

High-pressure x-ray crystallographic investigation of chalcogen bonding

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Keywords: High-pressure, Chalcogen Bonding, Organoselenium Molecules

Non-covalent interactions play a central role across a broad range of fields including drug design, molecular biology, and crystal engineering. Chalcogen bonding, a close relative of hydrogen and halogen bonding, is one such non-covalent interaction that is known to occur in crystalline solids.[1]

Ebselen is an organoselenium molecule that is known to exhibit anti-inflammatory and anti-viral properties,[2] and as a crystalline solid it has previously been shown to form chalcogen bonds in part due to its Se-N covalent bond.[3,4] Many derivatives of ebselen exist, and are also likely to form chalcogen bonding interactions, however not a lot is known about what would happen to these interactions under high-pressure conditions. Is there a shortening of the intermolecular chalcogen bond length, does the chalcogen bonding interaction become more stable, or is there a phase transition that alters the binding motif under high-pressure conditions?

To answer these questions, derivatives of ebselen have been investigated utilising high-pressure x-ray crystallography to better understand what happens to chalcogen bonding interactions when subjected to high-pressure conditions. Recently, the ebselen derivative 2-(3-pyridyl)-1,2-benziselenazol-3(2H)-one was investigated at the Australian Synchrotron, where structural information was determined at various pressures that range from ambient conditions up to 5.5 GPa, with a phase transition occurring at approximately 3 GPa. The chalcogen bond interaction was shown to occur between the pyridyl nitrogen and the selenium, with the intermolecular bond length decreasing under high pressure conditions.

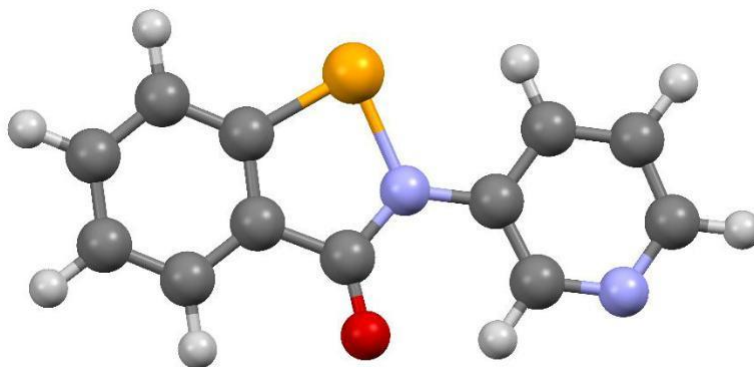


Figure 1. Structure of 2-(3-pyridyl)-1,2-benziselenazol-3(2H)-one, a derivative of ebselen, under ambient conditions.

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