

# **18-crown-6-sodium cholate complex: thermochemistry, structure and stability-SUPPORTING INFORMATION**

Tea Mihelj<sup>1\*</sup>, Vlasta Tomašić<sup>1\*</sup>, Nikola Biliškov<sup>2</sup>

<sup>1</sup>*Department of Physical Chemistry, Ruđer Bošković Institute, POB 180, HR-10002 Zagreb, Croatia*

<sup>2</sup>*Division of Materials Chemistry, Ruđer Bošković Institute, POB 180, HR-10002 Zagreb, Croatia*

\*To whom correspondence should be addressed:

Email: [tmihelj@irb.hr](mailto:tmihelj@irb.hr), [vlastom@irb.hr](mailto:vlastom@irb.hr),

Ruđer Bošković Institute, Department of Physical Chemistry

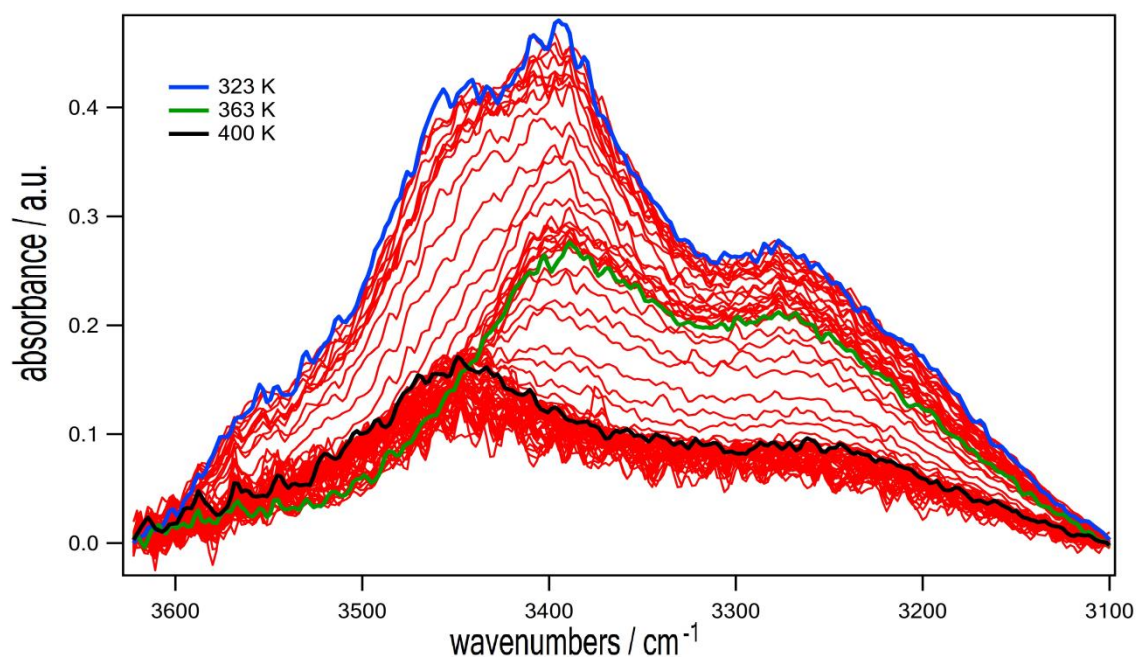
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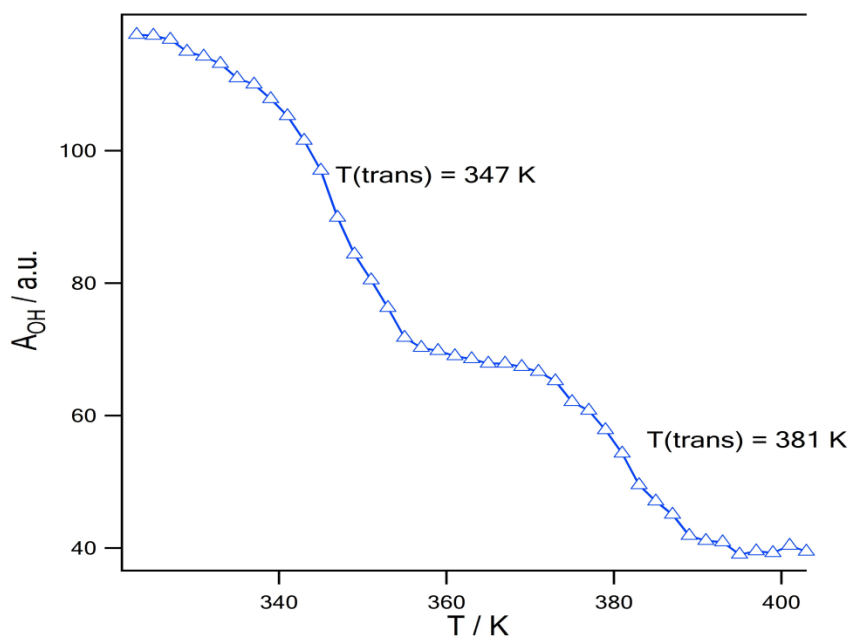
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Tel: +38514571211

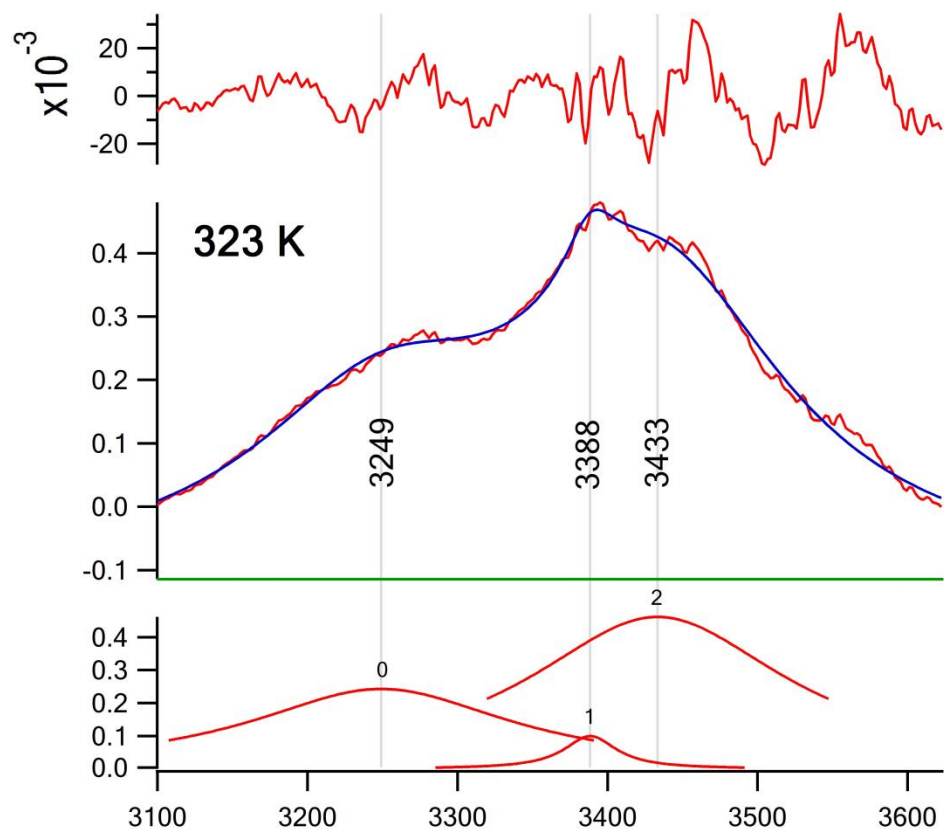
**Figure S1.** IR spectra of the 18C6NaCh complex in the 3700-3180  $\text{cm}^{-1}$  range, taken at different temperatures.



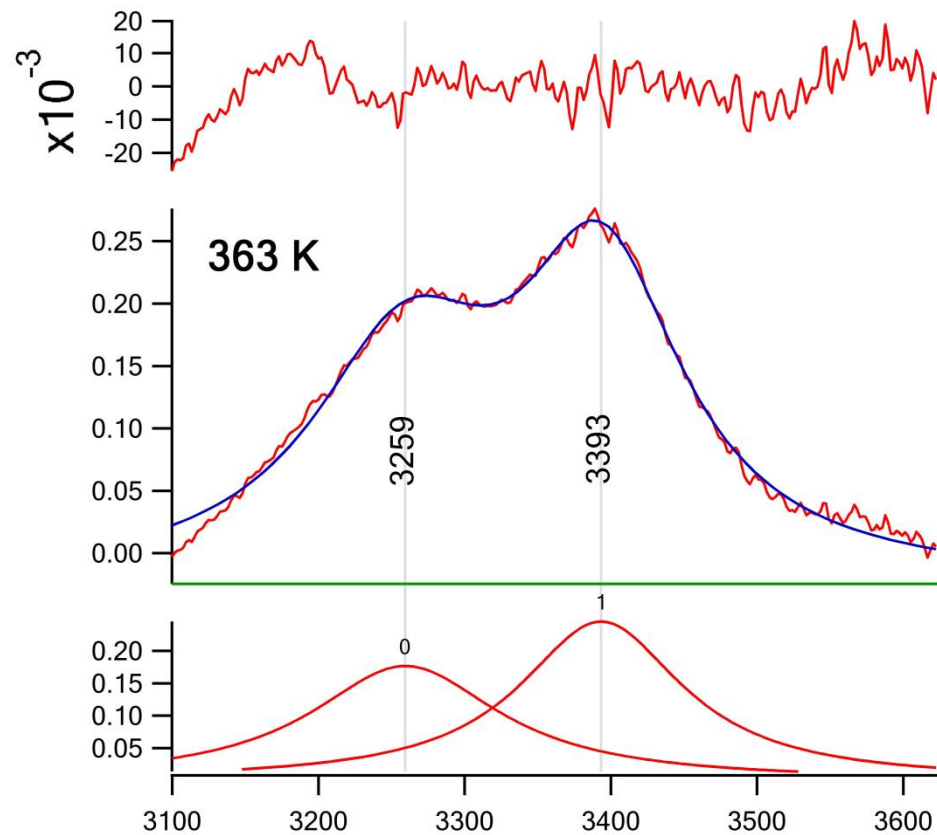
**a**



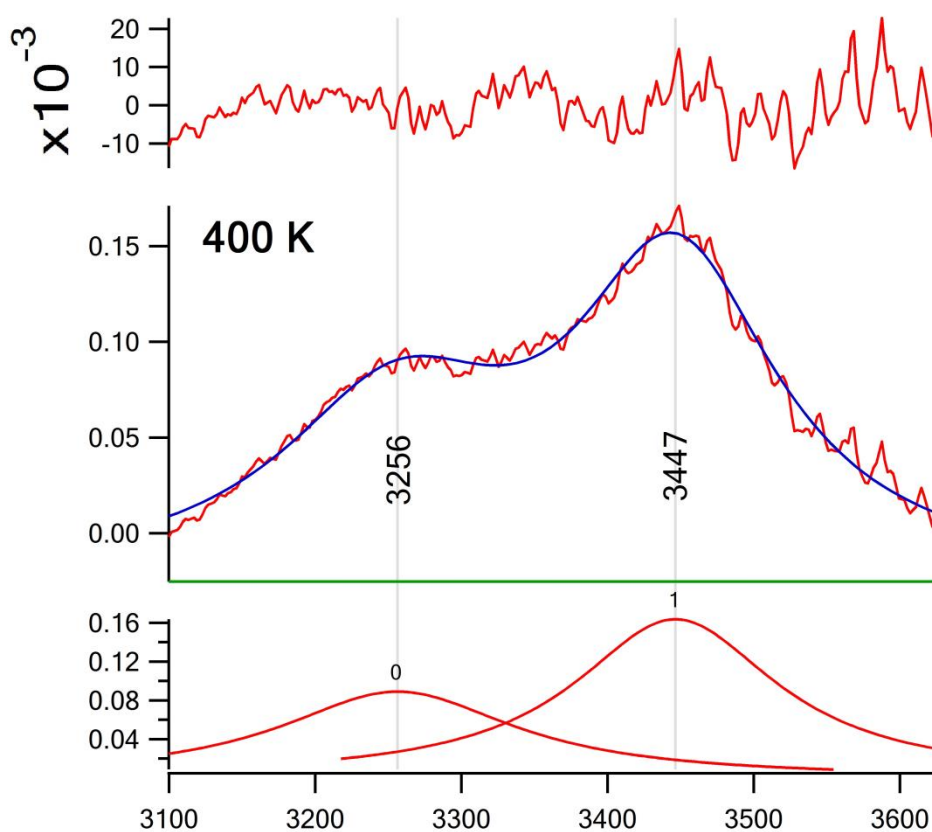
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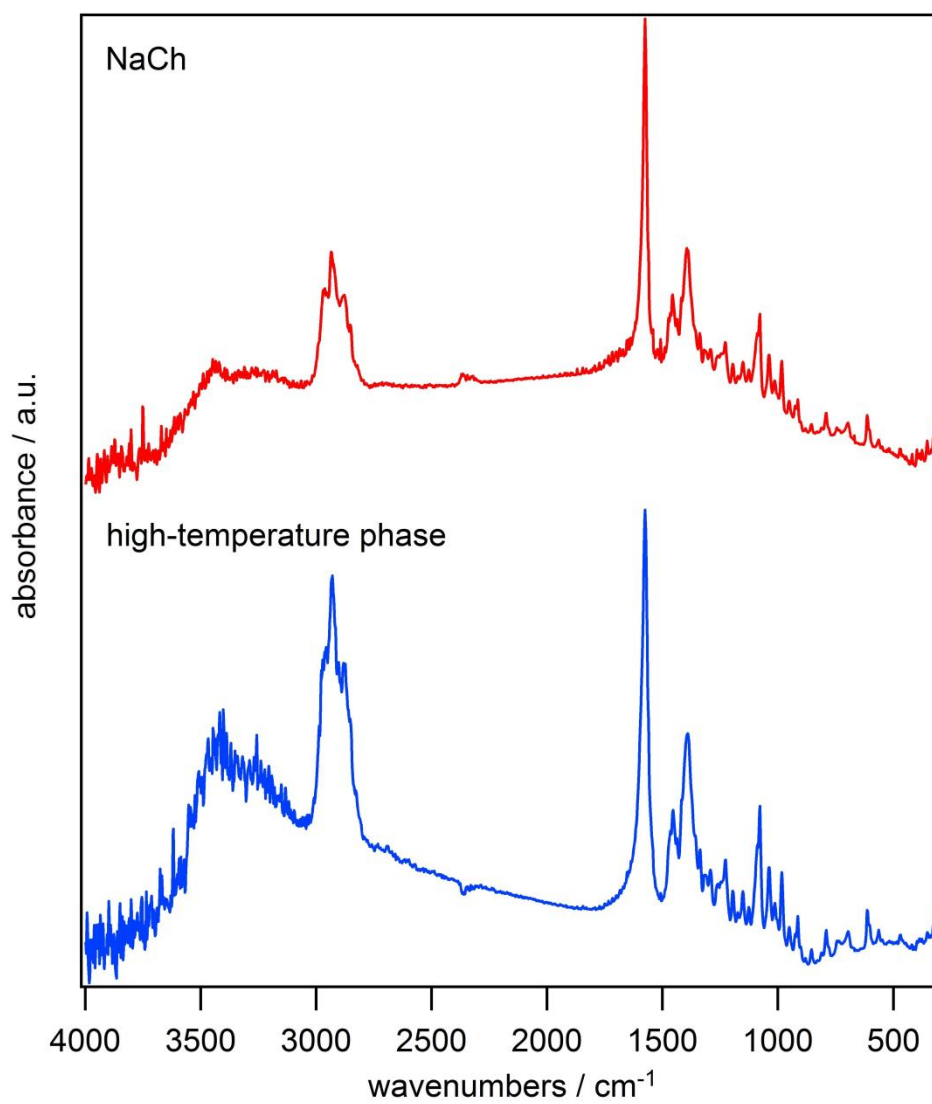
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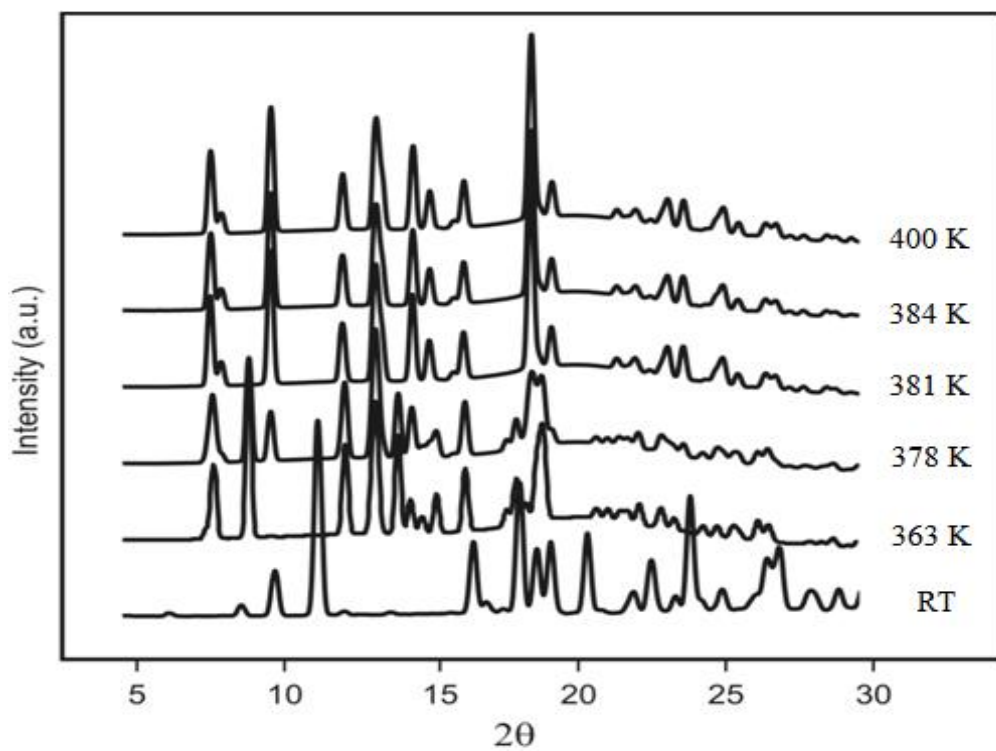
e

IR spectra of the 18C6NaCh complex suffer the most prominent change in the 3700-3180  $\text{cm}^{-1}$  range, attributed to hydrogen bonded water symmetric and antisymmetric OH stretching oscillators, but also to OH groups of cholate anion (Figure S1a). At room temperature, this spectral feature consists of three components, located at 3433, 3388 and 3249  $\text{cm}^{-1}$ , respectively (Figure S1c). Dehydration of the sample was followed by measurement of the area under the whole feature and the results are presented in Figure S1b.

**Figure S2.** The comparison of the room temperature IR spectrum of purchased sodium cholate (NaCh) and of the 18C6·NaCh high temperature phase confirmed the decomplexation of 18C6 from 18C6·NaCh above 400 K.



**Figure S3.** PXRD diffractograms of 18C6·NaCh at different temperatures. The sample is first recorded at RT, then at higher temperatures with the exposure time at each temperature of 10 minutes.



**Table S1.** Indexing of room temperature phase and higher temperature phases of 18C6-NaCh. The lattice is triclinic at room temperature,  $a = 15.45 \text{ \AA}$ ,  $b = 10.60 \text{ \AA}$ ,  $c = 6.84 \text{ \AA}$ ,  $\alpha = 91.7^\circ$ ,  $\beta = 105.6^\circ$ ,  $\gamma = 98.6^\circ$ . A monoclinic lattice is used at 363 K,  $a = 12.25 \text{ \AA}$ ,  $b = 12.65 \text{ \AA}$ ,  $c = 8.26 \text{ \AA}$ ,  $\gamma = 107.9^\circ$ . The lattice is also monoclinic at 390 K,  $a = 12.16 \text{ \AA}$ ,  $b = 11.60 \text{ \AA}$ ,  $c = 8.20 \text{ \AA}$ ,  $\gamma = 103.0^\circ$ .

RT			363 K			390 K		
<i>hkl</i>	$2\theta_{\text{exp}}/^\circ$	$2\theta_{\text{calc}}/^\circ$	<i>hkl</i>	$2\theta_{\text{exp}}/^\circ$	$2\theta_{\text{calc}}/^\circ$	<i>hkl</i>	$2\theta_{\text{exp}}/^\circ$	$2\theta_{\text{calc}}/^\circ$
(100)	5.99	6.01	(010)	7.35	7.34	(100)	7.45	7.45
(010)	8.47	8.45	(100)	7.57	7.58	(010)	7.80	7.81
(1 $\bar{1}$ 0)	9.62	9.54	(1 $\bar{1}$ 0)	8.78	8.78	(1 $\bar{1}$ 0)	9.51	9.51
(110)	11.09	11.15	(110)	12.09	12.07	(110)	11.96	11.96
(200)	12.00	12.04	(101)	13.10	13.13	(101)	13.10	13.12
(2 $\bar{1}$ 0)	13.58	13.54	(1 $\bar{1}$ 1)	13.88	13.86	(1 $\bar{1}$ 1)	14.37	14.39
(1 $\bar{1}$ 1)	15.63	15.63	(1 $\bar{2}$ 0)	14.31	14.32	(200)	14.93	14.94
(011)	16.41	16.43	(020)	14.71	14.70	(1 $\bar{2}$ 0)	15.76	15.76
(020)	16.87	16.94	(200)	15.19	15.19	(111)	16.10	16.13
(1 $\bar{1}$ 1)	17.43	17.36	(111)	16.20	16.16	(210)	18.41	18.38
(2 $\bar{1}$ 1)	18.00	18.05	(2 $\bar{2}$ 0)	17.61	17.62	(2 $\bar{1}$ 1)	18.72	18.69
(3 $\bar{1}$ 0)	18.59	18.70	(1 $\bar{2}$ 1)	17.95	17.91	(2 $\bar{2}$ 0)	19.11	19.08
(2 $\bar{2}$ 0)	19.07	19.15	(021)	18.26	18.22	(211)	21.33	21.36
(3 $\bar{1}$ 1)	20.32	20.34	(201)	18.62	18.62	(002)	21.68	21.65
(02 $\bar{1}$ )	20.82	20.90	(210)	18.83	18.83	(2 $\bar{2}$ 1)	21.97	21.97
(3 $\bar{1}$ 1)	21.90	21.94	(2 $\bar{2}$ 1)	20.67	20.66	(300)	22.48	22.49
(021)	22.51	22.47	(1 $\bar{3}$ 0)	21.07	21.07	(1 $\bar{3}$ 0)	23.06	23.07
(211)	23.33	23.29	(002)	21.47	21.50	(030)	23.60	23.58
(2 $\bar{2}$ 1)	23.84	23.69	(3 $\bar{1}$ 0)	21.77	21.75	(220)	24.05	24.05
(40 $\bar{1}$ )	24.26	24.25	(030)	22.13	22.13	(3 $\bar{2}$ 0)	24.37	24.39
(121)	24.93	24.94	(300)	22.86	22.87	(3 $\bar{1}$ 1)	24.68	24.63
(301)	25.51	25.50	(1 $\bar{1}$ 2)	23.30	23.26	(2 $\bar{3}$ 1)	24.96	24.96
(10 $\bar{2}$ )	26.02	26.06	(3 $\bar{1}$ 1)	24.33	24.30	(310)	25.48	25.48
(20 $\bar{2}$ )	26.47	26.43	(112)	24.80	24.73	(031)	25.95	25.99
(320)	26.88	26.88	(301)	25.36	25.31	(202)	26.42	26.41
(4 $\bar{2}$ 1)	27.96	27.93	(130)	25.60	25.58	(3 $\bar{2}$ 1)	26.77	26.73
(3 $\bar{3}$ 0)	28.92	28.89	(022)	26.20	26.15	(2 $\bar{3}$ 1)	27.25	27.25
			(3 $\bar{3}$ 0)	26.57	26.56	(311)	27.72	27.73
			(2 $\bar{2}$ 2)	27.97	27.93	(212)	28.51	28.55
			(311)	28.34	28.33	(3 $\bar{3}$ 0)	28.81	28.80
			(212)	28.76	28.73	(4 $\bar{1}$ 0)	29.33	29.37