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A flexible correlation group table (CGT) method for the relativistic configuration interaction wavefunctions

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A generalized correlation group table (CGT) method is described for the relativistic configuration interaction (RCI) wavefunctions of molecules containing heavy atoms. In this method first four keywords are defined and two properties are discussed in terms of spectroscopic states and double group theory. These definitions and properties are then used to summarize six principles to stipulate the relationship among relativistic states, nonrelativistic states, as well as RCI configurations. The definitions, properties, and principles comprise the generalized CGT method, which facilitates the classification and assignment of the RCI wavefunctions, and thus, provide a general technique for complex systems containing several open shells. Finally, the techniques are exemplified with a few computational models.

KEY WORDS: relativistic CI, double group, correlation group table

1. Introduction

Relativistic effects play an important role in the electronic structure and spectroscopy of molecules containing very heavy atoms [1–4]. The coupling of electron correlation effects and relativistic effects could be important, especially for molecules containing very heavy atoms [1]. While other relativistic effects and electron correlation effects can be introduced simultaneously by invoking the averaged relativistic effective core potentials (ARECPs) for large-scale CI calculations [1], the spin–orbit effects will have to be considered for molecules containing very heavy atoms. For example, for molecules such as IrC and IrCO, the spin–orbit effects have been found to be nonnegligible [5,6] due to the large spin–orbit splitting of the Ir atom. In order to address the coupling of spin–orbit and electron correlation effects, the relativistic configuration

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interaction (RCI) technique has been developed to include the electronic correlation effects and spin–orbit coupling simultaneously for such systems in the double group of the molecular point group [1,7,8].

It is well established that the RCI technique poses a major difficulty, especially for diatomics exhibiting several open-shell electronic configurations. For such systems, the classification and assignment of the RCI wavefunction patterns are the major bottlenecks. This stipulates the construction of a framework of wavefunctions as reference configurations that correlate into given nonrelativistic and relativistic states. In order to facilitate this, a series of correlation group tables, which mold the RCI wavefunctions in terms of the relativistic states of a given ω angular momentum, have been developed by one of the authors [1] for simple cases that contain only a few open shells. The current article is aimed at a systematic development of techniques for complex molecules containing any number of open shells.

We first provide a brief outline of the correlation group table (CGT) method starting with introduction to the basic principles used in [1]. Subsequently, we provide a framework of definitions and properties that result in important rules and tables for the assignment of the RCI wavefunctions arising from electronic states containing several open-shell electronic configurations. It is shown that the method can be used to conveniently classify the RCI wavefunctions derived from a given electronic configuration that leads to high spin multiplicities. Some specific calculations, results and correlation tables have been provided for convenient use in complex electronic states of very heavy molecules.

2. Method

2.1. Preliminaries

Once the spin–orbit operator is included into the Hamiltonian, neither the spatial symmetry operators nor the spin angular momentum operators commute with the Hamiltonian. Choosing the many-electron basis functions to transform according to the irreducible representations of the double group [1,7,9] may then block the Hamiltonian matrix. Note that the matrix elements may be real, imaginary or complex, although it is known that for molecules that exhibit $C_{2\mathrm{v}}$ or higher symmetries, the matrix elements are either purely real or purely imaginary [7].

Consider the simplest case of a singly occupied π orbital as an example. This electronic configuration generates a ${}^2\Pi$ nonrelativistic state. In the $C^2_{\infty\mathrm{v}}$ double group, the $\lambda = 1$ spatial state and the spin $1/2$ state correlate into Π and $E_{1/2}$ irreducible representations, respectively, as seen from tables 1 and 2.

Thus, for the ${}^2\Pi$ state under consideration, the overall relativistic states are obtained as

$$E_{1/2} \otimes \Pi = E_{1/2} \oplus E_{3/2} \quad \Longrightarrow \quad \Omega = \frac{1}{2}, \frac{3}{2}. \tag{1}$$

Table 1
Irreducible representations of diatomics and their ω–ω state designation in the $C^2_{\infty v}$ double group.

Irreducible representation	ω–ω state designation
Σ^+	0^+
Σ^-	0^-
Π	1
Δ	2
Φ	3
Γ	4
$E_{1/2}$	$1/2$
$E_{3/2}$	$3/2$
$E_{n/2}$	$n/2$

Table 2
Spin state correlation for diatomics in the $C^2_{\infty v}$ double group.

D^s	Irreducible representations
D^0	Σ^+
$D^{1/2}$	$E_{1/2}$
D^1	$\Sigma^- + \Pi$
$D^{3/2}$	$E_{1/2} + E_{3/2}$
D^n	$\Sigma^+ + \Pi + \cdots + \Gamma^n$, n even
D^n	$\Sigma^- + \Pi + \cdots + \Gamma^n$, n odd
$D^{n/2}$	$E_{1/2} + E_{3/2} + \cdots + E_{n/2}$

In terms of complex and real orbitals, the $1/2$ state can be expressed as

$$\frac{1}{2} = \pi^+\beta = (\pi_x\beta + \mathrm{i}\pi_y\beta) \quad \Longrightarrow \quad \begin{cases} \pi_x\beta, \\ \mathrm{i}\pi_y\beta. \end{cases} \tag{2}$$

Thus, the $1/2$ relativistic state arising from the π configuration consists of two configurations with β spin; $\pi_x\beta$ is real, while $\pi_y\beta$ is imaginary, but with the same sign, so that the net result is a $1/2$ angular-momentum state. Similarly, the $3/2$ relativistic state can be expressed as

$$\frac{3}{2} = \pi^+\alpha = (\pi_x\alpha + \mathrm{i}\pi_y\alpha) \quad \Longrightarrow \quad \begin{cases} \pi_x\alpha, \\ \mathrm{i}\pi_y\alpha. \end{cases} \tag{3}$$

Note that the difference of the configuration between $1/2$ and $3/2$ states is the spin direction, namely, β and α, respectively.

By correlating the patterns of the RCI wavefunctions in terms of the signs of the wavefunctions, and the corresponding nonrelativistic and relativistic states, one obtains the correlation group table for the π electronic configuration, as seen from table 3, where 00, 01, 10, and 11 represent null, β, α, and full occupations, respectively. This method

Table 3
RCI wavefunction patterns for π configuration.

λ–s state	ω–ω state	Case signs	Configuration π_x	π_y	C_{2v} (λ–s)
$^2\Pi$	$1/2$	$+$	01	00	$^2B_1$ or $^2B_2$
		$+$i	00	01	
	$3/2$	$+$	10	00	
		$+$i	00	10	

of describing the RCI wavefunctions can be generalized to more complex systems exhibiting multiple open shells, which we call the correlation group table (CGT) method.

For other nonrelativistic states with high multiplicities, for example, $^6\Pi$, which are often seen to be the low-lying states for species containing heavy transition metals, the construction of the CGT is more involved. As can be seen from tables 1 and 2, the $\lambda = 1$ spatial symmetry correlates with Π irreducible representation, but the $s = 5/2$ spin symmetry correlates into $E_{1/2}$, $E_{3/2}$, and $E_{5/2}$ irreducible representations. The overall states are obtained as

$$\begin{aligned} E_{1/2} \otimes \Pi = E_{1/2} \oplus E_{3/2} \quad &\Longrightarrow \quad \Omega = \frac{1}{2}, \frac{3}{2}, \\ E_{3/2} \otimes \Pi = E_{1/2} \oplus E_{5/2} \quad &\Longrightarrow \quad \Omega = \frac{1}{2}, \frac{5}{2}, \\ E_{5/2} \otimes \Pi = E_{7/2} \oplus E_{3/2} \quad &\Longrightarrow \quad \Omega = \frac{3}{2}, \frac{7}{2}. \end{aligned} \tag{4}$$

Consequently, a $^6\Pi$ nonrelativistic state generates two $1/2$, two $3/2$, one $5/2$, and one $7/2$ relativistic states. Since the two $1/2$ states and the $5/2$ state will inevitably lead to similar RCI patterns with the only exception of signs, one must differentiate them in terms of a generalized CGT technique, which we describe below.

2.2. Definitions and properties

Before describing the generalized CGT method, we first outline four definitions that are used to categorize the RCI wavefunctions. Subsequently, we introduce two useful properties by which more complicated RCI wavefunctions can be assigned relative to the given relativistic and nonrelativistic states.

Definition 1. A set of RCI wavefunctions is called a *RCI configuration* if the sign of the coefficient of each RCI wavefunction remains relatively unchanged after linearly combining the eigenfunction of a given relativistic state. Here "relatively unchanged" means the signs are the same with respect to every operation. Note that the sign may be either real or imaginary (that is, ± 1 or $\pm$i).

Definition 2. Among all the RCI configurations derived from an electronic configuration with the same overall angular momentum alongside the z axis, each of a set of RCI configurations is called a *characterized RCI configuration* of a given relativistic state if the set makes the greatest contribution to this state.

To illustrate, consider a π electronic configuration as an example. As can be seen from table 3, there are four RCI wavefunctions altogether derived from this electronic configuration, which can be expressed as $+\pi_x\beta$, $+\mathrm{i}\pi_y\beta$, $+\pi_x\alpha$, and $+\mathrm{i}\pi_y\alpha$. In this case, $+\pi_x\beta$ and $+\mathrm{i}\pi_y\beta$, and $+\pi_x\alpha$ and $+\mathrm{i}\pi_y\alpha$ comprise two RCI configurations, respectively. The first RCI configuration is the characterized RCI configuration of the $1/2$ state, while the second one is the characterized RCI configuration of the $3/2$ state.

Definition 3. A *spin configuration* refers to a distribution of electrons among complex molecular orbitals that includes spin–orbit coupling, for example, $\pi^+\alpha \cdot \pi^+\beta$ or $\pi^+\alpha \cdot \delta^{2+}\alpha$, etc. A spin configuration determines a set of RCI wavefunctions, namely, a RCI configuration.

Definition 4. A pair of spin configurations is said to be *coupled* if one transforms to the other by exchanging two electrons of different spin orientations between two different complex molecular orbitals. For example, $\pi^+\alpha \cdot \pi^-\beta$ and $\pi^-\alpha \cdot \pi^+\beta$ constitute a pair of *coupled spin configurations* which relate to the 0^+ or 0^- relativistic states.

Property 1. The number of spin configurations derived from a given nonrelativistic electronic configuration is equal to that of the relativistic states derived from the same electronic configuration.

To prove property 1, it may be observed that a spin configuration has one-to-one correspondence with an eigenfunction for the z component of the overall angular momentum, Ω, which is the sum of all of the individual angular-momentum projections. This well-known ω–ω coupling is expressed as

$$\Omega = \Sigma\omega_i, \tag{5}$$

where ω_i is the total angular momentum of the ith occupied electron, i.e.,

$$\omega_i = \lambda_{z_i} + s_{z_i}. \tag{6}$$

Note that Ω commutes with the total Hamiltonian including spin–orbit term (i.e., in the double group), or

$$[H, \Omega] = 0. \tag{7}$$

Thus, the set of spin configurations has one-to-one correspondence with the eigenfunctions of the Hamiltonian and the energy levels including spin–orbit splitting. Consequently, the total number of spin configurations is equal to the number of relativistic states.

Property 2. Nonrelativistically, a pair of coupled spin configurations has the same spatial symmetry if $\Lambda \neq 0$; for $\Lambda = 0$, the coupled spin configurations correspond to Σ^+, Σ^-, respectively.

Consider, for example, $\Lambda \neq 0$ case, namely, $\sigma\alpha \cdot \pi^{+}\alpha \cdot \pi'^{-}\beta$ (A) and $\sigma\alpha \cdot \pi^{+}\alpha \cdot \pi'^{-}\beta$ (B). They are both composed of the same type of complex molecular orbitals, thus leading to same overall spatial angular momentum

$$\Lambda = \Sigma\lambda_A = \Sigma\lambda_B. \tag{8}$$

For $\Lambda = 0$, according to the definition in diatomic molecular term symbols, a pair of wavefunctions with opposite orientation linearly constitutes Σ^+ or Σ^-. Usually, $A + B$ leads to Σ^+, while $A - B$ leads to Σ^-.

2.3. Generalized CGT method

The classification of the RCI wavefunctions can be simplified through the determination of the RCI configurations and characterized RCI configurations in terms of states. Thus, we have summarized some useful principles as follows:

1. Pauli's principle: electrons with the same ω and s cannot be in degenerate orbitals.

2. Relativistically, a pair of coupled spin configurations, namely, A and B, generates $A + B$ and $A - B$ linear combinations. We attribute 0^+ to $A + B$, while 0^- to $A - B$. Thus, the RCI wavefunction derived from a ${}^1\Sigma^+$ state is completely symmetric, and the sign for the RCI wavefunction of the ${}^1\Sigma^+$ state is identically positive. For nonrelativistic states with the same spatial symmetry, possible characterized RCI configurations corresponding to each state should be selected from the overall RCI configurations in terms of number, similarity, and degeneracy of the RCI wavefunctions.

3. If $\Omega + 2$ and Ω relativistic states contain the same type of RCI wavefunctions, but possess different signs, then these RCI wavefunctions build up different characterized RCI configurations, which belong to different nonrelativistic states. Basically, the nonrelativistic states are those with the same spin momentum, and differing in spatial momentum by 2.

4.1. The corresponding relationships between the characterized RCI configurations and nonrelativistic states are developed through the use of properties 1 and 2.

4.2. We stipulate that if an Ω state changes to $\Omega - 1$ by changing the spin orientation of an electron (from α to β) in the highest-occupied orbital, the characterized RCI configurations corresponding to the Ω and $\Omega - 1$ relativistic states, respectively, belong to the same nonrelativistic state.

5. All of the RCI wavefunctions corresponding to the characterized RCI configurations of a given relativistic state are to be fully considered with the exclusion of the "redundant" RCI wavefunctions.

6. The contributions of different nonrelativistic states to a given relativistic state depend on the MRSDCI energy values and spin–orbit coupling matrix elements.

2.4. Applications of the CGT method

The principles presented above could be applied to several complicated electronic configurations. We consider several such cases containing multiple open shells to illustrate the power of the CGT method and develop systematic tables for the classification of multiple open-shell wavefunctions that can be utilized in future computations and developments.

Example 1 ($\pi\pi'$ case). This electronic configuration is formed by placing two electrons in nonequivalent π molecular orbitals. According to the diatomic molecular term symbol rules [1,9] the $\pi\pi'$ electronic configuration generates nonrelativistic states including $^3\Delta_\mathrm{r}$ $(3, 2, 1)$, $^1\Delta$ (2), $^3\Sigma^+$ $(1, 0^-)$, $^1\Sigma^+$ (0^+), $^3\Sigma^-$ $(1, 0^+)$, $^1\Sigma^-$ (0^-), while those in parentheses are relativistic states corresponding to each nonrelativistic state. From property 1, the number of spin configurations should be $3 + 1 + 2 + 1 + 2 + 1 = 10$.

(1) For $\Omega = 3$, there is only one spin configuration, namely, $\pi^+\alpha \cdot \pi'^+\alpha$, which leads to a single characterized RCI configuration for the $^3\Delta_\mathrm{r}$ state.

(2) For $\Omega = 2$, there are two spin configurations, $\pi^+\alpha \cdot \pi'^+\beta$ and $\pi^+\beta \cdot \pi'^+\alpha$, thus generating a pair of coupled spin configurations. From definition 4 and property 2, the spatial symmetry for the two nonrelativistic states should be Δ, which is consistent with molecular term symbol rules. From principle 4, $\pi^+\alpha \cdot \pi'^+\beta$ and $\pi^+\beta \cdot \pi'^+\alpha$ correlate with $^3\Delta_\mathrm{r}$ and $^1\Delta$ states, respectively.

(3) For $\Omega = 1$, there are three spin configurations, $\pi^+\alpha \cdot \pi'^-\alpha$ (A), $\pi^-\alpha \cdot \pi'^+\alpha$ (B) and $\pi^+\beta \cdot \pi'^+\beta$ (C). From principle 2, A and B are more similar compared to C, suggesting that A and B should be chosen to form RCI configurations corresponding to the $^3\Sigma^-$ and $^3\Sigma^+$ states, while C is attributed to $^3\Delta_\mathrm{r}$. Specifically, $A + B$, or Re(A or B) provides the characterized RCI configuration for the $^3\Sigma^+$ state, while $A - B$, or Im(A or B) yields the $^3\Sigma^-$ state.

(4) For the $\Omega = 0^+$ or 0^- states, there are four spin configurations, $\pi^+\alpha \cdot \pi'^-\beta$ (A), $\pi^+\beta \cdot \pi'^-\alpha$ (B), $\pi^-\alpha \cdot \pi'^+\beta$ (C) and $\pi^-\beta \cdot \pi'^+\alpha$ (D), thus generating two pairs of coupled spin configurations, A and B, and C and D. From principle 2, Re($A + B$ or $C + D$) yields the characterized RCI configuration for the $^1\Sigma^+(0^+)$ state, while Re($A - B$ or $C - D$) is the characterized RCI configuration for $^3\Sigma^+(0^-)$. On the other hand, Im($A + B$ or $C + D$) yields the characterized RCI configuration for $^3\Sigma^-(0^+)$, and Im($A - B$ or $C - D$) provides the characterized RCI configuration for $^1\Sigma^-(0^-)$, respectively. All of the classifications derived above satisfy principle 3.

As a result, the CGT for the $\pi\pi'$ electronic configuration, shown in [1, table 5.15], has been generalized and shown in table 4. For the actual computations such as $\Omega = 0$ ($^+$ or $^-$), since A and B, and C and D are similar in the form of wavefunctions, thus, the redundant ones C and D are not necessary to be considered in construct-

Table 4
Correlation group table for the $\pi\pi'$ electronic configuration.

Ω	Spin configuration	Sign	RCI wavefunction π_x	π'_x	π_y	π'_y	Sign	RCI wavefunction π_x	π'_x	π_y	π'_y	λ–s
3	$\pi^+\alpha\pi'^+\alpha$	$+$	10	10			$-$			10	10	$^3\Delta_r$
		$+$i	10			10	$+$i		10	10		
2	$\pi^+\alpha\pi'^+\beta$	$+$	10	01			$-$			10	01	$^3\Delta_r$
		$+$i	10			01	$+$i		01	10		
	$\pi^+\beta\pi'^+\alpha$	$+$	01	10			$-$			01	10	$^1\Delta_r$
		$+$i	01			10	$+$i		10	01		
1	$\pi^+\alpha\pi'^-\alpha$ (A)	$+$	10	10			$+$			10	10	Re(A or B): $^3\Sigma^+$
		$+$i	10			10	$-$i		10	10		
	$\pi^-\alpha\pi'^+\alpha$ (B)	$+$	10	10			$+$			10	10	Im(A or B): $^3\Sigma^-$
		$-$i	10			10	$+$i		10	10		
	$\pi^+\beta\pi'^+\beta$	$+$	01	01			$-$			01	01	$^3\Delta_r$
		$+$i	01			01	$+$i		01		01	
0^+, 0^-	$\pi^+\alpha\pi'^-\beta$ (A)	$+$	10	01			$+$			10	01	Re($A+B$ or $C+D$)
		$-$i	10			01	$+$i		01	10		$^1\Sigma^+(0^+)$
	$\pi^+\beta\pi'^-\alpha$ (B)	$+$	01	10			$+$			01	10	Re($A-B$ or $C-D$)
		$-$i	01			10	$+$i		10	01		$^3\Sigma^+(0^-)$
	$\pi^-\alpha\pi'^+\beta$ (C)	$+$	10	01			$+$			10	01	Im($A+B$ or $C+D$)
		$+$i	10			01	$-$i		01	10		$^3\Sigma^-(0^+)$
	$\pi^-\beta\pi'^+\alpha$ (D)	$+$	01	10			$+$			01	10	Im($A-B$ or $C-D$)
		$+$i	01			10	$-$i		10	01		$^1\Sigma^-(0^-)$

ing reference configurations. The correlation between the nonrelativistic and relativistic states is then obtained according to the signs of the RCI wavefunctions listed in CGT.

Example 2 ($\sigma\pi^2\delta^2$). This electronic configuration results in electronic states with several spin multiplicities and, thus, a large array of electronic states. To determine the potential energy surfaces and the electronic structure for linear molecules containing very heavy atoms, such as Ta–CO, Re–CO, etc., these types of electronic configurations have to be considered since the ground states of these systems have very complex electronic states. Since the correlation of the $\sigma\pi^2\delta^2$ electronic configuration and the corresponding nonrelativistic states is not listed in Herzberg's equivalent and non-equivalent electronic configuration tables (see [9]), we, thus, obtain in table 5 the nonrelativistic states derived from the $\sigma\pi^2\delta^2$ electronic configuration by combining the term symbols.

The $\sigma\pi^2\delta^2$ electronic configuration can be envisaged as a direct product of $\sigma\pi^2$ and δ^2, i.e.,

$$\sigma\pi^2 \otimes \delta^2 \Rightarrow \sigma\pi^2\delta^2. \quad (9)$$

Table 5
The relativistic states and the nonrelativistic states derived from the $\sigma\pi^2\delta^2$ electronic configuration.

λ–s	$^2\Sigma^+(3)$	$^2\Sigma^-(2)$	$^2\Delta(3)$	$^4\Sigma^-(2)$	$^4\Sigma^+(2)$	$^4\Delta$	$^6\Sigma^+$	$^2\Gamma(2)$	$^4\Gamma$	^2I	Number of Ω
	$\frac{1}{2}(3)$	$\frac{1}{2}(2)$		$\frac{1}{2}(2)$	$\frac{1}{2}(2)$	$\frac{1}{2}$	$\frac{1}{2}$				11
			$\frac{3}{2}(3)$	$\frac{3}{2}(2)$	$\frac{3}{2}(2)$	$\frac{3}{2}$	$\frac{3}{2}$				9
			$\frac{5}{2}(3)$			$\frac{5}{2}$	$\frac{5}{2}$		$\frac{5}{2}$		6
ω–ω						$\frac{7}{2}$		$\frac{7}{2}(2)$	$\frac{7}{2}$		4
								$\frac{9}{2}(2)$	$\frac{9}{2}$		3
									$\frac{11}{2}$	$\frac{11}{2}$	2
										$\frac{13}{2}$	1

According to Herzberg's table [9], $\sigma\pi^2$ generates $^2\Sigma^+$, $^2\Sigma^-$, $^2\Delta$ and $^4\Sigma^-$ electronic states, and δ^2 generates $^1\Sigma^+$, $^3\Sigma^-$, $^1\Gamma$ states. Since

$$\begin{aligned} &^1\Sigma^+ \otimes \sigma\pi^2 \Rightarrow {}^2\Sigma^+, {}^2\Sigma^-, {}^2\Delta \text{ and } {}^4\Sigma^-, \\ &^3\Sigma^- \otimes \sigma\pi^2 \Rightarrow {}^2\Sigma^-, {}^4\Sigma^-, {}^2\Sigma^+, {}^4\Sigma^+, {}^2\Delta, {}^4\Delta, {}^2\Sigma^+, {}^4\Sigma^+ \text{ and } {}^6\Sigma^+, \\ &^1\Gamma \otimes \sigma\pi^2 \Rightarrow {}^2\Gamma, {}^2\Gamma, {}^2\Delta, {}^2I \text{ and } {}^4\Gamma, \end{aligned} \tag{10}$$

consequently, the relationship between the relativistic and nonrelativistic states derived from the $\sigma\pi^2\delta^2$ electronic configuration is easily determined, as seen from table 5.

Based on property 1 and table 5, the number of spin configurations corresponding to relativistic states from $\frac{1}{2}$ to $\frac{13}{2}$ are 11, 9, 6, 4, 3, 2, and 1, respectively. Suppose σ is the highest molecular orbital in energy, one obtains the assignment as follows:

(1) For $\Omega = \frac{13}{2}$, as can be seen from table 4, the spin configuration $\sigma\alpha\pi^+\alpha\pi^+\beta\,\delta^{2+}\alpha\delta^{2+}\beta$ is the only characterized RCI configuration for the ^2I state.

(2) For $\Omega = \frac{11}{2}$, there are two spin configurations, namely, $\sigma\beta\pi^+\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2+}\beta$ and $\sigma\alpha\pi^+\alpha\pi^-\alpha\delta^{2+}\alpha\delta^{2+}\beta$. From principle 4, the former is the only characterized RCI configuration for the ^2I state, while the latter characterizes $^4\Gamma$.

(3) For $\Omega = \frac{9}{2}$, there are three spin configurations, $\sigma\beta\pi^+\alpha\pi^-\alpha\delta^{2+}\alpha\delta^{2+}\beta$ (A), $\sigma\alpha\pi^+\alpha\pi^-\beta\delta^{2+}\alpha\delta^{2+}\beta$ (B), and $\sigma\alpha\pi^-\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2+}\beta$ (C). According to definition 4, A and B is a pair of coupled spin configurations, while B and C, and C and A are coupled spin configurations. In terms of similarity of the RCI wavefunctions, as stipulated from principle 2, the B and C configurations, which have the same form of RCI wavefunctions, are the characterized RCI configurations for $^2\Gamma$ and $^2\Gamma(\text{II})$, respectively. Thus, the A configuration is the characterized RCI configuration for the $^4\Gamma$ state. This assignment can be verified by the use of property 2, which stipulates that the spatial symmetries of the three nonrelativistic states are indeed the same as $\lambda = 4$. Moreover, the above assignment is in conformity with principles 3 and 4. For example, comparing $\sigma\alpha\pi^+\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2+}\beta$ of ^2I $(\Omega = \frac{13}{2})$ and $\sigma\alpha\pi^+\alpha\pi^-\beta\delta^{2+}\alpha\delta^{2+}\beta$ of $^2\Gamma$ $(\Omega = \frac{9}{2})$, one may deduce that the difference of spatial momenta between the two nonrelativistic states

is indeed 2, as in principle 3. Alternatively, one may obtain the same assignment from principles 3 and 4.

(4) For $\Omega = \frac{7}{2}$, the spin configurations include $\sigma\alpha\pi^{+}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2-}\alpha$ (A), $\sigma\beta\pi^{+}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2+}\beta$ (B), $\sigma\beta\pi^{-}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2+}\beta$ (C) and $\sigma\alpha\pi^{-}\beta\pi^{+}\beta\delta^{2+}\alpha\delta^{2+}\beta$ (D). From definition 4, B and C, C and D, and B and D are pairs of coupled spin configurations, while B and C constitute a degenerate pair. Thus, from principle 2, the B and C configurations are the characterized RCI configurations for $^2\Gamma$ and $^2\Gamma$(II), respectively, while D characterizes $^4\Gamma$. Finally, the A configuration belongs to the $^4\Delta$ state.

(5) The spin configurations for $\Omega = \frac{5}{2}$ include $\sigma\alpha\pi^{+}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2-}\beta$ (A), $\sigma\alpha\pi^{+}\alpha\pi^{+}\beta\delta^{2-}\alpha\delta^{2+}\beta$ (B), $\sigma\beta\pi^{+}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2-}\alpha$ (C), $\sigma\alpha\pi^{+}\alpha\pi^{-}\alpha\delta^{2+}\alpha\delta^{2-}\alpha$ (D), $\sigma\beta\pi^{+}\beta\pi^{-}\beta\delta^{2+}\alpha\delta^{2+}\beta$ (E), and $\sigma\alpha\pi^{-}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2+}\beta$ (F). From principle 4, C and E yield the $^4\Delta$ and $^4\Gamma$ states, respectively. Since A, B and F are more similar in the form of the RCI wavefunctions, they are attributed to the $^2\Delta$, $^2\Delta$(II) and $^2\Delta$(III) states, respectively, which are also consistent with principle 3. Finally, the D configuration is attributed to the $^6\Sigma^+$ state.

(6) The spin configurations for $\Omega = \frac{3}{2}$ include $\sigma\beta\pi^{+}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2-}\beta$ (A), $\sigma\beta\pi^{+}\alpha\pi^{+}\beta\delta^{2-}\alpha\delta^{2+}\beta$ (B), $\sigma\beta\pi^{-}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2+}\beta$ (C), $\sigma\alpha\pi^{+}\alpha\pi^{+}\beta\delta^{2+}\beta\delta^{2-}\beta$ (D), $\sigma\alpha\pi^{+}\alpha\pi^{-}\alpha\delta^{2-}\alpha\delta^{2+}\beta$ (E), $\sigma\alpha\pi^{+}\alpha\pi^{-}\alpha\delta^{2+}\alpha\delta^{2-}\beta$ (F), $\sigma\alpha\pi^{-}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2-}\alpha$ (G), $\sigma\alpha\pi^{+}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2-}\alpha$ (H), and $\sigma\beta\pi^{-}\alpha\pi^{+}\alpha\delta^{2+}\alpha\delta^{2-}\alpha$ (I). Since the spatial symmetry for A–D is the same as Δ, the A, B, C configurations are attributed to the $^2\Delta$, $^2\Delta$(II) and $^2\Delta$(III) states, respectively, while D is attributed to the $^4\Delta$ state. The E and F, and G and H configurations are coupled spin configurations, and the RCI wave functions derived from E and F, and G and H are similar in form, respectively. Thus, we attribute Re(E or F) and Re(G or H) to $^4\Sigma^+$ and $^4\Sigma^+$(II), respectively, while Im(E or F) and Im(G or H) to $^4\Sigma^-$ and $^4\Sigma^-$(II), respectively. Finally, the configuration I belongs to the $^6\Sigma^+$ state.

(7) The spin configurations for $\Omega = \frac{1}{2}$ include $\sigma\alpha\pi^{+}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2-}\beta$ (A), $\sigma\beta\pi^{-}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2-}\beta$ (B), $\sigma\alpha\pi^{+}\alpha\pi^{-}\beta\delta^{2-}\alpha\delta^{2+}\beta$ (C), $\sigma\alpha\pi^{-}\alpha\pi^{+}\beta\delta^{2-}\alpha\delta^{2+}\beta$ (D), $\sigma\alpha\pi^{+}\alpha\pi^{-}\alpha\delta^{2+}\alpha\delta^{2-}\beta$ (E), $\sigma\beta\pi^{+}\alpha\pi^{-}\alpha\delta^{2-}\alpha\delta^{2+}\beta$ (F), $\sigma\beta\pi^{+}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2-}\alpha$ (G), $\sigma\beta\pi^{-}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2-}\alpha$ (H), $\sigma\alpha\pi^{+}\alpha\pi^{-}\alpha\delta^{2+}\beta\delta^{2-}\beta$ (I), $\sigma\alpha\pi^{+}\beta\pi^{-}\beta\delta^{2+}\alpha\delta^{2-}\alpha$ (J), and $\sigma\beta\pi^{+}\alpha\pi^{+}\beta\delta^{2+}\beta\delta^{2-}\beta$ (K). In accordance with principles 2–4, we attribute Re(A or D) and Re(B or C) to $^2\Sigma^+$ and $^2\Sigma^+$(II), Im(A or D) and Im(B or C) to $^2\Sigma^-$ and $^2\Sigma^-$(II), Re(E or F) and Re(G or H) to $^4\Sigma^+$ and $^4\Sigma^+$(II), and Im(E or F) and Im(G or H) to $^4\Sigma^-$ and $^4\Sigma^-$(II), respectively. On the basis of principles 3 or 4, K is the characterized RCI configuration for the $^4\Delta$ state. On the other hand, it is difficult to contrast J and I by using principles 2–4 alone, and thus, principle 6 will have to be invoked. Suppose that the Ith spin configuration is a preferable characterized RCI configuration for the $^6\Sigma^+$ state, and J is the one for the $^2\Sigma^+$(III) state. In this case, principle 6 is useful for the assignment of the RCI wavefunctions in the actual computations, since the $^6\Sigma^+$ and $^2\Sigma^+$ states have different MRSDCI relative energies. Consequently, the CGT for the $\sigma\pi^2\delta^2$ electronic configuration is summarized in table 6.

2.5. *Examples of calculations and results*

A series of intriguing systems in catalytic research comprises heavy transition metals interacting with CO that usually possess high spin states from complex electronic configurations as the low-lying states. As some of the spectroscopic results pertinent to Ta–CO, Re–CO and W–CO have been published elsewhere [10–12], we describe here only salient details as to how the generalized CGT method can be utilized for such complex molecular systems.

The nonrelativistic spectroscopic properties for Ta interaction with CO have been reported previously [1]. Due to the fact that a $\sigma\pi^2\delta^2$ electronic configuration appears to dominate the $^6\Sigma^+$ first excited state at the MRSDCI level, the generalized CGT method could be used to include spin–orbit coupling. Table 7 shows the RCI reference configurations for the Ta–CO system including spin–orbit coupling. Consider the $\Omega = \frac{1}{2}$ relativistic state as an example. As can be seen from tables 6 and 7, the characterized RCI configurations A–D are exactly the same in the RCI wavefunctions, thus, only one characterized RCI configuration such as A needs to be selected. Note that A contains 16 reference configurations. Similarly, the E, G, I, J, K configurations are also selected subsequent to A, all of which donate 30 RCI wavefunctions. For the second root of RCI, the RCI wavefunctions

$$\sigma, \pi_x, \pi_y, \delta_{x^2-y^2}, \delta_{xy}\colon +10, 10, 10, 01, 01,$$
$$\sigma, \pi_x, \pi_y, \delta_{x^2-y^2}, \delta_{xy}\colon +10, 01, 01, 10, 10$$

Table 6
RCI reference configurations for Ta–CO system including spin–orbit coupling.

Electronic configuration						λ–s state	ω–ω state			
1σ	2σ	3σ	1π	2π	1δ		1/2	3/2	5/2	...
2	2	1	4	2	2	$^6\Sigma^+$	30	29	25	...
2	2	2	4	2	1	$^4\Delta$	10	10	10	...
2	2	2	4	3	0	$^2\Pi$	2	2		...
2	2	1	4	3	1	$^4\Pi$	16	16	16	...
Number of RCI reference configurations							58	57	51	...
Number of CSFs							13697	13452	12237	...

Table 7
Correlation group table for the $\sigma\pi^2\delta^2$ electronic configuration. $\delta 1 = \delta_{x^2-y^2}$, $\delta 2 = \delta_{xy}$.

Ω	Spin configuration	Sign	RCI wavefunction					Sign	RCI wavefunction					λ–s
			σ	π_x	π_y	$\delta 1$	$\delta 2$		σ	π_x	π_y	$\delta 1$	$\delta 2$	
$\frac{13}{2}$	$\sigma\alpha\pi^+\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2-}\beta$	+	10	11		11		+i	10	10	01	11		^2I
		−	10		11	11		+i	10	01	10	11		
		−	10	11			11	−i	10	10	01		11	
		+	10		11		11	−i	10	01	10		11	

Table 7
(Continued.)

Ω	Spin configuration	Sign	RCI wavefunction					Sign	RCI wavefunction					λ–s
			σ	π_x	π_y	$\delta 1$	$\delta 2$		σ	π_x	π_y	$\delta 1$	$\delta 2$	
		−	10	10	01	10	01	+i	10	11		10	01	
		−	10	01	10	10	01	−i	10	11		10	01	
		−	10	10	01	01	10	+i	10		11	01	10	
		−	10	01	10	01	10	−i	10		11	01	10	
$\frac{11}{2}$	$\sigma\beta\pi^+\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	01	11		11		+i	01	10	01	11		^2I
		−	01		11	11		+i	01	01	10	11		
		−	01	11			11	−i	01	10	01		11	
		+	01		11		11	−i	01	01	10		11	
		−	01	10	01	10	01	+i	01	11		10	01	
		−	01	01	10	10	01	−i	01	11		10	01	
		−	01	10	01	01	10	+i	01		11	01	10	
		−	01	01	10	01	10	−i	01		11	01	10	
	$\sigma\alpha\pi^+\alpha\pi^-\alpha\delta^{2+}\alpha\delta^{2+}\beta$	+i	10	10	10	11		−	10	10	10	10	01	$^4\Gamma$
		−i	10	10	10		11	−	10	10	10	01	10	
$\frac{9}{2}$	$\sigma\beta\pi^+\alpha\pi^-\alpha\delta^{2+}\alpha\delta^{2+}\beta$	+i	01	10	10	11		−	01	10	10	10	01	$^4\Gamma$
		−i	01	10	10		11	−	01	10	10	01	10	
	$\sigma\alpha\pi^+\alpha\pi^-\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	10	11		11		−i	10	10	01	11		$^2\Gamma$
		+	10		11	11		+i	10	01	10	11		
		−	10	11			11	+i	10	10	01		11	
		−	10		11		11	−i	10	01	10		11	
		+	10	10	01	10	01	+i	10	11		10	01	
		−	10	01	10	10	01	+i	10	11		10	01	
		+	10	10	01	01	10	+i	10		11	01	10	
		−	10	01	10	01	10	+i	10		11	01	10	
	$\sigma\alpha\pi^-\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	10	11		11		+i	10	10	01	11		$^2\Gamma$(II)
		+	10		11	11		−i	10	01	10	11		
		−	10	11			11	−i	10	10	01		11	
		−	10		11		11	+i	10	01	10		11	
		−	10	10	01	10	01	+i	10	11		10	01	
		+	10	01	10	10	01	+i	10	11		10	01	
		−	10	10	01	01	10	+i	10		11	01	10	
		+	10	01	10	01	10	+i	10		11	01	10	
$\frac{7}{2}$	$\sigma\alpha\pi^+\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2-}\alpha$	+i	10	11		10	10	−	10	10	01	10	10	$^4\Delta$
		−i	10		11	10	10	−	10	01	10	10	10	
	$\sigma\beta\pi^+\alpha\pi^-\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	01	11		11		−i	01	10	01	11		$^2\Gamma$
		+	01		11	11		+i	01	01	10	11		
	$\sigma\beta\pi^-\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2+}\beta$	−	01	11			11	+i	01	10	01		11	$^2\Gamma$(II)
		−	01		11		11	−i	01	01	10		11	
		+	01	10	01	10	01	+i	01	11		10	01	
		−	01	01	10	10	01	+i	01	11		10	01	

Table 7
(Continued.)

Ω	Spin configuration	Sign	RCI wavefunction					Sign	RCI wavefunction					λ–s
			σ	π_x	π_y	$\delta 1$	$\delta 2$		σ	π_x	π_y	$\delta 1$	$\delta 2$	
		+	01	10	01	01	10	+i	01		11	01	10	
		−	01	01	10	01	10	+i	01		11	01	10	
		+	01	11		11		+i	01	10	01	11		
		+	01		11	11		−i	01	01	10	11		
		−	01	11			11	−i	01	10	01		11	
		−	01		11		11	+i	01	01	10		11	
		−	01	10	01	10	01	+i	01	11		10	01	
		+	01	01	10	10	01	+i	01	11		10	01	
		−	01	10	01	01	10	+i	01		11	01	10	
		+	01	01	10	01	10	+i	01		11	01	10	
	$\sigma\alpha\pi^{+}\beta\pi^{-}\beta\delta^{2+}\alpha\delta^{2+}\beta$	+i	10	01	01	11		−	10	01	01	10	01	$^{4}\Gamma$
		−i	10	01	01		11	−	10	01	01	01	10	
$\frac{5}{2}$	$\sigma\alpha\pi^{+}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	10	11		11		+i	10	10	01	11		$^{2}\Delta$
		−	10		11	11		+i	10	01	10	11		
		+	10	11			11	+i	10	10	01		11	
		−	10		11		11	+i	10	01	10		11	
		+	10	10	01	10	01	−i	10	11		10	01	
		+	10	01	10	10	01	+i	10	11		10	01	
		−	10	10	01	01	10	+i	10		11	01	10	
		−	10	01	10	01	10	−i	10		11	01	10	
	$\sigma\alpha\pi^{+}\alpha\pi^{+}\beta\delta^{2-}\alpha\delta^{2+}\beta$	+	10	11		11		+i	10	10	01	11		$^{2}\Delta$(II)
		−	10		11	11		+i	10	01	10	11		
		+	10	11			11	+i	10	10	01		11	
		−	10		11		11	+i	10	01	10		11	
		−	10	10	01	10	01	+i	10	11		10	01	
		−	10	01	10	10	01	−i	10	11		10	01	
		+	10	10	01	01	10	−i	10		11	01	10	
		+	10	01	10	01	10	+i	10		11	01	10	
	$\sigma\alpha\pi^{-}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	10	11		11		−i	10	10	01	11		$^{2}\Delta$(III)
		−	10		11	11		−i	10	01	10	11		
		−	10	11			11	+i	10	10	01		11	
		+	10		11		11	+i	10	01	10		11	
		+	10	10	01	10	01	+i	10	11		10	01	
		+	10	01	10	10	01	−i	10	11		10	01	
		+	10	10	01	01	10	+i	10		11	01	10	
		+	10	01	10	01	10	−i	10		11	01	10	
	$\sigma\beta\pi^{+}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2-}\alpha$	+i	01	11		10	10	−	01	10	01	10	10	$^{4}\Delta$
		−i	01		11	10	10	−	01	01	10	10	10	
	$\sigma\beta\pi^{+}\beta\pi^{-}\beta\delta^{2+}\alpha\delta^{2+}\beta$	+i	01	01	01	11		−	01	01	01	10	01	$^{4}\Gamma$
		−i	01	01	01		11	−	01	01	01	01	10	
	$\sigma\alpha\pi^{+}\alpha\pi^{-}\alpha\delta^{2+}\alpha\delta^{2+}\alpha$	+	10	10	10	10	10							$^{6}\Sigma^{+}$

Table 7
(Continued.)

Ω	Spin configuration	Sign	RCI wavefunction σ	π_x	π_y	$\delta 1$	$\delta 2$	Sign	RCI wavefunction σ	π_x	π_y	$\delta 1$	$\delta 2$	λ–s
$\frac{3}{2}$	$\sigma\beta\pi^{+}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2-}\beta$	+	01	11		11		+i	01	10	01	11		$^{2}\Delta$
		−	01		11	11		+i	01	01	10	11		
		+	01	11			11	+i	01	10	01		11	
		−	01		11		11	+i	01	01	10		11	
		+	01	10	01	10	01	−i	01	11		10	01	
		+	01	01	10	10	01	+i	01	11		10	01	
		−	01	10	01	01	10	+i	01		11	01	10	
		−	01	01	10	01	10	−i	01		11	01	10	
	$\sigma\beta\pi^{+}\alpha\pi^{+}\beta\delta^{2-}\alpha\delta^{2+}\beta$	+	01	11		11		+i	01	10	01	11		$^{2}\Delta$(II)
		−	01		11	11		+i	01	01	10	11		
		+	01	11			11	+i	01	10	01		11	
		−	01		11		11	+i	01	01	10		11	
		−	01	10	01	10	01	+i	01	11		10	01	
		−	01	01	10	10	01	−i	01	11		10	01	
		+	01	10	01	01	10	−i	01		11	01	10	
		+	01	01	10	01	10	+i	01		11	01	10	
	$\sigma\beta\pi^{-}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	01	11		11		−i	01	10	01	11		$^{2}\Delta$(III)
		−	01		11	11		−i	01	01	10	11		
		−	01	11			11	+i	01	10	01		11	
		+	01		11		11	+i	01	01	10		11	
		+	01	10	01	10	01	+i	01	11		10	01	
		+	01	01	10	10	01	−i	01	11		10	01	
		+	01	10	01	01	10	+i	01		11	01	10	
		+	01	01	10	01	10	−i	01		11	01	10	
	$\sigma\alpha\pi^{+}\alpha\pi^{+}\beta\delta^{2+}\beta\delta^{2-}\beta$	+i	10	11		01	01	−	10	10	01	01	01	$^{4}\Delta$
		−i	10		11	01	01	−	10	01	10	01	01	
	$\sigma\alpha\pi^{+}\alpha\pi^{-}\alpha\delta^{2+}\alpha\delta^{2-}\beta$ (A)	+i	10	10	10	11		+	10	10	10	10	01	Re(A or B): $^{4}\Sigma^{+}$
		+i	10	10	10		11	−	10	10	10	01	10	
	$\sigma\alpha\pi^{+}\alpha\pi^{-}\alpha\delta^{2-}\alpha\delta^{2+}\beta$ (B)	+i	10	10	10	11		−	10	10	10	10	01	Im(A or B): $^{4}\Sigma^{-}$
		+i	10	10	10		11	+i	10	10	10	01	10	
	$\sigma\alpha\pi^{+}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2-}\alpha$ (C)	+i	10	11		10	10	+	10	10	01	10	10	Re(C or D): $^{4}\Sigma^{+}$(II)
		+i	10		11	10	10	−	10	01	10	10	10	
	$\sigma\alpha\pi^{-}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2-}\alpha$ (D)	+i	10	11		10	10	−	10	10	01	10	10	Im(C or D): $^{4}\Sigma^{-}$(II)
		+i	10		11	10	10	+	10	01	10	10	10	
	$\sigma\beta\pi^{+}\alpha\pi^{-}\alpha\delta^{2+}\alpha\delta^{2-}\alpha$	+	01	10	10	10	10							$^{6}\Sigma^{+}$
$\frac{1}{2}$	$\sigma\alpha\pi^{+}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2-}\beta$ (A)	+	10	11		11		−i	10	10	01	11		Re(A or D): $^{2}\Sigma^{+}$
		+	10		11	11		+i	10	01	10	11		
		+	10	11			11	−i	10	10	01		11	

Table 7
(Continued.)

Ω	Spin configuration	Sign	RCI wavefunction					Sign	RCI wavefunction					λ–s
			σ	π_x	π_y	$\delta 1$	$\delta 2$		σ	π_x	π_y	$\delta 1$	$\delta 2$	
		+	10		11		11	+i	10	01	10		11	
		−	10	10	01	10	01	−i	10	11		10	01	
		+	10	01	10	10	01	−i	10	11		10	01	
		+	10	10	01	01	10	+i	10		11	01	10	
		−	10	01	10	01	10	+i	10		11	01	10	
	$\sigma\alpha\pi^-\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2-}\beta$ (B)	+	10	11		11		+i	10	10	01	11		Im(A or D): $^2\Sigma^-$
		+	10		11	11		−i	10	01	10	11		
		+	10	11			11	+i	10	10	01		11	
		+	10		11		11	−i	10	01	10		11	
		+	10	10	01	10	01	−i	10	11		10	01	
		−	10	01	10	10	01	−i	10	11		10	01	
		−	10	10	01	01	10	+i	10		11	01	10	
		+	10	01	10	01	10	+i	10		11	01	10	
	$\sigma\alpha\pi^+\alpha\pi^-\beta\delta^{2-}\alpha\delta^{2+}\beta$ (C)	+	10	11		11		−i	10	10	01	11		Re(B or C): $^2\Sigma^+$(II)
		+	10		11	11		+i	10	01	10	11		
		+	10	11			11	−i	10	10	01		11	
		+	10		11		11	+i	10	01	10		11	
		+	10	10	01	10	01	+i	10	11		10	01	
		−	10	01	10	10	01	+i	10	11		10	01	
		−	10	10	01	01	10	−i	10		11	01	10	
		+	10	01	10	01	10	−i	10		11	01	10	
	$\sigma\alpha\pi^-\alpha\pi^+\beta\delta^{2-}\alpha\delta^{2+}\beta$ (D)	+	10	11		11		+i	10	10	01	11		Im(B or C): $^2\Sigma^-$(II)
		+	10		11	11		−i	10	01	10	11		
		+	10	11			11	+i	10	10	01		11	
		+	10		11		11	−i	10	01	10		11	
		−	10	10	01	10	01	+i	10	11		10	01	
		+	10	01	10	10	01	+i	10	11		10	01	
		+	10	10	01	01	10	−i	10		11	01	10	
		−	10	01	10	01	10	−i	10		11	01	10	
	$\sigma\beta\pi^+\alpha\pi^-\beta\delta^{2+}\alpha\delta^{2-}\beta$ (E)	+i	01	10	10	11		+	01	10	10	10	01	Re(E or F): $^4\Sigma^+$
		+i	01	10	10		11	−	01	10	10	01	10	
	$\sigma\beta\pi^+\alpha\pi^-\alpha\delta^{2-}\alpha\delta^{2+}\beta$ (F)	+i	01	10	10	11		−	01	10	10	10	01	Im(E or F): $^4\Sigma^-$
		+i	01	10	10		11	+	01	10	10	01	10	
	$\sigma\beta\pi^+\alpha\pi^-\beta\delta^{2+}\alpha\delta^{2-}\alpha$ (G)	+i	01	11		10	10	+	01	10	01	10	10	Re(G or H): $^4\Sigma^+$(II)
		+i	01		11	10	10	−	01	01	10	10	10	
	$\sigma\beta\pi^-\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2-}\alpha$ (H)	+i	01	11		10	10	−	01	10	01	10	10	Im(G or H): $^4\Sigma^-$(II)
		+i	01		11	10	10	+	01	01	10	10	10	
	$\sigma\alpha\pi^+\alpha\pi^-\alpha\delta^{2+}\beta\delta^{2-}\beta$ (I)	+	10	10	10	01	01							$^6\Sigma^+$ (preferable)
	$\sigma\alpha\pi^+\beta\pi^-\beta\delta^{2+}\alpha\delta^{2-}\alpha$ (J)	+	10	01	01	10	10							$^2\Sigma^+$(III)
	$\sigma\beta\pi^+\alpha\pi^+\beta\delta^{2+}\beta\delta^{2-}\beta$ (K)	+i	01	11		01	01	−	01	10	01	01	01	$^4\Delta$
		−	01		11	01	01	−	01	01	10	01	01	

were found to make significant contributions, with a total weight factor of 94%. Note that the $^2\Sigma^+$ state is too high in energy to be considered at the MRSDCI level [11], the $\Omega = \frac{1}{2}$(II) relativistic state is, thus, attributed to the $^6\Sigma^+$ state by using table 6. The $^4\Delta$ state, which yields $\Omega = \frac{1}{2}$, was found as the ground state of the Ta–CO molecule.

Example 3 (W–CO). The ground state of W–CO was found to be a $^7\Sigma^+$ state at the MRSDCI level, which originates from the $\sigma\sigma'\pi^2\delta^2$ electronic configuration [10]. By using the generalized CGT method, it is seen that

$$\sigma\pi^2\delta^2 \otimes \sigma' \Rightarrow \sigma\sigma'\pi^2\delta^2, \tag{11}$$

where σ' is the highest occupied molecular orbital mainly composed of $C(2p_z)$ and $O(2p_z)$. The CGT constructed for this case is shown as table 8.

Table 9 shows the RCI reference configurations for the W–CO system including spin–orbit coupling. Consider $\Omega = 0$ as an example; as can be seen from tables 8 and 9, since the characterized RCI configurations B–D, F–H, M–N, and Q–R are redundant, the remaining A, E, I–J, K–L, O–P, S–V donate 60 RCI reference configurations. Additionally, the I and J configurations can also be neglected, since they contribute to the energetically higher 0^+ or 0^- states derived from the $^5\Delta$ state. We have included those configurations corresponding to the Ith characterized RCI configuration in order to test if they are important [10]. Thus, the total number of RCI reference configurations for the 0^- state is 56.

According to the computational results, the 0^- state is dominated by those configurations derived from the Sth through Vth characterized RCI configurations, suggesting that this relativistic state is dominated by the $^7\Sigma^+$ ground state, with a weight factor of over 96%. The contributions of I and J configurations are negligible, as the weight factor is less than 10^{-5}.

3. Conclusions

In this investigation we have considered a generalized CGT method for the relativistic configuration interaction wavefunctions of the spin–orbit electronic states with high spin multiplicities. This was accomplished through a formulation of some definitions and a few properties of the RCI states and wavefunctions. Secondly, we formulated six principles to seek relationships among relativistic states, nonrelativistic states, as well as RCI configurations. As a matter of fact, these principles are not necessarily limited to linear systems, as properties 1 and 2 are applicable for nonlinear systems of polyatomic double groups. Finally, we exemplified the techniques with several computational models and summarized the results with several CGT tables for systems containing many open shells for future applications.

Table 8
Correlation group table for $\sigma\sigma'\pi^2\delta^2$ electronic configuration.

Ω	Spin configuration	Sign	RCI wavefunction σ	σ'	π_x	π_y	$\delta 1$	$\delta 2$	Sign	RCI wavefunction σ	σ'	π_x	π_y	$\delta 1$	$\delta 2$	λ–s
7	$\sigma\alpha\sigma'\alpha\pi^{+}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	10	10	11		11		+i	10	10	10	01	11		^3I
		−	10	10		11	11		+i	10	10	01	10	11		
		−	10	10	11			11	−i	10	10	10	01		11	
		+	10	10		11		11	−i	10	10	01	10		11	
		−	10	10	10	01	10	01	+i	10	10	11		10	01	
		−	10	10	01	10	10	01	−i	10	10	11		10	01	
		−	10	10	10	01	01	10	+i	10	10		11	01	10	
		−	10	10	01	10	01	10	−i	10	10		11	01	10	
6	$\sigma\alpha\sigma'\beta\pi^{+}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	10	01	11		11		+i	10	01	10	01	11		^3I
		−	10	01		11	11		+i	10	01	01	10	11		
		−	10	01	11			11	−i	10	01	10	01		11	
		+	10	01		11		11	−i	10	01	01	10		11	
		−	10	01	10	01	10	01	+i	10	01	11		10	01	
		−	10	01	01	10	10	01	−i	10	01	11		10	01	
		−	10	01	10	01	01	10	+i	10	01		11	01	10	
		−	10	01	01	10	01	10	−i	10	01		11	01	10	
	$\sigma\beta\sigma'\alpha\pi^{+}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	01	10	11		11		+i	01	10	10	01	11		^1I
		−	01	10		11	11		+i	01	10	01	10	11		
		−	01	10	11			11	−i	01	10	10	01		11	
		+	01	10		11		11	−i	01	10	01	10		11	
		−	01	10	10	01	10	01	+i	01	10	11		10	01	
		−	01	10	01	10	10	01	−i	01	10	11		10	01	
		−	01	10	10	01	01	10	+i	01	10		11	01	10	
		−	01	10	01	10	01	10	−i	01	10		11	01	10	
	$\sigma\alpha\sigma'\alpha\pi^{+}\alpha\pi^{-}\alpha\delta^{2+}\alpha\delta^{2+}\beta$	+i	10	10	10	10	11		−	10	10	10	10	10	01	$^5\Gamma$
		−i	10	10	10	10		11	−	10	10	10	10	01	10	
5	$\sigma\beta\sigma'\beta\pi^{+}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	01	01	11		11		+i	01	01	10	01	11		^3I
		−	01	01		11	11		+i	01	01	01	10	11		
		−	01	01	11			11	−i	01	01	10	01		11	
		+	01	01		11		11	−i	01	01	01	10		11	
		−	01	01	10	01	10	01	+i	01	01	11		10	01	
		−	01	01	01	10	10	01	−i	01	01	11		10	01	
		−	01	01	10	01	01	10	+i	01	01		11	01	10	
		−	01	01	01	10	01	10	−i	01	01		11	01	10	
	$\sigma\beta\sigma'\alpha\pi^{+}\alpha\pi^{-}\alpha\delta^{2+}\alpha\delta^{2+}\beta$	+i	01	10	10	10	11		−	01	10	10	10	10	01	$^5\Gamma$
		−i	01	10	10	10		11	−	01	10	10	10	01	10	
	$\sigma\alpha\sigma'\beta\pi^{+}\alpha\pi^{-}\alpha\delta^{2+}\alpha\delta^{2+}\beta$	+i	10	01	10	10	11		−	10	01	10	10	10	01	$^3\Gamma$
		−i	10	01	10	10		11	−	10	01	10	10	01	10	
	$\sigma\alpha\sigma'\alpha\pi^{+}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	10	10	11		11		−i	10	10	10	01	11		$^3\Gamma$(II)
		+	10	10		11	11		+i	10	10	01	10	11		
		−	10	10	11			11	+i	10	10	10	01		11	
		−	10	10		11		11	−i	10	10	01	10		11	

Table 8
(Continued.)

Ω	Spin configuration	Sign	RCI wavefunction σ	σ'	π_x	π_y	$\delta 1$	$\delta 2$	Sign	RCI wavefunction σ	σ'	π_x	π_y	$\delta 1$	$\delta 2$	λ–s
		+	10	10	10	01	10	01	+i	10	10	11		10	01	
		−	10	10	01	10	10	01	+i	10	10	11		10	01	
		+	10	10	10	01	01	10	+i	10	10		11	01	10	
		−	10	10	01	10	01	10	+i	10	10		11	01	10	
	$\sigma\alpha\sigma'\alpha\pi^-\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	10	10	11		11		+i	10	10	10	01	11		$^3\Gamma$(III)
		+	10	10		11	11		−i	10	10	01	10	11		
		−	10	10	11			11	−i	10	10	10	01		11	
		−	10	10		11		11	+i	10	10	01	10		11	
		−	10	10	10	01	10	01	+i	10	10	11		10	01	
		+	10	10	01	10	10	01	+i	10	10	11		10	01	
		−	10	10	10	01	01	10	+i	10	10		11	01	10	
		+	10	10	01	10	01	10	+i	10	10		11	01	10	
4	$\sigma\beta\sigma'\beta\pi^+\alpha\pi^-\alpha\delta^{2+}\alpha\delta^{2+}\beta$	+i	01	01	10	10	11		−	01	01	10	10	10	01	$^5\Gamma$
		−i	01	01	10	10		11	−	01	01	10	10	01	10	
	$\sigma\alpha\sigma'\alpha\pi^+\beta\pi^-\beta\delta^{2+}\alpha\delta^{2+}\beta$	+i	10	10	01	01	11		−	10	10	01	01	10	01	$^3\Gamma$
		−i	10	10	01	01		11	−	10	10	01	01	01	10	
	$\sigma\alpha\sigma'\beta\pi^+\alpha\pi^-\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	10	01	11		11		−i	10	01	10	01	11		$^3\Gamma$(II)
		+	10	01		11	11		+i	10	01	01	10	11		
		−	10	01	11			11	+i	10	01	10	01		11	
		−	10	01		11		11	−i	10	01	01	10		11	
		+	10	01	10	01	10	01	+i	10	01	11		10	01	
		−	10	01	01	10	10	01	+i	10	01	11		10	01	
		+	10	01	10	01	01	10	+i	10	01		11	01	10	
		−	10	01	01	10	01	10	+i	10	01		11	01	10	
	$\sigma\alpha\sigma'\beta\pi^-\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	10	01	11		11		+i	10	01	10	01	11		$^3\Gamma$(III)
		+	10	01		11	11		−i	10	01	01	10	11		
		−	10	01	11			11	−i	10	01	10	01		11	
		−	10	01		11		11	+i	10	01	01	10		11	
		−	10	01	10	01	10	01	+i	10	01	11		10	01	
		+	10	01	01	10	10	01	+i	10	01	11		10	01	
		−	10	01	10	01	01	10	+i	10	01		11	01	10	
		+	10	01	01	10	01	10	+i	10	01		11	01	10	
	$\sigma\beta\sigma'\alpha\pi^+\alpha\pi^-\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	01	10	11		11		−i	01	10	10	01	11		$^1\Gamma$
		+	01	10		11	11		+i	01	10	01	10	11		
		−	01	10	11			11	+i	01	10	10	01		11	
		−	01	10		11		11	−i	01	10	01	10		11	
		+	01	10	10	01	10	01	+i	01	10	11		10	01	
		−	01	10	01	10	10	01	+i	01	10	11		10	01	
		+	01	10	10	01	01	10	+i	01	10		11	01	10	
		−	01	10	01	10	01	10	+i	01	10		11	01	10	
	$\sigma\beta\sigma'\alpha\pi^-\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	01	10	11		11		+i	01	10	10	01	11		$^1\Gamma$(II)
		+	01	10		11	11		−i	01	10	01	10	11		

Table 8
(Continued.)

Ω	Spin configuration	Sign	RCI wavefunction						Sign	RCI wavefunction						λ–s
			σ	σ'	π_x	π_y	$\delta 1$	$\delta 2$		σ	σ'	π_x	π_y	$\delta 1$	$\delta 2$	
		−	01	10	11			11	−i	01	10	10	01		11	
		−	01	10		11		11	+i	01	10	01	10		11	
		−	01	10	10	01	10	01	+i	01	10	11		10	01	
		+	01	10	01	10	10	01	+i	01	10	11		10	01	
		−	01	10	10	01	01	10	+i	01	10		11	01	10	
		+	01	10	01	10	01	10	+i	01	10		11	01	10	
	$\sigma\alpha\sigma'\alpha\pi^+\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2+}\alpha$	+i	10	10	11		10	10	−	10	10	10	01	10	10	$^5\Delta$
		−	10	10		11	10	10	−	10	10	01	10	10	10	
3	$\sigma\beta\sigma'\alpha\pi^+\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2-}\alpha$	+i	01	10	11		10	10	−	01	10	10	01	10	10	$^3\Delta$
		−i	01	10		11	10	10	−	01	10	01	10	10	10	
	$\sigma\alpha\sigma'\beta\pi^+\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2-}\alpha$	+i	10	01	11		10	10	−	10	01	10	01	10	10	$^5\Delta$
		−i	10	01		11	10	10	−	10	01	01	10	10	10	
	$\sigma\beta\sigma'\alpha\pi^+\beta\pi^-\beta\delta^{2+}\alpha\delta^{2+}\beta$	+i	01	10	01	01	11		−	01	10	01	01	10	01	$^3\Gamma$
		−	01	10	01	01		11	−	01	10	01	01	01	10	
	$\sigma\alpha\sigma'\beta\pi^+\beta\pi^-\beta\delta^{2+}\alpha\delta^{2+}\beta$	+i	10	01	01	01	11		−	10	01	01	01	10	01	$^5\Gamma$
		−i	10	01	01	01		11	−	10	01	01	01	01	10	
	$\sigma\beta\sigma'\beta\pi^+\alpha\pi^-\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	01	01	11		11		−i	01	01	10	01	11		$^3\Gamma$(II)
		+	01	01		11	11		+i	01	01	01	10	11		
		−	01	01	11			11	+i	01	01	10	01		11	
		−	01	01		11		11	−i	01	01	01	10		11	
		+	01	01	10	01	10	01	+i	01	01	11		10	01	
		−	01	01	01	10	10	01	+i	01	01	11		10	01	
		+	01	01	10	01	01	10	+i	01	01		11	01	10	
		−	01	01	01	10	01	10	+i	01	01		11	01	10	
	$\sigma\beta\sigma'\beta\pi^-\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	01	01	11		11		+i	01	01	10	01	11		$^3\Gamma$(III)
		+	01	01		11	11		−i	01	01	01	10	11		
		−	01	01	11			11	−i	01	01	10	01		11	
		−	01	01		11		11	+i	01	01	01	10		11	
		−	01	01	10	01	10	01	+i	01	01	11		10	01	
		+	01	01	01	10	10	01	+i	01	01	11		10	01	
		−	01	01	10	01	01	10	+i	01	01		11	01	10	
		+	01	01	01	10	01	10	+i	01	01		11	01	10	
	$\sigma\alpha\sigma'\alpha\pi^+\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	10	10	11		11		+i	10	10	10	01	11		$^3\Delta$(II)
		−	10	10		11	11		+i	10	10	01	10	11		
		+	10	10	11			11	+i	10	10	10	01		11	
		−	10	10		11		11	+i	10	10	01	10		11	
		+	10	10	10	01	10	01	−i	10	10	11		10	01	
		+	10	10	01	10	10	01	+i	10	10	11		10	01	
		−	10	10	10	01	01	10	+i	10	10		11	01	10	
		−	10	10	01	10	01	10	−i	10	10		11	01	10	

Table 8
(Continued.)

Ω	Spin configuration	Sign	RCI wavefunction σ	σ'	π_x	π_y	$\delta 1$	$\delta 2$	Sign	RCI wavefunction σ	σ'	π_x	π_y	$\delta 1$	$\delta 2$	λ–s
	$\sigma\alpha\sigma'\alpha\pi^{+}\alpha\pi^{+}\beta\delta^{2-}\alpha\delta^{2+}\beta$	+	10	10	11		11		+i	10	10	10	01	11		$^{3}\Delta$(III)
		−	10	10		11	11		+i	10	10	01	10	11		
		+	10	10	11			11	+i	10	10	10	01		11	
		−	10	10		11		11	+i	10	10	01	10		11	
		−	10	10	10	01	10	01	+i	10	10	11		10	01	
		−	10	10	01	10	10	01	−i	10	10	11		10	01	
		+	10	10	10	01	01	10	−i	10	10		11	01	10	
		+	10	10	01	10	01	10	+i	10	10		11	01	10	
	$\sigma\alpha\sigma'\alpha\pi^{-}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	10	10	11		11		−i	10	10	10	01	11		$^{3}\Delta$(IV)
		−	10	10		11	11		−i	10	10	01	10	11		
		−	10	10	11			11	+i	10	10	10	01		11	
		+	10	10		11		11	+i	10	10	01	10		11	
		+	10	10	10	01	10	01	+i	10	10	11		10	01	
		+	10	10	01	10	10	01	−i	10	10	11		10	01	
		+	10	10	10	01	01	10	+i	10	10		11	01	10	
		+	10	10	01	10	01	10	−i	10	10		11	01	10	
	$\sigma\alpha\sigma'\alpha\pi^{+}\alpha\pi^{-}\alpha\delta^{2+}\alpha\delta^{2-}\alpha$	+	10	10	10	10	10	10								$^{7}\Sigma^{+}$
2	$\sigma\beta\sigma'\alpha\pi^{+}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2-}\beta$	+	01	10	11		11		+i	01	10	10	01	11		$^{1}\Delta$
		−	01	10		11	11		+i	01	10	01	10	11		
		+	01	10	11			11	+i	01	10	10	01		11	
		−	01	10		11		11	+i	01	10	01	10		11	
		+	01	10	10	01	10	01	−i	01	10	11		10	01	
		+	01	10	01	10	10	01	+i	01	10	11		10	01	
		−	01	10	10	01	01	10	+i	01	10		11	01	10	
		−	01	10	01	10	01	10	−i	01	10		11	01	10	
	$\sigma\beta\sigma'\alpha\pi^{+}\alpha\pi^{+}\beta\delta^{2-}\alpha\delta^{2+}\beta$	+	01	10	11		11		+i	01	10	10	01	11		$^{1}\Delta$(II)
		−	01	10		11	11		+i	01	10	01	10	11		
		+	01	10	11			11	+i	01	10	10	01		11	
		−	01	10		11		11	+i	01	10	01	10		11	
		−	01	10	10	01	10	01	+i	01	10	11		10	01	
		−	01	10	01	10	10	01	−i	01	10	11		10	01	
		+	01	10	10	01	01	10	−i	01	10		11	01	10	
		+	01	10	01	10	01	10	+i	01	10		11	01	10	
	$\sigma\beta\sigma'\alpha\pi^{-}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	01	10	11		11		−i	01	10	10	01	11		$^{1}\Delta$(III)
		−	01	10		11	11		−i	01	10	01	10	11		
		−	01	10	11			11	+i	01	10	10	01		11	
		+	01	10		11		11	+i	01	10	01	10		11	
		+	01	10	10	01	10	01	+i	01	10	11		10	01	
		+	01	10	01	10	10	01	−i	01	10	11		10	01	
		+	01	10	10	01	01	10	+i	01	10		11	10	01	
		+	01	10	01	10	01	10	−i	01	10		11	01	10	
	$\sigma\alpha\sigma'\beta\pi^{+}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	10	01	11		11		+i	10	01	10	01	11		$^{3}\Delta$(II)
		−	10	01		11	11		+i	10	01	01	10	11		

Table 8
(Continued.)

Ω	Spin configuration	Sign	RCI wavefunction σ	σ'	π_x	π_y	$\delta 1$	$\delta 2$	Sign	RCI wavefunction σ	σ'	π_x	π_y	$\delta 1$	$\delta 2$	λ–*s*
		+	10	01	11			11	+i	10	01	10	01		11	
		−	10	01		11		11	+i	10	01	01	10		11	
		+	10	01	10	01	10	01	−i	10	01	11		10	01	
		+	10	01	01	10	10	01	+i	10	01	11		10	01	
		−	10	01	10	01	01	10	+i	10	01		11	01	10	
		−	10	01	01	10	01	10	−i	10	01		11	01	10	
	$\sigma\alpha\sigma'\beta\pi^+\alpha\pi^+\beta\delta^{2-}\alpha\delta^{2+}\beta$	+	10	01	11		11		+i	10	01	10	01	11		$^3\Delta$(III)
		−	10	01		11	11		+i	10	01	01	10	11		
		+	10	01	11			11	+i	10	01	10	01		11	
		−	10	01		11		11	+i	10	01	01	10		11	
		−	10	01	10	01	10	01	+i	10	01	11		10	01	
		−	10	01	01	10	10	01	−i	10	01	11		10	01	
		+	10	01	10	01	01	10	−i	10	01		11	01	10	
		+	10	01	01	10	01	10	+i	10	01		11	01	10	
	$\sigma\alpha\sigma'\beta\pi^-\alpha\pi^-\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	10	01	11		11		−i	10	01	10	01	11		$^3\Delta$(IV)
		−	10	01		11	11		−i	10	01	01	10	11		
		−	10	01	11			11	+i	10	01	10	01		11	
		+	10	01		11		11	+i	10	01	01	10		11	
		+	10	01	10	01	10	01	+i	10	01	11		10	01	
		+	10	01	01	10	10	01	−i	10	01	11		10	01	
		+	10	01	10	01	01	10	+i	10	01		11	01	10	
		+	10	01	01	10	01	10	−i	10	01		11	01	10	
	$\sigma\beta\sigma'\beta\pi^+\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2-}\alpha$	+i	01	01	11		10	10	−	01	01	10	01	10	10	$^5\Delta$
		−i	01	01		11	10	10	−	01	01	01	10	10	10	
	$\sigma\alpha\sigma'\alpha\pi^+\alpha\pi^+\beta\delta^{2+}\beta\delta^{2-}\beta$	+i	10	10	11		01	01	−	10	10	10	01	01	01	$^3\Delta$
		−i	10	10		11	01	01	−	10	10	01	10	01	01	
	$\sigma\alpha\sigma'\beta\pi^+\alpha\pi^-\alpha\delta^{2+}\alpha\delta^{2-}\alpha$	+	10	01	10	10	10	10								$^7\Sigma^+$
	$\sigma\beta\sigma'\alpha\pi^+\alpha\pi^-\alpha\delta^{2+}\alpha\delta^{2-}\alpha$	+	01	10	10	10	10	10								$^5\Sigma^+$
	$\sigma\beta\sigma'\beta\pi^+\beta\pi^-\beta\delta^{2+}\alpha\delta^{2+}\beta$	+i	01	01	01	01	11		−	01	01	01	01	10	01	$^5\Gamma$
		−i	01	01	01	01		11	−	01	01	01	01	01	10	
	$\sigma\alpha\sigma'\alpha\pi^+\alpha\pi^-\alpha\delta^{2+}\alpha\delta^{2-}\beta$	+i	10	10	10	10	11		+	10	10	10	10	10	01	Re(*A* or *B*):
	(*A*)	+i	10	10	10	10		11	−	10	10	10	10	01	10	$^5\Sigma^+$(II)
	$\sigma\alpha\sigma'\alpha\pi^+\alpha\pi^-\alpha\delta^{2-}\alpha\delta^{2+}\beta$	+i	10	10	10	10	11		−	10	10	10	10	10	01	Im(*A* or *B*):
	(*B*)	+i	10	10	10	10		11	+	10	10	10	10	01	10	$^5\Sigma^-$
	$\sigma\alpha\sigma'\alpha\pi^+\alpha\pi^-\beta\delta^{2+}\alpha\delta^{2-}\alpha$	+i	10	10	11		10	10	+	10	10	10	01	10	10	Re(*C* or *D*):
	(*C*)	+i	10	10		11	10	10	−	10	10	01	10	10	10	$^5\Sigma^+$(III)
	$\sigma\alpha\sigma'\alpha\pi^+\alpha\pi^-\beta\delta^{2-}\alpha\delta^{2+}\alpha$	+i	10	10	11		10	10	−	10	10	10	01	10	10	Im(*C* or *D*):
	(*D*)	+i	10	10		11	10	10	+	10	10	01	10	10	10	$^5\Sigma^-$(II)

Table 8
(Continued.)

			RCI wavefunction							RCI wavefunction						
Ω	Spin configuration	Sign	σ	σ'	π_x	π_y	$\delta1$	$\delta2$	Sign	σ	σ'	π_x	π_y	$\delta1$	$\delta2$	λ–s
1	$\sigma\beta\sigma'\beta\pi^+\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2-}\beta$	+	01	01	11		11		+i	01	01	10	01	11		$^3\Delta$(II)
		−	01	01		11	11		+i	01	01	01	10	11		
		+	01	01	11			11	+i	01	01	10	01		11	
		−	01	01		11		11	+i	01	01	01	10		11	
		+	01	01	10	01	10	01	−i	01	01	11		10	01	
		+	01	01	01	10	10	01	+i	01	01	11		10	01	
		−	01	01	10	01	01	10	+i	01	01		11	01	10	
		−	01	01	01	10	01	10	−i	01	01		11	01	10	
	$\sigma\beta\sigma'\beta\pi^+\alpha\pi^+\beta\delta^{2-}\alpha\delta^{2+}\beta$	+	01	01	11		11		+i	01	01	10	01	11		$^3\Delta$(III)
		−	01	01		11	11		+i	01	01	01	10	11		
		+	01	01	11			11	+i	01	01	10	01		11	
		−	01	01		11		11	+i	01	01	01	10		11	
		−	01	01	10	01	10	01	+i	01	01	11		10	01	
		−	01	01	01	10	10	01	−i	01	01	11		10	01	
		+	01	01	10	01	01	10	−i	01	01		11	01	10	
		+	01	01	01	10	01	10	+i	01	01		11	01	10	
	$\sigma\beta\sigma'\beta\pi^-\alpha\pi^-\beta\delta^{2+}\alpha\delta^{2+}\beta$	+	01	01	11		11		−i	01	01	10	01	11		$^3\Delta$(IV)
		−	01	01		11	11		−i	01	01	01	10	11		
		−	01	01	11			11	+i	01	01	10	01		11	
		+	01	01		11		11	+i	01	01	01	10		11	
		+	01	01	10	01	10	01	+i	01	01	11		10	01	
		+	01	01	01	10	10	01	−i	01	01	11		10	01	
		+	01	01	10	01	01	10	+i	01	01		11	01	10	
		+	01	01	01	10	01	10	−i	01	01		11	01	10	
	$\sigma\beta\sigma'\alpha\pi^+\alpha\pi^+\beta\delta^{2+}\beta\delta^{2-}\beta$	+	01	10	11		01	01	−	01	10	10	01	01	01	$^3\Delta$ (suggested)
		−i	01	10		11	01	01	−	01	10	01	10	01	01	
	$\sigma\alpha\sigma'\beta\pi^+\alpha\pi^+\beta\delta^{2+}\beta\delta^{2-}\beta$	+i	10	10	11		01	01	−	10	10	10	01	01	01	$^5\Delta$ (suggested)
		−i	10	10		11	01	01	−	10	10	01	10	01	01	
	$\sigma\beta\sigma'\beta\pi^+\alpha\pi^-\alpha\delta^{2+}\alpha\delta^{2-}\alpha$	+	01	01	10	10	10	10								$^7\Sigma^+$
	$\sigma\alpha\sigma'\alpha\pi^+\alpha\pi^-\alpha\delta^{2+}\beta\delta^{2-}\beta$	+	10	10	10	10	01	01								$^5\Sigma^+$
	$\sigma\alpha\sigma'\alpha\pi^+\beta\pi^-\beta\delta^{2+}\alpha\delta^{2-}\alpha$	+	10	10	01	01	10	10								$^3\Sigma^+$
	$\sigma\alpha\sigma'\beta\pi^+\alpha\pi^-\alpha\delta^{2+}\alpha\delta^{2-}\beta$	+i	10	01	10	10	11		+	10	01	10	10	10	01	Re(A or B):
	(A)	+i	10	01	10	10		11	−	10	01	10	10	01	10	$^5\Sigma^+$(II)
	$\sigma\alpha\sigma'\beta\pi^+\alpha\pi^-\alpha\delta^{2-}\alpha\delta^{2+}\beta$	+i	10	01	10	10	11		−	10	01	10	10	10	01	Im(A or B):
	(B)	+i	10	01	10	10		11	+	10	10	10	10	01	10	$^5\Sigma^-$
	$\sigma\alpha\sigma'\beta\pi^+\alpha\pi^-\beta\delta^{2+}\alpha\delta^{2-}\alpha$	+i	10	01	11		10	10	+	10	01	10	01	10	10	Re(C or D):
	(C)	+i	10	01		11	10	10	−	10	01	01	10	10	10	$^5\Sigma^+$(III)
	$\sigma\alpha\sigma'\beta\pi^+\alpha\pi^-\beta\delta^{2-}\alpha\delta^{2+}\alpha$	+i	10	01	11		10	10	−	10	01	10	01	10	10	Im(C or D):
	(D)	+i	10	01		11	10	10	+	10	01	01	10	10	10	$^5\Sigma^-$(II)

Table 8
(Continued.)

Ω	Spin configuration	Sign	RCI wavefunction σ	σ'	π_x	π_y	$\delta 1$	$\delta 2$	Sign	RCI wavefunction σ	σ'	π_x	π_y	$\delta 1$	$\delta 2$	λ–s
	$\sigma\beta\sigma'\alpha\pi^{+}\alpha\pi^{-}\alpha\delta^{2+}\alpha\delta^{2-}\beta$	+i	01	10	10	10	11		+	01	10	10	10	10	01	Re(E or F):
	(E)	+i	01	10	10	10		11	−	01	10	10	10	01	10	$^3\Sigma^+$(II)
	$\sigma\beta\sigma'\alpha\pi^{+}\alpha\pi^{-}\alpha\delta^{2-}\alpha\delta^{2+}\beta$	+i	01	10	10	10	11		−	01	10	10	10	10	01	Im(E or F):
	(F)	+i	01	10	10	10		11	+	01	10	10	10	01	10	$^3\Sigma^-$
	$\sigma\beta\sigma'\alpha\pi^{+}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2-}\alpha$	+i	01	10	11		10	10	+	01	10	10	01	10	10	Re(G or H):
	(G)	+i	01	10		11	10	10	−	01	10	01	10	10	10	$^3\Sigma^+$(III)
	$\sigma\beta\sigma'\alpha\pi^{+}\alpha\pi^{-}\beta\delta^{2-}\alpha\delta^{2+}\alpha$	+i	01	10	11		10	10	−	01	10	10	01	10	10	Im(G or H):
	(H)	+i	01	10		11	10	10	+	01	10	01	10	10	10	$^3\Sigma^-$(II)
	$\sigma\alpha\sigma'\alpha\pi^{+}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2-}\beta$	+	10	10	11		11		−i	10	10	10	01	11		Re(I or L):
	(I)	+	10	10		11	11		+i	10	10	01	10	11		$^3\Sigma^+$(IV)
		+	10	10	11			11	−i	10	10	10	01		11	
		+	10	10		11		11	+i	10	10	01	10		11	
		−	10	10	10	01	10	01	−i	10	10	11		10	01	
		+	10	10	01	10	10	01	−i	10	10	11		10	01	
		+	10	10	10	01	01	10	+i	10	10		11	01	10	
		−	10	10	01	10	01	10	+i	10	10		11	01	10	
	$\sigma\alpha\sigma'\alpha\pi^{-}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2-}\beta$	+	10	10	11		11		+i	10	10	10	01	11		Im(I or L):
	(J)	+	10	10		11	11		−i	10	10	01	10	11		$^3\Sigma^-$(III)
		+	10	10	11			11	+i	10	10	10	01		11	
		+	10	10		11		11	−i	10	10	01	10		11	
		+	10	10	10	01	10	01	−i	10	10	11		10	01	
		−	10	10	01	10	10	01	−i	10	10	11		10	01	
		−	10	10	10	01	01	10	+i	10	10		11	01	10	
		+	10	10	01	10	01	10	+i	10	10		11	01	10	
	$\sigma\alpha\sigma'\alpha\pi^{+}\alpha\pi^{-}\beta\delta^{2-}\alpha\delta^{2+}\beta$	+	10	10	11		11		−i	10	10	10	01	11		Re(J or K):
	(K)	+	10	10		11	11		+i	10	10	01	10	11		$^3\Sigma^+$(V)
		+	10	10	11			11	−i	10	10	10	01		11	
		+	10	10		11		11	+i	10	10	01	10		11	
		+	10	10	10	01	10	01	+i	10	10	11		10	01	
		−	10	10	01	10	10	01	+i	10	10	11		10	01	
		−	10	10	10	01	01	10	−i	10	10		11	01	10	
		+	10	10	01	10	01	10	−i	10	10		11	01	10	
	$\sigma\alpha\sigma'\alpha\pi^{-}\alpha\pi^{+}\beta\delta^{2-}\alpha\delta^{2+}\beta$	+	10	10	11		11		+i	10	10	10	01	11		Im(J or K):
	(L)	+	10	10		11	11		−i	10	10	01	10	11		$^3\Sigma^-$(IV)
		+	10	10	11			11	+i	10	10	10	01		11	
		+	10	10		11		11	−i	10	10	01	10		11	
		−	10	10	10	01	10	01	+i	10	10	11		10	01	
		+	10	10	01	10	10	01	+i	10	10	11		10	01	
		+	10	10	10	01	01	10	−i	10	10		11	01	10	
		−	10	10	01	10	01	10	−i	10	10		11	01	10	

Table 8
(Continued.)

Ω	Spin configuration	Sign	RCI wavefunction						Sign	RCI wavefunction						λ–s
			σ	σ'	π_x	π_y	$\delta 1$	$\delta 2$		σ	σ'	π_x	π_y	$\delta 1$	$\delta 2$	
$0^+, 0^-$	$\sigma\alpha\sigma'\beta\pi^+\alpha\pi^-\beta\delta^{2+}\alpha\delta^{2-}\beta$	+	10	01	11		11		−i	10	01	10	01	11		Re($A+E$
	(A)	+	10	01		11	11		+i	10	01	01	10	11		or $D+H$): $^5\Sigma^+(0^+)$
		+	10	01	11			11	−i	10	01	10	01		11	
		+	10	01		11		11	+i	10	01	01	10		11	
		−	10	01	10	01	10	01	−i	10	01	11		10	01	
		+	10	01	01	10	10	01	−i	10	01	11		10	01	
		+	10	01	10	01	01	10	+i	10	01		11	01	10	
		−	10	01	01	10	01	10	+i	10	01		11	01	10	
	$\sigma\alpha\sigma'\beta\pi^-\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2-}\beta$	+	10	01	11		11		+i	10	01	10	01	11		Im($A+E$ or $D+H$):
	(B)	+	10	01		11	11		−i	10	01	01	10	11		$^3\Sigma^-(0^+)$
		+	10	01	11			11	+i	10	01	10	01		11	
		+	10	01		11		11	−i	10	01	01	10		11	
		+	10	01	10	01	10	01	−i	10	01	11		10	01	
		−	10	01	01	10	10	01	−i	10	01	11		10	01	
		−	10	01	10	01	01	10	+i	10	01		11	01	10	
		+	10	01	01	10	01	10	+i	10	01		11	01	10	
	$\sigma\alpha\sigma'\beta\pi^+\alpha\pi^-\beta\delta^{2-}\alpha\delta^{2+}\beta$	+	10	01	11		11		−i	10	01	10	01	11		Re($A-E$ or $D-H$):
	(C)	+	10	01		11	11		+i	10	01	01	10	11		$^3\Sigma^+(0^-)$
		+	10	01	11			11	−i	10	01	10	01		11	
		+	10	01		11		11	+i	10	01	01	10		11	
		+	10	01	10	01	10	01	+i	10	01	11		10	01	
		−	10	01	01	10	10	01	+i	10	01	11		10	01	
		−	10	01	10	01	01	10	−i	10	01		11	01	10	
		+	10	01	01	10	01	10	−i	10	01		11	01	10	
	$\sigma\alpha\sigma'\beta\pi^-\alpha\pi^+\beta\delta^{2-}\alpha\delta^{2+}\beta$	+	10	01	11		11		+i	10	01	10	01	11		Im($A-E$ or $D-H$):
	(D)	+	10	01		11	11		−i	10	01	01	10	11		$^5\Sigma^-(0^-)$
		+	10	01	11			11	+i	10	01	10	01		11	
		+	10	01		11		11	−i	10	01	01	10		11	
		−	10	01	10	01	10	01	+i	10	01	11		10	01	
		+	10	01	01	10	10	01	+i	10	01	11		10	01	
		+	10	01	10	01	01	10	−i	10	01		11	01	10	
		−	10	01	01	10	01	10	−i	10	01		11	01	10	
	$\sigma\beta\sigma'\alpha\pi^+\alpha\pi^-\beta\delta^{2+}\alpha\delta^{2-}\beta$	+	01	10	11		11		−i	01	10	10	01	11		Re($B+F$ or $C+G$):
	(E)	+	01	10		11	11		+i	01	10	01	10	11		$^5\Sigma^+(0^+)$(II)
		+	01	10	11			11	−i	01	10	10	01		11	
		+	01	10		11		11	+i	01	10	01	10		11	
		−	01	10	10	01	10	01	−i	01	10	11		10	01	
		+	01	10	01	10	10	01	−i	01	10	11		10	01	
		+	01	10	10	01	01	10	+i	01	10		11	01	10	
		−	01	10	01	10	01	10	+i	01	10		11	01	10	
	$\sigma\beta\sigma'\alpha\pi^-\alpha\pi^+\beta\delta^{2+}\alpha\delta^{2-}\beta$	+	01	10	11		11		+i	01	10	10	01	11		Im($B+F$ or $C+G$):
	(F)	+	01	10		11	11		−i	01	10	01	10	11		$^3\Sigma^-(0^+)$(II)

Table 8
(Continued.)

Ω	Spin configuration	Sign	RCI wavefunction						Sign	RCI wavefunction						λ–s
			σ	σ'	π_x	π_y	$\delta 1$	$\delta 2$		σ	σ'	π_x	π_y	$\delta 1$	$\delta 2$	
		+	01	10	11			11	+i	01	10	10	01		11	
		+	01	10		11		11	−i	01	10	01	10		11	
		+	01	10	10	01	10	01	−i	01	10	11		10	01	
		−	01	10	01	10	10	01	−i	01	10	11		10	01	
		−	01	10	10	01	01	10	+i	01	10		11	01	10	
		+	01	10	01	10	01	10	+i	01	10		11	01	10	
	$\sigma\beta\sigma'\alpha\pi^{+}\alpha\pi^{-}\beta\delta^{2-}\alpha\delta^{2+}\beta$	+	01	10	11		11		−i	01	10	10	01	11		Re($B-F$ or $C-G$):
	(G)	+	01	10		11	11		+i	01	10	01	10	11		$^{3}\Sigma^{+}(0^{-})$(II)
		+	01	10	11			11	−i	01	10	10	01		11	
		+	01	10		11		11	+i	01	10	01	10		11	
		+	01	10	10	01	10	01	+i	01	10	11		10	01	
		−	01	10	01	10	10	01	+i	01	10	11		10	01	
		−	01	10	10	01	01	10	−i	01	10		11	01	10	
		+	01	10	01	10	01	10	−i	01	10		11	01	10	
	$\sigma\beta\sigma'\alpha\pi^{-}\alpha\pi^{+}\beta\delta^{2-}\alpha\delta^{2+}\beta$	+	01	10	11		11		+i	01	10	10	01	11		Im($B-F$ or $C-G$):
	(H)	+	01	10		11	11		−i	01	10	01	10	11		$^{5}\Sigma^{-}(0^{-})$(II)
		+	01	10	11			11	+i	01	10	10	01		11	
		+	01	10		11		11	−i	01	10	01	10		11	
		−	01	10	10	01	10	01	+i	01	10	11		10	01	
		+	01	10	01	10	10	01	+i	01	10	11		10	01	
		+	01	10	10	01	01	10	−i	01	10		11	01	10	
		−	01	10	01	10	01	10	−i	01	10		11	01	10	
	$\sigma\beta\sigma'\beta\pi^{+}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2-}\beta$	+i	01	01	11		01	01	−	01	01	10	01	01	01	$I+J$: $^{5}\Delta(0^{+})$
	(I)	−i	01	01		11	01	01	−	01	01	01	10	01	01	
	$\sigma\alpha\sigma'\alpha\pi^{-}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2-}\alpha$	+i	10	10	11		10	10	+	10	10	10	01	10	10	$I-J$: $^{5}\Delta(0^{-})$
	(J)	−i	10	10		11	10	10	+	10	10	01	10	10	10	
	$\sigma\beta\sigma'\beta\pi^{+}\alpha\pi^{-}\beta\delta^{2+}\alpha\delta^{2-}\alpha$	+i	01	01	11		10	10	+	01	01	10	01	10	10	Re($K+L$ or $M+N$):
	(K)	+i	01	01		11	10	10	−	01	01	01	10	10	10	$^{1}\Sigma^{+}(0^{+})$
	$\sigma\alpha\sigma'\alpha\pi^{+}\alpha\pi^{-}\beta\delta^{2+}\beta\delta^{2-}\beta$	+i	10	10	11		01	01	+	10	10	10	01	01	01	Re($K-L$ or $M-N$):
	(L)	+i	10	10		11	01	01	−	10	10	01	10	01	01	$^{3}\Sigma^{+}(0^{-})$(III)
	$\sigma\beta\sigma'\beta\pi^{-}\alpha\pi^{+}\beta\delta^{2+}\alpha\delta^{2-}\alpha$	+i	01	01	11		10	10	−	01	01	10	01	10	10	Im($K+L$ or $M+N$):
	(M)	+i	01	01		11	10	10	+	01	01	01	10	10	10	$^{3}\Sigma^{-}(0^{+})$(III)
	$\sigma\alpha\sigma'\alpha\pi^{-}\alpha\pi^{+}\beta\delta^{2+}\beta\delta^{2-}\beta$	+i	10	10	11		01	01	−	10	10	10	01	01	01	Im($K-L$ or $M-N$):
	(N)	+i	10	10		11	01	01	+	10	10	01	10	01	01	$^{1}\Sigma^{-}(0^{-})$
	$\sigma\beta\sigma'\beta\pi^{+}\alpha\pi^{-}\alpha\delta^{2+}\alpha\delta^{2-}\beta$	+i	01	01	10	10	11		+	01	01	10	10	10	01	Re($O+P$ or $Q+R$):
	(O)	+i	01	01	10	10		11	−	01	01	10	10	01	10	$^{1}\Sigma^{+}(0^{+})$(II)
	$\sigma\alpha\sigma'\alpha\pi^{+}\beta\pi^{-}\beta\delta^{2+}\alpha\delta^{2-}\beta$	+i	10	10	01	01	11		+	10	10	01	01	10	01	Re($O-P$ or $Q-R$):
	(P)	+i	10	10	01	01		11	−	10	10	01	01	01	10	$^{3}\Sigma^{+}(0^{-})$(IV)

Table 8
(Continued.)

Ω	Spin configuration	Sign	RCI wavefunction σ σ' π_x π_y $\delta 1$ $\delta 2$	Sign	RCI wavefunction σ σ' π_x π_y $\delta 1$ $\delta 2$	λ–s
	$\sigma\beta\sigma'\beta\pi^{+}\alpha\pi^{-}\alpha\delta^{2-}\alpha\delta^{2+}\beta$	+i	01 01 10 10 11	–	01 01 10 10 10 01	Im($O+P$ or $Q+R$):
	(Q)	+i	01 01 10 10 11	+	01 01 10 10 01 10	$^{3}\Sigma^{-}(0^{+})$(IV)
	$\sigma\alpha\sigma'\alpha\pi^{+}\beta\pi^{-}\beta\delta^{2-}\alpha\delta^{2+}\beta$	+i	10 10 01 01 11	–	10 10 01 01 10 01	Im($O-P$ or $Q-R$):
	(R)	+i	10 10 01 01 11	+	10 10 01 01 01 10	$^{3}\Sigma^{-}(0^{-})$(II)
	$\sigma\beta\sigma'\alpha\pi^{+}\alpha\pi^{-}\alpha\delta^{2+}\beta\delta^{2-}\beta$ (S)	+	01 10 10 10 01 01		Suggested	$S+U+T+V$: $^{1}\Sigma^{+}(0^{+})$(III)
	$\sigma\beta\sigma'\alpha\pi^{+}\beta\pi^{-}\beta\delta^{2+}\alpha\delta^{2-}\alpha$ (T)	+	01 10 01 01 10 10			$(S-U)+(T-V)$: $^{3}\Sigma^{+}(0^{-})$(V)
	$\sigma\alpha\sigma'\beta\pi^{+}\alpha\pi^{-}\alpha\delta^{2+}\beta\delta^{2-}\beta$ (U)	+	10 01 10 10 01 01			$(S+U)-(T+V)$: $^{5}\Sigma^{+}(0^{+})$(III)
	$\sigma\alpha\sigma'\beta\pi^{+}\beta\pi^{-}\beta\delta^{2+}\alpha\delta^{2-}\alpha$ (V)	+	10 01 01 01 10 10			$(S-U)-(T-V)$: $^{7}\Sigma^{+}(0^{-})$

Table 9
RCI reference configurations for W–CO system including spin–orbit coupling.

Electronic configuration					λ–s state	ω–ω state				
1σ	2σ	3σ	1π	1δ		0^{+}	0^{-}	1	2	...
2	1	1	2	2	$^{7}\Sigma^{+}$		56	35	54	...
2	1	1	3	1	$^{5}\Phi$			32	32	...
2	2	0	2	2	$^{5}\Sigma^{+}$	18		12	17	...
2	2	0	3	1	$^{3}\Pi$	8	8	8	8	...
2	1	0	4	1	$^{3}\Delta$			2	4	...
2	2	0	4	0	$^{1}\Sigma^{+}$	1				...
2	0	0	4	2		4				...
Number of RCI reference configurations						31	64	89	115	...
Number of CSFs						5077	8560	9848	12762	...

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