Dissolution of BeO in acidic media

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Dissolution of beryllium oxide in low pH environments is a first step to aqueous beryllium exposure. Before studying how the dissolved beryllium particulates interact with the body, it is useful to know the structure of the dissolved beryllium complexes. Approaches starting from solid BeO and building from beryllium ions in solution give complementary structures. Since simulation of the dissolution of BeO is computationally intensive, the reverse process of adsorption of beryllium onto the BeO surface is considered. This process has identified an adsorbed beryllium structure reminiscent of $Be_3(H_2O)_5(OH)_4^{+3}$. Adding protons to each of the surface attached hydroxyls could liberate $Be(H_2O)_3(OH)^+$. Earlier quasi-chemical analysis finds that the beryllium ion is preferentially solvated by four waters and the solvated species has a pKa of 3.8. Figure 1 shows other possible beryllium complexes in solution, their hydrate structure and pKa. The pH in the vacuole of the pulmonary macrophage, which ingests the beryllium oxide particulates, is 4.8. The final column in Figure 1 shows the possible forms of beryllium in a 4.8 pH solution. Previous studies suggest that the first two forms are the most likely.

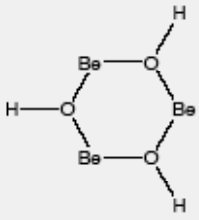
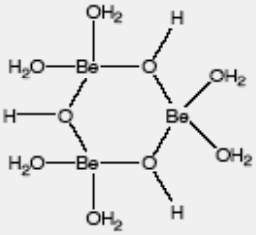
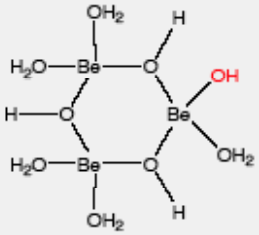
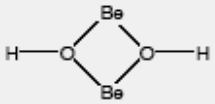
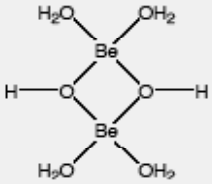
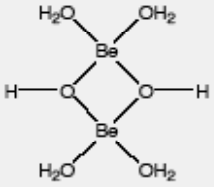
Base Structure	Hydrate	pKa	Structure in Solution (pH = 4.8)
Be^{2+}	$Be(H_2O)_4^{2+}$	3.8	$BeOH(H_2O)_3^{+}$
		3.9	
BeOH	$BeOH(H_2O)_3^{+}$	5.8	$BeOH(H_2O)_3^{+}$
		6.6	

Figure 1. The hydrated form of possible beryllium solutes and their pKa. Primitive quasi-chemical theory was used for the solvation free energies.