**Appendix E. Deposited as an electronic file only** Table 3. The main concepts introduced when preliminary considering inorganic crystal structures

			D C
Compounds	Examples of problems discussed	Concepts introduced	References
			(see Appendix C)
Binary and tertiary	What is the difference between a	Polymeric structures	Aslanov, 1989; Belov,
compounds	phase of $Fe_3O_4$ and a mixture of the	instead of individual	1947, 1951, 1986;
	two phases - $Fe_2O_3$ and $FeO?$	molecules.	Bokii 1972; Glusker <i>et</i>
	Describe a structure as i) a close-	Atomic and ionic radii.	<i>al.</i> , 2002; Mitchell,
	packing of balls, b) a set coordination	Close packing of different	2002; Navrotsky,
	polyhedra sharing vertices / edges /	balls.	1998; Shaskolskaya
	faces.	Coordination number.	1984; Tejuca, 1993
	Which parameters determine the	Coordination polyhedra.	
	crystal structure: the relative sizes of	Databases (revisited).	
	species, electronic structure, both?	Preferred coordination of	
	Correlate structures and properties.	an element (in relation to	
		coordination chemistry	
		and metal coordination in	
		proteins).	
		Structure-properties	
		relations (revisited).	
		Polymorphs and	
		polytypes (revisited)	
Perovskite and	The same as above +	Families of structures,	
ferrite families	Consider examples of the	"theme and variations"	
	chemical reactions "solid + solid",	Topotactic reactions.	
	"solid + gas",	Precursor techniques.	
	and discuss, which changes in the	Reconstructive and	Egger & Feitknecht,
	crystal structures they require.	destructive	1962; Feitknecht &
	Explain, why soft oxidation of small	transformations.	Mannweiler, 1967;
	Fe <sub>3</sub> O <sub>4</sub> particles gives $\gamma$ -polymorph		Gillot et al., 1978;
	of $Fe_2O_3$ , whereas the oxidation of		Yang & Yang, 2009
	large particles at high temperature		
	gives the $\alpha$ -polymorph		
	0 1 7 1		
Polymorphs of SiO <sub>2</sub> ,	Consider the structures as various	Families of structures,	Gibbs et al., 2009;
silicates	combinations of (SiO <sub>4</sub> ) <sup>4-</sup> in relation to	"theme and variations".	Dubrovinskaia, 2001;
	properties. Consider the structures, in	Structure-properties	Hazen et al., 1996;
	which Si has coordination higher	relations (continued)	Liebau, 1985;
	than 4. Under which conditions can		Pushcharovsky, 1986;
	these structures be expected to form		Thomson & Downs,
	and be stable?		2004, 2008, 2010
$CO_2$ in relation to	Compare the high-pressure	Pressure-induced	Santoro, 2010; Sun et
SiO <sub>2</sub>	framework structures of CO <sub>2</sub> with the	transitions "molecular	al., 2009
	ambient-pressure structures of SiO <sub>2</sub>	crystal - polymeric	
		structure" (revisited)	