

Regular article

A correlation-consistent basis set for Fe

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Abstract. A series of correlation-consistent basis sets are developed for Fe. Our best computed $^5F-^5D$ separation in the Fe atom is in excellent agreement with experiment. Our best estimate for the FeCO D_0 value is in good agreement with experiment. The $^5\Sigma^- - ^3\Sigma^-$ separation in FeCO has an error of 3.6 kcal/mol; while the origin of this error is not clear, it is probably not due to the basis set.

Key words: Basis set – Correlation-consistent – FeCO bond energies

1 Introduction

Correlation-consistent polarized valence (cc-pV) and augmented (aug) cc-pV basis sets [1–4] have been used extensively to obtain accurate dissociation energies and other molecular properties. Very recently developed sextuple-zeta basis sets [3, 4] yield N_2 and HF dissociation energies that are within 0.6–0.8 and 0.1 kcal/mol, respectively, of the estimated complete basis set (CBS) limits. The performance of the correlation-consistent basis sets relies on the fact that they are very systematic and therefore the energies can be extrapolated to the CBS limit. Most of the cc-pV basis sets have been developed for the elements of the main group, while only a few exist for transition-metal atoms [5]. Many applications require accurate bond energies for transition-metal systems and cc-pV basis sets are needed to obtain the desired chemical accuracy. In the present article we report on the development of a series of correlation-consistent basis sets for Fe; these sets are tested by computing the $^5F-^5D$ separation in the Fe atom and some molecular properties of the $^3\Sigma^-$ and $^5\Sigma^-$ states of FeCO.

2 Methods

The details of the development of the Fe basis set are given in Sect. 3. For C and O we use the triple-zeta (TZ), quadruple-zeta (QZ), and quintuple-zeta (5Z) aug-cc-pV sets [1, 2]. Most of the calculations were performed using the restricted coupled cluster singles and doubles approach [6, 7], including the effect of connected triples determined using perturbation theory [8, 9], RCCSD(T). In the valence treatment, we correlate the eight Fe 3d and 4s electrons and the 2s and 2p electrons of C and O. To improve the accuracy of the RCCSD(T) results, we extrapolate the TZ, QZ, and 5Z values to the CBS limit using the three-point ($n^{-4} + n^{-6}$) scheme described by Martin [10]. For FeCO, complete-active-space self-consistent-field (CASSCF) and internally contracted [11] multireference configuration interaction (ICMRCI) calculations were also performed. The active space is discussed in Sect. 4. The same number of electrons are correlated in the ICMRCI calculations as in the RCCSD(T) calculations.

Core-valence (CV) calculations were performed by adding the Fe 3s and 3p, C 1s, and O 1s electrons to the correlation treatment. We computed the CV effect using CV(TZ) basis sets and we did not correct the results for basis set superposition error. The CV(TZ) basis set for Fe is described in Sect. 3. The CV(TZ) basis sets for C and O were derived from the corresponding TZ set by contracting the first five s primitives to one function and by uncontracting the remaining s primitives and all the p, d, and f primitives. For C, three even-tempered tight d functions with exponents of 2.743, 6.856, and 17.141 were added and two even-tempered tight f functions with exponents of 2.283 and 6.849 were added. For O, two even-tempered tight d functions with exponents of 6.94 and 20.83 were added and one tight f function with an exponent of 4.284 was added. The CV effect was computed as the difference between the CCSD(T) treatments correlating only valence electrons and correlating the valence plus inner-shell electrons.

The scalar relativistic effect was computed at the modified coupled pair functional [12] (MCPDF) level of theory using the TZ basis set as the difference between the results using the nonrelativistic and the Douglas–Kroll (DK) approaches [13]. In the DK calculations, the same primitive basis sets were used and were contracted in the same manner as in the nonrelativistic calculations, but the contraction coefficients were taken from DK atomic calculations.

The atomic spin-orbit contribution to the dissociation energy was taken from experiment [14] and we used the difference between the lowest J component and the weighted average energy.

The zero-point energies (ZPEs) of the FeCO $^3\Sigma^-$ and $^5\Sigma^-$ states were taken to be half the sum of the harmonic frequencies, which were computed using density functional theory, in conjunction with the hybrid [15] B3LYP [16] approach. The 6-31G [17] basis set was used for C and O and the 6-31 + G basis set [18–20] was used for Fe.

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The B3LYP calculations were performed using Gaussian98 [21], the RCCSD(T) and ICMRCI calculations were performed using Molpro [22], and the MCPF calculations were performed using Molecule-Sweden [23]. The DK integrals were computed using a modified version of the program written by Hess [13].

3 Development of the Fe basis set

The first step in the development of the Fe basis set is to determine the contraction coefficients for the spd basis. We started from the (20s15p10d) primitive set optimized by Partridge [24]. The contraction coefficients were obtained from an SCF calculation of the 5D state. For the valence spd basis set we contracted the inner 18 s primitives to four functions. Note that contracting the inner 17 s primitives results in a large overlap between the third and fourth contracted functions, which could lead to linear dependencies in molecular calculations. For the p primitives, an inspection of the 3p coefficients indicates that one can contract the inner 9 p or the inner 10 p primitives. We decided to contract the inner 9 p functions because this leads to a 3p orbital with a TZ character. We contracted the inner five d primitives to one function. The exponents and the contraction coefficients are reported in Table 1. This valence set was used in all the cc-pV sets and only the polarization set was changed as done previously [5].

The next step is the optimization of the even-tempered polarization functions. The bonding in compounds containing Fe often involves mixtures of the Fe $^5D(3d^64s^2)$ and $^5F(3d^74s^1)$ states. To avoid any bias towards a specific state we optimized the polarization functions for the average of the Fe 5D and 5F states. We used a CCSD(T) treatment correlating the 3d and 4s valence electrons, denoted as 8e CCSD(T). The TZ, QZ, and 5Z polarization sets are 2f1g, 3f2g1h, and 4f3g2h1i, respectively, and are reported in Table 2.

The Fe CV basis set starts from the valence basis set and recontracts the s space, where the inner 16 s primitives are contracted to three functions. The remaining functions are the same as those used in the valence set. For Ti it was shown [5] that adding extra tight functions did not significantly improve the description of the CV wave functions, since the 3d orbital is rather compact, like the 3s and 3p orbitals.

4 Test of the Fe basis set

4.1 $^5F-^5D$ separation in Fe

We tested the Fe basis set by computing the Fe $^5F-^5D$ separation. Using the uncontracted Fe basis set, the SCF separation is 41.47 kcal/mol. This value is in very good agreement with the nonrelativistic numerical Hartree-Fock value of 41.51 kcal/mol [25]. Our contracted valence Fe basis set gives a separation of 41.89 kcal/mol, which is in very good agreement with the uncontracted basis set. To compare our results with the experimental Fe $^5F-^5D$ separation value of 20.1 kcal/mol [14], we need to account for electron correlation; we performed a CCSD(T) treatment correlating the 3d and

4s valence electrons [8e CCSD(T)] using the TZ, QZ, and 5Z basis sets. The values are reported in Table 3 and are extrapolated to the CBS limit using the three-point ($n^{-4} + n^{-6}$) scheme [10]. The CBS value of 17.35 kcal/mol is somewhat lower than obtained from experiment. Adding the 3s and 3p orbitals to the correlation treatment, denoted as 16e CCSD(T), decreases the separation even further. Our best result, denoted as 16e CCSD(T)+Rel, was obtained by adding the scalar relativistic effect, computed at the MCPF level, to the 16e CCSD(T) treatment. We obtained a computed Fe $^5F-^5D$ separation of 19.63 kcal/mol, in very good agreement with experiment.

4.2 $^3\Sigma^- - ^5\Sigma^-$ separation in FeCO

We studied the $^3\Sigma^-$ and $^5\Sigma^-$ states of FeCO as our second test of the Fe basis set. We optimized the geometry of the $^3\Sigma^-$ and $^5\Sigma^-$ states of FeCO at the CCSD(T) level of theory using a valence correlation treatment and a valence basis set. The geometrical values and the total energies are reported in Table 4. The geometrical parameters are practically converged for the QZ basis set. The geometry of the $^3\Sigma^-$ state is in good agreement with experiment [26].

Villalta and Leopold [27] showed that the ground state of FeCO is the $^3\Sigma^-$ state, with the $^5\Sigma^-$ state lying $1135 \pm 25 \text{ cm}^{-1}$ (3.2 kcal/mol) higher in energy. Both the MCPF [28] and CCSD(T) [29] approaches, without any relativistic corrections and using small basis sets, incorrectly found a $^5\Sigma^-$ ground state, with the $^3\Sigma^-$ state slightly higher in energy. This result was explained by the fact that the $^3\Sigma^-$ state has more multireference character than the $^5\Sigma^-$ state, so the single-reference-based MCPF and CCSD(T) methods are biased against the $^3\Sigma^-$ state; however, limitations in the basis sets may also have contributed to bias against the $^3\Sigma^-$ state. Very recently, Noro et al. [30] performed both CASSCF and MRCI calculations using atomic natural orbital (ANO) and segmented contracted Gaussian-type function (CGTF) basis sets. The MRCI approach favored the $^5\Sigma^-$ state despite the use of a multiconfigurational reference. It was only with the inclusion of the Davidson correction that they found a $^3\Sigma^-$ ground state, with the $^5\Sigma^-$ state lying 0.42 kcal/mol higher in energy for the CGTF basis, while for the ANO basis set the ground state was $^5\Sigma^-$ even after the addition of the Davidson correction. These MRCI calculations were performed using their medium-sized basis set, which has only a 1f polarization set. That is, their medium basis set has a polarization set smaller than our cc-pVTZ set. Since at the CASSCF level they found that basis set improvements to 2f1g favored the $^5\Sigma^-$ state, it is likely that their MRCI+Davidson approach in their large basis set would yield a very small separation, perhaps even a reversal of the states.

It is clearly of interest to obtain the CCSD(T) CBS value for the $^5\Sigma^- - ^3\Sigma^-$ separation to separate basis set effects from multireference effects. The $^5\Sigma^- - ^3\Sigma^-$ energy separation of FeCO as a function of the level of theory is summarized in Table 5 and other factors that can affect

Table 1. Exponents and contraction coefficients for the Fe valence spd basis set

Type	Exponents		Contraction coefficients						
s	4316265.300000	0.000009	-0.000003	0.000001	0.000000	0.0	0.0		
	646342.420000	0.000067	-0.000020	0.000008	0.000002	0.0	0.0		
	147089.730000	0.000354	-0.000108	0.000040	0.000009	0.0	0.0		
	41661.522000	0.001494	-0.000454	0.000168	0.000036	0.0	0.0		
	13590.765000	0.005411	-0.001650	0.000611	0.000131	0.0	0.0		
	4905.750000	0.017353	-0.005342	0.001984	0.000425	0.0	0.0		
	1912.745800	0.049540	-0.015619	0.005806	0.001242	0.0	0.0		
	792.604340	0.123034	-0.040888	0.015328	0.003284	0.0	0.0		
	344.806480	0.249291	-0.092907	0.035210	0.007553	0.0	0.0		
	155.899890	0.358569	-0.168937	0.066225	0.014272	0.0	0.0		
	72.230908	0.277479	-0.190991	0.078452	0.016996	0.0	0.0		
	32.725065	0.067201	0.043968	-0.018786	-0.004038	0.0	0.0		
	15.667622	-0.001155	0.515453	-0.305187	-0.069630	0.0	0.0		
	7.503483	0.001931	0.505163	-0.459338	-0.110096	0.0	0.0		
	3.312223	-0.000893	0.092375	0.127058	0.038472	0.0	0.0		
	1.558471	0.000385	-0.002403	0.729235	0.226240	0.0	0.0		
	0.683914	-0.000151	0.002246	0.399263	0.250661	0.0	0.0		
	0.146757	0.000056	-0.000494	0.016490	-0.319827	0.0	0.0		
	0.070583	0.0	0.0	0.0	0.0	1.0	0.0		
	0.031449	0.0	0.0	0.0	0.0	0.0	1.0		
p	7721.488600	0.000176	-0.000064	0.0	0.0	0.0	0.0	0.0	0.0
	1829.125800	0.001551	-0.000562	0.0	0.0	0.0	0.0	0.0	0.0
	593.627950	0.008639	-0.003156	0.0	0.0	0.0	0.0	0.0	0.0
	226.205360	0.035482	-0.013109	0.0	0.0	0.0	0.0	0.0	0.0
	95.261454	0.110805	-0.042283	0.0	0.0	0.0	0.0	0.0	0.0
	42.859203	0.251536	-0.099851	0.0	0.0	0.0	0.0	0.0	0.0
	20.049713	0.381669	-0.162046	0.0	0.0	0.0	0.0	0.0	0.0
	9.620885	0.309910	-0.114963	0.0	0.0	0.0	0.0	0.0	0.0
	4.541371	0.087864	0.181742	0.0	0.0	0.0	0.0	0.0	0.0
	2.113500	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
	0.947201	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
	0.391243	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
	0.156480	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
	0.062592	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0
	0.025037	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
d	217.368830	0.000945							
	64.999755	0.008060							
	24.773137	0.036504							
	10.436140	0.111034							
	4.679653	0.232545							
	2.125623	1.000000							
	0.945242	1.000000							
	0.402685	1.000000							
	0.156651	1.000000							
	0.062660	1.000000							

Table 2. The optimized even-tempered exponents for the correlation-consistent polarized valence polarization functions: triple-zeta (TZ), quadruple-zeta (QZ), quintuple-zeta (5Z)

	f	g	h	i
TZ	3.265953	2.248000		
	0.786787			
QZ	5.138777	3.705809	2.480000	
	1.519000			
	0.449010			
5Z	7.475917	5.713372	4.319745	3.210000
	2.569044			
	0.882833			
	0.303379			

this small energy separation are considered in Table 6. The CCSD(T) ${}^5\Sigma^- - {}^3\Sigma^-$ energy separation decreases as we improve the basis set from TZ to 5Z. We should note that our CBS separation is relatively insensitive to the extrapolation scheme, for example, if use the two-point method of Helgaker et al. [31] in conjunction with the QZ and 5Z basis sets the value is only 0.02 kcal/mol smaller. Thus, our basis sets appear as systematic for FeCO as for the Fe atom. We should note that Noro et al. found that basis set improvements lowered the ${}^5\Sigma^-$ state with respect to the ${}^3\Sigma^-$; however, their largest basis set contained a 2f1g polarization set, which is equivalent in size to our smallest TZ set. Our TZ separation is smaller than our previous [29] CCSD(T) value that used only a double-zeta plus polarization (DZP) basis set; this

Table 3. The Fe $^5F-^5D$ separation (kcal/mol). The complete basis set (CBS) values were computed using the three-point $n^{-4}+n^{-6}$ scheme. The experimental values are from Ref. [14]

Treatment	Basis	TZ	QZ	5Z	CBS
8e CCSD(T)	Val	21.71	19.46	18.41	17.35
16e CCSD(T)	3s3p	20.09	16.96	15.45	13.89
16e CCSD(T)+Rel					19.63
Experiment					20.1

Table 4. Summary of the optimized geometries of FeCO and their corresponding total energies computed at CCSD(T) level of theory using a valence correlation treatment and a valence basis set. The CBS values were computed using the three-point $n^{-4}+n^{-6}$ scheme. The experimental values are from Ref. [26]

	$r(\text{Fe-C})$ (Å)	$r(\text{C-O})$ (Å)	Total energies (hartrees)
$^3\Sigma^-$ state			
CCSD(T) TZ	1.746	1.163	-1375.80894015
CCSD(T) QZ	1.746	1.159	-1375.85342835
CCSD(T) 5Z	1.746	1.158	-1375.86920615
CBS			-1375.8830
Experiment	1.727	1.159	
$^5\Sigma^-$ state			
CCSD(T) TZ	1.853	1.155	-1375.81071127
CCSD(T) QZ	1.861	1.150	-1375.85442333
CCSD(T) 5Z	1.860	1.149	-1375.86988219
CBS			-1375.8834

Table 5. $^5\Sigma^- - ^3\Sigma^-$ energy separation for FeCO

	ΔE (kcal/mol)
CCSD(T) TZ	-1.11
CCSD(T) QZ	-0.62
CCSD(T) 5Z	-0.42
CCSD(T) CBS	-0.23
CASSCF TZ	-9.19
ICMRCI TZ	-1.92
ICMRCI+Q TZ	0.61

is consistent with our trend of a decrease in the separation with basis set improvement. The MCPF result [28] obtained in an approximately DZ basis is also consistent with the present results.

Using the TZ basis set we investigate multireference effects using the CASSCF/ICMRCI approach. The CASSCF active space consists of the Fe $3d$ and $4s$ orbitals and the CO π and π^* orbitals. All CASSCF configurations were included as references in the ICMRCI calculation which correlate all valence electrons. The reference comprises 94.4% of the $^5\Sigma^-$ ICMRCI wave function and 94.2% of that for the $^3\Sigma^-$ state. At the CASSCF and ICMRCI levels of theory the $^5\Sigma^-$ state is below the $^3\Sigma^-$ state (Table 5). It is only with the addition of the Davidson correction (denoted +Q) that the $^3\Sigma^-$ state is found to be below the $^5\Sigma^-$ state.

4.3 D_0 energy in the $^3\Sigma^-$ state of FeCO

In order to compute an accurate D_0 or T_0 we must account for other effects, which are summarized in Table 6, where we report the Fe-CO dissociation energies with respect to Fe 5D for both the $^3\Sigma^-$ and the $^5\Sigma^-$ states, and the separation between the states. We corrected our CBS D_e by taking into account ZPEs, scalar relativistic, spin-orbit, CV and thermal effects. T_0 was also corrected for multireference effects using the

Table 6. Summary of the Fe-CO dissociation energies (kcal/mol) with respect to Fe 5D for the $^3\Sigma^-$ and $^5\Sigma^-$ states and the separation between them

	$^3\Sigma^-$ state	$^5\Sigma^-$ state	Δ
CCSD(T) CBS	5.36	5.59	-0.23
Zero-point energy	-1.33	-0.63	-0.69
Scalar relativistic effect (MCPF)	-2.61	-2.09	-0.53
Spin orbit	-1.15	-1.15	0.00
Core-valence	0.98	1.61	-0.63
MRCI+Q-CCSD(T) TZ			1.72
Corrected D_0/T_0 (0 K)	1.25	3.33	-0.36
Thermal effects	0.96	0.45	0.51
Corrected D_0/T_0 (298 K)	2.20	3.78	0.15
Best estimate for D_0 (298 K)	6.98 ^a		
Experiment	10.5 \pm 3.7 ^b		3.2 ^b
	8.1 \pm 3.5 ^c		

^a Obtained by adding the experimental $^5\Sigma^- - ^3\Sigma^-$ separation [27] to the $^3\Sigma^- D_0$ (298 K) value

^b Ref. [27]

^c Ref. [32]

difference between the TZ CCSD(T) and ICMRCI+Q results. After making all these corrections, we find that our best computed T_0 value is -0.36 kcal/mol, which differs from experiment by 3.6 kcal/mol; clearly it is very difficult to accurately compute this separation. While it is very difficult to accurately compute the $^5\Sigma^- - ^3\Sigma^-$ separation, we believe that our approach should yield a very accurate description of the $^5\Sigma^-$ state, and therefore most of our error in our T_0 arises from errors in the $^3\Sigma^-$ state. Therefore we can improve our estimate of the $^3\Sigma^- D_0$ (298 K) value by correcting our $^5\Sigma^- D_0$ (298 K) value using the experimental $^5\Sigma^- - ^3\Sigma^-$ separation. Since we suspect that the $^5\Sigma^- D_0$ has an error bar of ± 3 kcal/mol, we assign this as the uncertainty in our best estimate for the $^3\Sigma^- D_0$. Thus, our best estimate for the $^3\Sigma^- D_0$ (298 K) is 7 ± 3 kcal/mol, which is in good agreement with the experimental values [27, 32].

5 Conclusions

We have developed a new correlation-consistent basis set for Fe which, in conjunction with a CCSD(T) theoretical treatment and an extrapolation to the CBS limit, has been able to reproduce the experimental Fe $^5\text{F}-^5\text{D}$ energy separation. We computed the geometry of the $^5\Sigma^-$ and $^3\Sigma^-$ states of FeCO, and the geometry of the $^3\Sigma^-$ state is in good agreement with experiment. Our computed $^5\Sigma^-$ - $^3\Sigma^-$ energy separation for FeCO differs from experiment by 3.6 kcal/mol, despite accounting for the scalar relativistic effect, CV correlation and multireference effects; clearly this separation is very difficult to compute. Our best estimate for the $^3\Sigma^- D_0$ (298 K) value, which is derived by combining our computed $^5\Sigma^- D_0$ with the experimental T_0 value, agrees with experiment to within their combined error bars.

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