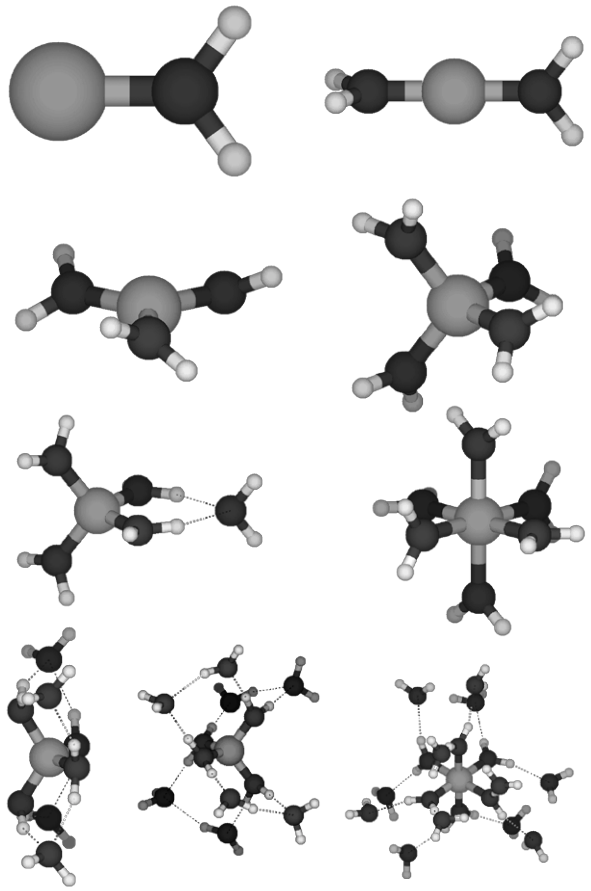
Beryllium hydration in aqueous solution. II. Correlation consistent basis set calculations

C.C. PYE*

Department of Chemistry, Saint Mary's University, 923 Robie St., Halifax NS, Canada B3H 3C3 (*correspondence: cory.pye@smu.ca)

The structures, energies, and vibrational frequencies of Be $(H_2O)_n^{2+}$, n=0-6, 8, 12, 18 have been calculated at the Hartree-Fock (HF), second-order Moller-Plesset (MP2), and density functional (B3LYP) levels of theory using the correlation-consistent basis sets [1]. Comparisons to the literature Raman spectra of aqueous beryllium solutions will be made [2].



[1] Pye (2009) *J. Mol. Struct. (Theochem)*, **913**, 210-214. [2] Rudolph, Fischer, Irmer & Pye (2009) *Dalton Trans.*, 6513-6527.

Uralian eclogites as exhumed ultrahigh-pressure paleoproterozoic rocks

A.M. PYSTIN AND J.I. PYSTINA

Institute of Geology, Komi Science Centre, Ural Branch of RAS, Syktyvkar, Russia (pystina@geo.komisc.ru)

In the Urals, the majority of dates obtained on eclogites falls within the interval 390-240 Ma. Taking this fact as a basis, many scientists limit the time of formation of eclogite-bearing rock associations (from the stage of high-pressure paragenesis crystallization in deep-seated zones till eclogite exhumation during the collision and post-collision stages of fold-orogenic belt development) by the above period.

However, there are more ancient dates on the objects to be studied. That is why, not denying the theoretical possibility of eclogite formation and exhumation during a single geodynamic cycle, we consider more realistic the models, which allow for a long time break between the eclogite formation and exhumation of the high-pressure associations out of the deep zones.

On the ground of the geochronological data yielded by Uralian eclogites, three age levels of the high-pressure metamorphic rocks formation (and alteration) can be distinguished: over 1560, 720-550, and 390-240 Ma.

Nowadays most researches think that conditions for metamorphic eclogite crystallization can occur only in subduction zones. We could agree to this hypothesis, however, repeated manifestation of high-pressure metamorphism in the same complexes in the course of more than 1 bln years seems unlikely. It appears that only the oldest eclogite ages (over 1560 Ma) point to the crystallization time of these rocks in subduction zones. Neoproterozoic and Paleozoic dates indicate the time of collision and post-collision processes at younger stages of geodynamic development. The dislocation of eclogite-bearing complexes to the lower levels of the Earth's crust is connected with them.