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On the use of small *d*-spaces in SCF and CI calculations on transition metals

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Summary. The possibility to use atomic basis sets with only two *d*-functions describing the metal atom has been investigated, both at the SCF and the CI levels, for the Ni and Pd atoms, their mono-hydrides and their mono-oxides. Using a general contraction scheme, two atomic *d*-orbitals, corresponding to two of the atomic configurations s^2d^8, s^1d^9 and s^0d^{10} were used as the two *d*-type basis functions. A surprisingly large part of the correlation effect on both atomic excitation energies and on the equilibrium distance and dissociation energies of the hydrides and the oxides was obtained using these small basis sets. It is argued that the reason for this is important "near-degeneracy" effects involving different atomic *d*-configurations and not dynamic correlation effects.

Key words: Transition metals – *d*-spaces – SCF–CI – Metal atom

1 Introduction

In calculations on transition metal complexes it is usually necessary to describe several *d*-configurations at the same time. This situation always occurs at the CI level where configurations involving a *d*-configuration other than that of the leading configuration become important (e.g. d^8-type and d^9-type configurations for Ni complexes). A similar situation occurs at the SCF level, both for complexes where the binding involves polarization of the *d*-orbitals which can be viewed as an admixture of other configurations and in metal clusters, where some metal atoms may have a *d*-configuration different from the expected one (usually $d^{n+1}s^1$). The remedy of this problem has usually been to increase the size of the *d*-basis, a procedure which always works but which may generate quite large basis sets. The minimum requirement is three *d*-type basis functions at the metal centre. It is evident that the basis sets soon get overwhelmingly large, in particular for metal clusters.

Two metals where the mixture of different atomic *d*-states is important are nickel and palladium. For Ni the $(d^8s^2)^3F$ and the $(d^9s^1)^3D$ states are nearly degenerate, and either configuration can dominate in complexes. Palladium has a $(d^{10}s^0)^1S$ ground state, but the d^9-configuration often becomes important. In the metallic state the d^9-configuration dominates for both Ni and Pd.

In a general contraction scheme, a balanced description of the different d-states of a metal can be obtained by simply using the appropriate atomic d-orbitals as explicit basis functions. This procedure should work at the SCF level, unless the atomic basis set becomes strongly linearly dependent. It is not evident if a basis set constructed in this way also is useful in CI applications, however.

The usefulness of small basis sets containing only two atomic d-orbitals and no polarizing functions with higher l-values is the subject of the present study. The investigation was done both at the SCF and the correlated levels. The investigated systems are the Ni and Pd atoms and their monohydrides and oxides. Relativistic effects are included for both metals, in the case of Ni by using explicit no-pair operators [1, 2], and for Pd through a relativistic Effective Core Potential (ECP).

Clearly, the overlap between a d-orbital from a $s^n d^m$ configuration and from a $s^{n-1} d^{m+1}$ configuration will be large. An evident question is whether basis sets containing two atomic d-orbitals will be too linearly dependent to be useful. This does not appear to be the case, although the overlap between the d-orbitals is sizeable, 0.987–0.998.

A surprising result is that a large part of the correlation energy contribution, both to the atomic excitation energies and to the molecular bonding, is described by these small basis sets. Even a notorious case like the $(d^9s^1)^3D - (d^{10}s^0)^1S$ splitting on the nickel atom [3] is reasonably well reproduced using a basis set with only 5 s-functions, 4 p-functions and 2 d-functions. For the molecules both dissociation energies and bond distances are satisfactory, compared to large basis set results.

2 Computational details

The Ni basis sets were obtained from the 14 s-type, 8 p-type, 5 d-type primitive basis set of Wachters [4], augmented with two diffuse p-functions [4] and one diffuse d-function (exponent 0.15), and contracted to 5 s-type, 4 p-type and 2 or 3 d-type functions using the general Rafenetti [5] contraction scheme. The contraction coefficients were obtained from relativistic atomic SCF calculations, using the spin free no-pair external field method suggested by Douglas and Kroll [1], as implemented in atomic and molecular calculations by Hess [2]. Several basis sets, with different d-orbitals (the remaining contractions being the same), were used. The contraction coefficients for the core orbitals were in all cases taken from calculations on the atomic $(d^9s^1)^3D$ state. Three of the basis sets contained two contracted d-functions: the d^8/d^9 basis with atomic d-orbitals obtained for the $(d^8s^2)^3F$ and the $(d^9s^1)^3D$ states, the d^9/d^{10} basis set with atomic d-orbitals from the $(d^9s^1)^3D$ and the $(d^{10}s^0)^1S$ states and the d^8/d^{10} basis set with atomic d-orbitals from the $(d^8s^2)^3F$ and the $(d^{10}s^0)^1S$ states. A fourth basis set containing all three d-type atomic orbitals, was also used (the $d^8/d^9/d^{10}$ basis set). In all cases the 4s AO:s of the $(d^8s^2)^3F$ and $(d^9s^1)^3D$ atomic states were used as the two outermost s-type basis functions.

For Pd an ECP was used for the inner core space, defined as the 1s-3s, 2p-3p and 3d-orbitals. The type of ECP used, which is similar to the ECP suggested by Bonifacic and Huzinaga [6], has been described in detail previously [7]. In the present case the outer core space, i.e. the 4s- and the 4p-orbitals, were allowed to relax instead of being frozen as in previous studies [7]. This relaxation of the core is inconsequential for all purposes except if gradient techniques are to be employed.

The primitive basis set used for Pd consisted of 8 *s*-type, 7 *p*-type and 5 *d*-type Cartesian gaussian functions. The exponents in the inner region and the expansion coefficients were determined by a least squares fit procedure to orbitals obtained from all-electron calculations. The contracted basis set contained 3*s*-type, 3*p*-type and 2*d*-type basis functions. All nodes were kept in the outer core and in the valence orbitals.

The valence basis set and the ECP parameters were derived from all-electron calculations using the 19 *s*-type, 16 *p*-type and 11 *d*-type primitive basis set suggested by Huzinaga [8], incremented by two *p*-functions (exponents 0.11 and 0.04), and one diffuse *d*-function (exponent 0.09). The ECP parameters were optimized in the uncontracted (8,7,5) basis, and the Rafenetti contraction coefficients were taken from the atomic ECP calculations. The *d*-orbital contraction coefficients were obtained from atomic (ECP) calculations on the d^9s^1 and $d^{10}s^0$ states on Pd. The atomic all-electron calculations were done using the relativistic no-pair procedure [1, 2]. At the ECP level relativistic effects were included in the ECP by fitting the parameters to the relativistic all-electron results. Spin-orbit effects were not considered.

The basis sets used for oxygen was Dunning's 4*s*, 3*p* basis [9], extended by one additional *p* and one *d* function. Hydrogen was described by contracting the 6 *s*-functions suggested by Huzinaga [10] to 3 basis functions, and adding two diffuse *p*-functions.

In the molecular calculations on both NiH and NiO only the d^8/d^9 basis set was used. Relativistic effects were accounted for by the no-pair external field method in the molecular calculations.

The calculations were carried out at several levels of approximation: SCF, CASSCF, internally contracted multireference ACPF [11], which is approximatively size-consistent, and one-configuration size-consistent MCPF [12]. The details of the calculations for each species is described in the respective sections below.

3 Results and discussion

3.1 Atomic results

The overlap between the *d*-orbitals of Ni range between 0.987 and 0.997, resulting in virtual orbital coefficients of the order of 50–70. Similarly for Pd the overlap between the *d*-orbitals is 0.998 resulting in coefficients among the virtual orbitals of the same size as for Ni. Coefficients of this order, which in fact also occur from time to time in normal large basis set calculations, are acceptable. Linear dependency is not a serious problem.

Results obtained for the d^8s^2, d^9s^1 and $d^{10}s^0$ states of Ni are shown in Table 1.

At the SCF level the computed excitation energies are very insensitive to the choice of basis set, as they should be.

At the CI level the small basis sets perform acceptably. Bauschlicher et al. [3] calculated the excitation energies of Ni using a (7*s*, 6*p*, 4*d*, 3*f*, 2*g*) ANO basis set and different correlation methods. At the single determinant level using the MCPF procedure, they obtained excitation energies of 2.26 eV and 0.33 eV for the $(d^9s^1)^3D - (d^{10}s^0)^1S$ and the $(d^8s^2)^3F - (d^9s^1)^3D$ transitions respectively. Our small basis set calculation (using the d^8/d^9 basis set) gives an excitation energy of 0.71 eV for the $(d^8s^2)^3F - (d^9s^1)^3D$ excitation, which is 0.38 eV too high compared to the

Table 1. Excitation energies for Ni. Energies in eV. SDCI is a single reference and MRCI is a multi-reference calculation. All CI energies include the Davidson correction

Basis	Method	$(d^8s^2) - (d^9s^1)$	$(d^9s^1) - (d^{10}s^0)$
d^8/d^9	SCF	1.56	
d^8/d^{10}	SCF		4.50
$d^8/d^9/d^{10}$	SCF	1.56	4.50
	HFR[a]	1.63	4.41
d^8/d^9	MCPF	0.71	
d^9/d^{10}	MCPF		2.42
$d^8/d^9/d^{10}$	MCPF	0.67	2.46
d^9/d^{10}	MRCI		2.12
	MCPF[b]	0.36	2.24
	MRCI[b]	0.20	1.84
	Exp[c]	− 0.03	1.71

[a] Ref [13]
[b] Ref [3]
[c] Ref [23]

value obtained by Bauschlicher et al. Similarly we get an excitation energy of 2.42 eV for the $(d^9s^1)^3F - (d^{10}s^0)^1S$ transition, or 0.16 eV too high. The inclusion of a third d-orbital in the basis set does not change the result significantly. The $(d^8s^2)^3F - (d^9s^1)^3$ excitation energy drops decreases to 0.67 eV, while the $(d^9s^1)^3D - (d^{10}s^0)^1S$ excitation energy actually increases to 2.46 eV. Our method for treating the relativistic effects is different from that used by Bauschlicher et al., who included relativistic effects by simply adding a correction term from the work of Martin and Hay [13]. However, since our results at the SCF level is in good agreement with the results of Hay and Martin, it seems safe to conclude that the differences between our results and the results obtained by Bauschlicher et al. is mainly due to the lack of functions with higher l-values in our basis set. This conclusion is also supported by the results of a multi-reference CI calculation. Bauschlicher et al. obtained an excitation energy for the $(d^9s^1)^3D - (d^{10}s^0)^1S$ transition of 1.84 eV from an MRCI calculation using both the $3d$ and a $3d'$ orbital as active orbitals in the reference state. We obtained 2.12 eV with a similar set of reference configurations using the d^9/d^{10} basis set.

Although our excitation energies are in error by 0.1–0.4 eV for Ni, we obtain a large fraction of the correlation energy contribution. The small basis sets are able to account for more than 90% of the correlation effect (compared to the results of Bauschlicher et al.) on the $(d^9s^1)^3D - (d^{10}s^0)^1S$ and about 70% of the correlation effect on the $(d^8s^2)^3F - (d^9s^1)^3D$ excitation energy.

One important point concerns the relative quality of the small basis sets. In fact it turns out that the d^8-orbital is particularly effective for calculating correlation energies. The total energy obtained for the $(d^9s^1)^3D$ state using the d^8/d^9 basis set is 1.04 eV lower than the energy obtained with the d^9/d^{10} basis. Similarly for the $(d^{10}s^0)^1S$ state the d^8/d^{10} basis gives an energy which is 0.64 eV lower than the energy obtained with the d^9/d^{10} basis. The excitation energy obtained by using the lowest total energies for the $(d^9s^1)^3D$ and the $(d^{10}s^0)^1S$ states is thus 2.8 eV (cf. Table 1). Consequently excitation energies should be computed using the same basis set for different states when basis sets of the present type are used, which anyway is the normal procedure in most calculations.

Table 2. Excitation energies for Pd

Basis	Method	$(d^9s^1) - (d^{10}s^0)$
d^9/d^{10}	SCF	− 0.10
d^9/d^{10}	MCPF	− 0.67
	AE-MCPF[a]	− 0.65
	AE-MCPF[b]	− 0.84
	HFR[c]	− 0.10
	Exp[d]	− 0.95

[a] Ref [25]. All-electron results, no *f*-functions in the basis set
[b] Ref [25]. All-electron results, three contracted *f*-functions in the basis set
[c] Ref [13]
[d] Ref [24]

In the case of Pd we only considered the $(d^9s^1)^3D - (d^{10}s^0)^1S$ excitation, and we only used one basis set, the d^9/d^{10}. The results are shown in Table 2. The SCF excitation energy agrees exactly with the value by Martin and Hay [13] (0.10 eV). The MCPF result, 0.67 eV, is in reasonable agreement with the result of Blomberg et al. [14] who obtained an excitation energy of 0.88 eV using a flexible basis set with two *f*-functions. Since the ground states of Ni and Pd are different, the ground state of Ni is $(d^9s^1)^3D$ while for Pd it is $(d^{10}s^0)^1S$, the small basis sets overestimate the excitation energy for Ni and underestimate it for Pd. In the Pd case the small basis sets account for almost 80% of the correlation energy contribution to the excitation energy compared with the results of Blomberg et al.

The reason why the small basis sets are able to account for such a large fraction of the correlation effect on the atomic excitations is not evident. The two *d*-functions in the basis set are strongly overlapping, and after orthogonalization the second *d*-function will have a node close to the maximum of the first one. It is possible that the correlation effect is largely dynamic, of the radial type, but this seems improbable since the results deteriorate drastically if the second *d*-function is truncated in any way, i.e. if one or more primitive *d*-functions are deleted from this orbital contraction. If the correlation was dynamic it seems reasonable that the sensitivity to the exact form of the correlating function should not be so large. The remaining hypothesis is that the effect is not due to dynamic correlation but rather to near degeneracy effects involving different *d*-configurations. The latter explanation seems to be the most probable one.

3.2 *The hydrides*

The results obtained for NiH and PdH are shown in Table 3.

The ground states of NiH and PdH and $^2\Delta$ and $^2\Sigma^+$. There are no evident near degeneracy effects in the hydrides which would make multi-reference CI methods necessary, and consequently we chose to use the size-consistent MCPF method for both hydrides.

The atomic electron configurations expected to be most important for the binding in the hydrides are d^8s^2 and d^9s^1 for NiH and d^9s^1 and $d^{10}s^0$ for PdH.

Table 3. NiH and PdH. The CI energies include the Davidson correction

System	Method	r_e	D_e	sup.err
NiH	SCF	2.88	1.44	0.013
NiH	MCPF	2.80	2.95	0.30
NiH	MRCI	2.77	2.82	0.30
PdH	SCF	3.10	1.55	0.004
PdH	MCPF	2.93	2.22	0.17
NiH[a]	MRCI	2.77		
NiH[b]	MCPF	2.81	2.69	
PdH	MCPF	2.91	2.22 eV	
NiH	Exp[d]	$\leqslant$ 73.5		
PdH	Exp			

[a] Ref [16]
[b] Ref [17], no relativistic effects included
[c] Ref [18]
[d] Ref [15]

Consequently we used the d^8s^2/d^9s^1 basis set in the calculations on NiH and the $d^9s^1/d^{10}s^0$ basis for PdH.

The CI effect obtained with the small basis sets on both the bond distance and the dissociation energy is remarkably large for both systems. In NiH the bond distance decreases from 2.88 to 2.80 a_0 and the binding energy increases from 1.45 eV to 3.24 eV (relative to the d^9s^1 state of Ni and a hydrogen atom). With such small basis sets the basis set superposition error (BSSE) may be expected to be large. A calculation with a hydrogen basis set at 2.80 a_0 gave a negligible BSSE at the SCF level but a CI BSSE of 0.3 eV. The latter value is rather but not remarkably large, and our corrected computed binding energy is thus 2.94 eV. These results compare favorably with experiment, $r_e = 2.76\ a_0$, $D_e \leqslant 3.07$ eV [15], and with previous theoretical results, $r_e = 2.76$ [16] a_0 and $D_e = 2.69$ eV [17] (the D_e value is nonrelativistic).

The PdH results are quite similar to those obtained for NiH. The bond distance and the dissociation energy obtained at the SCF level are 3.10 a_0 and 1.55 eV. At the MCPF level the binding energy increases to 2.21 eV, and the bond distance decreases to 2.99 a_0. The BSSE in PdH is 0.17 eV, and the binding energy has been corrected for this error. Previous MCPF calculations, in which relativistic ECP:s and large valence basis sets were used, gave a bond distance of 2.91 a_0 and a dissociation energy of 2.22 eV [18]. Compared to these results the small basis set performs remarkably well. The agreement with the experimental bond distance, 2.89 a_0 [15], is satisfactory.

3.3 The oxides

While multi-reference effects are not very important for the hydrides, this is not expected to be the case for the oxides, due to the importance of excitations in the π manifold. In view of this, the multi-reference correlation calculations were done

Table 4. NiO and PdO

System	Method	r_e	D_e [a]	sup.err
NiO	CAS	3.09	2.52	0.008
NiO	ACPF-MR	3.15	3.55	0.19
NiO	MRCI[b]	3.16		
PdO	SCF	3.64	1.44	0.004
PdO	ACPF-MR	3.57	2.12	0.16
PdO	CPF[c]	3.58	1.97	
PdO	MRCI[d]	3.49	2.39	
NiO	Exp[e]		3.87	
PdO	Exp[e]		2.87	

[a] D_e is calculated relative to the (d^9s^1) state of the Ni atom for NiO and relative to the $d^{10}s^0$ state of the Pd atom for PdO

[b] Refs [19, 20]

[c] Relativistic ECP results, Ref [26]

[d] Ref [22]

[e] Ref [15]

using internally contracted ACPF, which is an approximately size-consistent method.

The atomic electron configurations expected to be most important are the same as for the hydrides, i.e. d^8s^2 and d^9s^1 for NiO and d^9s^1 and $d^{10}s^0$ for PdO. The basis sets used were consequently the same as for the hydrides, i.e. d^8s^2/d^9s^1 for NiO and the $d^9s^1/d^{10}s^0$ for PdO.

The reference states used in the ACPF calculations were obtained from CASSCF calculations with an active space defined by distributing all the valence electrons on the metal and the $2p$ electrons on oxygen (a total of 14 electrons) among nine valence orbitals, defined by the *d*-orbitals on Ni and Pd, and the π and the σ orbitals which describe the oxygen $2p$ shell in an ionic picture. All configurations with coefficients larger than 0.05 were included in the CI reference space. The ground state for both species is $^3\Sigma^-$.

The results are shown in Table 4.

For NiO the bond distance and binding energy obtained at the CAS level were 3.09 a_0 and 2.52 eV (relative to the d^9s^1 state on Ni). At the CI level the bond distance increases to 3.15 a_0 and the binding energy to 3.55 eV. The BSSE at the CI level, 0.19 eV, was actually smaller than for NiH (0.30 eV). This value for the BSSE was obtained for the $(d^8s^2)^3F$ state of Ni with an oxygen basis set at 3.1 a.u. NiO has been studied previously by Bauschlicher et al. who obtained a bond distance of 3.16 a_0 for the $^2\Delta$ state using MRCI and large basis sets [19, 20]. The experimental values are 3.07 a_0 [21] and 3.87 eV [15].

While the bond distance in NiO increases as a result of correlation the reverse is true for PdO. In PdO the bond distance is decreased from 3.64 to 3.57 after CI. Since a multiconfigurational SCF mixes anti-bonding configurations with the ground state a decrease of the bond distance after CI is expected if near degeneracy effects are strong. Our result thus indicates that the near-degeneracy effects are more important in PdO than in NiO. The effect on the binding energies is weaker in PdO than in NiO; while the increase in PdO is 0.68 (from 1.44 eV to 2.12 eV) it is 1.03 eV for NiO. Siegbahn obtained a binding energy of 2.39 eV using large basis sets, first order perturbation theory for the relativistic effects and multireference CI, and a bond distance of 3.49 a_0 using MCPF and a somewhat smaller basis set [22]. The experimental binding energy is 2.87 eV [15].

The small basis set results compare favourably with previous large basis set calculations both for NiO and PdO. Our bond distance for NiO agrees almost exactly with the bond distance found by Bauschlicher et al. [19, 20] while we are too long by 0.09 a_0 for PdO. Our computed dissociation energy is too low by 0.27 eV compared to the result of Siegbahn [22]. Compared to experiment we are too low by 0.32 eV for NiO and 0.75 eV for PdO. For qualitative or semi-quantitative applications our small basis sets behave satisfactorily.

3.4 *The origin of the CI effects*

It is quite remarkable that such a large part of the CI effect is obtained using basis sets with only two *d*-functions and no correlating *f*:s.

The second *d*-functions used in the basis set will have a node close to the maximum density of the first one. This fact gives rise to two explanations regarding the origin of the CI effect. Either the effect is largely dynamic radial correlation or it is due to near degeneracy effects involving different *d*-configuration. The first interpretation is supported by a perturbation theory argument. Near degeneracy effects should, in second order perturbation theory, be more important the closer the states are in energy. However, the $d^{10}s^0$ state picks up more correlation energy with the $d^8s^2/d^{10}s^0$ basis set than with the $d^9s^1/d^{10}s^0$ basis (see above), in spite of the fact that the energy separation between the $d^{10}s^0$ state and the d^9s^1 state is smaller than the energy separation between the $d^{10}s^0$ state and the d^8s^2 state. The second interpretation is supported by the effects of truncating the correlating *d*-orbital. If a primitive function is removed from the contraction of the correlating d^9-orbital in a calculation on the d^{10}-state, keeping the remaining coefficients unchanged, 85% of the correlation effect is lost (the contraction coefficient of this primitive function is 0.02). It seems unlikely that the effects of this modified correlating orbital could be so drastic if the first interpretation was correct, i.e. if the correlation is dynamic. We therefore conclude that dynamical correlation effects, in the traditional sense, are not very important to describe either the binding or the low excited states in the present systems. Instead, the correlation effects are due to the interaction between "real" states with varying *d*-occupations. Dunning et al. [23] have previously drawn a similar conclusion from a study of Ti, where large correlation effects were found in an MCSCF calculation using a 3*d* and a 3*d*′ orbital. The 3*d*′ orbital used in that study was considerably more diffuse than our correlating orbital, however.

4 Conclusions

In the present article we have shown that it is possible to describe both atomic excitations and molecular properties, at both the SCF and the CI levels of approximation, with a reasonably high level of accuracy with quite small basis sets built from real atomic orbitals describing different atomic states. We also argue that the major part of the *d* correlation effect is due to strong interactions (near degeneracy effects) involving different atomic *d*-configurations.

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