450000\\ 0.28750000\\ -0.481100000\\ 0.895100000\\ 1.7940000\\ 1.735700000\\ 0.33690000\\ 0.971100000\\ -0.433100000\end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.138600000 -2.138600000 -2.865500000 -0.806900000 -1.187400000 0.467100000 1.295900000 0.312700000	-0.69430000 0.54100000 -1.85890000 -1.53990000 -3.20590000 -3.96030000 -3.13400000 -3.66300000 -4.917200000 -4.917200000 -4.917200000 -4.555500000
$ \begin{array}{c} 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 7 \\ 6 \\ 7 \\ $	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.97450000\\ 0.28750000\\ -0.481100000\\ 0.895100000\\ 1.79400000\\ 1.735700000\\ 0.33690000\\ 0.971100000\\ -0.433100000\\ 2.270800000\end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.138600000 -2.138600000 -2.865500000 -0.806900000 -1.187400000 0.467100000 1.295900000 0.312700000 -0.576100000	-0.69430000 0.54100000 -1.85890000 -3.20590000 -3.20590000 -3.96030000 -3.13400000 -3.66630000 -4.91720000 -3.79550000 -4.11950000 -4.55450000 -2.61710000
$ \begin{array}{c} 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 1 \\ $	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.97450000\\ 0.28750000\\ -0.481100000\\ 0.895100000\\ 1.179400000\\ 1.735700000\\ 0.33690000\\ 0.971100000\\ -0.433100000\\ 2.270800000\\ 2.873200000\end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.138600000 -2.138600000 -2.865500000 -0.806900000 -1.187400000 0.467100000 0.312700000 -0.576100000 -1.483100000	-0.69430000 0.54100000 -1.85890000 -3.20590000 -3.96030000 -3.13400000 -3.66630000 -4.91720000 -3.79550000 -4.11950000 -2.61710000 -2.53170000
$ \begin{array}{c} 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ $	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.97450000\\ 0.28750000\\ -0.48110000\\ 0.895100000\\ 1.79400000\\ 1.735700000\\ 0.336900000\\ 0.971100000\\ -0.433100000\\ 2.270800000\\ 2.873200000\\ 2.929900000\end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.138600000 -2.138600000 -2.865500000 -0.806900000 -1.187400000 0.467100000 0.312700000 -0.576100000 -1.483100000 0.233800000	-0.69430000 0.54100000 -1.85890000 -1.53990000 -3.20590000 -3.96030000 -3.13400000 -3.66630000 -4.91720000 -3.79550000 -4.11950000 -2.61710000 -2.53170000 -2.93810000
$ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 1 \\ 6 \\ 1 \\ $	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.97450000\\ 0.287500000\\ -0.481100000\\ 0.895100000\\ 1.179400000\\ 1.735700000\\ 0.336900000\\ 0.971100000\\ -0.433100000\\ 2.270800000\\ 2.873200000\\ 2.929900000\\ 1.635300000\\ 1.635300000\end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.138600000 -2.138600000 -2.865500000 -0.806900000 -1.187400000 0.467100000 1.295900000 0.312700000 -0.5761000000 -1.483100000 0.233800000 -0.234200000	-0.69430000 0.54100000 -1.85890000 -3.20590000 -3.20590000 -3.266030000 -3.3400000 -3.79550000 -4.91720000 -3.79550000 -4.11950000 -4.55450000 -2.61710000 -2.93810000 -1.270300000
$ \begin{array}{c} 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 1 \\ 6 \\ 1 \\ $	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.97450000\\ 0.28750000\\ -0.481100000\\ -0.481100000\\ 1.73570000\\ 1.73570000\\ 0.33690000\\ 0.97110000\\ -0.43310000\\ 2.27080000\\ 2.873200000\\ 2.873200000\\ 1.635300000\\ 2.43220000\end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.138600000 -2.865500000 -3.865500000 -3.865900000 -1.187400000 0.467100000 1.295900000 0.312700000 -0.576100000 -1.483100000 -0.234200000 -0.068000000	-0.69430000 0.54100000 -1.85890000 -1.53990000 -3.20590000 -3.20590000 -3.13400000 -3.66300000 -4.91720000 -4.91720000 -4.5450000 -2.61710000 -2.53170000 -2.93810000 -1.27030000 -0.535300000
$ \begin{array}{c} 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.97450000\\ 0.28750000\\ -0.481100000\\ 1.7940000\\ 1.7940000\\ 1.73570000\\ 0.33690000\\ 0.33690000\\ 0.971100000\\ -0.43310000\\ 2.27080000\\ 2.87320000\\ 2.92990000\\ 1.635300000\\ 2.43220000\\ 0.78150000\\ 0.78150000\\ \end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.138600000 -2.138600000 -2.865500000 -0.806900000 -1.187400000 0.467100000 0.467100000 0.312700000 -0.576100000 -1.483100000 -0.234200000 -0.068000000 1 031000000	-0.69430000 0.54100000 -1.85890000 -1.53990000 -3.20590000 -3.20590000 -3.66300000 -3.66300000 -4.91720000 -4.91720000 -4.91720000 -4.5450000 -2.61710000 -2.53170000 -2.93810000 -1.270300000 -1.389800000 -1.38980000
$ \begin{array}{c} 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.34450000\\ -0.97450000\\ 0.28750000\\ -0.481100000\\ 0.895100000\\ 1.79400000\\ 1.735700000\\ 0.33690000\\ 0.971100000\\ -0.433100000\\ 2.270800000\\ 2.873200000\\ 2.873200000\\ 2.929900000\\ 1.635300000\\ 2.432200000\\ 0.781500000\\ 0.14020000\end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.138600000 -2.138600000 -2.865500000 -0.806900000 -1.187400000 0.467100000 0.312700000 -0.576100000 -1.483100000 -0.233800000 -0.234200000 -0.068000000 1.260200002	-0.69430000 0.54100000 -1.85890000 -1.53990000 -3.20590000 -3.20590000 -3.96030000 -3.13400000 -3.66630000 -4.91720000 -4.91720000 -4.91720000 -4.55450000 -2.61710000 -2.53170000 -2.93810000 -1.27030000 -0.53530000 -1.389800000 0.04520000
$ \begin{array}{c} 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 6 \\ 6 \\ \end{array} $	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.97450000\\ 0.28750000\\ -0.481100000\\ 0.895100000\\ 1.179400000\\ 1.735700000\\ 0.336900000\\ 0.971100000\\ -0.43100000\\ 2.270800000\\ 2.873200000\\ 2.873200000\\ 2.432200000\\ 1.635300000\\ 2.432200000\\ 0.781500000\\ 0.14030000\\ 0.14030000\\ 0.14030000\\ 0.14030000\\ 0.14030000\\ 0.14030000\\ 0.14030000\\ 0.1403000\\ 0.1403000\\ 0.1403000\\ 0.1403000\\ 0.140300\\ 0.140300\\ 0.140300\\ 0.140300\\ 0.140300\\ 0.140300\\ 0.140300\\ 0.140300\\ 0.140300\\ 0.140300\\ 0.140300\\ 0.140300\\ 0.140300\\ 0.140300\\ 0.14030\\ 0.14000\\ 0.1400\\ 0.1400\\ 0.1400\\ 0.1400\\ 0.1400\\ 0.14$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.138600000 -2.138600000 -2.865500000 -0.806900000 -1.187400000 0.467100000 0.312700000 0.312700000 -0.576100000 -0.234200000 -0.234200000 -0.068000000 1.0310000000 1.369300000	-0.69430000 0.54100000 -1.85890000 -3.20590000 -3.20590000 -3.96030000 -3.96030000 -3.96030000 -3.96630000 -4.91720000 -4.91720000 -4.91720000 -4.55450000 -2.61710000 -2.53170000 -2.93810000 -1.27030000 -0.53530000 -1.38980000 -0.045500000 -0.045500000 -0.045500000
$ \begin{array}{c} 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.37450000\\ 0.28750000\\ -0.481100000\\ 0.895100000\\ 1.179400000\\ 1.735700000\\ 0.336900000\\ 0.971100000\\ -0.433100000\\ 2.270800000\\ 2.873200000\\ 2.873200000\\ 2.635300000\\ 2.432200000\\ 0.781500000\\ 0.140300000\\ 1.417700000\\ \end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.462300000 -2.138600000 -2.865500000 -0.806900000 -1.187400000 0.467100000 1.295900000 0.312700000 -0.576100000 -0.234200000 1.031000000 1.369300000 1.8708000000	-0.69430000 0.54100000 -1.858900000 -3.20590000 -3.20590000 -3.266030000 -3.400000 -3.79550000 -4.91720000 -3.79550000 -4.11950000 -2.53170000 -2.53170000 -2.93810000 -1.27030000 -0.53530000 -1.38980000 -0.63550000 -1.69350000 -1.69350000
$ \begin{array}{c} 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.34450000\\ -0.97450000\\ 0.28750000\\ -0.481100000\\ 0.895100000\\ 1.179400000\\ 1.735700000\\ 0.336900000\\ 0.971100000\\ -0.433100000\\ 2.270800000\\ 2.873200000\\ 2.873200000\\ 2.873200000\\ 2.432200000\\ 0.781500000\\ 0.781500000\\ 0.140300000\\ 1.417700000\\ -0.301300000\end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.462300000 -2.138600000 -2.865500000 -3.865500000 -3.865900000 -1.187400000 0.467100000 1.295900000 0.312700000 -0.5761000000 -0.5761000000 -0.234200000 -0.234200000 -0.31000000 1.369300000 1.870800000 0.797300000	-0.69430000 0.54100000 -1.85890000 -3.20590000 -3.20590000 -3.26030000 -3.13400000 -3.66300000 -4.91720000 -3.79550000 -4.91720000 -3.79550000 -4.11950000 -2.61710000 -2.53170000 -2.53170000 -2.53170000 -1.27030000 -1.38980000 -0.04550000 -1.69350000 -2.44770000
$ \begin{array}{c} 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.37450000\\ -0.97450000\\ -0.8750000\\ -0.481100000\\ 1.73500000\\ 1.73570000\\ 0.33690000\\ 0.33690000\\ 0.971100000\\ -0.43310000\\ 2.27080000\\ 2.873200000\\ 2.873200000\\ 2.929900000\\ 1.635300000\\ 2.43220000\\ 0.78150000\\ 0.781500000\\ 0.14030000\\ 1.417700000\\ -0.30130000\\ -0.907100000\\ \end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.462300000 -2.138600000 -2.865500000 -2.865500000 -1.187400000 0.467100000 0.467100000 0.312700000 -0.576100000 -0.576100000 -0.234200000 -0.234200000 1.31000000 1.369300000 1.870800000 0.797300000 1.705200000	-0.69430000 0.54100000 -1.85890000 -1.53990000 -3.20590000 -3.20590000 -3.96030000 -3.13400000 -3.66300000 -4.91720000 -4.91720000 -4.55450000 -2.61710000 -2.93810000 -2.93810000 -1.38980000 -0.04550000 -1.69350000 -2.44770000 -2.54910000
$ \begin{array}{c} 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.34450000\\ -0.3450000\\ -0.8750000\\ -0.481100000\\ -0.481100000\\ 1.73570000\\ 0.33690000\\ 0.33690000\\ 0.971100000\\ -0.43310000\\ 2.27080000\\ 2.87320000\\ 2.87320000\\ 2.87320000\\ 2.432200000\\ 1.635300000\\ 2.432200000\\ 1.43200000\\ 0.78150000\\ 0.14030000\\ 0.14030000\\ -0.301300000\\ -0.907100000\\ -1.197200000\\ \end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.138600000 -2.138600000 -2.865500000 -0.806900000 -1.187400000 0.467100000 1.295900000 0.312700000 -0.576100000 -0.234200000 -0.234200000 -0.31000000 1.369300000 1.870800000 0.797300000 1.705200000 -0.357200000	-0.69430000 0.54100000 -1.85890000 -1.53990000 -3.20590000 -3.96030000 -3.13400000 -3.66630000 -4.91720000 -4.91720000 -4.91720000 -4.55450000 -2.61710000 -2.53170000 -2.93810000 -1.27030000 -1.38980000 -0.4550000 -1.69350000 -2.54910000 -2.54910000 -1.98810000
$ \begin{array}{c} 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.34450000\\ -0.97450000\\ 0.28750000\\ -0.481100000\\ 0.895100000\\ 1.79400000\\ 1.735700000\\ 0.33690000\\ 0.971100000\\ -0.433100000\\ 2.270800000\\ 2.873200000\\ 2.873200000\\ 2.873200000\\ 2.432200000\\ 1.635300000\\ 2.432200000\\ 0.781500000\\ 0.140300000\\ -0.401300000\\ -0.907100000\\ -0.907100000\\ -1.97200000\\ -1.846200000\\ \end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.138600000 -2.138600000 -2.865500000 -0.806900000 -1.187400000 0.467100000 1.295900000 0.312700000 -0.576100000 -0.234200000 -0.234200000 -0.369300000 1.369300000 1.369300000 1.705200000 -0.357200000 -0.016500000	-0.69430000 0.54100000 -1.85890000 -1.53990000 -3.20590000 -3.20590000 -3.96030000 -3.13400000 -3.66630000 -4.91720000 -4.91720000 -4.91720000 -4.91720000 -2.53170000 -2.53170000 -2.53170000 -2.53310000 -1.27030000 -1.38980000 -0.64950000 -2.54910000 -1.98810000 -0.64960000
$\begin{array}{c} 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 6$	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.34450000\\ -0.97450000\\ 0.28750000\\ -0.481100000\\ 0.895100000\\ 1.179400000\\ 1.735700000\\ 0.336900000\\ 0.971100000\\ -0.433100000\\ 2.270800000\\ 2.873200000\\ 2.873200000\\ 2.873200000\\ 2.432200000\\ 0.781500000\\ 0.140300000\\ -0.301300000\\ -0.301300000\\ -0.301300000\\ -0.907100000\\ -1.846200000\\ -1.846200000\\ -2.449800000\\ \end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.462300000 -2.138600000 -2.865500000 -0.806900000 -1.187400000 0.467100000 1.295900000 0.312700000 -0.234200000 -0.234200000 -0.234200000 -0.31000000 1.369300000 1.369300000 1.870800000 0.797300000 0.357200000 -0.016500000 -5.500900000	-0.69430000 0.54100000 -1.85890000 -3.20590000 -3.20590000 -3.2630000 -3.13400000 -3.1400000 -3.79550000 -4.91720000 -3.79550000 -4.11950000 -2.617100000 -2.53170000 -2.93810000 -1.27030000 -1.27030000 -1.38980000 -0.4550000 -1.69350000 -2.44770000 -2.54910000 -2.54910000 -0.64960000 0.32880000
$\begin{array}{c}1\\6\\6\\1\\6\\1\\1\\6\\8\\6\\1\\1\\6\\1\\6\\6\\1\\6\\6\\1\\6\\6\\1\\6\\6\\1\end{array}$	1.34900000 0.09480000 -0.34450000 -0.974500000 0.287500000 -0.481100000 0.895100000 1.179400000 1.735700000 0.336900000 0.971100000 -0.433100000 2.270800000 2.873200000 2.873200000 2.432200000 0.781500000 0.140300000 1.417700000 -0.301300000 -1.197200000 -1.846200000 -2.49800000 -2.49800000 -2.301300000	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.462300000 -2.138600000 -2.865500000 -3.865500000 -3.865500000 -1.187400000 1.295900000 -0.467100000 -0.5761000000 -0.234200000 -0.234200000 -0.368000000 1.369300000 1.369300000 1.369300000 1.705200000 -0.357200000 -0.357200000 -0.550090000 -5.500900000 -5.500900000	-0.69430000 0.54100000 -1.85890000 -3.20590000 -3.20590000 -3.26630000 -3.3400000 -3.79550000 -4.91720000 -3.79550000 -4.11950000 -2.61710000 -2.61710000 -2.53170000 -2.53170000 -1.27030000 -0.53530000 -1.69350000 -0.44770000 -2.54910000 -2.54910000 -0.52880000 0.32880000 0.65590000
$\begin{matrix} 1 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 8 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1$	1.34900000 0.09480000 -0.34450000 -0.97450000 0.28750000 -0.481100000 0.895100000 1.179400000 1.73570000 0.336900000 0.971100000 -0.433100000 2.873200000 2.873200000 2.873200000 2.432200000 0.781500000 0.140300000 1.417700000 -0.301300000 -1.97200000 -1.846200000 -2.301300000 -2.301300000 -2.301300000 -1.241700000	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.462300000 -2.138600000 -2.865500000 -2.865500000 -1.187400000 0.467100000 1.295900000 0.312700000 -0.5761000000 -0.34200000 -0.34200000 1.369300000 1.369300000 1.369300000 1.705200000 0.357200000 -0.358600000 -0.357200000 -0.358600000 -0.358600000 -0.357200000 -0.3586000000 -0.3586000000 -0.3586000000 -0.3586000000 -0.3586000000 -0.3586000000 -0.3586000000 -0.3586000000000000000000000000000000000000	-0.69430000 0.54100000 -1.85890000 -1.53990000 -3.20590000 -3.2630000 -3.13400000 -3.13400000 -3.79550000 -4.91720000 -3.79550000 -4.91720000 -3.79550000 -4.11950000 -2.61710000 -2.53170000 -2.53170000 -2.53170000 -1.27030000 -1.38980000 -0.04550000 -1.98810000 -1.98810000 0.64960000 0.32880000 0.65690000 -0.0820000
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$\begin{matrix} 1 & 6 & 6 \\ 1 & 6 & 1 \\ 1 & 1 & 6 \\ 8 & 6 & 1 \\ 1 & 1 & 6 \\ 1 & 6 & 1 \\ 6 & 1 & 6 \\ 1 & 6 & 6 \\ 1 & 8 & 6 \\ 1 \\ 8 & 6 \\ 1 \\ 8 \\ 1 \\ 8 \\ 1 \\ 8 \\ 1 \\ 8 \\ 1 \\ 8 \\ 1 \\ 1$	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.34450000\\ -0.97450000\\ 0.28750000\\ -0.481100000\\ 0.895100000\\ 1.179400000\\ 1.735700000\\ 0.336900000\\ 0.971100000\\ -0.433100000\\ 2.270800000\\ 2.873200000\\ 2.873200000\\ 2.873200000\\ 2.432200000\\ 0.781500000\\ 0.140300000\\ -1.417700000\\ -0.301300000\\ -0.907100000\\ -1.197200000\\ -1.846200000\\ -2.301300000\\ -2.449800000\\ -2.449800000\\ -2.41700000\\ -3.436400000\\ -4.319700000\\ -3.78750000\\ -3.7875000\\ -3.78750000\\ -3.78750000\\ -3.7875000$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.462300000 -2.138600000 -2.865500000 -2.865500000 -1.187400000 -1.487400000 -0.467100000 -0.312700000 -0.312700000 -0.23800000 -0.234200000 -0.234200000 -0.234200000 -0.357200000 -0.357200000 -0.357200000 -5.500900000 -5.500900000 -5.500900000 -5.487100000 -5.487100000 -6.075700000	-0.69430000 0.54100000 -1.85890000 -3.20590000 -3.20590000 -3.26630000 -3.79550000 -4.91720000 -3.79550000 -4.91720000 -3.79550000 -4.11950000 -2.61710000 -2.53170000 -2.53170000 -1.27030000 -1.27030000 -1.27030000 -1.59350000 -1.4770000 -2.54910000 -2.54910000 -2.54910000 -0.64960000 0.32880000 0.65690000 -0.85460000 -0.85460000 -0.85460000 -0.85460000 -0.564500
$\begin{array}{c}1\\6\\6\\1\\6\\1\\1\\6\\8\\6\\1\\1\\6\\1\\6\\1\\6\\6\\1\\8\\6\\1\\8\\6\\1\\8\\.\end{array}$	1.34900000 0.09480000 -0.34450000 0.287500000 0.287500000 0.287500000 1.179400000 1.735700000 0.336900000 0.971100000 -0.433100000 2.270800000 2.873200000 2.873200000 2.432200000 0.781500000 0.140300000 1.417700000 -0.301300000 -1.197200000 -1.846200000 -2.449800000 -2.301300000 -2.41700000 -3.436400000 -2.787500000 -2.787500000	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.462300000 -2.138600000 -2.865500000 -2.865500000 -3.865900000 -1.187400000 1.295900000 -0.467100000 -0.5761000000 -0.5761000000 -0.234200000 -0.234200000 -0.357200000 -0.357200000 -0.357200000 -5.500900000 -5.538600000 -5.538600000 -5.487100000 -6.074900000 -6.074900000 -6.074900000	-0.69430000 0.54100000 -1.85890000 -3.20590000 -3.20590000 -3.26630000 -3.3400000 -3.79550000 -4.91720000 -3.79550000 -4.91720000 -3.79550000 -4.11950000 -2.61710000 -2.53170000 -2.53170000 -2.53170000 -1.27030000 -0.53530000 -0.53530000 -0.45500000 -1.69350000 -2.54910000 -2.54910000 -0.52880000 0.65690000 -0.85460000 -0.85460000 -0.85460000 -0.56450000 -1.949200000 -1.9492
$\begin{array}{c} 1 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 6 \\ 8 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 8 \\ 6 \\ 1 \\ 8 \\ 1 \\ 8 \\ 1 \\ 8 \\ 1 \\ 8 \\ 1 \\ 1$	1.34900000 0.09480000 -0.34450000 -0.974500000 -0.87500000 -0.481100000 0.895100000 1.179400000 1.735700000 0.336900000 0.971100000 -0.433100000 2.873200000 2.873200000 2.873200000 2.432200000 0.781500000 0.140300000 -1.417700000 -0.301300000 -1.197200000 -1.846200000 -2.449800000 -2.449800000 -2.449800000 -3.436400000 -3.436400000 -3.373500000 -3.373500000	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.462300000 -2.138600000 -2.865500000 -2.865500000 -2.865500000 -1.187400000 0.467100000 -1.295900000 -0.576100000 -0.576100000 -0.234200000 -0.234200000 -0.234200000 -0.68000000 1.369300000 1.369300000 1.369300000 1.357200000 -0.357200000 -0.357200000 -6.538600000 -5.50090000 -5.50990000 -5.5487100000 -6.075700000 -6.074900000 -6.075700000 -6.03500000	-0.69430000 0.54100000 -1.85890000 -3.20590000 -3.20590000 -3.26030000 -3.13400000 -3.13400000 -3.13400000 -3.6630000 -4.91720000 -3.79550000 -4.91720000 -3.79550000 -4.11950000 -2.61710000 -2.53170000 -2.53170000 -2.53170000 -2.53170000 -2.5310000 -1.27030000 -1.38980000 -0.55500000 -2.54910000 -2.54910000 -3.580000 0.649600000 0.64960000 0.68540000 -0.85460000 -0.85460000 -0.56450000 -1.94920000 -2.71950000 -2.71950000
$\begin{matrix} 1 & 6 & 6 \\ 1 & 6 & 1 \\ 1 & 1 & 6 & 8 \\ 6 & 1 & 1 & 6 & 1 \\ 1 & 6 & 1 & 6 & 6 & 1 \\ 1 & 6 & 6 & 1 & 8 & 6 \\ 1 & 8 & 6 & 1 & 8 \\ 1 & 8 & 1 & 6 \\ 1 & 8 & 6 & 1 \\ 1 & 8 & 6 & 1 \\ 1 & 8 & 6 & 1 \\ 1 & 1 & 6 & 1 \\ 1 & 1 & 6 & 1 \\ 1 & 1 & 6 & 1 \\ 1 & 1 & 6 & 1 \\ 1 & 1 & 6 & 1 \\ 1 & 1 & 6 & 1 \\ 1 & 1 & 6 & 1 \\ 1 & 1 & 6 & 1 \\ 1 & 1 & 6 & 1 \\ 1 & 1 & 6 & 1 \\ 1 & 1 & 6 & 1 \\ 1 & 1 & 6 & 1 \\ 1 & 1 & 6 & 1 \\ 1 & 1 & 6 & 1 \\ 1 & 1 & 6 & 1 \\ 1 & 1 & 6 & 1 \\ 1 & 1 & 6 & 1 \\ 1 & 1 & 1 & 6 \\ 1 & 1 & 1 & 6 \\ 1 & 1 & 1 & 6 \\ 1 & 1 & 1 & 6 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 &$	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.37450000\\ -0.3750000\\ -0.481100000\\ -0.481100000\\ 1.735700000\\ 1.73570000\\ 0.33690000\\ 0.33690000\\ 0.971100000\\ -0.43310000\\ 2.270800000\\ 2.873200000\\ 2.873200000\\ 2.873200000\\ 2.432200000\\ 1.635300000\\ 2.432200000\\ 0.781500000\\ 0.781500000\\ 0.140300000\\ -1.417700000\\ -0.301300000\\ -1.97200000\\ -1.846200000\\ -2.301300000\\ -2.449800000\\ -2.301300000\\ -1.241700000\\ -3.436400000\\ -3.375500000\\ -3.908100000\\ -3.908100000\\ \end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.462300000 -2.138600000 -2.865500000 -2.865500000 -0.806900000 -1.187400000 0.467100000 -1.295900000 -0.576100000 -0.576100000 -0.234200000 -0.234200000 -0.234200000 -0.234200000 -0.357200000 -0.357200000 -0.357200000 -0.357200000 -5.580900000 -5.580900000 -5.580900000 -5.580900000 -5.487100000 -6.075700000 -6.075700000 -6.075700000 -6.03500000 -4.060000000	$\begin{array}{l} -0.69430000\\ 0.54100000\\ -1.858900000\\ -1.858900000\\ -3.205900000\\ -3.205900000\\ -3.960300000\\ -3.960300000\\ -3.13400000\\ -3.666300000\\ -4.917200000\\ -4.917200000\\ -4.917200000\\ -4.554500000\\ -2.617100000\\ -2.531700000\\ -2.531700000\\ -2.938100000\\ -1.389800000\\ -0.545500000\\ -1.389800000\\ -0.649500000\\ -2.549100000\\ -1.988100000\\ -0.649600000\\ -0.854600000\\ -0.854600000\\ -0.854600000\\ -0.564500000\\ -0.564500000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.59800000\\ -1.59800000\\ -1.59800000\\ -1.59800000\\ -1.59800000\\ -1.59800000\\ -1.59800000\\ -1.59800000\\ -1.59800000\\ -1.59800000\\ -1.59800000\\ -1.5980000\\ -1.59800000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.598000\\ -1.598000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.5980000\\ -1.598000\\ -1.598000\\ -1.598000\\ -1.598000\\ -1.598000\\ -1.598000\\ -1.598000\\ -1.59800\\ -1.598000\\ -1.598000\\ -1.598000\\ -1.598000\\ -1.$
$\begin{array}{c}1\\6\\6\\1\\6\\1\\1\\6\\8\\6\\1\\1\\6\\1\\6\\1\\6\\1\\6\\1\\$	$\begin{array}{c} 1.34900000\\ 0.09480000\\ -0.34450000\\ -0.34450000\\ -0.97450000\\ 0.28750000\\ -0.481100000\\ 1.73500000\\ 1.73570000\\ 0.33690000\\ 0.33690000\\ 0.971100000\\ -0.43310000\\ 2.27080000\\ 2.873200000\\ 2.87320000\\ 2.87320000\\ 2.432200000\\ 1.635300000\\ 2.432200000\\ 1.43200000\\ 0.781500000\\ 0.14030000\\ 0.14030000\\ 0.14030000\\ 0.14030000\\ -1.97200000\\ -1.84620000\\ -2.301300000\\ -2.301300000\\ -2.449800000\\ -2.301300000\\ -3.436400000\\ -3.373500000\\ -3.908100000\\ -3.066500000\\ \end{array}$	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.462300000 -2.865500000 -2.865500000 -2.865500000 -0.806900000 0.467100000 0.467100000 0.312700000 -0.576100000 -0.576100000 -0.234200000 -0.234200000 -0.68000000 1.369300000 1.369300000 1.369300000 0.797300000 0.797300000 0.797300000 -0.357200000 -0.357200000 -5.580900000 -5.580900000 -6.075700000 -6.075700000 -6.075700000 -6.075700000 -6.03500000 -4.060000000 -3.480900000	$\begin{array}{l} -0.69430000\\ 0.54100000\\ -1.85890000\\ -1.85890000\\ -1.53990000\\ -3.20590000\\ -3.20590000\\ -3.96030000\\ -3.66630000\\ -3.66630000\\ -3.79550000\\ -4.91720000\\ -4.91720000\\ -4.91720000\\ -2.53170000\\ -2.53170000\\ -2.53170000\\ -2.53170000\\ -2.53170000\\ -2.53170000\\ -2.53170000\\ -2.53170000\\ -2.53170000\\ -2.53170000\\ -2.53170000\\ -2.53170000\\ -2.53170000\\ -2.53170000\\ -2.53170000\\ -2.53170000\\ -2.54910000\\ -3.2880000\\ -0.64960000\\ -0.8540000\\ -0.85460000\\ -0.56450000\\ -1.5980000\\ -1.59910000\\ -1.59910000\\ -1.59910000\\ -1.59910000\\ \end{array}$
$\begin{matrix} 1 & 6 & 6 \\ 1 & 6 & 1 \\ 1 & 1 & 6 \\ 8 & 6 & 1 \\ 1 & 1 & 6 \\ 1 & 6 & 1 \\ 6 & 1 & 6 \\ 1 & 6 & 6 \\ 1 & 8 & 6 \\ 1 & 8 \\ 1 & 1 & 1 \\ 1 $	1.34900000 0.09480000 -0.34450000 -0.974500000 0.287500000 0.287500000 1.179400000 1.179400000 1.735700000 0.336900000 0.971100000 -0.433100000 2.270800000 2.873200000 2.873200000 1.635300000 2.43220000 0.781500000 0.140300000 -1.97200000 -1.97200000 -1.846200000 -2.301300000 -2.301300000 -2.449800000 -2.449800000 -2.449800000 -2.4787500000 -3.787500000 -3.9081000000 -3.90810	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.462300000 -2.138600000 -2.865500000 -2.865500000 -1.187400000 0.467100000 1.295900000 -0.312700000 -0.576100000 -0.234200000 -0.234200000 -0.234200000 -0.234200000 -0.357200000 0.797300000 1.369300000 1.870800000 0.357200000 -0.357200000 -5.500900000 -5.500900000 -5.487100000 -6.075700000 -6.075700000 -6.075700000 -6.075700000 -6.074900000 -4.060000000 -3.480900000 -4.156500000	-0.69430000 0.54100000 -1.85890000 -3.20590000 -3.20590000 -3.20590000 -3.26630000 -3.13400000 -3.79550000 -4.91720000 -3.79550000 -4.11950000 -2.61710000 -2.53170000 -2.53170000 -1.27030000 -1.27030000 -1.27030000 -1.49350000 -1.49350000 -2.44770000 -2.44770000 -2.54910000 -0.64960000 0.65690000 -0.85460000 -0.85460000 -0.85460000 -0.56450000 -1.5980000 -1.56910000 -2.10530000 -2.10530000
$\begin{matrix} 1 & 6 & 6 \\ 1 & 6 & 1 \\ 1 & 1 & 6 \\ 8 & 6 & 1 \\ 1 & 1 & 6 \\ 1 & 6 & 1 \\ 6 & 1 & 6 \\ 1 & 6 & 6 \\ 1 & 8 & 6 \\ 1 & 8 & 1 \\ 1 & 8 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\$	1.34900000 0.09480000 -0.34450000 -0.974500000 0.287500000 -0.481100000 0.895100000 1.179400000 1.179400000 0.336900000 0.971100000 -0.433100000 2.270800000 2.432200000 1.635300000 2.43220000 0.781500000 0.140300000 -1.417700000 -1.39700000 -1.846200000 -2.449800000 -2.449800000 -2.449800000 -2.449800000 -2.787500000 -3.373500000 -3.908100000 -3.908100000 -3.908100000 -3.908100000 -3.908100000 -3.908100000 -3.943500000 -3.958200000	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.462300000 -2.138600000 -2.138600000 -2.865500000 -3.865500000 -1.187400000 0.467100000 -1.295900000 -0.576100000 -0.576100000 -0.234200000 -0.234200000 -0.234200000 -0.357200000 1.369300000 1.369300000 1.357200000 -0.357200000 -5.500900000 -5.50090000 -5.538600000 -5.487100000 -6.075700000 -6.075700000 -6.075700000 -3.48900000 -3.48900000 -3.283100000	-0.69430000 0.54100000 -1.85890000 -1.53990000 -3.20590000 -3.20590000 -3.26630000 -3.79550000 -4.91720000 -3.79550000 -4.11950000 -2.61710000 -2.53170000 -2.53170000 -2.53170000 -0.53530000 -0.3550000 -1.69350000 -0.4550000 -0.64550000 -0.64500000 -0.56450000 -0.56450000 -0.56450000 -1.5980000 -1.5980000 -1.5980000 -1.5980000 -1.5980000 -1.5980000 -1.5980000 -1.5980000 -1.5980000 -1.5980000 -1.5910000 -2.22510000 -2.22510000
$\begin{array}{c}1\\6\\6\\1\\6\\1\\1\\6\\8\\6\\1\\8\\1\\1\\8\\1\\1\\8\\1\\1\\8\\1\\1\\8\\1\\1\\8\\1\\1\\8\\1\\1\\8\\1$	1.34900000 0.09480000 -0.34450000 -0.974500000 0.287500000 -0.481100000 0.895100000 1.179400000 1.179400000 0.336900000 0.971100000 -0.433100000 2.873200000 2.873200000 2.873200000 2.432200000 0.781500000 0.140300000 -1.417700000 -1.397100000 -1.197200000 -1.449800000 -2.449800000 -2.449800000 -2.449800000 -2.787500000 -3.373500000 -3.373500000 -3.908100000 -3.375500000 -3.908100000 -3.375500000 -3.908100000 -3.375500000 -3.908100000 -3.375500000 -3.908100000 -3.375500000 -3.908100000 -3.375500000 -3.908100000 -3.375200000 -3.375500000 -3.37	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.462300000 -2.138600000 -2.865500000 -2.865500000 -2.865500000 -3.12700000 -0.467100000 -1.187400000 -0.576100000 -0.576100000 -0.234200000 -0.234200000 -0.234200000 -0.368000000 -1.369300000 -3.57200000 -0.357200000 -0.357200000 -6.538600000 -5.500900000 -5.509900000 -6.538600000 -5.5487100000 -6.075700000 -6.075700000 -6.074900000 -3.283100000 -3.283100000 -3.377700000	-0.69430000 0.54100000 -1.85890000 -1.53990000 -3.20590000 -3.20590000 -3.26630000 -3.13400000 -3.79550000 -4.91720000 -3.79550000 -4.11950000 -2.61710000 -2.61710000 -2.53170000 -2.53170000 -2.53170000 -1.27030000 -0.53530000 -0.53530000 -0.45500000 -1.69350000 -2.54910000 -2.54910000 -0.5850000 0.65690000 -0.85460000 -0.85460000 -0.56450000 -1.5980000 -1.5980000 -1.5910000 -2.71950000 -1.5930000 -2.251000000 -2.251000000 -2.251000000 -2.25100000 -2.25100000000 -2.251000000 -2.25
$\begin{matrix} 1 & 6 & 6 \\ 1 & 6 & 1 \\ 1 & 6 & 8 & 6 \\ 1 & 1 & 6 & 1 \\ 1 & 6 & 1 & 6 & 1 \\ 1 & 6 & 6 & 1 \\ 1 & 8 & 6 & 1 \\ 1 & 8 & 1 & 6 \\ 1 & 1 & 1 & 6 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 &$	1.34900000 0.09480000 -0.34450000 -0.97450000 0.28750000 0.28750000 -0.481100000 0.895100000 1.179400000 0.33690000 0.971100000 -0.433100000 2.270800000 2.873200000 2.873200000 2.873200000 2.432200000 0.781500000 0.140300000 -1.417700000 -0.301300000 -1.44700000 -1.846200000 -1.846200000 -2.449800000 -2.301300000 -2.787500000 -3.373500000 -3.908100000 -3.908100000 -3.908100000 -3.94500000 -3.96500000 -3.96500000 -3.96500000 -4.376300000 -5.358200000 -5.254100000	-2.289200000 -1.046200000 -1.623300000 -2.462300000 -2.462300000 -2.138600000 -2.865500000 -2.865500000 -2.865500000 -1.187400000 0.467100000 -1.295900000 -0.576100000 -0.576100000 -0.34200000 -0.234200000 -0.234200000 -0.369300000 -1.369300000 1.369300000 -1.369300000 -3.57200000 -0.357200000 -6.358600000 -5.38600000 -5.38600000 -5.487100000 -6.075700000 -6.075700000 -6.075700000 -3.480900000 -3.480900000 -3.480900000 -3.283100000 -3.283100000 -3.283100000 -3.377700000	-0.69430000 0.54100000 -1.85890000 -3.20590000 -3.20590000 -3.26630000 -3.13400000 -3.13400000 -3.13400000 -3.79550000 -4.91720000 -3.79550000 -4.91720000 -2.61710000 -2.63170000 -2.53170000 -2.53170000 -2.53170000 -2.53170000 -3.5300000 -1.27030000 -1.38980000 -0.45500000 -1.98810000 -0.564500000 -0.85460000 -0.85460000 -0.56450000 -1.5980000 -1.5990000 -1.5990000 -2.21050000 -2.22510000 0.136700000 0.52590000
$\begin{smallmatrix} 1 & 6 & 6 \\ 1 & 6 & 1 \\ 1 & 6 & 8 & 6 \\ 1 & 1 & 6 & 1 \\ 1 & 6 & 1 & 6 & 1 \\ 1 & 6 & 1 & 6 & 6 & 6 \\ 1 & 8 & 6 & 1 & 8 & 1 \\ 1 & 6 & 1 & 6 & 1 \\ 1 & 6 & 1 & 6 & 1 \\ 1 & 6 & 1 & 6 & 1 \\ 1 & 6 & 1 & 6 & 1 \\ 1 & 6 & 1 & 6 & 1 \\ 1 & 6 & 1 & 6 & 1 \\ 1 & 6 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1$	1.34900000 0.09480000 -0.34450000 -0.97450000 0.28750000 -0.481100000 1.7940000 1.735700000 0.33690000 0.33690000 0.971100000 -0.43310000 2.270800000 2.873200000 2.873200000 2.873200000 1.635300000 0.781500000 0.140300000 -1.97200000 -1.197200000 -1.846200000 -2.301300000 -2.301300000 -2.449800000 -2.301300000 -3.373500000 -3.37500000 -3.908100000 -3.908100000 -3.908100000 -3.908100000 -3.908100000 -3.908100000 -3.908100000 -3.96500000 -4.943500000 -3.254100000 -5.254100000 -3.246300000	-2.289200000 -1.046200000 -1.046200000 -1.623300000 -2.462300000 -2.462300000 -2.865500000 -2.865500000 -0.806900000 -1.187400000 0.467100000 1.295900000 -0.576100000 -0.34200000 -0.34200000 -0.369300000 1.369300000 1.369300000 1.369300000 -3.57200000 -0.357200000 -0.357200000 -5.580900000 -5.580900000 -5.580900000 -5.487100000 -5.487100000 -6.075700000 -6.075700000 -6.075700000 -3.480900000 -3.480900000 -3.283100000 -3.283100000 -3.283100000 -3.4572000	-0.69430000 0.54100000 -1.85890000 -3.20590000 -3.20590000 -3.26630000 -3.13400000 -3.66630000 -3.13400000 -3.79550000 -4.91720000 -4.91720000 -4.91720000 -2.53170000 -2.53170000 -2.53170000 -2.53170000 -2.53170000 -2.53170000 -2.53170000 -2.53170000 -2.53170000 -2.53170000 -2.53170000 -2.53170000 -2.53170000 -2.54910000 -1.3880000 -0.64960000 -0.64960000 -0.56450000 -0.56450000 -0.56450000 -1.5910000 -1.5910000 -1.56910000 -2.22510000 0.13670000 0.52590000 1.175200000

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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
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8	4.921600000	-0.021000000	0.270100000
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8	6.795300000	-1.355800000	-1.190400000
1	7.009300000	-2.022400000	-1.863000000
6	4.991700000	-2.845600000	-0.538800000
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8	5.452800000	-3.872100000	-1.382200000
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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
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8	4.846400000	3.903100000	-2.481100000
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6	1.546200000	5.262000000	-1.314700000
1	1.011500000	4.322800000	-1.520800000
8	2.331100000	5.638000000	-2.419/00000
6	2 398500000	5.054500000	-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
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1	3.328300000	4.809200000	2.334700000
8	2.095400000	3.436600000	3.101200000
1	1.141900000	3.2/4300000	3.225800000
1	-4.910/00000	3.538500000	1.043300000
8	-4.666200000	2.299500000	0.029800000
6	-4.751900000	4.629700000	-0.440800000
ĩ	-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./55500000	1.384400000
1	-2.446600000	2.795400000	1.723000000
6	-4.009300000	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
6	-5.682300000	-0.933100000	-2.937200000
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	-5.594600000	0.946500000	2./10100000
1	-4./98200000 -5.046200000	0.239600000	2.77300000
8	-6.72860000	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	-1.8/4500000	0.873100000
1	-2.305300000	-0.829300000	-0.333100000
1	-2.434100000 -1 349700000	0.888300000	-0.738900000
0	-1.760400000	-0.208600000	2.05900000
1	1., 00400000	0.20000000	2.037000000
1-A	dOH·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

-3,989200000 -2,459100000 -0.918300000 -3,020200000 -3,02760000 -1.962400000 -7,55200000 -3,800100000 2,057300000 -3,13270000 -3,743900000 0.903900000 -3,14300000 -2,057500000 -1,629800000 -3,46800000 -4,227500000 -2,529400000 -5,782200000 3,833300000 -0,690200000 -6,47000000 3,225800000 -3,0330000 -6,117100000 0.988800000 -3,03300000 -6,117100000 1,98800000 -3,00330000 -5,47200000 -1,267400000 -0,227500000 -5,47200000 -0,267400000 -0,277800000 -5,47200000 5,29400000 -3,31700000 -2,461500000 5,294700000 -0,33700000 -2,47800000 5,294700000 -3,33300000 -3,417300000 5,294700000 -2,83200000 -3,417300000 5,294700000 -2,93400000 -2,25400000 5,695900000 1,447000000 -2,25400000 5,6959000000 1,447000000				
-3.02020000-3.02760000-1.962400000-7.55200000-3.8001000002.057300000-5.83260000-3.743900000.90390000-5.154300000-2.057500000-1.629800000-5.782200003.833300000-0.690200000-6.47000003.225800000.43050000-6.1216000001.815400000.737800000-6.1216000001.708300000-1.648300000-5.143000001.708300000-1.648300000-5.1448600000.99850000-3.003300000-6.6705000001.026740000-0.227500000-5.8068000003.03340000-1.83850000-5.8468000003.03340000-1.838500000-5.8468000005.94600000.247800000-2.4615000006.928300000-0.247800000-2.779000005.242700000-2.83200000-3.8486000005.1034000002.83300000-4.254000005.659000001.98330000-4.255000006.191700000-3.317300000-4.255000006.191700000-3.337800000-4.255000006.291400000-2.328900003.572900005.5935000001.484000001.483000005.6698000001.4911000000.4761000005.93500000-1.457600000-4.757000005.291400000-2.725900003.572900005.935000001.148000001.4676000005.935000001.348000001.4676000005.817900000.1848000001.475000005.9249000005.9249000003.572900005.92490000	6	-3.989200000	-2.459100000	-0.918300000
,352000000 ,3500000 ,13500000	6	-3.020200000	-3.027600000	-1.962400000
-3.13200000 -3.743900000 0.90390000 -3.142700000 -3.743900000 -2.529400000 -3.46800000 -4.22750000 -2.52940000 -5.782200000 3.83330000 -0.690200000 -6.47000000 3.22580000 0.43050000 -6.47000000 1.81540000 0.73780000 -6.47000000 1.81540000 -3.0330000 -5.44860000 0.98850000 -3.03330000 -5.47200000 1.577400000 -5.67500000 -5.84600000 0.82280000 -3.41120000 -5.84600000 0.822800000 -3.41300000 -3.44500000 5.249700000 -0.335700000 -3.44500000 5.23200000 -1.44000000 -3.417300000 5.69900000 -1.435700000 -4.25500000 6.19170000 -3.117300000 -4.25500000 6.3360000 -1.445760000 -4.25500000 5.43700000 -3.37800000 -4.477300000 5.69800000 -1.445760000 -4.25500000 6.33800000 -1.4457600000 -4.477300000	8	-7.552000000	-1.737500000 -3.800100000	1.105900000
-5.154300000 -2.057500000 -1.629800000 -3.468000000 -4.227500000 -2.529400000 -5.782200000 3.83330000 -0.69020000 -6.647000000 3.22580000 0.43050000 -6.117100000 0.98880000 -0.55050000 -5.316700000 1.70830000 -1.64830000 -5.44860000 0.998500000 -3.03300000 -6.670500000 4.02760000 0.227500000 -5.847200000 -0.26740000 -0.227500000 -5.86800000 3.03340000 -1.838500000 -5.77200000 5.94600000 -0.34780000 -2.461500000 6.92830000 -0.34780000 -2.45900000 5.23200000 -1.44000000 -3.448600000 5.23400000 -2.83200000 -4.477300000 5.69900000 -1.45760000 -4.25500000 6.19170000 -3.17300000 -4.25400000 5.638300000 -1.9480000 -4.25400000 5.64800000 1.537800000 -4.477300000 5.9350000 -1.944500000 -4.7790	8 8	-3.132700000	-3.800100000 -3.743900000	2.037300000
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-5.782200003.83330000-0.69020000-6.647000003.225800000.43050000-6.121600001.815400000-0.555500000-5.316700001.70830000-1.648300000-5.316700000.988800000-3.00330000-6.670500004.0276000001.577400000-6.927000001.151500000.688100000-5.947200000.267400000-0.227500000-5.806800003.033400000-1.838500000-7.8464000006.7836000000.87700000-7.846500005.249700000-0.247800000-3.2094000005.249700000-0.335700000-3.4173000005.103400000-2.0330000-4.2254000005.659000001.983300000-4.4255000006.191700000-3.317300000-4.4255000006.98630000-1.9457600000-4.255000006.191700000-3.3173000003.6549000005.6698000001.98330000-4.255000006.291400002.328900001.457000005.817900000.1484800001.6676000005.817900000.148400001.4676000005.817900000.148500003.0786000005.9224000000.2735000003.0786000005.9228000002.7325000003.7795000005.9228000000.1445000005.924900001.409000005.588600003.475000002.718000000.4449000005.588000003.778000000.1435000005.5945000002.718000000.4449000005.5945000002.71800000	8	-3.468000000	-4.227500000	-2.529400000
-6.6470000003.2258000000.430500000-6.1216000001.815400000-0.550500000-5.3167000001.708300000-1.648300000-5.448600000.998500000-3.003300000-6.6705000004.027600000-1.577400000-6.92790000-0.26740000-0.27500000-5.806800003.03340000-1.838500000-5.847200000-0.26740000-0.27500000-1.4214000006.783600000-3.411200000-2.4615000006.9283000000.879700000-3.2094000005.5946000001.012300000-3.4173000005.232200000-1.44000000-3.4173000005.69900000-2.93400000-4.255000007.3204000002.033400000-4.255000006.191700000-3.81860000-4.4773000005.698000001.4957600000-4.255000006.191700000-3.81300000-4.4773000005.698000001.4911000003.6549000005.698000001.4911000000.8675000006.291400000-2.328900001.4833000005.593500002.723500000.7757000006.22940000-2.328900003.5729000005.92240000-1.4465000003.586000005.817900000.1445000005.5886000005.817900000.1445000005.5886000005.271800000-2.316300005.5886000003.81100000-2.414000005.5886000003.81100000-4.444900005.5886000003.881100000-4.444900005.588600000-2.	6	-5.782200000	3.833300000	-0.690200000
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-5.806800003.03340000-1.83850000-6.786400000.88280000-3.41120000-1.421400006.78360000-0.24780000-2.461500006.928300000.879700000-3.209400005.594600001.012300000-3.848600005.24970000-0.335700000-2.779000005.223200000-1.44000000-3.4173000005.1034000002.09340000-4.254000005.659000001.983300000-4.254000005.65900000-1.457600000-2.031900006.43730000-1.457600000-4.255500006.191700000-3.1173000003.6549000005.6698000001.537800001.4833000005.6698000001.4911000000.8875000006.29140000-2.328900001.4570000005.5935000002.7235000000.757000005.9240000-0.8886000001.415000007.68080000-2.316300000.4761000005.817900000.144500005.924000001.445000005.924000001.541600004.6214000002.9780000-2.316300005.7295000003.34150000-3.41300005.586000003.88110000-1.445000005.586000003.88110000-1.445000005.7295000002.77080000-0.4464000006.43500000-2.31630000-1.445000005.7295000003.3560000-1.445000005.729500000-3.55590000-1.445000005.729500000-3.77580000-1.918600005.729500000-1.44600	8	-5.547200000	-0.267400000	-0.227500000
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$\begin{array}{c} -3.29400000 & 5.29400000 & -1.01250000 \\ -3.417300000 & 5.223200000 & -1.440000000 \\ -3.417300000 & 5.103400000 & 2.83200000 \\ -1.886800000 & 7.320400000 & 2.093400000 \\ -4.225400000 & 5.659000000 & 1.983300000 \\ -4.225400000 & 5.659000000 & -0.194500000 \\ -2.031900000 & 6.437300000 & -1.457600000 \\ -4.255500000 & 6.191700000 & -3.117300000 \\ 3.654900000 & 5.450100000 & 0.283300000 \\ 2.973300000 & 6.033600000 & 1.537800000 \\ 1.483300000 & 5.669800000 & 1.491100000 \\ 0.887500000 & 6.201800000 & 0.184800000 \\ 1.667600000 & 5.638300000 & -1.014800000 \\ 1.215000000 & 6.291400000 & -2.328900000 \\ 3.572900000 & 5.817900000 & 0.140800000 \\ 3.058600000 & 5.922400000 & -0.888600000 \\ 0.476100000 & 5.817900000 & 0.140800000 \\ 3.058600000 & 5.922400000 & -0.388600000 \\ 1.410500000 & 7.680800000 & -2.316300000 \\ 6.329200000 & 0.925800000 & 0.134500000 \\ 5.924900000 & 1.400900000 & 1.541600000 \\ 4.621400000 & 2.199500000 & 1.446500000 \\ 4.621400000 & 2.199500000 & 0.444900000 \\ 5.58800000 & 3.881100000 & -1.918600000 \\ 5.729500000 & 0.335600000 & 2.431900000 \\ 4.252900000 & 2.751800000 & 0.44490000 \\ 5.58800000 & 4.043100000 & 0.346300000 \\ 6.43800000 & 4.74360000 & -1.441600000 \\ 5.88600000 & -3.555900000 & -1.441600000 \\ 5.88600000 & -3.555900000 & -1.443700000 \\ 6.643500000 & -3.555900000 & -1.916800000 \\ 5.943500000 & -1.95800000 & -0.749800000 \\ 5.943500000 & -1.95800000 & -0.749800000 \\ 5.551000000 & -3.555900000 & -0.446400000 \\ 6.43800000 & -0.749800000 \\ 5.943500000 & -1.769600000 & -0.327900000 \\ 5.943500000 & -1.95600000 & -3.127600000 \\ 5.943500000 & -1.769600000 & -3.127600000 \\ 5.384500000 & -3.01040000 & -2.422700000 \\ 5.343900000 & -5.756200000 & -3.122100000 \\ 2.684300000 & -5.756200000 & -3.122100000 \\ 2.11200000 & -5.756200000 & -1.681600000 \\ 3.211600000 & -5.756200000 & -1.681600000 \\ 3.211600000 & -5.756200000 & -1.681600000 \\ 3.211600000 & -5.756200000 & -1.681600000 \\ 3.211600000 & -5.756200000 & -1.681600000 \\ 3.211600000 & -5.756200000 & -1.681600000 \\ 3.211200000 & -5.756200000 & -1.6816000$	6	-2.461500000	6.928300000 5.594600000	0.8/9/00000
$\begin{array}{c} -2.779000000 & 5.223200000 & -1.440000000\\ -3.417300000 & 5.203200000 & -2.832000000\\ -1.886800000 & 7.320400000 & 2.093400000\\ -4.225400000 & 5.659000000 & 1.983300000\\ -4.225400000 & 6.437300000 & -1.457600000\\ -2.031900000 & 6.437300000 & -1.457600000\\ -4.255500000 & 6.191700000 & -3.117300000\\ 3.654900000 & 5.450100000 & 0.283300000\\ 2.973300000 & 6.033600000 & 1.537800000\\ 1.483300000 & 5.669800000 & 1.491100000\\ 0.887500000 & 6.201800000 & 0.184800000\\ 1.667600000 & 5.638300000 & -1.014800000\\ 1.215000000 & 6.291400000 & -2.328900000\\ 3.572900000 & 5.593500000 & 2.723500000\\ 0.775700000 & 6.229800000 & 2.570400000\\ -0.476100000 & 5.817900000 & 0.140800000\\ 3.058600000 & 5.922400000 & -0.888600000\\ 1.410500000 & 7.680800000 & 2.316300000\\ 6.329200000 & 0.925800000 & 0.134500000\\ 5.924900000 & 1.400900000 & 1.541600000\\ 4.621400000 & 2.199500000 & 0.444900000\\ 5.258900000 & 2.770800000 & -0.911900000\\ 5.588600000 & 3.881100000 & -1.918600000\\ 5.729500000 & 2.751800000 & 2.431900000\\ 4.252900000 & 2.751800000 & 2.431900000\\ 6.438600000 & -3.959100000 & -1.443700000\\ 6.438600000 & -3.959100000 & -1.443600000\\ 5.551000000 & -3.959100000 & -1.916800000\\ 5.551000000 & -3.959100000 & -1.916800000\\ 5.588600000 & -1.95600000 & -0.749800000\\ 6.43800000 & -1.747600000 & -1.916800000\\ 5.551000000 & -3.55900000 & -0.446400000\\ 6.643500000 & -3.55900000 & 0.23127600000\\ 5.943500000 & -1.769600000 & -3.127600000\\ 5.362800000 & -1.769600000 & -3.127600000\\ 5.362800000 & -7.033300000 & -2.42200000\\ 5.943500000 & -7.07300000 & -3.122100000\\ 2.55900000 & -5.520800000 & -1.681600000\\ 5.38300000 & -5.52080000 & -1.681600000\\ 3.24200000 & -5.7500000 & -3.122100000\\ 2.684300000 & -5.75020000 & -3.122100000\\ 2.684300000 & -5.750200000 & -1.681600000\\ 3.211600000 & -5.756200000 & -1.681600000\\ 3.211600000 & -5.756200000 & -1.681600000\\ 3.211600000 & -5.756200000 & -1.681600000\\ 3.211600000 & -5.756200000 & -1.681600000\\ 3.211200000 & -5.756200000 & -1.681600000\\ 3.211200000 & -5.756200000 & -1.681600000\\ 3.211200000 & -5.75$	6	-3.209400000	5 249700000	-0.335700000
$\begin{array}{c} -3.417300000 & 5.103400000 & -2.832000000 \\ -1.886800000 & 7.320400000 & 2.093400000 \\ -4.225400000 & 5.659000000 & 1.983300000 \\ -4.225400000 & 6.437300000 & -0.194500000 \\ -2.031900000 & 6.437300000 & -1.457600000 \\ -4.255500000 & 6.191700000 & -3.117300000 \\ 3.654900000 & 5.450100000 & 0.283300000 \\ 2.973300000 & 6.033600000 & 1.537800000 \\ 1.483300000 & 5.669800000 & 1.491100000 \\ 0.887500000 & 6.201800000 & 0.184800000 \\ 1.667600000 & 5.638300000 & -1.014800000 \\ 1.215000000 & 6.291400000 & -2.328900000 \\ 3.572900000 & 5.93500000 & 2.723500000 \\ 0.775700000 & 6.29800000 & 2.570400000 \\ -0.476100000 & 5.817900000 & 0.140800000 \\ 3.058600000 & 5.922400000 & -0.888600000 \\ 1.410500000 & 7.680800000 & -2.316300000 \\ 6.329200000 & 0.925800000 & 1.34500000 \\ 5.924900000 & 1.400900000 & 1.541600000 \\ 5.258900000 & 2.77080000 & -0.911900000 \\ 5.258900000 & 2.751800000 & 2.431900000 \\ 4.252900000 & 2.751800000 & 2.431900000 \\ 4.252900000 & 2.05400000 & -0.749800000 \\ 6.438600000 & -3.990100000 & -1.443700000 \\ 6.438600000 & -3.990100000 & -1.443700000 \\ 6.43500000 & -3.555900000 & -0.3890900000 \\ 5.943500000 & -1.196600000 & -0.399090000 \\ 5.943500000 & -1.747600000 & -1.918600000 \\ 5.943500000 & -3.990100000 & -1.443700000 \\ 6.438600000 & -2.24200000 & 0.203900000 \\ 5.943500000 & -3.990100000 & -1.443700000 \\ 5.943500000 & -3.555900000 & -0.446400000 \\ 6.193600000 & -2.24200000 & 0.519700000 \\ 5.943500000 & -1.196600000 & -0.399090000 \\ 5.943500000 & -1.747600000 & -1.443700000 \\ 5.943500000 & -1.747600000 & -1.443700000 \\ 5.943500000 & -1.747600000 & -1.443700000 \\ 5.943500000 & -3.555900000 & -0.446400000 \\ 5.943500000 & -3.555900000 & -0.446400000 \\ 5.943500000 & -3.555900000 & -0.446400000 \\ 5.943500000 & -3.552800000 & -0.673700000 \\ 5.943500000 & -7.033300000 & 0.519700000 \\ 5.443800000 & -5.528800000 & -1.681600000 \\ 5.924200000 & -7.033300000 & 0.85500000 \\ 5.443500000 & -5.52800000 & -1.681600000 \\ 5.7112000000 & -5.756200000 & -1.681600000 \\ 5.112000000 & -5.756200000 & -1.681600000 \\ 5.714000000 $	6	-2.779000000	5.223200000	-1.440000000
-1.88680000 7.32040000 2.093400000 -4.225400000 5.65900000 1.983300000 -4.225400000 6.437300000 -1.457600000 -4.255500000 6.191700000 -3.117300000 3.654900000 5.450100000 0.283300000 2.973300000 6.033600000 1.537800000 1.483300000 5.669800000 1.491100000 0.887500000 6.201800000 -1.014800000 1.667600000 5.638300000 -1.014800000 1.215000000 6.291400000 -2.328900000 3.572900000 5.593500000 2.773500000 0.775700000 6.229800000 2.570400000 -0.476100000 5.817900000 -1.40800000 3.058600000 5.922400000 -0.888600000 4.621400000 2.199500000 1.34500000 4.621400000 2.199500000 1.446500000 4.813700000 3.341500000 -0.911900000 5.588600000 3.881100000 -1.918600000 5.729500000 2.751800000 2.686500000 3.588000000 4.743600000 -1.441600000 5.551000000 -3.990100000 -1.443700000 6.43500000 -1.747600000 -1.443700000 6.43500000 -1.747600000 -1.442700000 6.193600000 -2.32200000 -3.127600000 5.94900000 -3.127600000 -3.990100000 5.94900000 -3.199100000 -3.489800000 6.193600000 -3.555900000 -1.443700000 <td>6</td> <td>-3.417300000</td> <td>5.103400000</td> <td>-2.832000000</td>	6	-3.417300000	5.103400000	-2.832000000
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$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	8	-4.225400000	5.659000000	1.983300000
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	8	4.478100000	-5.704000000	1.606800000
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6 8 8	5.615300000 4.025400000 3.145200000	-1.229200000 -3.592100000 4.657200000	-2.833500000 -3.035100000 0.665300000
6 8 8 8	5.615300000 4.025400000 3.145200000	-1.229200000 -3.592100000 -4.657200000	-2.833500000 -3.035100000 -0.665300000
6 8 8 8 8	5.048500000 5.615300000 4.025400000 3.145200000 6.135200000	-1.229200000 -3.592100000 -4.657200000 -2.813300000	-2.833500000 -3.035100000 -0.665300000 0.429400000
6 8 8 8 8 8	5.615300000 4.025400000 3.145200000 6.135200000 5.1136000000	-1.229200000 -3.592100000 -4.657200000 -2.813300000 -3.906600000	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000
6 8 8 8 8 8 8 6	5.645300000 5.615300000 4.025400000 3.145200000 6.135200000 5.113600000 5.705100000	-1.229200000 -3.592100000 -4.657200000 -2.813300000 -3.906600000 3.225800000	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000
6 8 8 8 8 8 8 8 8 6 6	5.048300000 5.615300000 4.025400000 3.145200000 6.135200000 5.113600000 5.705100000 6.748000000	-1.229200000 -3.592100000 -4.657200000 -2.813300000 -3.906600000 3.225800000 2.712300000	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000
6 8 8 8 8 8 8 8 6 6 6	5.645300000 5.615300000 3.145200000 6.135200000 5.113600000 5.705100000 6.748000000 6.199100000	-1.229200000 -3.592100000 -4.657200000 -2.813300000 -3.906600000 3.225800000 2.712300000 1.424900000	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.675700000
6 8 8 8 8 8 8 6 6 6 6	5.615300000 5.615300000 4.025400000 3.145200000 5.113600000 5.705100000 6.748000000 6.199100000 5.90700000	-1.229200000 -3.592100000 -3.592100000 -2.813300000 -3.906600000 3.225800000 2.712300000 1.424900000 0.412800000	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.675700000 0.437000000
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6 8 8 8 8 8 8 6 6 6 6 6 6	5.048300000 5.615300000 4.025400000 3.145200000 6.135200000 5.705100000 6.748000000 6.199100000 5.900700000 4.965500000	-1.229200000 -3.592100000 -3.592100000 -2.813300000 -3.906600000 3.225800000 2.712300000 1.424900000 0.412800000 1.034300000	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.675700000 0.437000000 1.484300000
6 8 8 8 8 8 8 6 6 6 6 6 6	5.048300000 5.615300000 4.025400000 3.145200000 6.135200000 5.113600000 5.705100000 6.748000000 6.199100000 5.900700000 4.965500000 4.826300000	$\begin{array}{c} -1.29200000\\ -1.29200000\\ -3.592100000\\ -4.657200000\\ -2.813300000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 0.412800000\\ 1.034300000\\ 0.120900000\\ \end{array}$	$\begin{array}{c} -2.833500000\\ -3.035100000\\ -0.665300000\\ 0.429400000\\ 2.977100000\\ 0.962100000\\ -0.050400000\\ -0.675700000\\ 0.437000000\\ 1.484300000\\ 2.710200000\end{array}$
6 8 8 8 8 8 6 6 6 6 6 6 8	5.048300000 5.615300000 4.025400000 3.145200000 6.135200000 5.705100000 6.748000000 6.748000000 6.199100000 4.965500000 4.826300000 7.070600000	$\begin{array}{c} -1.229200000\\ -1.229200000\\ -3.592100000\\ -4.657200000\\ -2.813300000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 0.412800000\\ 0.412800000\\ 0.120900000\\ 3.657700000\end{array}$	$\begin{array}{c} -2.833500000\\ -3.035100000\\ -0.665300000\\ 0.429400000\\ 2.977100000\\ 0.962100000\\ -0.050400000\\ -0.675700000\\ 0.437000000\\ 1.484300000\\ 2.710200000\\ -1.030100000\end{array}$
6 8 8 8 8 8 6 6 6 6 6 8 8	5.048300000 5.615300000 4.025400000 3.145200000 5.113600000 5.705100000 6.748000000 6.199100000 5.900700000 4.965500000 4.826300000 7.070600000 7.122100000	$\begin{array}{c} -1.229200000\\ -1.229200000\\ -3.592100000\\ -4.657200000\\ -2.813300000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 1.424900000\\ 1.034300000\\ 0.120900000\\ 3.657700000\\ 0.869100000\\ \end{array}$	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.675700000 0.437000000 1.484300000 2.710200000 -1.030100000 -1.589100000
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6888866666688888	5.048300000 5.615300000 4.025400000 3.145200000 5.113600000 5.705100000 6.748000000 6.748000000 6.199100000 5.900700000 4.965500000 4.826300000 7.0706000000 7.1221000000 5.2659000000 5.4793000000	$\begin{array}{c} -1.29200000\\ -1.29200000\\ -3.592100000\\ -3.592100000\\ -2.813300000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 0.412800000\\ 1.034300000\\ 0.120900000\\ 3.657700000\\ 0.869100000\\ -0.734600000\\ 2.274500000\\ -0.115500000\\ \end{array}$	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 -0.050400000 -0.050400000 -0.675700000 0.437000000 1.484300000 -1.030100000 -1.589100000 -0.107600000 1.961600000 3.337000000
688888666666888886	5.615300000 5.615300000 4.025400000 5.135200000 5.13600000 5.705100000 6.748000000 6.748000000 6.99100000 6.990700000 4.965500000 7.070600000 7.122100000 5.265900000 5.479300000 6.056300000 1.082500000	-1.229200000 -3.592100000 -3.592100000 -3.657200000 -2.813300000 -3.906600000 3.225800000 2.712300000 1.424900000 1.424900000 1.034300000 0.120900000 3.657700000 0.869100000 -0.734600000 2.274500000 -0.115500000 6.720000000	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.675700000 0.437000000 1.484300000 2.710200000 -1.030100000 -1.589100000 -0.107600000 1.961600000 3.337900000 0.281200000
688886666668888866	5.048300000 5.615300000 4.025400000 3.145200000 5.113600000 5.705100000 6.748000000 6.748000000 6.1991000000 4.965500000 4.8263000000 7.0706000000 7.1221000000 5.2659000000 5.4793000000 6.0563000000 1.9825000000	-1.229200000 -1.229200000 -3.592100000 -3.592100000 -3.906600000 3.225800000 2.712300000 1.424900000 0.412800000 0.412800000 0.412800000 0.557700000 0.869100000 -0.734600000 2.274500000 -0.115500000 6.729900000	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.675700000 0.437000000 1.484300000 2.710200000 -1.030100000 -1.589100000 -0.107600000 1.961600000 3.337900000 -0.281300000
6 8 8 8 8 8 6 6 6 6 6 8 8 8 8 8 8 8 6 6 6 6 6 6 6 6 8 8 8 8 8 8 8 6	5.048300000 5.615300000 4.025400000 3.145200000 5.113600000 5.705100000 6.748000000 6.748000000 6.199100000 5.9007000000 4.9655000000 4.9655000000 7.0706000000 7.1221000000 5.2659000000 5.4793000000 6.0563000000 1.9825000000 3.1028000000	$\begin{array}{c} -1.29200000\\ -1.29200000\\ -3.592100000\\ -3.592100000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 0.412800000\\ 1.034300000\\ 0.120900000\\ 3.657700000\\ 0.869100000\\ 0.869100000\\ 0.734600000\\ 2.274500000\\ -0.734600000\\ 2.274500000\\ 6.729900000\\ 6.562000000\\ \end{array}$	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.675700000 0.437000000 1.484300000 2.710200000 -1.030100000 -1.589100000 -0.107600000 1.961600000 3.337900000 -0.281300000 -1.325500000
68888666666888886666	5.048300000 5.615300000 4.025400000 3.145200000 5.113600000 5.705100000 6.748000000 6.748000000 6.199100000 4.9655000000 4.8263000000 7.0706000000 7.1221000000 5.2659000000 5.4793000000 6.0563000000 1.9825000000 3.1028000000 3.6214000000	$\begin{array}{c} -1.29200000\\ -1.29200000\\ -3.592100000\\ -3.592100000\\ -3.592100000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 0.412800000\\ 1.034300000\\ 0.120900000\\ 3.657700000\\ 0.869100000\\ -0.734600000\\ 2.274500000\\ -0.115500000\\ 6.729900000\\ 6.562000000\\ 5.119000000\end{array}$	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 -0.050400000 -0.050400000 -0.675700000 0.437000000 1.484300000 -1.030100000 -1.030100000 -1.589100000 -0.107600000 1.961600000 3.337900000 -0.281300000 -1.325500000 -1.235500000
088886666668888866666	5.648300000 5.615300000 4.025400000 3.145200000 5.113600000 5.705100000 6.748000000 6.748000000 6.748000000 4.965500000 4.965500000 7.070600000 7.070600000 5.265900000 5.4793000000 5.4793000000 3.102800000 3.6214000000	$\begin{array}{c} -1.229200000\\ -1.229200000\\ -3.592100000\\ -3.592100000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 1.424900000\\ 1.034300000\\ 0.120900000\\ 3.657700000\\ 0.869100000\\ -0.734600000\\ 2.274500000\\ -0.715500000\\ 6.562000000\\ 5.119000000\\ 4.863700000\\ \end{array}$	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.675700000 0.437000000 1.484300000 -1.030100000 -1.030100000 -1.589100000 -0.107600000 1.961600000 -0.281300000 -1.325500000 0.195500000
688886666668888866666	5.648300000 5.615300000 4.025400000 3.145200000 5.113600000 5.705100000 6.748000000 6.748000000 6.1991000000 4.9655000000 4.8263000000 7.0706000000 7.0706000000 5.2659000000 5.4793000000 6.0563000000 1.9825000000 3.1028000000 3.6214000000 4.1010000000	$\begin{array}{c} -1.229200000\\ -1.229200000\\ -3.592100000\\ -3.592100000\\ -3.592100000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 1.034300000\\ 0.412800000\\ 1.034300000\\ 0.120900000\\ 3.657700000\\ 0.869100000\\ -0.734600000\\ 2.274500000\\ -0.734600000\\ 2.274500000\\ -0.115500000\\ 6.729900000\\ 6.562000000\\ 5.119000000\\ 4.863700000\\ 5.161200000\\ \end{array}$	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.050400000 0.437000000 1.484300000 2.710200000 -1.030100000 -1.589100000 -0.107600000 1.961600000 3.337900000 -0.281300000 -1.235500000 0.195500000 0.195500000
68888666666888886666666	5.648300000 5.615300000 4.025400000 3.145200000 5.113600000 5.705100000 6.748000000 6.748000000 6.1991000000 4.9655000000 4.9655000000 7.0706000000 7.0706000000 5.2659000000 5.4793000000 5.4793000000 3.1028000000 3.62140000000 4.9746000000 3.4819000000	$\begin{array}{c} -1.29200000\\ -1.29200000\\ -3.592100000\\ -3.592100000\\ -3.592100000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 0.412800000\\ 0.412800000\\ 0.412800000\\ 0.412800000\\ 0.565700000\\ 0.569100000\\ -0.734600000\\ 2.274500000\\ -0.734600000\\ -0.734600000\\ 5.15500000\\ 5.119000000\\ 5.161200000\\ 5.085400000\\ 5.085400000\\ \end{array}$	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.050400000 1.484300000 2.710200000 -1.030100000 -1.030100000 -1.030100000 -0.107600000 1.961600000 3.337900000 -0.281300000 -1.235500000 -1.235500000 0.195500000 1.199100000 2.645900000
0888866666688888666666	5.645300000 5.615300000 4.025400000 3.145200000 6.135200000 5.705100000 6.748000000 6.748000000 6.748000000 4.9655000000 4.9655000000 7.0706000000 7.122100000 5.265900000 5.479300000 6.056300000 1.982500000 3.102800000 3.621400000 4.101000000 2.974600000 3.481900000 3.481900000 3.624400000 3.624400000 3.624400000 3.624400000 3.624400000 3.624400000 3.624400000 3.624400000 3.624400000 3.624400000 3.624400000 3.624400000 3.624400000 3.624400000 3.624400000 3.624400000 3.624400000 3.624400000 3.624400000 3.644000000 3.644000000 3.644000000 3.64400000000000000000000000000000000000	$\begin{array}{c} -1.29200000\\ -1.29200000\\ -3.592100000\\ -3.592100000\\ -3.592100000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 0.412800000\\ 1.424900000\\ 0.412800000\\ 0.412800000\\ 0.57700000\\ 0.657700000\\ 0.869100000\\ -0.734600000\\ -0.734600000\\ -0.734600000\\ -0.734600000\\ -0.734600000\\ -0.734600000\\ -0.734600000\\ -0.734600000\\ -0.734600000\\ -0.734600000\\ -0.734600000\\ -0.734600000\\ -0.115500000\\ -0.58200000\\ -0.88540000\\ -0.88540000\\ -0.88540000\\ -0.88540000\\ -0.88540000\\ -0.88540000\\ -0.88540000\\ -0.88540000\\ -0.88540000\\ -0.88540000\\ -0.88540000\\ -0.88540000\\ -0.88540000\\ -0.88540000\\ -0.8854000\\ -0.885400\\ $	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 -0.050400000 -0.050400000 -0.675700000 0.437000000 1.484300000 -1.030100000 -1.030100000 -1.589100000 -0.281300000 -0.281300000 -1.235500000 -1.235500000 0.195500000 1.199100000 2.645900000 2.645900000
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088886666668888666668888	5.615300000 5.615300000 4.025400000 3.145200000 5.113600000 5.705100000 6.748000000 6.748000000 6.748000000 4.9655000000 4.9655000000 7.7026000000 7.122100000 5.265900000 5.479300000 5.265900000 3.621400000 3.621400000 3.621400000 4.101000000 2.974600000 3.481900000 2.684400000 4.506700000 2.462000000	$\begin{array}{c} -1.29200000\\ -1.29200000\\ -3.592100000\\ -3.592100000\\ -3.592100000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 0.412800000\\ 1.034300000\\ 0.12090000\\ 3.657700000\\ 0.869100000\\ 0.657700000\\ 0.869100000\\ -0.734600000\\ 2.274500000\\ -0.734600000\\ 5.161200000\\ 5.161200000\\ 5.161200000\\ 5.161200000\\ 5.161200000\\ 5.82700000\\ 4.906600000\\ 3.509400000\\ 6.478100000\\ \end{array}$	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 -0.050400000 -0.050400000 -0.675700000 0.437000000 1.484300000 -1.030100000 -1.030100000 -1.030100000 -0.281300000 -0.281300000 -1.235500000 -1.235500000 -1.235500000 -1.235500000 -1.235500000 -1.235500000 -2.6208000000 -2.110800000 0.280000000 1.011000000
0 8 8 8 8 6 6 6 6 6 6 6 6 6 6 8 8 8 8 8	5.615300000 5.615300000 4.025400000 5.11360000 5.11360000 5.705100000 6.74800000 6.74800000 6.74800000 6.799100000 7.070600000 7.070600000 7.070600000 7.122100000 5.265900000 5.479300000 5.479300000 3.102800000 3.621400000 3.62500000 3.62500000 3.62500000 3.62500000 3.62500000 3.62500000 3.62500000 3.62500000 3.62500000 3.62500000 3.62500000 3.62500000 3.62500000 3.62000000 3.62500000 3.625000000 3.625000000 3.625000000 3.625000000 3.625000000 3.625000000 3.625000000 3.625000000 3.625000000 3.625000000 3.625000000 3.625000000 3.625000000 3.625000000 3.625000000 3.625000000 3.625000000 3.625000000 3.625000000000000000000000000000000000000	$\begin{array}{c} -1.229200000\\ -1.229200000\\ -3.592100000\\ -3.592100000\\ -3.657200000\\ -2.813300000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 0.412800000\\ 1.034300000\\ 0.120900000\\ 3.657700000\\ 0.3657700000\\ 0.869100000\\ -0.734600000\\ 2.274500000\\ -0.734600000\\ -0.72900000\\ -0.73400000\\ -0.73400000\\ -0.72900000\\ -0.7290000\\ -0.72000\\ $	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.050400000 -0.437000000 1.484300000 -1.030100000 -1.030100000 -1.589100000 -0.107600000 -1.235500000 -1.235500000 -1.235500000 -1.235500000 -1.235500000 -2.620800000 -2.620800000 -2.110800000 0.280000000 -0.101000000 2.879000000
088886666668888666666888886	5.615300000 5.615300000 4.025400000 5.11360000 5.11360000 5.705100000 6.748000000 6.748000000 6.74800000 4.965500000 4.826300000 7.070600000 7.070600000 5.265900000 5.479300000 5.265900000 3.02800000 3.621400000 3.621400000 3.621400000 3.481900000 2.684400000 4.506700000 2.684400000 4.506700000 2.462000000 3.181100000	$\begin{array}{c} -1.229200000\\ -1.229200000\\ -3.592100000\\ -3.592100000\\ -3.657200000\\ -2.813300000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 0.412800000\\ 1.034300000\\ 0.120900000\\ 3.657700000\\ 0.869100000\\ -0.734600000\\ 2.274500000\\ -0.734600000\\ 2.274500000\\ -0.115500000\\ 6.729900000\\ 6.56200000\\ 5.161200000\\ 5.085400000\\ 5.085400000\\ 5.085400000\\ 6.882700000\\ 4.906600000\\ 3.509400000\\ 6.478100000\\ 5.962200000\\ 5.85780000\\ 5.85780000\\ 5.8$	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.050400000 -0.437000000 1.484300000 -1.030100000 -1.030100000 -1.030100000 -1.235500000 -1.235500000 -1.235500000 -1.235500000 -1.235500000 -2.620800000 -2.620800000 -2.110800000 -2.81000000 -2.620800000 -2.620800000 -2.110800000 -2.80000000 -2.879000000 -2.879000000 -2.879000000 -2.879000000 -1.038500000
0888866666688888666666888866	5.615300000 5.615300000 4.025400000 3.145200000 5.135200000 5.705100000 6.748000000 6.748000000 6.748000000 4.965500000 4.826300000 7.070600000 7.070600000 5.265900000 5.479300000 5.265900000 3.102800000 3.621400000 3.621400000 3.621400000 3.621400000 3.481900000 2.684400000 4.506700000 2.462000000 4.552900000 -3.1811000000 2.370500000	$\begin{array}{c} -1.229200000\\ -1.229200000\\ -3.592100000\\ -3.592100000\\ -3.592100000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 0.412800000\\ 1.034300000\\ 0.412800000\\ 0.412800000\\ 0.412800000\\ 0.5657700000\\ 0.5657700000\\ -0.734600000\\ 2.274500000\\ -0.734600000\\ -0.790000\\ -0.790000\\ -0.790000\\ -0.790000\\ -0.79000\\ -0.79000\\ -0.79000\\ -0.79000\\ -0.7900\\ -0.7$	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.050400000 1.484300000 2.710200000 -1.030100000 -1.030100000 -1.030100000 -0.107600000 -1.235500000 -1.235500000 -1.235500000 -1.235500000 -2.620800000 -2.620800000 -2.110800000 -2.879000000 -2.879000000 -2.879000000 -2.879000000 -2.879000000 -2.75400000
088888666666888886666668888866	5.615300000 5.615300000 4.025400000 3.145200000 6.135200000 5.705100000 6.748000000 6.748000000 6.748000000 4.9655000000 4.9655000000 7.0706000000 7.0706000000 5.479300000 5.2659000000 3.6214000000 3.6214000000 4.1010000000 2.9746000000 4.5067000000 4.5067000000 2.462000000 4.552900000 -3.181100000 -2.3705000000 -2.3705000000 -2.3705000000 -2.3705000000 -2.3705000000 -2.3705000000 -2.3705000000 -2.3705000000 -2.3705000000 -2.3705000000 -2.3705000000 -2.3705000000 -2.3705000000 -2.3705000000 -2.370500000 -2.370500000 -2.370500000 -2.370500000 -2.370500000 -2.370500000 -2.370500000 -2.370500000 -2.370500000 -2.370500000 -2.370500000 -2.370500000 -2.370500000 -2.370500000 -2.370500000	$\begin{array}{c} -1.29200000\\ -1.29200000\\ -3.592100000\\ -3.592100000\\ -3.592100000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 0.412800000\\ 0.412800000\\ 0.412800000\\ 0.412800000\\ 0.657700000\\ 0.657700000\\ 0.869100000\\ 0.657700000\\ 0.869100000\\ 0.657700000\\ 0.657700000\\ 0.869100000\\ 0.56200000\\ 5.119000000\\ 5.161200000\\ 5.161200000\\ 5.857800000\\ 6.478100000\\ 5.962200000\\ 5.857800000\\ 6.289200000\\ 5.857800000\\ 6.289200000\\ 5.962200000\\ 5.85780000\\ 5.8578000$	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.050400000 -0.437000000 1.484300000 -1.030100000 -1.030100000 -1.030100000 -0.281300000 -1.235500000 -1.235500000 -1.235500000 -1.235500000 -2.108000000 -2.110800000 0.2879000000 -1.038500000 -2.275400000 -2.275400000 -2.275400000
088888666668888866666888886666	5.615300000 5.615300000 4.025400000 5.11360000 5.135200000 5.705100000 6.748000000 6.748000000 6.74800000 6.799100000 7.070600000 7.070600000 7.070600000 7.070600000 5.479300000 5.479300000 5.479300000 3.02800000 3.621400000 3.621400000 3.621400000 2.684400000 4.704800000 2.684400000 4.704800000 2.684400000 4.506700000 2.462000000 4.5052900000 -3.181100000 -3.70500000 -0.913400000	$\begin{array}{c} -1.229200000\\ -1.229200000\\ -3.592100000\\ -3.592100000\\ -3.906600000\\ -2.813300000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 0.412800000\\ 1.034300000\\ 0.129900000\\ 0.129900000\\ 0.3657700000\\ 0.869100000\\ -0.734600000\\ 2.274500000\\ -0.734600000\\ 0.115500000\\ 6.562000000\\ 6.562000000\\ 5.119000000\\ 4.863700000\\ 5.161200000\\ 5.085400000\\ 5.085400000\\ 6.882700000\\ 6.478100000\\ 5.962200000\\ 5.857800000\\ 6.289200000\\ 5.837700000\\ \end{array}$	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.050400000 -0.437000000 1.484300000 -1.32100000 -1.030100000 -1.589100000 -0.281300000 -0.281300000 -1.325500000 -1.325500000 -1.235500000 -2.620800000 -2.620800000 -2.110800000 -2.81000000 -2.875400000 -2.275400000 -2.2106500000
088888666668888866666888886666	5.615300000 4.025400000 3.145200000 6.135200000 5.705100000 5.705100000 6.748000000 6.748000000 4.965500000 4.965500000 7.070600000 7.070600000 7.070600000 5.265900000 5.479300000 5.265900000 3.621400000 3.621400000 4.506700000 2.684400000 4.506700000 2.684400000 4.52900000 3.1811000000 -2.370500000 -0.913400000	$\begin{array}{c} -1.229200000\\ -1.229200000\\ -3.592100000\\ -3.592100000\\ -3.592100000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 0.412800000\\ 1.034300000\\ 0.129900000\\ 0.3657700000\\ 0.869100000\\ -0.734600000\\ 2.274500000\\ -0.734600000\\ -0.734600000\\ -0.734600000\\ -0.734600000\\ 5.62000000\\ 5.62000000\\ 5.119000000\\ 5.161200000\\ 5.85700000\\ 6.882700000\\ 6.478100000\\ 5.962200000\\ 5.857800000\\ 6.289200000\\ 5.857800000\\ 6.382100000\\ \end{array}$	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.057700000 0.437000000 -1.484300000 -1.030100000 -1.030100000 -1.589100000 -0.107600000 -1.235500000 -1.235500000 -1.235500000 -2.620800000 -2.620800000 -2.110800000 -2.8100000 -2.275400000 -2.275400000 -2.2106500000 -2.2106500000 -2.2106500000 -2.2106500000 -0.784700000
088886666668888666668888666668888666666	5.615300000 5.615300000 4.025400000 5.11360000 5.135200000 5.705100000 6.748000000 6.748000000 6.748000000 4.965500000 7.070600000 7.070600000 7.070600000 7.070600000 5.265900000 5.479300000 5.265900000 3.102800000 3.621400000 4.506700000 2.684400000 4.506700000 2.462000000 4.552900000 -3.181100000 -3.70500000 -0.913400000 -1.273700000	$\begin{array}{l} -1.229200000\\ -1.229200000\\ -3.592100000\\ -3.592100000\\ -3.592100000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 1.424900000\\ 1.034300000\\ 0.412800000\\ 1.034300000\\ 0.3657700000\\ 3.657700000\\ 0.869100000\\ -0.734600000\\ 2.274500000\\ -0.734600000\\ 2.274500000\\ -0.734600000\\ 5.161200000\\ 5.161200000\\ 5.161200000\\ 5.161200000\\ 5.85700000\\ 6.478100000\\ 5.962200000\\ 5.857800000\\ 6.289200000\\ 5.857800000\\ 6.382100000\\ 5.97000000\\ \end{array}$	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.050400000 -0.675700000 0.437000000 -1.484300000 -1.030100000 -1.030100000 -1.589100000 -1.235500000 -1.235500000 -1.235500000 -1.235500000 -1.235500000 -2.620800000 -2.620800000 -2.620800000 -2.110800000 -2.879000000 -2.275400000 -2.275400000 -2.106500000 -0.784700000 0.383700000
088886666688888666668888666666666666666	5.615300000 5.615300000 4.025400000 3.145200000 5.135200000 5.705100000 6.748000000 6.748000000 6.748000000 4.965500000 4.826300000 7.070600000 7.070600000 5.265900000 5.479300000 5.265900000 3.102800000 3.621400000 4.506700000 2.684400000 4.506700000 2.462000000 4.552900000 -3.181100000 -3.370500000 -0.363700000 -0.363700000 -1.273700000 -0.854500000	$\begin{array}{l} -1.29200000\\ -1.29200000\\ -3.592100000\\ -3.592100000\\ -3.592100000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 0.412800000\\ 1.034300000\\ 0.412800000\\ 0.412800000\\ 0.412800000\\ 0.412800000\\ 0.412800000\\ 0.412800000\\ 0.55700000\\ 0.562000000\\ 5.11900000\\ 6.562000000\\ 5.11900000\\ 6.562000000\\ 5.11900000\\ 6.56200000\\ 5.11900000\\ 6.56200000\\ 5.11900000\\ 5.857800000\\ 6.88270000\\ 6.88270000\\ 5.857800000\\ 5.97000000\\ 5.970000000\\ 5.970000000\\ 5.97000000\\ 5.97000000\\ 5.97000000\\ 5.97000000\\ 5.970000000\\ 5.97000000\\ 5.970000000\\ 5.97000000\\ 5.970000000\\ 5.97000000\\ 5.970000000\\ 5.97000000\\ $	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.675700000 0.437000000 1.484300000 -1.030100000 -1.030100000 -1.030100000 -0.281300000 -0.281300000 -0.281300000 -1.235500000 -1.235500000 -1.235500000 -2.620800000 -2.620800000 -2.110800000 0.2879000000 -1.038500000 -2.275400000 -2.275400000 -2.275400000 -0.784700000 0.383700000 -0.583700000 -0.583700000 -0.583700000 -0.583700000 -2.645900000 -2.106500000 -2.275400000 -2.275400000 -2.275400000 -2.2784000000 -2.2784000000 -2.2784000000 -2.2784000000 -2.2784000000 -2.2784000000000000000000000000000000000000
08888866666688886666668888666668888666666	5.615300000 5.615300000 4.025400000 5.11360000 5.11360000 5.705100000 6.748000000 6.748000000 6.74800000 6.799100000 4.965500000 7.070600000 7.070600000 7.070600000 5.265900000 5.479300000 5.265900000 5.479300000 3.621400000 4.96200000 3.621400000 4.96400000 2.684400000 4.506700000 2.684400000 4.552900000 -3.181100000 -3.70500000 -0.913400000 -0.363700000 -0.854500000 -2.925700000	$\begin{array}{c} -1.229200000\\ -1.229200000\\ -3.592100000\\ -3.592100000\\ -3.657200000\\ -2.813300000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.034300000\\ 0.412800000\\ 0.412800000\\ 0.412800000\\ 0.3657700000\\ 0.869100000\\ -0.734600000\\ 2.274500000\\ -0.734600000\\ -0.734600000\\ -0.734600000\\ 5.657700000\\ 6.562000000\\ 5.119000000\\ 5.085400000\\ 5.161200000\\ 5.085400000\\ 5.085400000\\ 5.962200000\\ 5.857800000\\ 6.478100000\\ 5.962200000\\ 5.837700000\\ 6.382100000\\ 5.837700000\\ 6.382100000\\ 5.970000000\\ 5.801500000\\ 5.801500000\\ \end{array}$	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.050400000 -0.675700000 0.437000000 -1.3200000 -1.32500000 -1.235500000 -1.235500000 -1.235500000 -1.235500000 -1.235500000 -2.620800000 -2.620800000 -2.110800000 -2.879000000 -1.038500000 -2.2754000000 -2.2754000000 -2.2754000000 -2.2754000000 -2.2754000000 -2.2754000000 -2.2754000000 -2.27540000000000 -2.2754000000000000000000000000000000000000
08888866666688886666668888866666888866666	5.615300000 5.615300000 4.025400000 5.11360000 5.135200000 5.705100000 6.748000000 6.748000000 6.748000000 4.965500000 7.070600000 7.070600000 7.070600000 7.122100000 5.265900000 5.479300000 6.0563000000 1.982500000 3.621400000 3.621400000 3.621400000 4.506700000 2.684400000 4.704800000 4.506700000 2.684400000 4.552900000 -3.181100000 -3.370500000 -0.913400000 -0.854500000 -0.854500000 -0.854500000 -0.854500000 -0.854500000 -0.9200000 -0.854500000 -0.920000 -0.9200000 -0.9200000 -0.9200000 -0.9200000 -0.9200000 -0.920000 -0.9200000 -0.9200000 -0.9200000 -0.9200000 -0.9200000 -0.9200000 -0.9200000 -0.	$\begin{array}{c} -1.229200000\\ -1.229200000\\ -3.592100000\\ -3.592100000\\ -3.592100000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 0.412800000\\ 1.034300000\\ 0.129900000\\ 3.657700000\\ 0.869100000\\ -0.734600000\\ 2.274500000\\ -0.734600000\\ 2.274500000\\ -0.734600000\\ 5.62000000\\ 6.562000000\\ 5.161200000\\ 5.085400000\\ 5.161200000\\ 5.085400000\\ 5.857800000\\ 6.382100000\\ 5.857800000\\ 6.382100000\\ 5.970000000\\ 6.671500000\\ 5.970000000\\ 5.080000\\ 5.970000000\\ 5.09100000\\ 5.970000000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.0910000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.0910000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.09100000\\ 5.0910000\\ 5.0910000\\ 5.0910000\\ 5.0910000\\ 5.0910000\\ 5.0910000\\ 5.0910000\\ 5.0910000\\ 5.0910000\\ 5.0910000\\ 5.0910000\\ 5.0910000\\ 5.091000\\ 5.0910000\\ 5.0910000\\ 5.0910000\\ 5.0910000\\ 5.0910000\\ 5.0910000\\ 5.091000\\ 5.091000\\ 5.0910000\\ 5.0910000\\ 5.0910000\\ 5.0910000\\ 5.0910000\\ 5.091000\\ 5.091000\\ 5.091000\\ 5.091000\\ 5.00$	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.050400000 -0.675700000 0.437000000 -1.030100000 -1.030100000 -1.030100000 -1.235500000 -1.235500000 -1.235500000 -1.235500000 -1.235500000 -2.620800000 2.645900000 -2.620800000 -2.110800000 -2.275400000 -2.275400000 -2.275400000 -2.275400000 -2.275400000 -2.275400000 -3.83700000 -3.464700000 -3.464700000 -3.464700000 -3.464700000 -3.464700000 -3.464700000
0888866666688888666668888866666888866666888	5.615300000 5.615300000 4.025400000 3.145200000 6.135200000 5.705100000 6.748000000 6.748000000 6.748000000 4.965500000 7.070600000 7.070600000 7.070600000 7.070600000 5.479300000 5.479300000 5.479300000 6.056300000 1.982500000 3.102800000 3.621400000 4.506700000 2.684400000 4.506700000 2.462000000 4.552900000 -3.181100000 -3.63700000 -0.913400000 -0.913400000 -0.913400000 -0.925700000 -0.925700000 -0.109200000 -0.925700000 -0.925700000 -0.925700000 -0.925700000 -0.9200000 -0.9200000 -0.9200000 -0.925700000 -0.9200000 -0.	$\begin{array}{c} -1.229200000\\ -1.229200000\\ -3.592100000\\ -3.592100000\\ -3.592100000\\ -3.906600000\\ 3.225800000\\ 2.712300000\\ 1.424900000\\ 0.412800000\\ 1.034300000\\ 0.120900000\\ 3.657700000\\ 0.869100000\\ -0.734600000\\ 2.274500000\\ -0.734600000\\ 2.274500000\\ -0.734600000\\ 5.6200000\\ 6.729900000\\ 6.82700000\\ 6.882700000\\ 6.882700000\\ 5.085400000\\ 6.882700000\\ 5.857800000\\ 6.882700000\\ 5.857800000\\ 6.882700000\\ 5.801500000\\ 6.8260000\\ 6.82600000\\ 6.82600000\\ 6.82600000\\ 6.82600000\\ 6.82600000\\ 6.82600000\\ 6.82600000\\ 6.82600000\\ 6.82600000\\ 6.8200000\\ 6.82700000\\ 6.82700000\\ 6.8200000\\ 6.8000$	-2.833500000 -3.035100000 -0.665300000 0.429400000 2.977100000 0.962100000 -0.050400000 -0.050400000 -0.675700000 0.437000000 -1.484300000 -1.030100000 -1.030100000 -1.589100000 -1.235500000 -1.235500000 -1.235500000 -1.235500000 -2.620800000 -2.620800000 -2.620800000 -2.110800000 -2.275400000 -2.275400000 -2.275400000 -2.275400000 -2.106500000 -0.784700000 0.383700000 -3.464700000 -3.464700000 -3.464700000 -3.464700000 -2.11020000
8	-2.622800000	6.357900000	0.141600000
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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./03/00000	0.990200000
6	-3.11/500000	-6.864800000	0.039400000
6	-3./46300000	-5.481400000	-0.169600000
6	-4.11/100000	-4.883900000	1.190100000
6	-2.899200000	-4.8/2200000	2.128400000
6	-3.299/00000	-4.4/2400000	3.555200000
8	-2./64100000	-7.459800000	-1.17/000000
8	-4.913600000	-5.550300000	-0.953100000
8	-4.585000000	-3.30/800000	0.94/800000
0	-2.311900000	-0.108/00000 5 226200000	2.218000000
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6	0.288900000	-6.438200000	0.031000000
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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
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1	4.184400000	-5.160000000	1.721600000
1	5.954100000	-5.0/5/00000	1.493500000
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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	4.17/300000	-0.157600000
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8	2 199700000	6 797300000	-1.938900000
8	2.199700000	4 156200000	-0.890300000
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o Q	-6 03000000	2 833800000	-2.003+00000
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6	-5.921600000	-2.400500000	-0.568800000
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