

## Wasserstoffbrückenbindungen mit Cyanidionen? Die Strukturen von 1,3-Diisopropyl-4,5-dimethylimidazoliumcyanid und 1-Isopropyl-3,4,5-trimethylimidazoliumcyanid

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### Abstract

#### Hydrogen Bonds with Cyanide Ions? The Structures of 1,3-Diisopropyl-4,5-dimethylimidazolium Cyanide and 1-Isopropyl-3,4,5-trimethylimidazolium Cyanide

1,3-Diisopropyl-4,5-dimethylimidazolium cyanide (**2a**) and 1-isopropyl-3,4,5-trimethylimidazolium cyanide (**2b**) are obtained from the reaction of the corresponding 2,3-dihydrodimethylimidazol-2-ylidenes (**1**) and hydrogen cyanide in excellent yield. Their crystal structure analyses reveal the presence of ion pairs linked by hydrogen bonds. The crystal structure analysis of **2a** reveals a near colinear orientation of the C(1)-H bond axis and the cyanide ion while in **2b** this orientation is perpendicular. In both cases, the interionic distances are in the expected range for hydrogen bonds. Ab-initio calculations of the total energy of the salts **2** indicate small differences in energy between the colinear and perpendicular orientation of the ions as well as between the colinear C-H...C-N and C-H...N-C orientations. The comparison of calculated and measured <sup>13</sup>C and <sup>15</sup>N NMR chemical shifts does not allow the distinction between the possible orientations.