$Li_{2.3}CuFeS_2$: A Novel Lithium Intercalated Compound

Jaime Llanos,* Marcelo Tejeda, Carlos Contreras-Ortega and Carlos Mujica

Departamento de Química, Universidad Católica del Norte, Casilla 1280, Antofagasta, Chile

Reaction of Li_2S with $CuFeS_2$ gives the compound $Li_{2.3}CuFeS_2$, which has a layered structure with intercalated lithium atoms.

In the course of investigations on the chemistry of copper–iron sulphide cathodes for use in secondary batteries,[1] we found that the reaction of Li_2S with $CuFeS_2$ at 1173 K in graphite crucibles, gives a new sulphide phase with the composition $Li_{2.3}CuFeS_2$. (Elemental analysis, calc.: Cu, 32.02; Fe, 28.00; S, 32.14; Li, 8.00%. Found: Cu, 31.88; Fe, 26.83; S, 33.33; Li, 7.96%).

$Li_{2.3}CuFeS_2$ forms grey crystals with metallic lustre. These crystals can be easily cleaved. The growth direction is [010] and the cleavage plane is (100). X-Ray powder diagrams and Buerguer precession photographs show that $Li_{2.3}CuFeS_2$ is hexagonal with $a = 3.86$ and $c = 6.56$ Å. Further structural investigations are in progress.

$Li_{2.3}CuFeS_2$ shows remarkable reactivity to air and moisture. The reactivity depends on the degree of crystallization; fine grained powder samples react fast, but larger crystals decompose only over a period of several hours. Protic solvents such as water or alcohol react topotactically with $Li_{2.3}CuFeS_2$ with hydrogen evolution parallel to (100) planes and the crystals decompose into graphite-like flashes of another new material that contains less than 0.34% Li, indicating that lithium simultaneously oxidizes and leaves the crystal. Reflection electron microscopy (REM) photographs show that both compounds are layered.

The easy cleavage along planes and the softness that we observe in the delithiated phase, rule out the possibility that normal valence forces are operative between planes. Preliminary coulometric titration experiments, carried out in propylene carbonate, showed that it is possible to insert lithium atoms in these compounds, probably due to the virtual lack of bonding between planes.

The above facts allow us to assume that reduction of Li^+ (Li_2S) to Li^0 occurs in the formation of $Li_{2.3}CuFeS_2$. In addition, the atom ratio of Cu : Fe = 1 : 1 and the laminar structure of $Li_{2.3}CuFeS_2$ leads us to discard a substitution of Cu by Li as was reported for other Li–Cu–Fe sulphide phases.[2,3] Hence, we conclude that lithium atoms are intercalated in a copper–iron sulphide framework. These results show the new $Li_{2.3}CuFeS_2$ compound as a very promising cathode material for lithium batteries.

More work to evaluate the properties of this new phase as a cathode in lithium batteries using molten salts or organic solvents, is in progress.

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