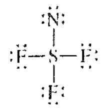
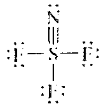
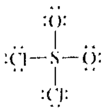
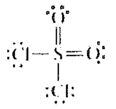
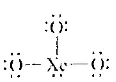
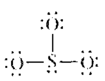
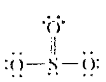
第一大題（Q1－Q27）：單選題（一個答案，答對給分，每題2.5分）不倒扣

1. About electromagnetic radiation, which description is incorrect?
   (a) It includes magnetic and electric fields.
   (b) Gamma ray, X-ray, visible light, electron beam, microwave, and radio waves all are electromagnetic radiations.
   (c) Electromagnetic radiation is a kind of energy.
   (d) The propagation directions of electric and magnetic fields in the electromagnetic radiation are in 90°.
   (e) The velocity of visible light from an illuminator in the vacuum environment is always the same in the two conditions when the illuminator is moving toward and away from the observer.

2. The development of the theories for describing the molecular formulas and geometries is a long history. Taking PF_5 as the example, please check which one below is correct.
   (a) P has higher electronegativity than that of F.
   (b) It has the trigonal bipyramidal structure according to the rule demonstrated by G. N. Lewis.
   (c) The formal charge of P in the structure is 1+.
   (d) The symmetry operation elements of PF_5 include E, C_3, C_2, σ_h, σ_v, S_3.
   (e) The point group of PF_5 is D_3.

3. O_2 gas is active while N_2 gas is inert. Please pick the correct explanations for the difference.
   (a) Both of their highest occupied molecular orbitals (HOMOs) are $\sigma_g(2p)$.
   (b) N_2 has unpaired electrons while O_2 doesn't.
   (c) The bond order of N_2 is 2 and O_2 is 3.
   (d) There is significant 2s-2p orbital mixing in the O atom due to their small energy difference.
   (e) The lowest unoccupied molecular orbital (LUMO) of O_2 is $\sigma_u^*(2p)$.

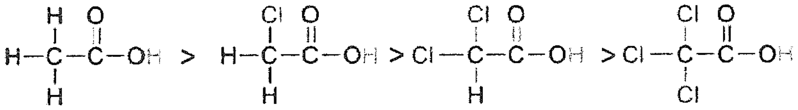
4. The table below records the formal charges and expanded electron counts on the central atoms of the listed molecules. Please pick the correct values of formal charges in the options for the molecules.

	Octet			*Expanded*			
Molecule		*Atom*	*Formal Charge*		*Atom*	*Formal Charge*	*Expanded to:*
SNF_3		S N	$\boxed{a}$		S N	0 0	12
SO_2Cl_2		S O	$\boxed{b}$		S O	$\boxed{e}$	12
XeO_3		Xe O	$\boxed{c}$		Xe O	0 0	14
SO_3^{2-}		S O	$\boxed{d}$		S O	0 0, 1−	10

(a) S:2+, N:2−; (b) S:2+, O:2−; (c) Xe: 2+, O:1−; (d) S:1+, O:1+; (e) S:0, O:0

5. There are two kinds of close packing in crystal structures. Some of the following information about the close packing may not be true. Please point the incorrect answer out.
   (a) The types of close packing are ccp and hcp.
   (b) The atomic packing factor (APF) for the close packing is 74%.
   (c) The body-centered cubic crystal structure is the type of ccp.
   (d) The layer stacking for ccp is ABCABC, and that for hcp is ABABAB.
   (e) There are 4 atoms in the unit cell of ccp.

6. There are different kinds of demonstrations for the definitions of acids and bases. Checking which expression below is incorrect.
   (a) In 1884, Arrhenius proposed the concept of acid and base based on the theory of ionization in aqueous solution.
   (b) The Brønsted–Lowry acid–base theory is to declare the concept of conjugated acid and base.
   (c) For the pKa values of the carboxylic acids, the order is as below.



$H_3C-COOH > ClH_2C-COOH > Cl_2HC-COOH > Cl_3C-COOH$

   (d) The order in the basicities of nitrogen-based compounds is listed.
   $NH_3 < NH_2Me < NH_2Et < NHME_2 < NHEt_2 < NHBu_2$
   (e) Both of CO and CO_2 are Lewis acids.

7. NCS^- is a kind of ambidentate ligands. Both of N and S can serve as the Lewis base to coordinate with Lewis acids, but N is more hard base than S. In this regard, please pick the Lewis acids more reactive to N than S.
   (a) Hg_2^{2+}, (b) Fe^{3+}, (c) Cu^+, (d) Hg^{2+}, (e) Ag^+.

8. The four lattice types of unit cells, primitive (P), face-centered (F), body-centered (I), and side-centered (A, B, or C) can be observed in the seven crystal systems. Which crystal system has all the lattice types?
   (a) cubic, (b) monoclinic, (c) hexagonal, (d) orthorhombic, (e) tetragonal.

9. About the periodic table, which description is incorrect?
   (a) The group of alkali elements are of lithophiles.
   (b) Cu and Au are chalcophiles.
   (c) The element with the highest electronegativity is F.
   (d) Ge and As are metalloids.
   (e) Soft acidity: $F^- < Cl^- < Br^- < I^-$

10. $CH_3COOH_{(aq)} + H_2O_{(l)} \rightarrow H_3O^+_{(aq)} + CH_3COO^-_{(aq)}$, which description is incorrect?
   (a) $K_a = [H_3O^+][CH_3COO^-]/[CH_3COOH]$
   (b) $pH = \log K_a$
   (c) H_3O^+ is the conjugate base to CH_3COOH.
   (d) The K_a value of CH_3COOH is 1.7×10^{-5}, indicating it's a kind of weak acids.
   (e) pKa = 4.76

11. $A\ I_2 + B\ OH^- \rightarrow C\ I^- + D\ IO_3^- + E\ H_2O$, please confirm which value is not right for A, B, C, D, and E.
   (a) A = 3 (b) B = 4 (c) C = 5 (d) D = 1 (e) E = 3

12. Isomerism is important in the coordination chemistry. Which description is correct?
   (a) Linkage isomers: $[Pt\mathbf{Cl_2}(NH_3)_4]\mathbf{Br_2}$ vs $[Pt\mathbf{Br_2}(NH_3)_4]\mathbf{Cl_2}$
   (b) Coordination isomers: $[Co(NH_3)_5(\mathbf{NO_2})]^{2+}$ -O—N—O or $-NO_2$
   (c) Hydrate isomers: $[Cr(H_2O)_6]Cl_3$; $[Cr(H_2O)_5Cl]Cl_2 \cdot H_2O$; $[Cr(H_2O)_4Cl_2]Cl \cdot 2H_2O$
   (d) Ionization isomers: $[\mathbf{Co}(NH_3)_6][\mathbf{Cr}(CN)_6]$ and $[\mathbf{Cr}(NH_3)_6][\mathbf{Co}(CN)_6]$
   (e) None of above is correct.

注意：背面有試題

13. X-ray is discovered by Wilhelm Conrad Röntgen and widely used in different areas. About the X-ray, which one is incorrect?
    - (a) The wavelength of X-ray is shorter than that of visible light.
    - (b) X-ray was discovered when Röntgen operated the cathodic tube.
    - (c) X-ray diffraction (XRD) over the crystal is a kind of inelastic scattering.
    - (d) The soft X-ray dissipates quickly at ambient.
    - (e) Bragg equation: $2d\sin\theta = n\lambda$

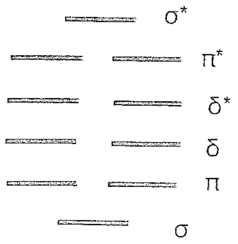
14. A chemical bond length is closed to:
    (a) 10 nm, (b) 1 nm, (c) 0.1 nm (d) 0.1 pm or (e) 1 pm.

15. A C–C bond dissociation energy is closed to:
    (a) 1 kcal/mol, (b) 10 kcal/mol, (c) 100 kcal/mol, or (d) 1000 kcal/mol.

16. The complex that does not obey 18-electron rule is:
    - (a) $[(\eta^5\text{-}C_5H_5)FeCl(CO)(PPh_3)]$
    - (b) $[Cr(CO)_3(SiMe_3)(Cl)(NCMe)_2]$
    - (c) $[Co(PPh_3)_2(AsPh_2)Cl_3]^-$
    - (d) $[Os(N)Br_2(PMe_3)(NMe_2)]^-$
    - (e) $[Fe(NMe_3)_6]^{2+}$

17. Complexes of general formula, *fac*-$[Mo(CO)_3(\text{phosphine})_3]$ have the C–O stretching frequencies as given below.
    Phosphines: (A) PMe_3; (B) PPh_2Cl; (C) PF_3; (D) PCl_3
    One of ν_{CO} (cm^{-1}) of higher frequency: (i) 2090; (ii) 2040; (iii) 1977; (iv) 1945
    The correct combination of phosphine and stretching frequency is
    - (a) (A)-(i); (B)-(ii); (C)-(iii); (D)-(iv)
    - (b) (A)-(iv); (B)-(iii); (C)-(ii); (D)-(i)
    - (c) (A)-(iv); (B)-(i); (C)-(iii); (D)-(ii)
    - (d) (A)-(iv); (B)-(iii); (C)-(i); (D)-(ii)
    - (e) (A)-(i); (B)-(iv); (C)-(iii); (D)-(ii)

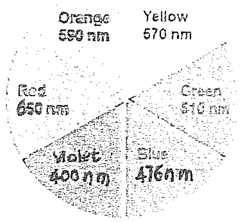
18. Given a qualitative *d* orbital splitting diagrams of three-fold symmetric homobimetallic complexes shown on the right. The metal-metal bond order of $[W_2Cl_6]$ is likely to be:
    (a) 1, (b) 2, (c) 3, (d) 4, or (e) 5.



19. The complex ion $[Cr(CN)_6]^{4-}$ has magnetic properties that correspond to how many unpaired electrons?
    (a) 0, (b) 1, (c) 2, (d) 3, (e) 4.

20. Ethylenediaminetetraacetic acid (EDTA) is:
    - (a) not useful as a chelating agent.
    - (b) an effective antidote for heavy metal poisoning (e.g., Pb^{2+} and Hg^{2+}).
    - (c) a monodentate ligand.
    - (d) known to form unstable complex ions with Fe^{3+}, Hg^{2+}, and Zn^{2+}.
    - (e) known to form complexes with platinum that inhibit the growth of cancerous cells.

21. Solutions of the complexes $[Co(NH_3)_6]^{3+}$ (A), $[Co(H_2O)_6]^{3+}$ (B), and $[CoCl_4]^{4-}$ (C) are colored. One is purple, another is yellow, and the third is blue. Which of the following combination is correct? A color wheel shown below is helpful in determining this relationship.
    - (a) A: bule; B: yellow; C: purple
    - (b) A: yellow; B: blue; C: purple
    - (c) A: purple; B: yellow; C: blue
    - (d) A: yellow; B: purple; C: blue
    - (e) A: bule; B: purple; C: yellow



注意：背面有試題

22. The compound that can undergo oxidative addition reaction with Cl_2 is:
(a) $[(\eta^5\text{-}C_5H_5)_2Fe]$, (b) $[Mn(CO)_5]^-$, (c) $PtCl_4$, (d) $[(\eta^5\text{-}C_5H_5)Mo(CO)_3]^-$, or (e) $[Ir(CO)Cl(PPh_3)_2]$.

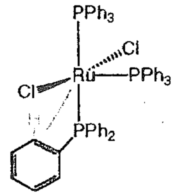
23. What are the states (with J values) of ^3D term?
(a) $^3D_3$, $^3D_2$, $^3D_1$.
(b) $^3D_2$, $^3D_3$, $^3D_4$.
(c) $^3P_1$, $^3P_2$, $^3P_3$.
(d) $^3P_2$, $^3P_3$, $^3P_4$.
(e) $^3F_2$, $^3F_3$, $^3F_4$.

24. Which of the following is labile?
(a) $[(\eta^5\text{-}C_5H_5)_2Ru]$, (b) $[Mn(CN)_6]^{3-}$, (c) $[V(H_2O)_6]^{2+}$, (d) $[CoF_6]^{3-}$, or (e) $[Pt(CN)_4]^{2-}$

25. $[Cu(H_2O)_6]^{2+}$ has ^2D ground state term that splits into two energy levels, the state with lower energy is?
(a) $^2A_{1g}$, (b) $^3T_1$, (c) $^3B_1$, (d) ^2E_g, or (e) $^2T_{2g}$

26. For the hexaaqua complexes of Mn(II), Fe(II), Co(II), Ni(II), Cu(II), and Zn(II), How many of them are expected to exhibit geometric distortions based on Jahn-Teller Theorem?
(a) 0, (b) 1, (c) 2, (d) 3, or (e) 4.

27. The following statements are given regarding the complex $[Ru(PPh_3)_3Cl_2]$ showing an agostic Ru–H–C interaction (structure shown on the right).



I. This complex is an 18-electron species.
II. The ^1H NMR shift of Ru–<u>H</u>–C shows in upfield region as compared to other protons.
III. The agostic C–H bonds shows ν_{CH} that shifts to lower wavenumber as compared to other C–H bonds.
IV. Increased acidity observed for the agostic C–H proton.
How many of these statements are true: (a) 0, (b) 1, (c) 2, (d) 3, or (e) 4

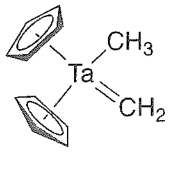
第二大題（Q28－Q40）：複選題（多個答案，全對才給分，每題2.5分） 不倒扣

28. Exchange of an H_2O ligand on $[(CO)_3Mn(H_2O)_3]^+$ is much more rapid than on $[(CO)_3Re(H_2O)_3]^+$. The activation volume for the Mn case is -4.5 ± 0.4 cm^3 mol^{-1}. The Mn complex has infrared bands at 2051 and 1944 cm^{-1} that can be attributed to C–O stretching vibrations. Which of the following are correct?
    (a) First row transition metal complexes are generally more substitutionally labile, thus more "weak-field" than second and third row complexes.
    (b) The negative volume of activation is consistent with a D (or I_d) mechanism.
    (c) Occurrence of two infrared bands of $[(CO)_3Mn(H_2O)_3]^+$ is more consistent with a fac isomer.
    (d) *mer*-$[(CO)_3Mn(H_2O)_3]^+$ is isostructural with *mer*-$[(CO)_3Re(H_2O)_3]^+$.
    (e) The C–O stretching vibrations observed in $[(CO)_3Mn(H_2O)_3]^+$ should have higher vibrational frequencies as compared to free CO.

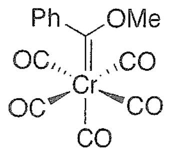
29. Two well-known complex ions containing Ni are $[Ni(H_2O)_6]^{2+}$, which is green, and $[Ni(en)_3]^{2+}$ (en = ethylenediamine), which is purple. Which of these statements are true?
    (a) The green complex absorbs green light.
    (b) The reaction of $[Ni(H_2O)_6]^{2+}$ with excess of en should afford $[Ni(en)_3]^{2+}$.
    (c) Both complex ions are paramagnetic.
    (d) Both complex ions are 18-electron species.
    (e) The crystal field splitting energy is smaller for $[Ni(en)_3]^{2+}$ than for $[Ni(H_2O)_6]^{2+}$.

30. A complex of dihydrogen, such as $[Ir(P^iPr_3)_2Cl_3(H_2)]$, is a metal compound with H_2 as ligands. Which of the following statements are correct for this dihydrogen complex?
    (a) H_2 is a σ-donor.
    (b) The H–H bond length of $[Ir(P^iPr_3)_2Cl_3(H_2)]$ is longer than that of molecular dihydrogen.
    (c) This complex is an 18-electron species.
    (d) The formal oxidation state of Ir should be +3.
    (e) H_2 molecule of $[Ir(P^iPr_3)_2Cl_3(H_2)]$ forms π-bonding interaction with the Ir.

31. Consider the two structures A and B, which of the following statements are correct?
    (a) A is a Fischer Carbene and B is a Schrock Alkylidene.
    (b) The carbene ligand in A should be described as a dianionic, 4-electron donor, and the carbene ligand in B should be described as a neutral, 2-electron donor.
    (c) A can be prepared via α-H elimination.
    (d) A tends to react with a nucleophile.
    (e) B could react with BF_3 to yield a carbide product.



A



B

32. For the reaction show below, which of the following statements are correct?

$$Ni^0L_4 + CO \rightleftharpoons Ni^0L_3CO + L$$

    (a) The forward reaction is likely to go by the Dissociative (D) mechanism.
    (b) The forward reaction should possess a large positive $\Delta H^\ddagger$ and a large negative $\Delta S^\ddagger$.
    (c) To obtain the ΔG for the reaction, you can measure rates of forward reaction at different temperatures to determine rate constants, and plot ln k vs. 1/T.
    (d) PPh_3 would yield the largest value of K_{eq} and ΔG for the reaction as compared to PMe_3 and $P(OEt)_3$. This statement should be attributed to the electronic argument.
    (e) The presence of higher concentration of CO should shift the equilibrium to the right.

33. Which of the following techniques could provide electronic information of a metal complex?
    (a) UV-vis spectroscopy
    (b) IR spectroscopy
    (c) Cyclic Voltammetry
    (d) Mass spectrometry
    (e) EPR spectroscopy

The atom was regarded the smallest unit to compose all kinds of objects in nature by Dalton; however, it was subverted by the discovery of electron followed by the demonstrations for the real atomic structure. Please answer the following groups of questions about the atom and electron. Please answer the following questions 34-36.

34. About the atom, which descriptions are correct?
    (a) J. J. Thomson asserted the plum budding model for the atomic structure.
    (b) J. J. Thomson concluded the charge of an electron in his cathode-ray experiment.
    (c) In Robert A. Millikan's oil drop experiment, the ratio of charge/mass for an electron is -1.76×10^8 C/g.
    (d) By Ernest Rutherford, the concept of the atomic structure formed with the dense nucleus and the loose electron cloud was demonstrated.
    (e) The Bohr hydrogen atomic structure is a model based on quantum mechanics.

35. In the Bohr's model of the hydrogen atom, please find the correct explanations.
    (a) Only the Lyman series in the emission spectrum of hydrogen fits the range of visible light.
    (b) The electron moves in a circular path around the nucleus.
    (c) The energy of the electron can take on only certain quantized values.
    (d) The only allowed orbitals are those in which the angular momentum of the electron is an integer multiple of $h/2\pi$.
    (e) The electron can only absorb or emit electromagnetic radiation when it moves from one orbital to another.

36. Louis de Broglie's postulation that a particle has wave-like properties, together with Heisenberg's uncertainty principle, successfully rectified the major flaw in the Bohr-Sommerfeld model. (quantized energy states, and, electrons orbit around nucleus with well-defined values of momentum and position). However, it could not provide quantitative description of objects. Erwin Schrödinger developed the wave equation to mathematically describe the energy and position of the electron in space and time, taking into account the matter wave nature of the electron inside an atom. What are correct in the descriptions below?
    (a) The de Broglie wavelength is $\lambda = h/p$ where h is the Planck constant and p is the momentum.
    (b) The Schrödinger wavefunction includes two parts which are about the kinetic energy and the potential energy of an electron.
    (c) The wavefunction of an electron in an atom contains radial and angular distribution functions.
    (d) When the radial distribution function R(r) is zero, it means the radial nodes (nodal surfaces) take place over "l", where "l" is the angular momentum.
    (e) The Hund's rule mentions the spin multiplicity, the number of unpaired electron plus one, $2n(1/2)+1$.

TiO_2 is a very famous semiconductor widely applied for photocatalysis and nanotechnology. It has several different crystal structures which exhibit certain extent of different properties. Please answer the following group of questions 37-39 about TiO_2.

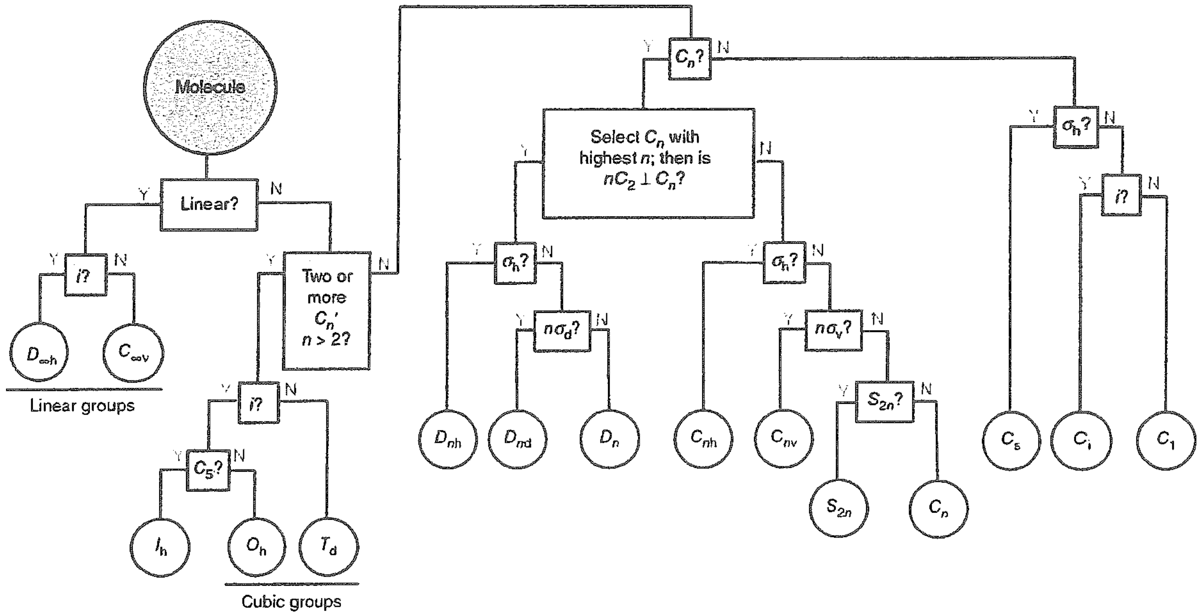
37. Which options are of TiO_2 crystal structures?
    (a) perovskite (b) rutile (c) wurtzite (d) anatase (e) brookite

38. Which descriptions below are not correct?
    (a) In typical, TiO_2 is a n-type semiconductor.
    (b) Anatase TiO_2 has a direct bandgap and thus is able to emit fluorescence.
    (c) There is partial positive charge over the O-deficient sites.
    (d) TiO_2 can not be dissolved in aqueous acids.
    (e) Sol-gel process is one of the methods for synthesizing TiO_2.

39. About the photocatalyst of TiO_2, which are correct statements?
    (a) TiO_2 photocatalysts are at nanoscale.
    (b) TiO_2 photocatalysts exhibit radicals after light excitation to achieve sterilization.
    (c) TiO_2 can be used as the material for water proof.
    (d) TiO_2 is one of the important materials in the applications of solar cells.
    (e) TiO_2 is very toxic and hence it is not allowed to be used in the food additives.

注意：背面有試題

40. The scheme below shows the way for determining the point groups of molecules. Please use it to check which options are correct.



(a) CH_4 is D_{4h}. (b) CO_2 is $D_{\infty h}$. (c) XeF_4 is C_{4h}. (d) H_2O_2 is C_2. (e) SO_2Cl_2 has the same point group to H_2O.