

<p>COMPONENTS:</p> <p>(1) Potassium iso.butanoate (potassium iso.butyrate); ($\text{i.C}_4\text{H}_7\text{O}_2$)K; [19455-20-0]</p> <p>(2) Sodium iso.butanoate (sodium iso.butyrate); ($\text{i.C}_4\text{H}_7\text{O}_2$)Na; [996-30-5]</p>	<p>EVALUATOR:</p> <p>Schiraldi, A., Dipartimento di Chimica Fisica Universita' di Pavia (ITALY).</p>
<p>CRITICAL EVALUATION:</p> <p>This system was studied only by Sokolov and Pochtakova (Ref. 1) who suggested the phase diagram to be of the eutectic type, the invariant point occurring at 521 K (248 °C) and $100x_1 = 7.5$.</p> <p>Component 1, however, forms liquid crystals. Therefore the temperature of 633 K (360 °C) given in Ref. 1 should be identified with the clearing (and not the fusion) temperature of this component, and compared with the $T_{\text{clr}}(1)$ value (625.6 ± 0.8 K) reported in Table 2.</p> <p>For the same component, three phase transition temperatures are quoted in Ref. 1 from Ref. 2, i.e., 621, 546, and 481 K, the second of which can be reasonably identified with the fusion temperature [$T_{\text{fus}}(1) = 553.9 \pm 0.5$ K] listed in Preface, Table 2. Consequently: (i) the transition temperature at 621 K (if actually existing) might correspond to some kind of transformation (undetected by DSC, see Preface, Table 2) within the liquid crystal field; and (ii) only the transition at 481 K should correspond to a solid state transformation, although the latter figure is almost 60 K higher than the single $T_{\text{trs}}(1)$ value (424 ± 3 K) listed in Table 2 of the Preface.</p> <p>Concerning component 2, the fusion temperature of 535 K (262 °C; Ref. 1) is in reasonable agreement with that (526.9 ± 0.7 K) reported in Table 2 of the Preface. In this Table, however, no mention is made of other phase transformations, although three solid state transitions are quoted for this component in Ref. 1 (from Ref. 2), at 493, 364, and 340 K (220, 91, and 67 °C), respectively. Duruz et al. (Ref. 3) report in turn: fusion at 527 K (in agreement with the fusion temperature from Table 2), and solid state transitions at 493 K (in agreement with the highest transition temperature from Ref. 2), and at 468 K (a figure which has no correspondence in Ref. 2). Finally, Ferloni et al. (Ref. 4) are inclined to think that Sokolov's transformation at 340 K (Ref. 2) actually represents a transition of a hydrated form of the salt.</p> <p>In the evaluator's opinion, a re-investigation of the phase relations in solid sodium iso.butanoate would be desirable. At any rate, the phase diagram suggested by Sokolov and Pochtakova (Ref. 1) has to be modified (due to the occurrence of liquid crystals in component 1) with reference to Schemes A.1, or A.3, of the Preface according to the kind of solid state miscibility between components, the eutectic point actually being an M'_E point.</p> <p>REFERENCES:</p> <p>(1) Sokolov, N.M.; Pochtakova, E.I. Zh. Obshch. Khim. <u>1960</u>, 30, 1405-1410 (*); Russ. J. Gen. Chem. (Engl. Transl.) <u>1960</u>, 30, 1433-1437.</p> <p>(2) Sokolov, N.M. Tezisy Dokl. X Nauch. Konf. S.M.I. <u>1956</u>.</p> <p>(3) Duruz, J.J.; Michels, H.J.; Ubbelohde, A.R. Proc. Roy. Soc. London <u>1971</u>, A 322, 281-299.</p> <p>(4) Ferloni, P.; Sanesi, M.; Tonelli, P.L.; Franzosini, P. Z. Naturforsch. <u>1978</u>, A 33, 240-242.</p>	

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<p>VARIABLES:</p> <p>Temperature.</p>	<p>PREPARED BY:</p> <p>Baldini, P.</p>																																																																					
<p>EXPERIMENTAL VALUES:</p> <table data-bbox="123 520 368 1098"> <thead> <tr> <th>$t/^\circ\text{C}$</th> <th>T/K^a</th> <th>$100x_1$</th> </tr> </thead> <tbody> <tr><td>262</td><td>535</td><td>0</td></tr> <tr><td>254</td><td>527</td><td>5</td></tr> <tr><td>248</td><td>521</td><td>7.5</td></tr> <tr><td>255</td><td>528</td><td>10</td></tr> <tr><td>266</td><td>539</td><td>15</td></tr> <tr><td>277</td><td>550</td><td>20</td></tr> <tr><td>285</td><td>558</td><td>25</td></tr> <tr><td>293</td><td>566</td><td>30</td></tr> <tr><td>302</td><td>575</td><td>35</td></tr> <tr><td>308</td><td>581</td><td>40</td></tr> <tr><td>315</td><td>588</td><td>45</td></tr> <tr><td>320</td><td>593</td><td>50</td></tr> <tr><td>325</td><td>598</td><td>55</td></tr> <tr><td>331</td><td>604</td><td>60</td></tr> <tr><td>335</td><td>608</td><td>65</td></tr> <tr><td>338</td><td>611</td><td>70</td></tr> <tr><td>342</td><td>615</td><td>75</td></tr> <tr><td>345</td><td>618</td><td>80</td></tr> <tr><td>348</td><td>621</td><td>85</td></tr> <tr><td>353</td><td>626</td><td>90</td></tr> <tr><td>357</td><td>630</td><td>95</td></tr> <tr><td>360</td><td>633</td><td>100</td></tr> </tbody> </table> <div data-bbox="769 546 1131 1038"> </div> <p>^a T/K values calculated by the compiler.</p> <p>Characteristic point(s): Eutectic, E, at 248 °C and $100x_1 = 7.5$ (authors).</p>		$t/^\circ\text{C}$	T/K^a	$100x_1$	262	535	0	254	527	5	248	521	7.5	255	528	10	266	539	15	277	550	20	285	558	25	293	566	30	302	575	35	308	581	40	315	588	45	320	593	50	325	598	55	331	604	60	335	608	65	338	611	70	342	615	75	345	618	80	348	621	85	353	626	90	357	630	95	360	633	100
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<p>METHOD/APPARATUS/PROCEDURE:</p> <p>Visual polythermal analysis.</p>	<p>SOURCE AND PURITY OF MATERIALS:</p> <p>Both components were prepared from commercial "pure" grade iso.butanoic acid, distilled before use, and the proper "chemically pure" hydrogen carbonate (Ref. 1); then recrystallized from n-butanol. Component 1 undergoes phase transitions at $t_{\text{trs}}(1)/^\circ\text{C} = 208, 273, 348$ (Ref. 2). Component 2 undergoes phase transitions at $t_{\text{trs}}(2)/^\circ\text{C} = 67, 91, 220$ (Ref. 2).</p>																																																																					
<p>REFERENCES:</p> <p>(1) Sokolov, N.M. Zh. Obshch. Khim. 1954, 24, 1150-1156.</p> <p>(2) Sokolov, N.M. Tezisy Dokl. X Nauch. Konf. S.M.I. 1956 (this is Ref. 6 in the original paper, and not Ref. 5 as erroneously quoted in the text; compiler).</p>	<p>ESTIMATED ERROR:</p> <p>Temperature: accuracy probably ± 2 K (compiler).</p>																																																																					