Advanced Inorganic Chemistry part Inorganic Molecules

Exercises 1 to 22 (electronic and molecular structures, building reactions, and chemical and physical properties, and symmetry of inorganic molecules and molecular ions and of main group IV, V, and VI elements, hydrogen bonding, packing of molecules, structure determination methods)

Exercise 1

For 3 of the molecules and ions listed below, give the oxidation numbers of the non-ligand atoms, draw a suitable Lewis structure with the formal charges (if necessary) by using lines for bonds and free electron pairs and dots for single electrons, the ψ-type AL_mE_n (m = number of ligands, n = number of free electron pairs or single electrons) the resulting ψ-polyhedron, the gas phase structure/shape and the symmetry of the molecule (in form of a draw or description), and mark those with a star which have no resonance structures (no other electronic structure).
Give the result in form of a table as given below.

Formula	**Ox. no.**	**Lewis struct.**	**ψ-type**	**ψ-polyhedron**	**Mol. struct.**	**Sym.**
NF_3	3+	draw it	AL_3E	tetrahedron	trig. pyr.	C_{3v}

Exercise 2

For the same molecules and ions treated in Exercise 1, give the formula, the names, a suitable building reaction, the reactivity, the color, the state of matter under normal conditions (if possible), and the magnetic properties (d for dia- and p for paramagnetic).
As far as possible, give the result in form of a table.

Molecules/ions to be treated in exercises 1 and 2.

No	**Name**				**No**	**Name**			
1	Quimeng	AsX_3	N_2	SeX_2	18	Bontu	ClF_5	SO_2	TeX_2
2	Jia	AsX_4^+	N_2O	SeX_4	19	??? Murthay	CO_2	OX_2	S_2
3	Suriev	$BeCl_2$	$N_2O_2^{2-}$	SF_4	20	Klein	CO_3^{2-}	$P_2O_6^{4-}$	S_2Cl_2
4	Lu	BeX_4^{2-}	N_2O_3	SF_6	21	Baskara	CX_4	$P_2O_7^{4-}$	S_2F_{10}
5	Jiang	BrF_3	N_2O_4	SiF_6^{2-}	22	Hameed	GaI_3	P_2Se_5	S_2F_2
6	Li	BrF_4^-	N_2O_5	SiX_4	23	Kothapally	GeX_4	$P_4(NR)_6$	$S_2O_3^{2-}$
7	Zhang	BrF_5	NO	$SnCl_2$	24	Kölsch	$H_2PO_2^-$	P_4O_{10}	$S_2O_4^{2-}$
8	Tran	BX_3	NO^+	ZnX_2	25	Krämer	HgX_2	P_4O_6	$S_2O_6^{2-}$
9	Khairalla	BX_4^-	NO_2	SO_3	26	Jasper	HPO_3^{2-}	P_4S_6	$SbCl_5$
10	Fazuldjanova	$[(CH_3)_2PN]_3$	NO_2^-	SO_3^{2-}	27	Lai	I_2Cl_6	PCl_3F_2	SbF_5
11	Pithan	$[(CH_3)_2SiO]_3$	NO_2^+	SO_4^{2-}	28	Lucke	I_3^-	PCl_5	SbX_3
12	Steinhoff	$[Cl_2PN]_3$	NO_3^-	SX_2	29	Nischal	ICl_2^-	PCl_6^-	XeF_3^+
13	Steinbrück	$[Cl_2PN]_4$	NX_3	$Te(OH)_6$	30	Salah Uddin	ICl_4^-	PF_5	XeF_4
14	Schmidt	CdX_2	NX_4^+	TeF_4	31	Stephan	IF_5	PF_6^-	Se_2F_{10}
15	Höfer	ClF_3	OH_3^+	TeF_6	32	Cleiton	IF_7	PO_4^{3-}	XeF_5^+
16	v. Gradowski	SCl_4	SeF_4	XeF_2	33	Roesener	TeF_7^-	PX_3	XeF_6
17	Staudt	SCl_2	SeF_6	XeO_4	34		$BrCl_3$	NO_3^-	XeO_3

* X = F, Cl, Br, and/or I

Every student has to treat the 3 molecules/ions given in the table (going down from No 1 to No 34).

For help, information, and further exercises, refer to the given textbook(s) of inorganic chemistry and to our corresponding website (http://anorganik.chemie.uni-siegen.de, then "Advanced Inorg. Chem." and "Inorganic Molecules").

Exercise 3
Please explain why P_4O_6, and P_4O_{10} are built instead of P_2O_3 and P_2O_5, respectively.

Exercise 4
Please sketch suitable Lewis formula of potential non-cyclic and cyclic P_4S_6 (no exo S atoms).

Exercise 5
$(Cl_2PN)_3$ was found to have symmetry D_{3h}. Sketch a Lewis formula and explain why it is not aromatic.

Exercise 6
Name and describe structurally two forms each of the elements C, P, and S.

Exercise 7
Name and describe structurally the allotropic forms of the main group IV elements.

Exercise 8
Name and describe structurally the allotropic forms of the main group V elements.

Exercise 9
Name and describe structurally the allotropic forms of the main group VI elements.

Exercise 10
Name and describe structurally the thermodynamically stable forms of the elements C, P, and S.

Exercise 11
Name the number of covalent bonds, the elements N, P, S, and Cl can build, and explain why the compounds or ions SiF_6^{2-}, PF_5, SF_6 do exist and CF_6^{2-}, NF_5, OF_6 do not.

Exercise 12
Sketch the Lewis structures of N_2, NH_3, and S_2 and explain why these molecules do not have different resonance structures.

Exercise 13
Sketch the Lewis structures and the expected and found molecular structures and give the names and the symmetry groups (Schönflies or Hermann/Mauguin) of "P_2O_3". "P_2O_5", P_4S_6, and P_2Se_5.

Exercise 14
Sketch and explain the VB wavefunctions and MO's of N_2 and HF.

Exercise 15
Give a short definition of a hydrogen bond and name and explain the factors affecting the strength of a hydrogen bond.

Exercise 16
Name the factors affecting the acceptor capability of a hydrogen-bond acceptor and order the given anions according to their relative acceptor capability (staring with the weakest and ending with the strongest): Br^-, ClO_4^-, F^-, SO_3^{2-}, SO_4^{2-}, H_2O, H_3O^+, $HSeO_3^-$, and OH^-.

Exercise 17
Assign the hydrogen bond enthalpies of 7, 22, and 55 kJ/mol to the hydrogen bonds $HO\text{-}H\cdot\cdot OH_2$, $HO\text{-}H\cdot\cdot Cl^-$, and $HS\text{-}H\cdot\cdot SH_2$, respectively.

Exercise 18
Give the ranges of energies and wavelengths of X-ray, UV/Vis, and IR radiation. Name and describe the structure determination methods based on these radiations and explain the respective physical processes.

Exercise 19
Sketch the principle parts of an IR spectrometer and a X-ray diffraction device and describe the main differences between IR spectroscopy and X-ray diffraction concerning the principle processes, selection rules, changes of energy etc., and their meaning for the structure determination of inorganic molecules.

Exercise 20
Sketch the principle parts of an IR and a Raman spectrometer and describe the main differences between IR and Raman spectroscopy concerning the principle processes, selection rules, and their meaning for the structure determination of inorganic molecules.

Exercise 21
Name and describe/scetch two common structure determination methods based on different types of electromagnetic radiation with their ranges of energies and wavelengths each and the respective physical processes.

Exercise 22
Name and specify the factors and forces affecting the crystal structures of molecular solids.

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