description using the default parameters, the molecule is essentially ionic (Rn^{2+}, $2F^-$) so that the difference of 2.1 eV in these two energies is approximately twice the 1.2 eV atomic spin–orbit destabilization of $6p_{3/2}$ from −11.6 eV (EHT) to −10.4 eV (REX).

Summary

Comparisons of REX orbital energies to those calculated by other theoretical methods and to those obtained from PES data indicate the usefulness of the REX method for obtaining semiquantitative estimates of spin–orbit splittings of valence molecular orbitals in compounds of uranium. The "crystal-field" splittings of the 5f levels in these compounds are also adequately accounted for by the REX method. There are some particularly interesting features of the REX descriptions of uranium compounds: the occurrence of a mostly 5f MO as the HOMO in UO_2^{2+}; spin–orbit splittings of at least 1 eV for the t_{1u} HOMO's of UF_6 and UCl_6; essentially ionic descriptions of the bonding in $U(BH_4)_4$ and $U(COT)_2$; nearly degenerate $|m| = {}^1/_2$ and ${}^5/_2$ mostly $5f_{5/2}$ levels as HOMO's in $U(COT)_2$, so that a "high-spin" $|M| = 3$ ground state is expected, in accord with earlier ligand field calculations.[46]

Comparative studies for some compounds of Po, At, and Rn with the use of the relativistic (REX) and nonrelativistic (EHT) parameterizations suggest a number of relativistic trends in bonding. The REX description of PoH_2, and to a greater extent that of (eka)PoH_2, is characterized by a tendency toward $p_{1/2}$ rather than p_σ bonding. A substantial relativistic stabilization of the $D_{\infty h}$ structure of collinear AtI_2^- relative to the $C_{\infty v}$ structure is predicted. In contrast to results for compounds of Tl or Pb, the REX description of RnF_2 involves a relativistic enhancement of bond strength arising from the spin–orbit destabilization of the $6p_{3/2}$ orbitals. These and other results obtained by our method[1,3] indicated its usefulness in establishing guidelines as to the significance of relativistic effects in chemistry.

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Appendix

The atomic orbital energies α_i and the Slater exponents ζ_i used in this study are listed in Table III. For Cl(3p) our double-ζ functions[3] were used. See the parameterization section for discussion of the parameters and their modifications.

Registry No. UO_2^{2+}, 16637-16-4; $UO_2Cl_4^{2-}$, 19160-32-8; UF_6, 7783-81-5; UCl_4, 10026-10-5; UCl_6, 13763-23-0; $U(BH_4)_4$, 12523-77-2; $U(COT)_2$, 11079-26-8; LaI_3, 13813-22-4; GdI_3, 13450-91-4; LaI_3, 13813-45-1; PoH_2, 31060-73-8; I_3^-, 14900-04-0; AtI_2^-, 77189-82-3; RnF_2, 18976-85-7.

Supplementary Material Available: A listing of the relativistic and nonrelativistic atomic orbital energies and Slater exponents for all elements (3 pages). Ordering information is given on any current masthead page.

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Use of the Jahn–Teller Theorem in Inorganic Chemistry

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The observed distortions from octahedral geometry in Cu^{II} complexes of local stoichiometry MY_6 and *trans*-$MY_4Y'_2$ are well described in qualitative terms by (a) s–d mixing and (b) the relative stabilization energies of square-planar MY_4 and $MY_2Y'_2$ units via the angular-overlap model. No recourse is made to the enigmatic symmetry results of the first- and second-order Jahn–Teller approaches within the d-orbital manifold.

Introduction

Many structural and dynamic aspects of transition-metal chemistry are currently rationalized with use of the Jahn–Teller theorem,[2] which asserts that a molecule in an orbitally degenerate electronic state will distort to remove the degeneracy. Present usage of the theorem[3] in this area may be summarized by two comments. (a) In most point groups, asymmetric occupation of degenerate orbitals leads to a degenerate electronic state. An exception occurs in groups such as D_{4h} and D_{8h} where no degenerate state is so produced. The classic case of singlet cyclobutadiene[4] is an example of this type. (b) Substituted octahedral compounds (for example, *cis*-$MY_4Y'_2$, where the point symmetry is low and degenerate representations do not occur, are structurally very similar to their totally substituted parent (MY_6), where a degenerate electronic state is possible at the undistorted geometry.

Where the first-order Jahn–Teller theorem (applicable to degenerate electronic states only) may not be used, higher order variants[5] often allow rationalization of the structural results. Equation 1 shows a perturbation theoretic expansion

$$E(0) = \langle 0|\mathcal{H}_q|0\rangle q + \frac{1}{2}\left[\langle 0|\mathcal{H}_{qq}|0\rangle - 2{\sum_n}' \frac{|\langle 0|\mathcal{H}_q|n\rangle|^2}{\Delta E_{0n}}\right]q^2 \tag{1}$$

for the energy of the electronic ground state (0) as a function of a distortion coordinate, q. $\mathcal{H}_q$ and $\mathcal{H}_{qq}$ are the first and second derivatives with respect to q of the electronic Hamil-

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[1] Fellow of the Alfred P. Sloan Foundation and Camille and Henry Dreyfus Teacher-Scholar.

[2] (a) Jahn, H. A.; Teller, E. *Proc. R. Soc. London, Ser. A* **1937**, *161*, 220. (b) Jahn, H. A. *Ibid.* **1938**, *164*, 117.

[3] Burdett, J. K. "Molecular Shapes"; Wiley: New York, 1980.

[4] (a) Dewar, M. J. S.; Gleicher, G. J. *J. Am. Chem. Soc.* **1965**, *87*, 3255. (b) Maier, G. *Angew. Chem. Int. Ed. Engl.* **1974**, *13*, 425.

[5] (a) Liehr, A. D. *J. Phys. Chem.* **1963**, *67*, 389, 471. (b) Pearson, R. G. *J. Phys. Chem. Soc.* **1969**, *91*, 1252, 4947. (c) Pearson, R. G. *J. Chem. Phys.* **1970**, *52*, 2167; **1970**, *53*, 2986. (d) Bartell, L. S. *J. Chem. Educ.* **1968**, *64*, 457.

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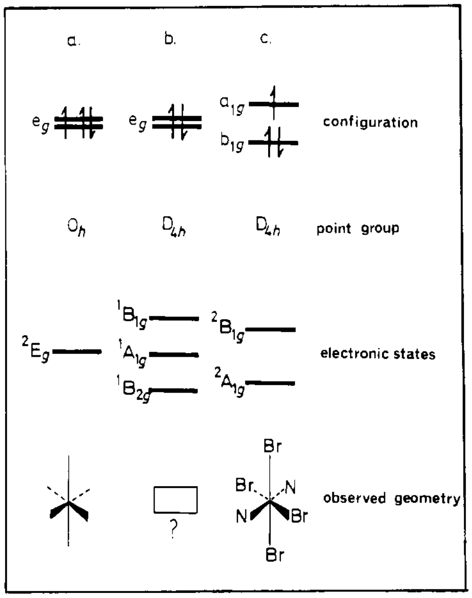
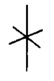


Figure 1. Some distorted molecules with "Jahn–Teller" explanations: (a) first-order Jahn–Teller distortion in a regular octahedral complex, e.g., solid $CuCl_2$; (b) pseudo-Jahn–Teller distortion in cyclobutadiene; (c) second-order Jahn–Teller distortion in a *trans*-$MY_4Y'_2$ species, e.g., $Cu(NH_3)_2Br_2$.

tonian. The term in eq 1 containing q is the true or first-order Jahn–Teller contribution, nonzero only for degenerate electronic states.[6] The term containing q^2 gives the second-order or pseudo-Jahn–Teller contribution and can give rise to a stabilization of the system on distortion if there is a low-lying state n (small ΔE_{0n}) of the correct symmetry such that $\langle 0|\mathcal{H}_q|n\rangle$ is nonzero. (I.e., $a_1 \epsilon \Gamma_0 \times \Gamma_q \times \Gamma_n$ where the Γ's are the symmetry species of the relevant functions.

Figure 1 shows the three electronic possibilities we have just mentioned and their explanation as a first-order Jahn–Teller effect (e.g., Cu^{II} in solid $CuCl_2$), as a pseudo-Jahn–Teller effect (e.g., cyclobutadiene) where the (nondegenerate) electronic states derived from the same electronic configuration may couple together on distortion (eq 1), and as a second-order Jahn–Teller effect (e.g., α-$Cu(NH_3)_2Br_2$) where the ground and first excited electronic states (both nondegenerate) derived from different electronic configurations may mix together on distortion. At an orbital, or one-electron, level the second-order Jahn–Teller effect is usually regarded as mixing of the HOMO and the LUMO on distortion.[3,5b–d]

There are two items of specific interest concerning these distorted molecules that will allow an evaluation of the use of these Jahn–Teller ideas in understanding the electronic factors behind molecular structures. First, the distortion of octahedral molecules in E_g states is almost invariably an e_g tetragonal elongation rather than a compression[7–9] (**1** rather than **2**). Second, there are many systems for which the second-order Jahn–Teller prescription of eq 1 and Figure 1c give the wrong answer. While the observed distortion in $CuCl_2 \cdot H_2O$ or α-$Cu(NH_3)_2Br_2$ of Figure 1 is compatible with a b_{1g} motion (**3**) of the D_{4h} parent (which couples the a_{1g} and b_{1g} levels of the undistorted molecule), that in a wide range of $Cu^{II}O_2N_4$ complexes,[8] with oxygen- and nitrogen-containing donor ligands, is not (**4**). The a_{1g} distortion of the parent is not in accord with the symmetry restrictions imposed by a nonzero element $\langle 0|\mathcal{H}_q|n\rangle$ in eq 1.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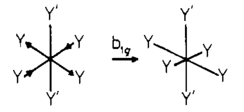

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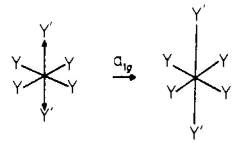

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The Distortion Route

From the symmetry properties the first term in eq 1, for E_g electronic states, of octahedral Cu^{II} systems for example, an e_g symmetry distortion removes the degeneracy. A continuous series of distortions, representing linear combinations of the two e_g components and involving lengthening and shortening of various bonds, is possible and is described by the traditional "Mexican hat" potential-energy surface, shown in ref 8 for example. (I.e., the Jahn–Teller theorem gives the symmetry species of the distortion, but there is an ambiguity as to the exact geometrical configuration a particular system will adopt.) Which particular distortion is actually preferred will then depend upon other electronic and stereochemical factors. The result will be a "crimped" Mexican hat containing local minima. Bersuker and co-workers[8] have emphasized the importance of the crystalline environment in favoring one arrangement over another, but there are two fundamental electronic effects associated with the details of the orbitals themselves that we believe are of major importance. They do not rely on the presence of any *symmetry-determined* "Jahn–Teller distortion energy" arising from the first term of eq 1 at all.

As we have recently pointed out,[3] inclusion of the central-atom s orbital into the molecular orbital picture allows an understanding of the prevalence of the tetragonal elongation route.[10] In lower-than-octahedral geometries, the $(n + 1)$s orbital transforms as the same symmetry species as does the nz^2 orbital. The two may then mix together to form a hybrid orbital, of lower energy than that of the original z^2 orbital. (This s–d (and also p–d) mixing is of crucial importance[11] in understanding structural features of many, especially organometallic, transition-metal complexes.) Such effects have

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[6] We ignore totally symmetric motions q that do not change the molecular point symmetry.

[7] (a) It is probably true to say that tetragonal elongations are always observed in Cu^{II} systems if the following conditions are met. (i) The six pseudooctahedral ligands must be identical. (ii) The site containing the Cu^{II} species in a solid-state structure is undistorted when it contains a non-Jahn–Teller-active ion. In $Ba_2Zn_{1-x}Cu_xF_6$ ($x \leq 0.3$), for example, the octahedral sites are tetragonally compressed when occupied by Zn^{II} ($x = 0$) itself (but somewhat more strongly distorted when occupied by Cu^{II}) (Friebel, C.; Propach, V.; Reinen, D. *Z. Naturforsch, B: Anorg. Chem., Org. Chem.* **1976**, *31B*, 1574). (b) One system often quoted as containing a tetragonally compressed Cu^{II} environment is K_2CuF_4. A reinvestigation of the structure (Haegele, V. R.; Babel, D. *Z. Anorg. Allg. Chem.* **1974**, *409*, 11) shows four short (1.92 Å) and two long (2.22 Å) Cu–F linkages.

[8] For a comprehensive review of Cu^{II} data see: Gazo, J.; Bersuker, I. B.; Garaj, J.; Kabesova, M.; Kohout, J.; Langfelderova, H.; Melnik, M.; Serator, M.; Valach, V. *Coord. Chem. Rev.* **1976**, *19*, 253.

[9] (a) Hathaway, B. J.; Hodgson, P. G. *J. Inorg. Nucl. Chem.* **1973**, *35*, 4071. (b) Tomlinson, A. A. G.; Hathaway, B. J.; Billing, B. E.; Nicholls, P. *J. Chem. Soc. A* **1969**, 65.

[10] Such ideas have been in the chemical literature for some years. See: Pearson, R. G. "Symmetry Rules for Chemical Reactions"; Wiley: New York, 1976.

[11] Hoffmann, R. *Science* **1981**, *211*, 995.

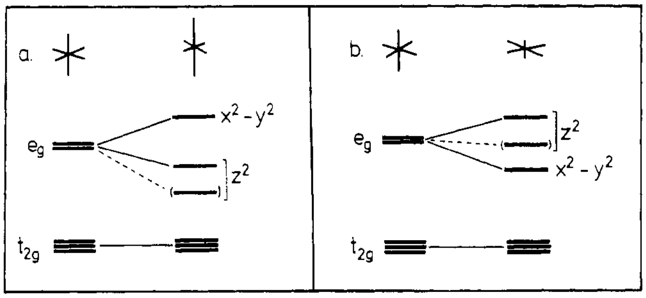


Figure 2. Energetic behavior of the metal d orbitals of an MY_6 complex on tetragonal distortions: (a) elongation; (b) compression. The behavior of the $x^2 - y^2$ and z^2 orbitals on a d-orbital model is shown by solid lines and may readily be derived using either the crystal field or the angular-overlap model[3]. The effect of s–d mixing is shown via a dashed line. With three electrons initially in the e_g pair of orbitals (e.g., Cu^{II}, d^9), a is clearly favored over b on this simple model. For simplicity no splitting of the metal t_{2g} orbitals is shown.

been spectroscopically studied in square-planar Ni^{II} complexes[12a] where this stabiization is dramatic (5000–6000 cm^{-1}).[12b] On tetragonal elongation (**1**) of an octahedral complex z^2 drops to lower energy on a d-orbital-only model as antibonding effects with the axial ligands are reduced. On tetragonal compression (**2**) the reverse is true (Figure 2). The z^2 orbital however, is stabilized in addition by s–d mixing in the distorted structure. With three electrons occupying the z^2, x^2–y^2 pair of orbitals (e.g., Cu^{II}), from Figure 2 the overall result is clearly a better stabilization via the elongation route. In this way the distortion of such systems may well be best described as a second-order Jahn–Teller process, via coupling of nz^2 and $(n + 1)$s orbitals on distortion.

The second consideration employs the angular-overlap model to view the problem. As we have noted,[3,13] the molecular orbital stabilization energies (MOSE) for square-planar four-, square-pyramidal five-, and octahedral six-coordinate d^9 (and low-spin d^8) systems are equal. This implies that the binding energy of one or two axial ligands to the square plane is identically zero on a d-orbital-only model or, alternatively, that the axial linkages of a pseudooctahedral complex should be much weaker, and hence longer, than their equatorial counterparts. If the total MOSE for this geometry is partitioned between equatorial and axial linkages in the usual way[3] for the d^9 configuration, that for the latter is identically zero, and the axial ligands are attached purely as a result of interaction between central-atom s and p orbitals and the ligand orbitals.

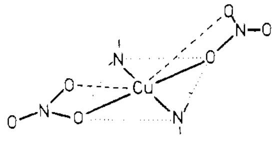
In order to determine which metal–ligand linkages may be elongated in a given system, all we need to do on this model is to compare, numerically, MOSE values for the possible square-planar alternatives. Good e_σ and e_π values for Cu^{II} systems are sparse, simply because of the distorted nature of the complexes, but recent spectral measurements of systems containing the adjacent element Ni^{II} have allowed a reasonable compilation of values for various ligands[15] (Table I). We use the relative ordering of these numbers to ask under what circumstances distortions of type **3** and type **4** will occur. In *trans*-$MY_4Y'_2$ the two possible square-planar structures with weakly coordinated axial ligands are MY_4 with a MOSE of $3e_\sigma(Y)$ and $MY_2Y'_2$ with a MOSE of $^3/_2(e_\sigma(Y) + e_\sigma(Y'))$. MY_4 will clearly be energetically favored over MY_2Y_2' in those cases where $e_\sigma(Y) > e_\sigma(Y')$. The CuO_2N_4 complexes described above, whose structures ran counter to second-order Jahn–Teller arguments, are examples of this type. The distortions are simply rationalized if oxygen donors have smaller e_σ values than nitrogen donors, as is certainly the case for water itself in Table I. $MY_2Y'_2$ will be favored in those cases where $e_\sigma(Y') > e_\sigma(Y)$ as shown in the structure of $CuCl_2{\cdot}H_2O$ and in the chain structures of α-$Cu(NH_3)_2X_2$ (X = Cl Br), all of which contain long metal–halogen distances. From Table I we can see that these two halogens do indeed have smaller e_σ values than both water and ammonia.

Table I. e_σ Values for Ligands Coordinated to Ni^{II} [a] and Cr^{III} [b]

ligand	e_σ, cm^{-1}	
	Ni^{II}	Cr^{III}
NH_3	4000	7030
NH_2	4010	
pyridine		5850
NHMe	4125	
NHEt	3890	
NMe_2	3535	
NEt_2	2599	
NCS	3890	
OH_2	1980	7900
F^-		7390
Cl^-	1710	5540
Br^-	1180	4920

[a] Reference 15. [b] Glerup, J.; Mønsted, O.; Schäffer, C. E. *Inorg. Chem.* 1976, *15*, 1399.

Similar arguments apply to the wide spectrum of other distorted Cu^{II} systems. One intersting example is the nitrato complex $Cu(2\text{-picoline})_2(NO_3)_2$ (**5**) where two long pseudoaxial Cu–O distances are found along with two pairs of short Cu–O and Cu–N distances. The alternative would be the square-planar structure containing two nitrato groups and two long Cu–N distances. The observed structure is consistent with our approach since $e_\sigma(N) > e_\sigma(O)$. In the chain structure of $Cu(SCN)_2(NH_3)_2$ (**6**) containing SCN groups bridging via sulfur- and nitrogen–metal coordination, the Cu–N(H_3) and Cu–N(CS) distances are short but the Cu–S(CN) distance is long. Although there are no e_σ data for sulfur-coordinated SCN, chemical intuition leads us to expect that the values should be considerably smaller than those for nitrogen donors. In principle we then have a way of ordering ligands in terms of their e_σ values, independent of spectroscopic studies.[16] The



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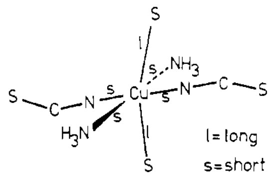

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(12) (a) For example: Hitchman, M. A.; Bremner, J. B. *Inorg. Chim. Acta* **1978**, *27*, L61. (b) L. G. Vanquickenborne and A. Ceulemans (unpublished) have pointed out that the size of the stabilization in general is numerically close to e_σ itself.

(13) (a) Burdett, J. K. *Inorg. Chem.* **1975** *14*, 931. (b) See also: DeKock, R. L.; Gray, H. B. "Chemical Structure and Bonding"; Benjamin/Cummings: Menlo Park, N.J., 1980.

(14) Interestingly the same result is not found if the crystal field model is used instead.

(15) Lever, A. B. P.; London, G.; McCarthy, P. J. *Can. J. Chem.* **1977**, *55*, 3172. Lever, A. B. P.; Walker, I. M.; McCarthy, P. J. *Spectrosc. Lett.* **1979**, *12* (*10*), 739; *Inorg. Chim. Acta* **1980**, *44*, L143. Lever, A. B. P., personal communication, 1980.

(16) Numerically, e_σ values have been obtained in other ways that do not employ spectroscopic methods. That for Me_2SO was obtained via substitution-rate data at Pt^{II} centers: Burdett, J. K. *Inorg. Chem.* **1977**, *16*, 3013.

result may well be somewhat different for various metal centers. Use of the spectroscopic parameters for Cr^{III}, for example, in our discussion above, would have resulted in the opposite conclusion for the distortion route of the CuO_2N_4 systems since, for this metal, $e_\sigma(H_2O) > e_\sigma(NH_3)$ (Table I).

Discussion

The two very simple ideas outlined above are capable of rationalizing qualitatively most of the available data on octahedrally distorted Cu^{II} species without using *any* symmetry arguments of the Jahn–Teller sort that involve the d-orbital manifold—the traditional way to view such effects. (Our approach at present, however, is not able to rationalize the great variations in the size of the distortions observed.) Our previous discussion[13] showed why such distortions are larger for the d^9 case compared to similar "Jahn-Teller" distortions of high-spin d^4 Cr^{II} complexes for example. The MOSE associated with the axial linkages is less than that for the equatorial ones but importantly, in contrast to the d^9 case, is not zero. We may also comment on the small distortions, if any, found for orbitally degenerate systems containing asymmetric occupation of the octahedral t_{2g} orbitals. For a $(t_{2g})^5(e_g)^2$ moiety (e.g., high-spin Co^{II}) the MOSE for square-planar, square-pyramidal, and octahedral geometries is simply $ne_\sigma + 4e_\pi$, where n is the number of ligands. So while the π contribution is coordination number independent, just like the corresponding MOSE values for the d^9 systems (which contain only σ contributions for this electronic configuration), analogous distortion arguments do no apply. The ligands are each bound (with a MOSE of e_σ per linkage) in all three structures. The details of the structure in this case will surely be dominated by the σ manifold.

To conclude, this paper provides a unified way to view distorted Cu^{II} complexes irrespective of which particular variant of the Jahn–Teller approach is conventionally[17] used. This one-electron approach is similar to the one we have used to understand angular geometries in transition-metal systems.[3,18,19]

Acknowledgment. I thank Professor A. B. P. Lever for his compilation of Ni^{II} e_σ values used in Table I.

Registry No. Cu, 7440-50-8.

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(17) It is interesting to recall Kettle and Jotham's comment: "It is possible that it [a static first-order Jahn–Teller distortion] has never been observed" (Kettle, S. F. A.; Jotham, R. W. *Inorg. Chim. Acta* **1971**, *5*, 183).

(18) Burdett, J. K. *Inorg. Chem.* **1975**, *14*, 931.

(19) Burdett, J. K. *Chem. Soc. Rev.* **1978**, *7*, 507.

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Electronic Structure and Photoelectron Spectrum of Tris(π-allyl)chromium, $Cr(\eta^3\text{-}C_3H_5)_3$

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The He I and He II photoelectron spectra of $Cr(\eta^3\text{-}C_3H_5)_3$ have been recorded for the gaseous material at ca. 17 °C. The details observed have been interpreted with reference to the intensity changes observed from He I to He II ionization and to the results of ab initio molecular orbital calculations, which included consideration of configuration interaction to allow for the effects of orbital relaxation upon ionization. The two lowest spectral features, at 7.13 (4) and 7.76 (3) eV, are attributed to ionization from the metal localized $(6a')^1$ and $(6e')^2$ levels. The latter ionization is considered to overlap with the ionization from the highest filled ligand level, $(4e'')^4$, which correlates with the $1a_2$ π molecular orbital of the allyl group; the other level which correlates with this ligand orbital, $(4a'')^2$, is considered to be responsible for the ionization at 8.69 (3) eV. There is a significant amount of metal character in the 4e″ and 4a″ orbitals, arising from the interaction of the $1a_2$ ligand orbitals with empty chromium 3d and 4p orbitals; these overlaps are considered to be primarily responsible for the metal–ligand bonding interactions. The remaining peaks in the photoelectron spectra are attributed to ionizations from orbitals which are essentially localized on the ligands: the features at 10.37 (4) and 11.47 (6) eV are attributed to ionizations from the 5e′ and 5a′ molecular orbitals which correlate with the $1b_1$ allyl π orbital; the peaks at 12.62 (6), 14.11 (2), 15.41 (5), 18.15 (15), and 21.90 (15) eV are attributed to ionizations from the molecular orbitals which correlate with the $3b_2$, $4a_1$, $3a_1$ and $2b_2$, $2a_1$, and $1b_2$ allyl σ orbitals, respectively.

Introduction

Transition-metal complexes involving the allyl ligand are amongst the simplest organometallic complexes known. For this reason, they have been the subject of many experimental and theoretical studies[1] to elucidate their electronic structure. In particular, the low-energy photoelectron (PE) spectra of $Ni(\eta^3\text{-}C_3H_5)_2$ and its methyl-substituted derivatives have been extensively studied, and the PE spectrum of $Pd(\eta^3\text{-}C_3H_5)_2$ has also been measured.[2,3] Calculations of the ionization energies (IE) of $Ni(\eta^3\text{-}C_3H_5)_2$ by the ab initio SCF–MO method have revealed the inadequacy of Koopmans' theorem for describing metal orbital ionization of this complex,[1] a feature also found in many other transition-metal complexes. In spite of these studies, there is no unambiguous assignment of the PE spectrum of $Ni(\eta^3\text{-}C_3H_5)_2$ nor is there an ab initio calculation that agrees with the most likely assignment.[2] Although the nickel complex has the advantage of a small number of ligands, which should assist in the interpretation of its PE spectrum, the large number of d electrons and the large degree of electron reorganization accompanying d electron ionization complicate the assignment of the PE spectrum. We have encountered

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(1) Rohmer, M.-M.; Demuynck, J.; Veillard, A. *Theor. Chim. Acta* **1974**, *36*, 93. Rohmer, M.-M.; Veillard, A. *J. Chem. Soc., Chem. Commun.* **1973**, 250. Brown, D. A.; Owens, A. *Inorg. Chim. Acta* **1971**, *5*, 675. King, R. B.; "Transition Metal Chemistry—An Introduction"; Academic Press: New York, 1969; p 31.

(2) Batich, C. D. *J. Am. Chem. Soc.* **1976**, *98*, 7585.

(3) Lloyd, D. R.; Lynaugh, N. In "Electron Spectroscopy"; Shirley, D. E., Ed; North-Holland Publishing Co.: Amsterdam, 1972; p 445.

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