

※請在答案卡內作答

選擇題（只有一個答案對，答錯不倒扣，每一題兩分，總分 100）

- In a transition metal complex having O_h symmetry, which configurations in the followings can be classified as E ?
(A) t_{2g}^3 (B) $t_{2g}^4 e_g^2$ (C) t_{2g}^5 (D) $t_{2g}^3 e_g^3$ (E) $t_{2g}^5 e_g^2$
- For a free ion with d^2 configuration determine the order of term energy levels:
(A) $^3P < ^1S < ^1D$ (B) $^3P < ^1D < ^1S$ (C) $^1G < ^3P < ^1D$
(D) $^3P < ^1D < ^3F$ (E) $^3P < ^1F < ^1D$
- Which of the following salts has the highest lattice energy?
(A) LiI (B) LiF (C) CsI (D) CsF
- Both ZnS and CaF₂ have a face-centered cubic unit cell where the S²⁻ and Ca²⁺ ions are closest packed in each structure. Which of the following is true?
(A) There are 4 tetrahedral holes empty in each structure.
(B) In both compounds, one-half of the tetrahedral holes are filled.
(C) In both compounds, all the tetrahedral holes are filled.
(D) There are 8 Zn²⁺ ions and 4 F⁻ ions in the unit cell.
(E) In ZnS, one-half of the tetrahedral holes are filled by Zn²⁺ ions, whereas in CaF₂ all the tetrahedral holes are filled with F⁻ ions.
- If the radius of an atom is r , what is the length of the side of the body-centered cubic unit cell?
(A) $4r/3^{1/2}$ (B) $2.25r$ (C) r (D) $2r$ (E) $8^{1/2}r$
- Which of the followings is incorrect regarding applications of Tanabe-Sugano diagram?
(A) Tanabe-Sugano diagrams can be used for both high-spin and low-spin complexes
(B) Orgel diagrams apply only to high spin complexes
(C) Based on Tanabe-Sugano diagram, the ground state of $[\text{Mn}(\text{H}_2\text{O})_6]^{2+}(\text{aq})$ is 6A_1
(D) The D_0 and B of a complex can be obtained by the absorption maxima from the spectra
(E) According to Tanabe-Sugano diagram, $[\text{Cr}(\text{H}_2\text{O})_6]^{2+}$ generally shows two spin-allowed transitions.
- Which of the followings is the consequence of selection rules in spectroscopy?
(A) Complexes with $d-d$ transition tend to show large extinction coefficient.
(B) The optical transition observed in IrBr_6^{3-} is parity-forbidden.
(C) Tetrahedral complexes have more intense absorption than octahedral complexes.
(D) $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$ shows both spin- and Laporte-forbidden transitions.
- Which of the following has the largest Δ_{tet} ?
(A) CrO_4^{4-} (B) MnO_4^{3-} (C) FeO_4^{2-} (D) RuO_4^{2-}
- What of the following complexes shows metal-to-ligand charge transfer (MLCT)?
(A) $[\text{Fe}(\text{SCN})(\text{H}_2\text{O})_5]^{2+}$ (B) $[\text{IrBr}_6]^{3-}$ (C) $[\text{Cu}(\text{phen})_2]^+$ (D) $[\text{Cu}(\text{NH}_3)_4]^{2+}$
- Which of the following electron configurations does not show single spin-allowed $t_{2g} \rightarrow e_g$ transitions?
(A) d^1 (B) d^1 (high-spin) (C) d^1 (low-spin) (D) d^6 (high-spin) (E) d^9

參考用

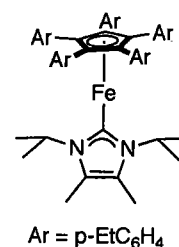
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11. Which of the following complexes do you expect to be colorless?
(A) $K_3[CrCl_6]$ (B) $[Cd(NH_3)_4Cl_2]$ (C) $[Fe(H_2O)_6]SO_4$ (D) $Na_3[Co(CN)_6]$
12. Which one of the following complexes has the lowest ligand exchange rate?
(A) $[Sr(H_2O)_6]^{2+}$ (B) $[Mg(H_2O)_6]^{2+}$ (C) $[Ca(H_2O)_6]^{2+}$ (D) $[Na(H_2O)_6]^+$
13. Which of the following complexes do you expect to be kinetically inert?
(A) $[CoCl_4]^{2-}$ (B) $[ZnCl_4]^{2-}$ (C) $[CrCl_6]^{3-}$ (D) $[TiCl_4]^{2-}$
14. The following complexes are formed upon reaction of $[Ni(H_2O)_6]^{2+}$ with the corresponding ligand(s) in water. For which complex do you expect the greatest positive entropy change (ΔS) in the corresponding complex formation reaction?
(A) $[Ni(NH_3)_6]^{2+}$ (B) $[Ni(en)(NH_3)_4]^{2+}$ (C) $[Ni(en)_3]^{2+}$ (D) $[Ni(en)_2(NH_3)_2]^{2+}$
15. Which of the following complexes do you expect to be kinetically inert?
(A) $[Co(NH_3)_4]^{2+}$ (B) $[Zn(CN)_4]^{2-}$ (C) $[Fe(CN)_6]^{4-}$ (D) $[Ti(H_2O)_6]^{3+}$
16. Which of the following complexes do you expect to be brightly colored?
(A) $Cs_2(TiCl_6)$ (B) $[Zn(pic)Cl_2]$ (C) $[Mn(H_2O)_6]SO_4$ (D) $[Fe(H_2O)_4(SCN)_2]$
17. Put in order of increasing rate of substitution by H_2O the complexes $[Co(NH_3)_6]^{3+}$, $[Rh(NH_3)_6]^{3+}$, $[Ir(NH_3)_6]^{3+}$, $[Mn(H_2O)_6]^{2+}$, $[Ni(H_2O)_6]^{2+}$.
(A) $[Ir(NH_3)_6]^{3+} < [Rh(NH_3)_6]^{3+} < [Co(NH_3)_6]^{3+} < [Ni(OH_2)_6]^{2+} < [Mn(OH_2)_6]^{2+}$.
(B) $[Ir(NH_3)_6]^{3+} < [Rh(NH_3)_6]^{3+} < [Co(NH_3)_6]^{3+} < [Mn(OH_2)_6]^{2+} < [Ni(OH_2)_6]^{2+}$.
(C) $[Co(NH_3)_6]^{3+} < [Mn(OH_2)_6]^{2+} < [Ni(OH_2)_6]^{2+} < [Ir(NH_3)_6]^{3+} < [Rh(NH_3)_6]^{3+}$.
(D) $[Ni(OH_2)_6]^{2+} < [Mn(OH_2)_6]^{2+} < [Ir(NH_3)_6]^{3+} < [Rh(NH_3)_6]^{3+} < [Co(NH_3)_6]^{3+}$.
18. Which of the following complexes has the greatest thermodynamic stability (en = $H_2N-CH_2CH_2-NH_2$)? Note: assume a high-spin configuration for Mn in these complexes.
(A) $[Mn(NH_3)_6]^{2+}$ (B) $[Zn(NH_3)_6]^{2+}$ (C) $[Mn(en)_3]^{2+}$ (D) $[Zn(en)_3]^{2+}$
19. Among the $[M(H_2O)_6]^{n+}(aq)$ (M: 3d-transition metal ion) complexes, why is the $[Mn(H_2O)_6]^{2+}$ shows the much weaker UV-Vis absorption than solution of other metal ions?
(A) because other transition metal ions
(B) because Mn^{2+} is high-spin d^5 but other transition metal ions are low-spin
(C) because the UV-Vis absorption of other transition metal ions are parity-allowed
(D) because there are no excited states of the same spin multiplicity and no spin-allowed absorption
(E) None of the above is correct
20. Which of the following configuration can NOT be classified as E in complexes having O_h symmetry?
(A) $t_{2g}^3 e_g^1$ (B) $t_{2g}^3 e_g^3$ (C) $t_{2g}^4 e_g^2$ (D) $t_{2g}^6 e_g^3$ (E) none of the above is correct
21. Given the four complexes (A) $[Co(H_2O)_6]^{3+}$, (B) $[Co(NH_3)_6]^{3+}$, (C) $[Co(NH_3)_6]^{2+}$ and (D) $[Co(NH_3)_4]^{2+}$, which order of ligand field splitting (D) of Co-complexes is correct?
(A) $A > B > D > C$ (B) $B > A > C > D$ (C) $A > B > C > D$ (D) $C > A > B > D$
(E) None of the above is correct.

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22. Given the following complexes, predict which two are labile?
 A: $(\text{NH}_4)_2\text{Cr}(\text{=O})\text{Cl}_5$ B: K_2MnI_6 C: $\text{K}_3[\text{Fe}(\text{CN})_6]$ D: $[\text{Fe}(\text{NH}_3)_6]\text{Cl}_2$
 (A) A, C (B) B, C (C) A, D (D) B, D (E) None of the above is correct
23. Indicate that which of the following electron transfer reactions is inner-sphere type?
 (A) $[\text{Cr}(\text{H}_2\text{O})_6]^{2+} + [\text{Co}(\text{NH}_3)_5\text{Cl}]^{2+} \rightarrow$ (B) $[\text{Cr}(\text{bipy})_3]^{2+} + [\text{Co}(\text{NH}_3)_5\text{Cl}]^{2+} \rightarrow$
 (C) $[\text{Ru}(\text{NH}_3)_6]^{2+} + [\text{Co}(\text{NH}_3)_5\text{OH}]^{2+} \rightarrow$ (D) $[\text{Ru}(\text{NH}_3)_6]^{2+} + [\text{Co}(\text{NH}_3)_5(\text{H}_2\text{O})]^{2+} \rightarrow$
 (E) None of the above is correct.
24. Which of the followings regarding d^8 square-planar complex is incorrect?
 (A) The electron count of most stable d^8 square-planar complexes is 16.
 (B) The MOs derived primarily from d_{xy} and d_{z^2} orbitals of the metal are slightly bonding and slightly antibonding, respectively.
 (C) Additional electrons will occupy the orbitals derived from the antibonding interaction of an M $d_{x^2-y^2}$ orbital
 (D) The MOs derived primarily from d_{yz} and d_{xz} orbitals of the metal are non-bonding.
 (E) All of the above is correct.
25. Which of the following is INCORRECT regarding the M-N-O conformation in metal nitrosyl complexes?
 (A) The M-N-O angle can strongly deviate from 180° when back-bonding is less important.
 (B) Linear NO complex has a lower IR vibrational frequency in most cases.
 (C) The complex *trans*- $[\text{Co}(\text{en})_2(\text{NO})\text{Cl}]^+$ adopts a bent NO ligand geometry.
 (D) The $[\text{Fe}(\text{CN})_5(\text{NO})]^{3-}$ adopts a linear NO ligand geometry.
26. The Nobel Prize in Chemistry 2010 was awarded to the topic “for palladium-catalyzed cross couplings in organic synthesis”. Who are the recipients for this award:
 (A) Jacques Dubochet, Joachim Frank and Richard Henderson
 (B) Richard F. Heck, Ei-ichi Negishi and Akira Suzuki
 (C) William S. Knowles, Ryoji Noyori and K. Barry Sharpless
 (D) Yves Chauvin, Robert H. Grubbs and Richard R. Schrock
 (E) Jean-Pierre Sauvage, Sir J. Fraser Stoddart and Bernard L. Feringa
27. A newly prepared iron species (*Angew. Chem. Int. Ed.* **2017**, *56*, 7995–7999) was structurally characterized shown on the right. What is the electron count for this complex?
 (A) 14 (B) 15 (C) 16 (D) 17 (E) 18.
28. Following Q 27, what would be the possible spin states for this complex?
 (A) 0 and 1; (B) 0 and 1/2; (C) 1 and 2; (D) 1/2 and 3/2; (E) 3/2 and 2.
29. The molecular geometry of $\text{I}(\text{CF}_3)_2\text{Cl}_2$ is?
 (A) Trigonal (B) Square pyramidal (C) Trigonal bipyramidal (D) tetrahedral (E) octahedral
30. Following Q 29, the Cl–I–Cl bond angle in $\text{I}(\text{CF}_3)_2\text{Cl}_2$ would be close to
 (A) 60° (B) 90° (C) 109° (D) 120° (E) 180°
31. Consider SF_6 molecule, what is the bond order for each S–F bond if only 3s and 3p valence shell of S are considered in forming bonds with F?
 (A) 1/3 (B) 2/3 (C) 1/2 (D) 1 (E) 3/2



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32. What is the point group for 1,3,5,7-cyclooctatetraene (COT)?
 (A) C_{2h} (B) S_4 (C) D_{4h} (D) D_{2d} (E) C_{2v}



1,3,5,7-cyclooctatetraene

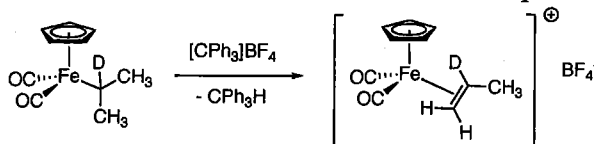
33. Match list I (compounds) with list II (structures), and select the correct answer using the codes given below.

List I	List II
(a) XeO_4	(i) square planar
(b) BrF_4^-	(ii) tetrahedral
(c) $SeCl_4$	(iii) distorted tetrahedral.

- (A) (a-iii) (b-i) (c-ii). (B) (a-ii) (b-iii) (c-i). (C) (a-ii) (b-i) (c-iii). (D) (a-i) (b-ii) (c-iii)
 (E) (a-i) (b-iii) (c-ii)

34. In metalloenzymes, the metal centres are covalently linked through the side chains of the amino acid residues. The correct set of amino acids which are involved in the primary coordinates spheres of metalloenzymes is
 (A) Ala, Leu, His (B) Glu, His, Cys (C) Leu, Glu, Cys (D) Ala, His, Glu (E) Val, Phe, Asn

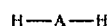
35. For the formation of an iron alkene complex shown below, what is the role of $[CPh_3]BF_4$?



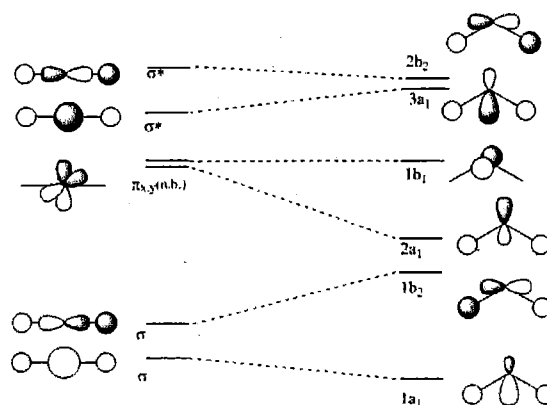
- (A) Hydride scavenger (B) Brønsted base (C) Catalyst (D) Brønsted acid (E) Hydrogen scavenger

36. Which of the following reaction does NOT go forward?

- (A) $MgCO_3 + Hg_2I_2 \rightarrow MgI_2 + Hg_2CO_3$
 (B) $ZnO + 2LiC_4H_9 \rightarrow Zn(C_4H_9)_2 + Li_2O$
 (C) $NaCN + AgF \rightarrow NaF + AgCN$
 (D) $2HI + FeBr_2 \rightarrow 2HBr + FeI_2$
 (E) $Fe + 2CF_3SO_3H \rightarrow H_2 + Fe(CF_3SO_3)_2$



37. The Walsh diagram (on the right) shows the correlation of the molecular orbital diagram of AH_2 system ($A = 2^{nd}$ period elements) in conversion between linear and bent geometries. Predict which of the molecules or ions, BeH_2 , CH_2 , NH_2^- , FH_2^- , are linear?
 (A) BeH_2 , CH_2 , FH_2^- (B) NH_2^- , FH_2^-
 (C) BeH_2 , FH_2^- (D) None of them are linear
 (E) All of them are linear



38. Following Q37, triplet carbene (CH_2) has two unpaired electrons and it can adopt either a bent or linear geometry, which would you predict is more stable?
 (A) Bent (B) Linear (C) Both have the same stability

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39. Which amine would you expect to form the least stable adducts with BMe_3 ?

- (A) NEt_3 (B) NH_2Me_2 (C) $NHMe_2$
(D) NH_3 (E) Quinuclidine (on the right)

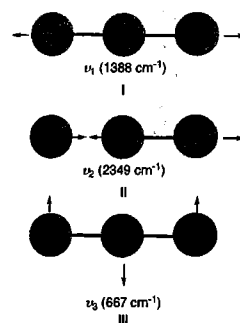


40. What does the HOMO of CO look like?



41. Of the vibrational normal modes of CO_2 shown on right, which are infrared active?

- (A) I and II only (B) I and III only (C) II and III only (D) I, II, and III (E) None

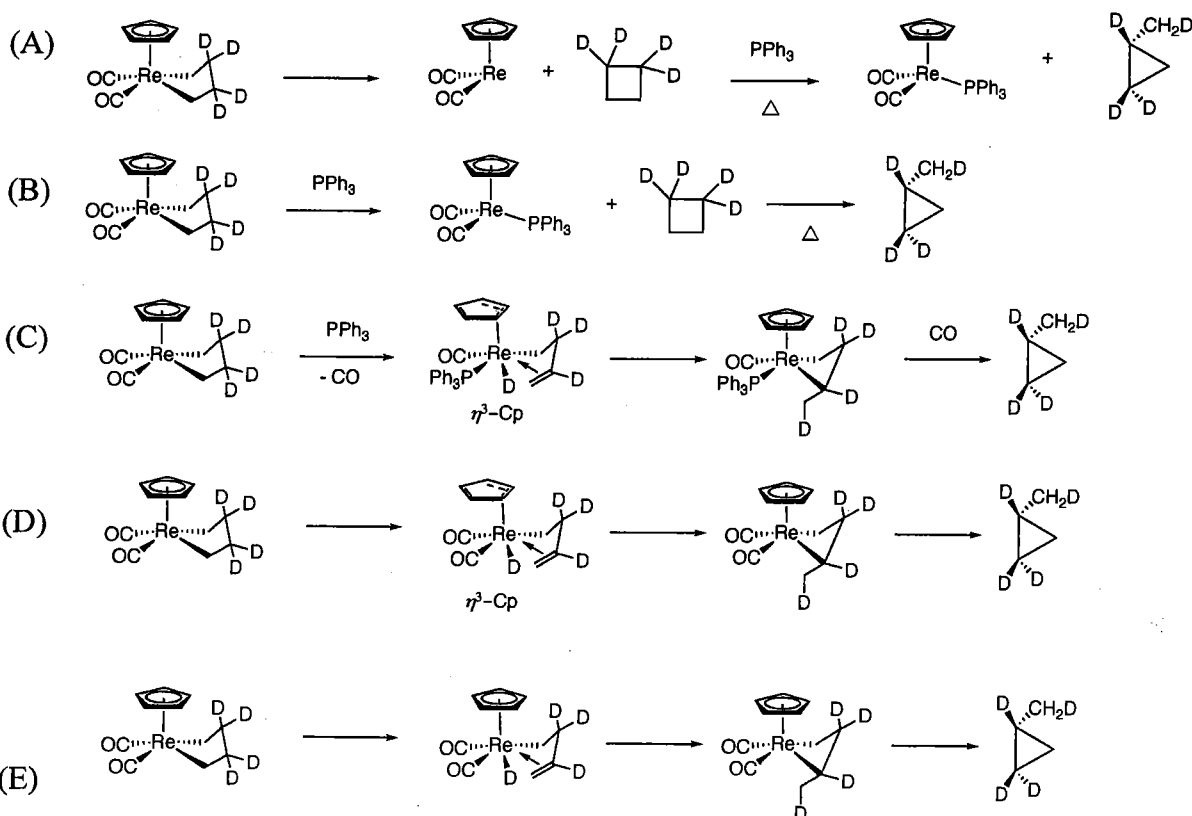
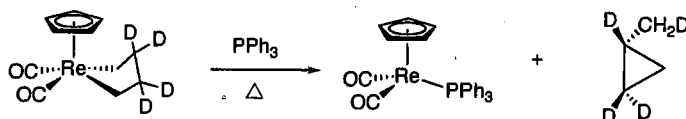


42. Which of the following is *nido*?

- (A) $C_2B_3H_5(CoCp)_2$ (B) $B_4H_6(CoCp)_2$ (C) $C_2B_8H_{10}^{4-}$ (D) SB_9H_{11} (E) $CPB_{10}H_{11}$

43. Which of the following mechanism for the illustrated reaction is consistent with these observations?

- The reaction is first order in $[Cp(CO)_2Re(CH_2CD_2CD_2CH_2)]$
- The reaction is zero order in PPh_3
- CO dissociation does NOT occur during the reaction



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44. Which complex would be expected to have the highest C–O stretching frequency?
 (A) $\text{Fe}(\text{PMe}_3)(^{13}\text{CO})_4$ (B) $\text{Fe}(\text{PMe}_3)(\text{CO})_4$ (C) $\text{Fe}(\text{PF}_3)(^{13}\text{CO})_4$
 (D) $\text{Fe}(\text{PF}_3)(\text{CO})_4$ (E) $\text{Fe}(\text{CO})_5$
45. Which is the strongest acid in dilute aqueous solutions?
 (A) HNO_3 (B) HCl (C) HBr (D) HClO_4 (E) All have the same acidity in aqueous solution.
46. The wavefunction of one of the 3d orbitals for the hydrogen atom is

$$\psi(r, \theta, \phi) = R_{nl}(r) \cdot Y_{lm_l}(\theta, \phi) = \frac{1}{81\sqrt{30}} \left(\frac{z}{a_0}\right)^{\frac{3}{2}} \left(\frac{zr}{a_0}\right)^2 e^{-Zr/3a_0} \cdot \left(\frac{15}{16\pi}\right)^{\frac{1}{2}} \sin^2\theta \sin 2\phi$$
, where
 $R_{nl}(r)$ is the radial function and $Y_{lm_l}(\theta, \phi)$ is the angular function. How many radial nodes and angular nodes are there in this orbital?
 (A) 0 and 1 (B) 0 and 2 (C) 1 and 1 (D) 1 and 2 (E) 2 and 2
47. What is the Mo–Mo bond order for $[\text{Mo}_2(\text{SO}_4)_4]^{3-}$?
 (A) 2.5 (B) 3 (C) 3.5 (D) 4 (E) 5
48. Amongst the following which is *not* isolobal pairs
 (A) $\text{Mn}(\text{CO})_5$ and CH_3 (B) $\text{Fe}(\text{CO})_4$ and O (C) $\text{Co}(\text{CO})_3$ and R_2Si (D) $\text{Mn}(\text{CO})_5$ and RS
49. 12-Crown-4 binds with the alkali metal ions in the following order: $\text{Li}^+ \gg \text{Na}^+ > \text{K}^+ > \text{Cs}^+$. It is due to the
 (A) Right size of cation (B) Conformational flexibility of crown ether (C) Hydrophobicity of crown ether (D) Change in entropy being positive
50. The reaction between SbF_5 and two equivalents of HF leads to the formation of
 (A) $\text{SbF}_3 + \text{H}_2 + 2\text{F}_2$ (B) $[\text{SbF}_6]^- [\text{H}_2\text{F}]^+$ (C) $\text{HSbF}_2 + 3\text{F}_2$ (D) $\text{H}_2\text{SbF}_3 + 2\text{F}_2$
 (E) $[\text{SbF}_4]^+ [\text{HF}_2]^-$

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Character table for O_h

O_h	E	$8C_3$	$6C_2$	$6C_4$	$3C_2=(C_4)^2$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$	linear functions, rotations	quadratic functions	cubic functions
A_{1g}	+1	+1	+1	+1	+1	+1	+1	+1	+1	+1	-	$x^2+y^2+z^2$	-
A_{2g}	+1	+1	-1	-1	+1	+1	-1	+1	+1	-1	-	-	-
E_g	+2	-1	0	0	+2	+2	0	-1	+2	0	-	$(2z^2-x^2-y^2, x^2-y^2)$	-
T_{1g}	+3	0	-1	+1	-1	+3	+1	0	-1	-1	(R_x, R_y, R_z)	-	-
T_{2g}	+3	0	+1	-1	-1	+3	-1	0	-1	+1	-	(xz, yz, xy)	-
A_{1u}	+1	+1	+1	+1	+1	-1	-1	-1	-1	-1	-	-	-
A_{2u}	+1	+1	-1	-1	+1	-1	+1	-1	-1	+1	-	-	xyz
E_u	+2	-1	0	0	+2	-2	0	+1	-2	0	-	-	-
T_{1u}	+3	0	-1	+1	-1	-3	-1	0	+1	+1	(x, y, z)	-	$(x^3, y^3, z^3) [x(z^2+y^2), y(z^2+x^2), z(x^2+y^2)]$
T_{2u}	+3	0	+1	-1	-1	-3	+1	0	+1	-1	-	-	$[x(z^2-y^2), y(z^2-x^2), z(x^2-y^2)]$

Character table for D_{4h}

D_{4h}	E	$2C_4(z)$	C_2	$2C_2$	$2C_2'$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$	linear functions, rotations	quadratic functions	cubic functions
A_{1g}	+1	+1	+1	+1	+1	+1	+1	+1	+1	+1	-	x^2+y^2, z^2	-
A_{2g}	+1	+1	+1	-1	-1	+1	+1	+1	-1	-1	R_z	-	-
B_{1g}	+1	-1	+1	+1	-1	+1	-1	+1	+1	-1	-	x^2-y^2	-
B_{2g}	+1	-1	+1	-1	+1	+1	-1	+1	-1	+1	-	xy	-
E_g	+2	0	-2	0	0	+2	0	-2	0	0	(R_x, R_y)	(xz, yz)	-
A_{1u}	+1	+1	+1	+1	+1	-1	-1	-1	-1	-1	-	-	-
A_{2u}	+1	+1	+1	-1	-1	-1	-1	-1	+1	+1	z	-	$z^3, z(x^2+y^2)$
B_{1u}	+1	-1	+1	+1	-1	-1	+1	-1	-1	+1	-	-	xyz
B_{2u}	+1	-1	+1	-1	+1	-1	+1	-1	+1	-1	-	-	$z(x^2-y^2)$
E_u	+2	0	-2	0	0	-2	0	+2	0	0	(x, y)	-	$(xz^2, yz^2) (xy^2, x^2y), (x^3, y^3)$

Character table for T_d

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$	linear functions, rotations	quadratic functions	cubic functions
A_1	+1	+1	+1	+1	+1	-	$x^2+y^2+z^2$	xyz
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)	-	$[x(z^2-y^2), y(z^2-x^2), z(x^2-y^2)]$
T_2	+3	0	-1	-1	+1	(x, y, z)	(xy, xz, yz)	$(x^3, y^3, z^3) [x(z^2+y^2), y(z^2+x^2), z(x^2+y^2)]$