Recently I have found that $[H_2B(NH_3)_2]BH_4$ will convert to H_3BNH_3 *without* H_2 evolution in a polyether solution containing B_2H_6. The data support the new equation

$$[H_2B(NH_3)_2]BH_4 \xrightarrow[B_2H_6\text{(small amount)}]{\text{polyether}} 2H_3BNH_3$$

With diglyme as solvent 91% of the original $[H_2B(NH_3)_2]BH_4$ was converted in one run to H_3BNH_3 after 40 hr at 25°. In a second run 80% of the original salt was converted after an equivalent time. When monoglyme was used as solvent, the reaction was much slower, and in two runs only 22% and 37% of H_3BNH_3 were formed after 60 hr.

It appears that NH_3 in diethyl ether catalyzes decomposition with H_2 generation while diborane in polyether yields H_3BNH_3 as the sole product of decomposition.

Contrary to earlier literature reports[1,2] I found that solid H_3BNH_3 of high purity did not undergo conversion to $[H_2B(NH_3)_2]BH_4$ even when the H_3BNH_3 was held at 50° for 13 days.

Experimental Section

General Information. Ether solvents were vacuum distilled from $LiAlH_4$ suspensions into the reaction flask. $H_2B(NH_3)_2BH_4$ was prepared in liquid ammonia[3] and extracted with diethyl ether before use to remove any H_3BNH_3 impurities. H_3BNH_3 was prepared from B_2H_6 and NH_3 in diethyl ether.[4]

$H_2B(NH_3)_2BH_4$ in Diglyme with B_2H_6. Diglyme (20 ml) was condensed onto 2.45 mmol of $H_2B(NH_3)_2BH_4$ (0.12 *M*) and 0.26 mmol of B_2H_6 was added. The evacuated system was stirred at −23° until $H_2B(NH_3)_2BH_4$ had dissolved completely. Afterward, the clear solution was warmed to room temperature and stirred with a magnetic bar for 40 hr. A 0.090-mmol amount of H_2 was formed after this period and only a trace of precipitate was formed. Diglyme was pumped off quantitatively and fractionated. A 0.21-mmol amount of B_2H_6 was recovered. From the solid nonvolatile residue 4.45 mmol of H_3BNH_3 (1.82 $H_3BNH_3/H_2B(NH_3)_2BH_4$) was extracted with diethyl ether. After pumping off the ether solvent H_3BNH_3 was washed with *n*-hexane to remove any grease impurities and characterized by its X-ray powder pattern and infrared spectrum. The ether-insoluble residue consisted of 0.22 mmol of unreacted $H_2B(NH_3)_2BH_4$ as was shown by its X-ray powder pattern. No evidence was found for the formation of any other reaction products.

In another experiment 1.36 mmol of $H_2B(NH_3)_2BH_4$ was dissolved in 15 ml of diglyme (0.091 *M*) and 0.15 mmol of B_2H_6 added. After 40 hr of reaction time at room temperature 0.045 mmol of H_2 was formed. A 0.13-mmol amount of B_2H_6 was recovered and 2.16 mmol of H_3BNH_3 (1.59 $H_3BNH_3/H_2B(NH_3)_2BH_4$) could be isolated.

$H_2B(NH_3)_2BH_4$ in Monoglyme with B_2H_6. The reaction was carried out as described above with diglyme as solvent. $H_2B(NH_3)_2BH_4$ (0.99 mmol) was dissolved in 15 ml of monoglyme (0.067 *M*) and 0.14 mmol of B_2H_6 was added. After 60 hr of reaction time at 25° 0.01 mmol of H_2 was formed. A 0.12-mmol amount of B_2H_6 was recovered and 0.44 mmol of H_3BNH_3 was isolated (0.44 $H_3BNH_3/H_2B(NH_3)_2BH_4$). The diethyl ether insoluble residue consisted again of unreacted $H_2B(NH_3)_2BH_4$.

In a second experiment a more concentrated solution was used (1.15 mmol of $H_2B(NH_3)_2BH_4$ in 5 ml of monoglyme, 0.23 *M*) and 0.15 mmol of B_2H_6. After an equivalent reaction time, 0.094 mmol of H_2 and 0.13 mmol of B_2H_6 were isolated. A 0.84-mmol amount of H_3BNH_3 was formed (0.73 $H_3BNH_3/H_2B(NH_3)_2BH_4$).

Attempted Conversion of H_3BNH_3 into $H_2B(NH_3)_2BH_4$. A sample of 1.27 mmol of pure H_3BNH_3 was stored at room temperature over 4 months in an evacuated glas ampoule. No trace of H_2 was formed over this period and H_3BNH_3 was completely soluble in diethyl ether.

Another sample of 1.91 mmol of H_3BNH_3 was heated for 13 days at 50°. Higher temperatures could not be used because H_2 formation became considerable. A 0.16-mmol amount of H_2 (0.084 H_2/H_3BNH_3) was formed. The solid residue was extracted with diethyl ether and 1.74 mmol of H_3BNH_3 recovered (91% of originally used material). The decomposition of 9% H_3BNH_3 corresponds well with the formation of 8.4% H_2 indicating decomposition of H_3BNH_3 into polymeric borazane. The X-ray patterns of the sample stored at room temperature and of the sample heated at 50° contained no reflections of $H_2B(NH_3)_2BH_4$.

Registry No. $H_2B(NH_3)_2BH_4$, 17125-97-2; H_3BNH_3, 17596-45-1; B_2H_6, 19287-45-7; hydrogen, 1333-74-0.

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(2) E. Wiberg and E. Amberger, "Hydrides of the Elements of Main Groups I-IV," Elsevier, Amsterdam, 1971, p 151; K. Niedenzu and J. W. Dawson, "Boron-Nitrogen Compounds," Springer-Verlag, Berlin, 1965.

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(4) E. Mayer, *Inorg. Chem.*, 11, 866 (1972).

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Synthetic Procedure for Some Acidotetraaminechromium(III) Complexes

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Received January 26, 1973

In 1970, Vaughn, DeJovine, and Seiler published a paper in this journal describing the synthesis of *trans*-$[Cr(en)_2FCl]ClO_4$.[1] This molecule was of great interest to us so we have repeated the above-referenced synthesis. In the course of our investigation we have modified the conditions of the original technique somewhat and have found our modification to be of great utility for the synthesis of a variety of Cr(III) complexes. We have not established the limits of the applicability of the synthesis but have satisfied ourselves that the method is powerful and should be described. In this report we describe in detail the syntheses of *trans*-$[Cr(en)_2FCl]ClO_4$, *trans*-$[Cr(en)_2FBr]ClO_4$, *trans*-$[Cr(NH_3)_4F_2]ClO_4$, and *trans*-$[Cr(NH_3)_4FCl]ClO_4$ and indicate how the method of synthesis can be applied in other cases.

Experimental Section

Synthesis of *trans*-$[Cr(en)_2FCl]ClO_4$. A 10-g sample of *trans*-$[Cr(en)_2FH_2O](ClO_4)_2 \cdot H_2O$, prepared as described by Vaughn, Stvan, and Magnuson,[2] was slurried with 5 g of NH_4Cl in 150 ml of methanol and stirred in the dark at 40° for 18–24 hr. The crude product was removed by filtration and recrystallized from warm water by addition of $NaClO_4$ followed by cooling. Spectral data are given in Table I. *Anal.* Calcd for *trans*-$[Cr(en)_2FCl]ClO_4$: Cr, 15.95. Found: Cr, 15.96.

Synthesis of *trans*-$[Cr(en)_2FBr]ClO_4$. A 3.5-g sample of *trans*-$[Cr(en)_2FH_2O](ClO_4)_2 \cdot H_2O$ was treated with 3.5 g of NH_4Br in 25 ml of methanol. The mixture was stirred vigorously at 40° for 24 hr after which it was filtered and the precipitate dried. The crude complex was dissolved in 15° water in order to decrease the amount of complex that aquates during the recrystallization.[3] After addition of $NaClO_4$ to the filtered solution it was cooled to 0°; this yielded a precipitate that was washed with ethanol and dried *in vacuo*. The yield was 1.4 g, 45%. Spectral data are given in Table I. *Anal.* Calcd for *trans*-$[Cr(en)_2FBr]ClO_4$: Cr, 14.03; F, 5.13. Found: Cr, 14.11; F, 5.13.

Synthesis of *trans*-$[Cr(NH_3)_4F_2]ClO_4$. The starting material for this synthesis was *trans*-$[Cr(NH_3)_4ClH_2O]Cl_2$, prepared as described.[4] A sample of 6 g of this complex was treated with 6 g of finely ground NH_4F in 120 ml of methanol and the slurry was stirred at 40° in the dark for 17 hr. The solid was removed by filtration and washed with ethanol; it was then dissolved in warm, dilute HCl. The solution was filtered into solid $NaClO_4$ and cooled. The solid that resulted from this procedure was still a mixture of compounds, but a final recrystal-

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(1) J. W. Vaughn, J. M. DeJovine, and G. J. Seiler, *Inorg. Chem.*, 9, 684 (1970).

(2) J. W. Vaughn, O. J. Stvan, and V. E. Magnuson, *Inorg. Chem.*, 7, 736 (1968).

(3) A detailed report of the aquation kinetics of this complex as well as several related complexes will appear elsewhere.

(4) D. W. Hoppenjans and J. B. Hunt, *Inorg. Chem.*, 8, 505 (1969).

lization from warm 0.5 *N* $HClO_4$ yielded a precipitate of pure *trans*-$[Cr(NH_3)_4F_2]ClO_4$. The yield was 1.8 g, 28%. Spectral data are in Table I. *Anal.* Calcd for *trans*-$[Cr(NH_3)_4F_2]ClO_4$: Cr, 20.20; N, 21.75; F, 14.77. Found: Cr, 19.91; N, 22.33; F, 14.66.

Synthesis of *trans*-$[Cr(NH_3)_4FCl]ClO_4$. A 2.0-g sample of *trans*-$[Cr(NH_3)_4F_2]ClO_4$ was treated with 10 ml of concentrated $HClO_4$ and allowed to stand in a Teflon beaker for about 1 hr. *Caution! HF is formed. A fume hood should be used.* During this time a precipitate formed. This solution was cooled and filtered, and the precipitate was washed with cold absolute ethanol. *Caution! Concentrated perchloric acid is known to form explosive esters.* The solid sample was then dried *in vacuo*; this sample was not characterized in the solid state, but the method of preparation and the observation that solutions of it exhibit spectral bands very similar to those of *trans*-$[Cr(en)_2FH_2O]^{2+}$ (Table I) suggest that this solid contains the cation *trans*-$[Cr(NH_3)_4FH_2O]^{2+}$. A 1.8-g sample of this solid was mixed with 2.0 g of NH_4Cl and 40 ml of methanol and stirred at 40° for 16 hr. The sample was filtered, and the solid was dissolved in warm water, filtered onto solid $NaClO_4$, and cooled. The resulting solid was recrystallized from 40° water by cooling. The yield was 0.64 g, 46%. Spectral data are given in Table I. *Anal.* Calcd for *trans*-$[Cr(NH_3)_4FCl]ClO_4$: Cr, 18.97; N, 20.40; F, 6.94. Found: Cr, 18.94; N, 21.03; F, 7.05.

Techniques. The analysis for Cr was performed by basic peroxide decomposition and spectrophotometric determination of the resulting CrO_4^{2-} at 3730 Å;[5] F^- was determined by an ion-selective electrode using a standard solution of NaF to establish a calibration curve. Before reading $[F^-]$, the complex was decomposed by treatment of a sample with warm EDTA solution in either a HPO_4^{2-}–$H_2PO_4^-$ or an acetate–acetic acid buffer. The standard was treated similarly. Nitrogen was determined by basic decomposition of the complex and distillation of the liberated NH_3 into a standard acid solution. All spectra were recorded on a Cary Model 14 recording spectrophotometer.

Results and Discussion

Vaughn, *et al.*,[1] treated *trans*-$[Cr(en)_2FH_2O](ClO_4)_2 \cdot H_2O$ with NH_4Cl in methanol but chose to carry out the reaction in a homogeneous solution. Our modification involves the use of heterogeneous reaction conditions, gentle warming, and vigorous stirring of the mixture. Under these conditions we not only have been able to synthesize the previously reported *trans*-$[Cr(en)_2FCl]ClO_4$ but also have successfully prepared *trans*-$[Cr(en)_2FBr]ClO_4$, a substance that Vaughn, *et al.*,[1] were unable to synthesize by their procedure. In addition, we have been successful in causing the reaction

$$trans\text{-}[Cr(NH_3)_4H_2OCl]^{2+} + 2F^- = trans\text{-}[Cr(NH_3)_4F_2]^+ + Cl^- + H_2O \tag{1}$$

to take place. Although *trans*-$[Cr(NH_3)_4F_2]^+$ has been reported previously in the literature,[6] the synthesis involves reaction of *trans*-$[Cr(py)_4F_2]I$[7] with NH_3 in an autoclave. We were unable to reproduce this synthesis using a variety of conditions. The synthesis of *trans*-$[Cr(NH_3)_4FCl]^{2+}$, a previously unknown molecule, is also easily carried out by our procedure.

In addition to these carefully controlled experiments, we have also explored other reactions qualitatively. Reaction of *cis*-$[Cr(NH_3)_4(H_2O)_2](ClO_4)_3$[4] with 1 equiv of NH_4NCS produced a solid that is a mixture of at least three complexes. Two recrystallizations yielded a material with constant spectrum, but ion exchange revealed the presence of a small amount of impurity. The dominant species was, however, *cis*-$Cr(NH_3)_4H_2ONCS^{2+}$.[8] On the other hand, reaction of *cis*-$[Cr(en)_2Cl_2]ClO_4$ with NH_4F did not proceed smoothly to *cis*-$[Cr(en)_2F_2]ClO_4$.[9] It seems possible that the insolubility of the dichloro salt in methanol is the cause of the failure of this synthesis. In all of our successful syntheses, there was at least some color imparted to the methanolic solution of the starting complex. In addition, it is to be noted that although the driving force for reaction is probably a lowering of net charge, the method may yield an undesirable result if the entering anionic ligand is a more strongly bonding ligand than some other anion in the coordination shell. For instance, although reaction of *trans*-$[Cr(NH_3)_4FH_2O]^{2+}$ with NH_4Cl proceeds smoothly to *trans*-$[Cr(NH_3)_4FCl]^+$, reaction of *trans*-$[Cr(NH_3)_4ClH_2O]^{2+}$ with NH_4F produces a mixture containing *trans*-$[Cr(NH_3)_4F_2]^+$, but little, if any, *trans*-$[Cr(NH_3)_4FCl]^+$. Presumably the strong interaction between Cr(III) and F^- is sufficient to displace the Cl^- from the coordination shell.

Table I. Spectral Data for Some Acidotetraaminechromium(III) Complexes

Complex	λ (ε)[a] This work	λ (ε)[a] Lit.	Ref
trans-$Cr(en)_2FCl^+$	5505 (19.3)	5530 (19.9)	1
	4600 (21.1)	4600 (21.5)	
	3810 (27.6)	3810 (27.4)	
trans-$Cr(NH_3)_4FCl^+$	5670 (17.9)		
	4760 (14.5)		
	3880 (23.7)		
trans-$Cr(en)_2FBr^+$	5630 (22.7)		
	4660[b] (23.2)		
	≃4600 (22.2)		
	3850 (30.1)		
trans-$Cr(en)_2FH_2O^{2+}$	5190 (23.1)	5190 (24.2)	2
	4570 (23.9)	4540 (25.6)	
	3690 (29.9)	3710 (31.2)	
trans-$Cr(NH_3)_4FH_2O^{2+}$	5290 (21.6)		
	4850 sh (20.2)		
	3770 (27.9)		
trans-$Cr(en)_2F_2^+$		5250 sh (16.3)	11
		4660 (21.1)	
		4000 sh (12.8)	
		3500 (14.5)	
trans-$Cr(NH_3)_4F_2^+$	5400 sh (13.7)	5520 (12.1)[c]	10
	4900 (15.4)	4780 (12.8)[c]	
	4030 (11.3)	4050 (9.5)[c]	
	3580 (11.6)	3550 (10.0)[c]	

[a] Wavelength is given in Å; ε in M^{-1} cm^{-1}; sh denotes shoulder. [b] See text. [c] The data for both λ and ε reflect the result of a gaussian analysis of the original spectrum. See ref 10.

Of the four complexes whose preparation is described herein, the spectrum of one has previously been reported. In the case of *trans*-$Cr(NH_3)_4F_2^+$, the observed spectrum has not been reported, but a gaussian analysis of this system has been.[10] These literature data as well as our observed data are listed in Table I.[1,2,10,11] As shown there, our data are in reasonable accord with the values in the literature. The spectral data for *trans*-$Cr(en)_2FBr^+$, in particular the three distinct bands, have been used to assign to the complex a trans configuration. As expected, if one moves down the series F^-, Cl^-, Br^- as the X^- ligand in *trans*-$Cr(en)_2FX^+$, the lowest energy peak, ${}^4B_1 \rightarrow {}^4E$ (assuming tetragonal symmetry), shifts to lower energies: F^-, 19,000 cm^{-1}; Cl^-, 18,200 cm^{-1}; Br^-, 17,800 cm^{-1}. On the other hand, the second band in the spectra of these three complexes is relatively unaffected by a change in X^- (21,400, 21,750, and about 21,750 cm^{-1} for $X^- = F^-$, Cl^-, and Br^-, respectively) since the transition involved, ${}^4B_1 \rightarrow {}^4B_2$, affects principally changes of electron density in the *x,y* plane.[12] One peculiarity in

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(5) G. Haupt, *J. Res. Nat. Bur. Stand.*, 48, 414 (1952).

(6) J. Glerup and C. E. Schaffer, *Chem. Commun.*, 38 (1968).

(7) J. Glerup, J. Josephsen, K. Michelsen, E. Pedersen, and C. E. Schaffer, *Acta Chem. Scand.*, 24, 247 (1970).

(8) E. Zinato, R. D. Lindholm, and A. W. Adamson, *J. Amer. Chem. Soc.*, 91, 1076 (1969).

(9) We have been, however, able to synthesize this molecule by reaction of NH_4F with *cis*-$Cr(en)_2Cl_2^+$ in aqueous solution.

(10) J. Glerup and C. E. Schaffer in "Progress in Coordination Chemistry," M. Cais, Ed., Elsevier, New York, N. Y., 1968, p 500.

(11) S. C. Pyke and R. G. Linck, *Inorg. Chem.*, 10, 2445 (1971).

the spectrum of *trans*-$Cr(en)_2FBr^+$ is the appearance of a narrow, weak transition, superimposed on the second broad band, at 21,400 cm^{-1}. The position and intensity of this spectral band suggests that it is a transition to a doublet, ^2E or $^2B_2$, arising out of the $^2T_{2g}(t^3{}_{2g})$ manifold of the parent octahedral $Cr(en)_3{}^{3+}$ complex. Its appearance in the spectrum of *trans*-$Cr(en)_2FBr^+$ may be due to a combination of large spin-orbit coupling in this complex and near degeneracy of this transition with the $^4B_1 \rightarrow {}^4B_2$ transition.

The spectral data for *trans*-$Cr(NH_3)_4FCl^+$ is completely compatible with that of the corresponding ethylenediamine complex when the slightly smaller value of the splitting parameter 10*Dq* for NH_3 (compared to en) is taken into account. On this basis we believe the assignment of the trans structure to this molecule is valid. It is interesting to note that the extinction coefficients observed for *trans*-$Cr(NH_3)_4FX^{n+}$, where X = F^-, Cl^-, or H_2O, are all somewhat, but distinctly, lower than the values for the corresponding complexes of ethylenediamine. The data are in Table I. This phenomenon is also true of $Cr(NH_3)_6{}^{3+}$ compared to $Cr(en)_3{}^{3+}$, as well as a number of *cis*-CrN_4X_2 complexes[13] in which cases the effect is more dramatic. Whether this effect is simply a lowering of symmetry restrictions in the ethylenediamine complexes compared to ammonia complexes or arises from the nature of the vibronic combinations[14] is not clear to us.

Registry No. *trans*-$[Cr(en)_2FCl]ClO_4$, 26748-18-5; *trans*-$[Cr(en)_2FH_2O](ClO_4)_2$, 15688-01-4; *trans*-$[Cr(en)_2FBr]ClO_4$, 40029-15-0; *trans*-$[Cr(NH_3)_4F_2]ClO_4$, 40029-16-1; *trans*-$[Cr(NH_3)_4ClH_2O]Cl_2$, 18737-53-6; *trans*-$[Cr(NH_3)_4FCl]ClO_4$, 40029-18-3; *trans*-$[Cr(NH_3)_4FH_2O]^{2+}$, 40029-19-4.

Acknowledgment. This work was supported by a grant from the Academic Senate, University of California at San Diego. We are grateful for that support and wish also to thank George Malouf for help in analyzing some of the samples. C. B. acknowledges financial support from CONICIT, Caracas, Venezuela.

(12) J. R. Perumareddi, *Coord. Chem. Rev.*, 4, 73 (1969).

(13) See the data in C. S. Garner and D. A. House, *Transition Metal Chem.*, 6, 200 (1970).

(14) See, for instance, L. Dubicki and P. Day, *Inorg. Chem.*, **10**, 2043 (1971).

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Photochemical Implications of Configuration Interaction in d^3 Complexes

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Received February 8, 1973

In recent publications, a model based on the antibonding properties of excited electronic states was presented which rationalized and predicted the types of photoreactions and relative quantum yields of chromium(III)[1] and cobalt(III) and rhodium(III)[2] complexes. The effects of the medium on the model's predictions have also been discussed.[3] In the case of the d^3 complexes, the model used quartet-state symmetry functions and doublet-state energy considerations when the photoeffects of the two types of states were considered.[1] In this note the photochemical consequences of configuration interaction, CI, are considered in detail. The primary importance of CI to the model is the result, derived herein, that the *fractional composition* of the lowest photoactive states vary in a regular manner. The relevance of fractional composition to the prediction of relative quantum yields in a series of chromium(III) complexes is discussed.

Symmetry Wave Functions

Symmetry functions for the doublet and quartet states of a d^3 configuration are tabulated or may be constructed from Table A24 in ref 4. Wave functions and energy matrices have also been published by Perumareddi.[5] The quartet states have been discussed elsewhere[1] and are reproduced here for convenience.

$$^4B_{1g}(^4A_{2g}) \qquad \phi_1 = |(xz)(yz)(xy)| \qquad (1)$$

$$^4B_{2g}(^4T_{2g}) \qquad \phi_2 = |(xz)(yz)(x^2-y^2)| \qquad (2)$$

$$^4E_g(^4T_{2g}) \quad \left\{ \begin{array}{ll} \phi_3 = -(1/2)\,|(yz)(xy)(x^2-y^2)| + & \\ \quad (\sqrt{3}/2\,|(yz)(xy)(z^2)| & (3) \\ \phi_4 = -(1/2)\,|(xy)(xz)(x^2-y^2)| - & \\ \quad (\sqrt{3}/2)\,|(xy)(xz)(z^2)| & (4) \end{array} \right.$$

$$^4A_{2g}(^4T_{1g}) \qquad \phi_5 = |(xz)(yz)(z^2)| \qquad (5)$$

$$^4E_g(^4T_{1g}) \quad \left\{ \begin{array}{ll} \phi_6 = -(1/2)\,|(yz)(xy)(z^2)| - & \\ \quad (\sqrt{3}/2)\,|(yz)(xy)(x^2-y^2)| & (6) \\ \phi_7 = -(1/2)\,|(xy)(xz)(z^2)| + & \\ \quad (\sqrt{3}/2)\,|(xy)(xz)(x^2-y^2)| & (7) \end{array} \right.$$

The members of the lowest manifold of doublet states with which we will be concerned are those which could lead to photochemical activity, *i.e.*, those which represent a substantial change in orbital population compared to the ground state $(d_{xz})^1(d_{yz})^1(d_{xy})^1$. As has been pointed out, the photoactive states can only involve the configurations $(d_{xz})^2(d_{yz})^1$, $(d_{xz})^1(d_{yz})^2$, $(d_{xy})^2(d_{xz})^1$, and $(d_{xy})^2(d_{yz})^1$. The former two represent an increase in electron population in the *z* direction; the latter two represent a decrease compared to the ground state. The symmetry functions involving the above four configurations are

$$^2E(^2T_1) \quad \left\{ \begin{array}{ll} \psi_1 = \dfrac{1}{\sqrt{2}}\left[(d_{xz})^2(d_{yz})^1 - (d_{xy})^2(d_{yz})^1\right] & (8) \\ \psi_2 = \dfrac{1}{\sqrt{2}}\left[(d_{xy})^2(d_{xz})^1 - (d_{yz})^2(d_{xz})^1\right] & (9) \end{array} \right.$$

$$^2E(^2T_2) \quad \left\{ \begin{array}{ll} \psi_3 = \dfrac{1}{\sqrt{2}}\left[(d_{xy})^2(d_{yz})^1 + (d_{xz})^2(d_{yz})^1\right] & (10) \\ \psi_4 = \dfrac{1}{\sqrt{2}}\left[(d_{xy})^2(d_{xz})^1 + (d_{yz})^2(d_{xz})^1\right] & (11) \end{array} \right.$$

The *symmetry functions* contain equal admixtures of increase and decrease of electronic population along the *z* direction and thus could not lead to photochemical consequences. The energies of the symmetry states are shown in Figure 1.

Configuration Interaction

For two wave functions, ψ_a and ψ_b, of the same irreducible

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(1) J. I. Zink, *J. Amer. Chem. Soc.*, **94**, 8039 (1972).

(2) J. I. Zink, *Inorg. Chem.*, **12**, 1018 (1973).

(3) J. I. Zink, *Mol. Photochem.*, **5**, 151 (1973).

(4) J. S. Griffith, "The Theory of Transition Metal Ions," Cambridge University Press, Cambridge, U. K., 1964, pp 396–407.

(5) J. R. Perumareddi, *J. Phys. Chem.*, **71**, 3144 (1967).