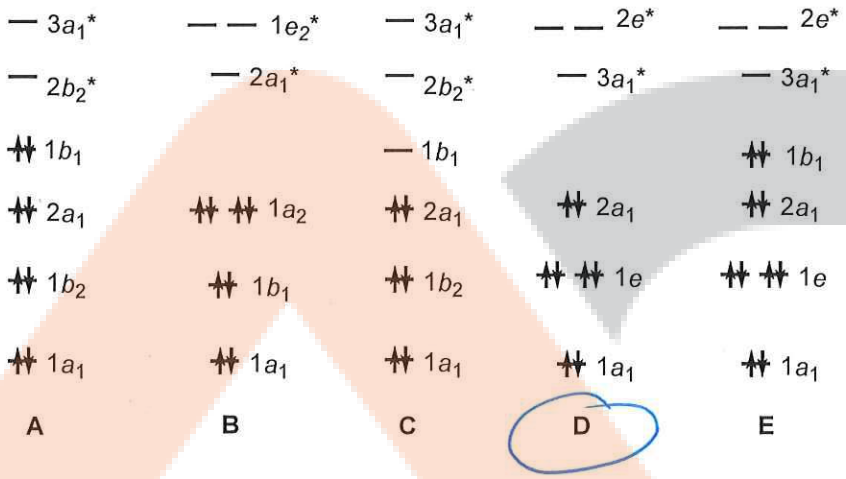
1. Identify the point groups of the following species in their predicted geometry. **(4 p)**

XeF_4	B_2H_6	SO_3^{2-}	SF_6
D_{4h}	D_{2h}	C_{3v}	O_h

2. Identify the correct simplified MO diagram for the hydronium ion, OH_3^+ **(4p)**.



$3 \times 1S(H) + 2S(O) + 3 \times 2p(O) = 7$ atomic orbitals $\Rightarrow$ 7 MO $\Rightarrow$ B or D

$OH_3^{\oplus} \Rightarrow C_{3v} \Rightarrow$ no S_1 symmetry as in B $\Rightarrow$ D

There are other justifications as well.

3. Identify the elements that are oxidized and reduced during the discharge of a secondary (rechargeable) lithium ion battery of your choice. A chemical equation is not necessary. (**2 p**)

carbon (or graphite) is oxidised.

cobalt or iron is reduced.

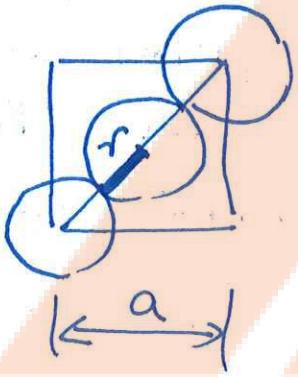
4. Determine the percentage carbon (by mass) in 18-crown-6. (**2 p**)

$(CH_2-CH_2-O)_6$

$$\frac{12.1 \times 2 \times 100}{12.1 \times 2 + 16.00 + 1.008 \times 4} = 54.71\ \%$$

5. Calcium crystallizes in a face centered cubic structure with the unit cell edge of 536.04 pm. Using this data, calculate the density of calcium metal in g/cm^3 and the metallic radius of calcium in pm. Avogadro's number is 6.022×10^{23}. (**4 p**)

$$d = \frac{M}{V} = \frac{4 \times 40.08}{6.022 \times 10^{23}} \cdot \frac{1}{5.36^3 \times 10^{-24}} = 1.729\ g/cm^3.$$



$$a^2 + a^2 = (4r)^2$$

$$2a^2 = (4r)^2 \Rightarrow r = \frac{a\sqrt{2}}{4} =$$

$$= \frac{536.04\sqrt{2}}{4} = 189.52\ pm.$$

6. Define a Lewis acid (**2 p**).

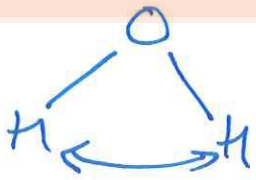
A Lewis acid is an electron pair acceptor.

7. The H-E-H bond angles of Group 16 hydrides and fluorides are provided in the table below. Explain why water has a) a wider bond angle than hydrogen sulfide and b) a slightly wider bond angle than oxygen fluoride. **(2 p)**.

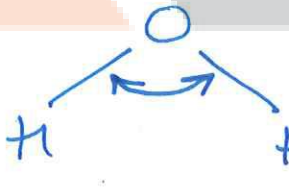
	H_2O	H_2S	H_2Se	H_2Te
H-E-H angle, °	104.45	92.1	91.0	90.0
F-E-F angle, °	103.1	98.2	94.0	

a) Major factor: the smaller, more electronegative O brings the O-H bonding electrons in close proximity, causing repulsion.
Minor factor: the O-H bonds are shorter, resulting in steric interactions between the two H's.

b) F is more electronegative than O, hence the bond is polarized towards F.
The bonding electrons are further away from each other and their reciprocal electrostatic repulsion is reduced.



steric repulsion



electrostatic repulsion of bonding electrons.

****

RR

C_{2v}	E	C_2	σ_v	σ_v‘		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	-1	R_z	
E	2	-1	0	(x, y), (R_x, R_y)	($x^2 - y^2$, xy), (xz, yz)

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$		
A_1	1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	-1	-1	R_z	
B_1	1	-1	1	1	-1		$x^2 - y^2$
B_2	1	-1	1	-1	1		xy
E	2	0	-2	0	0	(x, y)(R_x, R_y)	(xz, yz)

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	*i*	σ(xy)	σ(xz)	σ(yz)		
A_g	1	1	1	1	1	1	1	1		x^2, y^2, z^2
B_{1g}	1	1	-1	-1	1	1	-1	-1	R_z	xy
B_{2g}	1	-1	1	-1	1	-1	1	-1	R_y	xz
B_{3g}	1	-1	-1	1	1	-1	-1	1	R_x	yz
A_u	1	1	1	1	-1	-1	-1	-1		
B_{1u}	1	1	-1	-1	-1	-1	1	1	z	
B_{2u}	1	-1	1	-1	-1	1	-1	1	y	
B_{3u}	1	-1	-1	1	-1	1	1	-1	x	

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1’	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2’	1	1	-1	1	1	-1	R_z	
E’	2	-1	0	2	-1	0	(x,y)	($x^2 - y^2$, xy)
A_1”	1	1	1	-1	-1	-1		
A_2”	1	1	-1	-1	-1	1	z	
E”	2	-1	0	-2	1	0	(R_x,R_y)	(xz, yz)

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$		
A_1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0		($2z^2 - x^2 - y^2$, $x^2 - y^2$)
T_1	3	0	-1	1	-1	(R_x, R_y, R_z)	
T_2	3	0	-1	-1	1	(x, y, z)	(xz, yz, xy)

1 1A																	18 8A
1 H 1.008	2 2A											13 3A	14 4A	15 5A	16 6A	17 7A	2 He 4.003
3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
11 Na 22.99	12 Mg 24.31	3	4	5	6	7	8	9	10	11	12	13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.38	31 Ga 69.72	32 Ge 72.59	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
55 Cs 132.9	56 Ba 137.3	57* La 138.9	72 Hf 178.5	73 Ta 180.9	74 W 183.9	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.6	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra 226.0	89** Ac (227)	104 Rf (261)	105 Ha (262)	106 Sg (263)	107 Ns (262)	108 Hs (265)	109 Mt (266)	110 Uun (269)	111 Uuu (272)