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Calcolo completo delle matrici di energia per la configurazione d^4 a sim m etria D_{4h}

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Chimica. — *Calcolo completo delle matrici di energia per la configurazione d^4 a simmetria* D_{4h} (*). Nota di FRANCA MORAZZONI, FRANCO CARIATI e VENANZIO VALENTI, presentata (**) dal Corrisp. L. MALATESTA.

SUMMARY. — The aim of the present paper is to extend the point bond model to metal complexes with d^4 electronic configuration. The energy matrices have been calculated according to the strong field model also taking into account the interelectronic repulsion and *spin*–orbit coupling perturbations.

L'interesse allo studio delle proprietà elettroniche e magnetiche del complesso $[Re(DPE)_2X_2]X$, *trans*, con X = Cl, Br e DPE = difenilfosfinoetano [1] ci ha condotto al calcolo delle matrici di energia secondo il formalismo del campo forte in simmetria D_{4h}.

Si può infatti ammettere che questi composti presentino legami Me—X ed DPE diretti ai vertici di un ottaedro, ma differenti per la diversa forza dei leganti X e DPE.

Nel calcolo che rende le matrici diagonali rispetto all'operatore di campo si è tenuto conto anche delle perturbazioni minori di repulsione interelettronica e di accoppiamento *spin* orbita; le energie di repulsione interelettronica sono state calcolate utilizzando le Tabelle A 26 di Griffith [2], mentre per il calcolo delle energie di interazione *spin* orbita ci siamo serviti degli operatori riportati in letteratura [3].

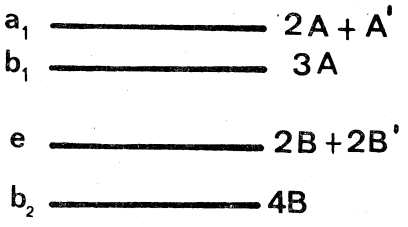

Fig. 1. – Termini di campo monoelettronici.

I termini diagonali di campo, espressi in funzione dei parametri A, B per l'alogeno, A', B' per il legante, secondo l'approssimazione del point bond model [4], possono essere dedotti per tutte le 23 configurazioni dalla fig. 1, nella quale sono riportati i termini di campo monoelettronici.

Nelle Tabelle I, II, III, IV e V riportiamo le matrici dei termini di repulsione elettrostatica interelettronica e di accoppiamento *spin*–orbita, espresse per comodità in unità ζ (costante di accoppiamento *spin*–orbita).

Il controllo dei termini è stato effettuato riproducendo, per la simmetria ottaedrica, gli autovalori calcolati da Schroeder [5].

(*) Lavoro eseguito con il contributo del C.N.R. nell'Istituto di Chimica generale dell'Università di Milano.

(**) Nella seduta del 14 novembre 1970.

TABELLA I. – *Elementi di matrice di interazione elettrostatica ed interazione* spin-*orbita. Rappresentazione* B_1.

	e^3b_2	$e^2b_2^2$	$e^2b_2a_1$			e^3a_1	e^3b_1	$eb_2^2a_1$	$eb_2^2b_1$	$e^2b_2b_1$			$e^2a_1^2$	$e^2b_1^2$	$eb_2a_1^2$	$eb_2b_1^2$	$b_2^2a_1b_1$	$e^2a_1b_1$			$eb_2a_1b_1$				$eb_1^2a_1$	$ea_1^2b_1$	$b_2b_1^2a_1$
	^3E	$^1B_1$	$^5B_1$	$^1B_1$	$^3B_2$	^3E	^3E	^3E	^3E	$^5A_1$	$^1B_1$	$^3B_2$	$^1B_1$	$^1B_1$	^3E	^3E	$^1B_1$	$^1B_1$	$^3B_2$	$^3B_2$	^3E	^3E	^3E	^5E	^3E	^3E	$^3B_2$
	$-15B+5C+\frac{1}{2}$	$-\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	$-\frac{1}{2}$	$-\frac{\sqrt{3}}{2}$	$-2\sqrt{3}B$	-1	$-\sqrt{3}B$	$3B$	$-\frac{1}{\sqrt{2}}$	$\frac{1}{2}$	$-\frac{1}{2}$	0	0	$-B-C$	$-3B-C$	0	0	0	0	$-\sqrt{6}B$	0	0	0	0	0	0
		$-9B+7C$	0	$3\sqrt{2}B$	0	0	0	$-\sqrt{\frac{3}{2}}$	$\frac{1}{\sqrt{2}}$	0	$-3\sqrt{2}B$	$-\sqrt{2}$	$4B+C$	C	0	0	$2\sqrt{3}B$	0	0	0	0	0	0	0	0	0	0
			$-21B$	0	$-\frac{2}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	0	$\frac{1}{\sqrt{6}}$	0	0	0	0	0	0	$-\frac{1}{\sqrt{2}}$	0	0	0	$\frac{1}{\sqrt{3}}$	$\sqrt{\frac{2}{3}}$	$\frac{1}{2\sqrt{3}}$	0	$-\frac{1}{2\sqrt{6}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	0	0	0
				$-9B+6C$	$\frac{1}{\sqrt{3}}$	$-\frac{1}{2\sqrt{3}}$	0	$-\frac{1}{2\sqrt{3}}$	0	0	$-3B$	0	$-3\sqrt{2}B$	0	$\frac{1}{2}$	0	$3\sqrt{6}B$	$3\sqrt{3}B$	$\sqrt{\frac{2}{3}}$	$-\frac{1}{\sqrt{3}}$	$-\frac{1}{2\sqrt{6}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{3}}$	0	0	0	0
					$-5B+6C$	$\frac{1}{2}$	0	$-\frac{1}{2}$	0	0	0	$-5\sqrt{3}B$	0	0	$-\frac{\sqrt{3}}{2}$	0	0	-1	$\frac{6}{\sqrt{2}}B$	$3B$	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	0	$\frac{1}{2}$	0	0	$\sqrt{2}(3B+C)$
						$B+5C-\frac{1}{2}$	$2\sqrt{3}B$	$3B+C$	0	0	0	0	$\sqrt{\frac{3}{2}}$	0	$\sqrt{3}B$	0	0	$\frac{1}{2}$	0	$-\frac{1}{2}$	$-\frac{3}{\sqrt{2}}B$	$-\frac{9}{\sqrt{2}}B$	$3B$	0	$3B+C$	$\sqrt{3}B$	0
							$-15B+5C+\frac{1}{2}$	0	$3B+C$	$\frac{1}{\sqrt{2}}$	$-\frac{1}{2}$	$-\frac{1}{2}$	0	$-\frac{1}{\sqrt{2}}$	0	$-3B$	0	$-\frac{\sqrt{3}}{2}$	0	$-\frac{\sqrt{3}}{2}$	$\sqrt{\frac{3}{2}}B$	$\sqrt{\frac{3}{2}}B$	$\sqrt{3}B$	0	$\sqrt{3}B$	$B+C$	0
								$-14B+5C+\frac{1}{2}$	$-3\sqrt{3}B$	0	0	0	0	0	$2\sqrt{3}B$	0	$\frac{1}{\sqrt{2}}$	0	0	0	$\frac{1}{\sqrt{2}}$	$-\frac{6}{\sqrt{2}}B+\frac{1}{\sqrt{2}}$	0	1	C	0	0
									$5C-\frac{1}{2}$	$\frac{1}{\sqrt{2}}$	$-\frac{1}{2}$	$-\frac{1}{2}$	0	0	0	-1	$-\sqrt{\frac{3}{2}}$	0	0	0	$\sqrt{6}B$	$4\sqrt{\frac{3}{2}}B$	$2\sqrt{3}B$	0	0	$4B+C$	0
										$-21B$	0	0	0	0	0	$\frac{1}{\sqrt{2}}$	0	0	0	0	$-\frac{\sqrt{3}}{2}$	0	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	0	0	0
											$-9B+6C$	0	0	$\frac{6}{\sqrt{2}}B$	0	$-\frac{1}{2}$	$-\sqrt{6}B$	$-5\sqrt{3}B$	0	0	$\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2}$	0	0	0	0
												$-9B+4C$	0	$-\sqrt{2}$	0	$+\frac{1}{2}$	0	0	$-\sqrt{6}B$	$\sqrt{3}B$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	0	$\frac{\sqrt{3}}{2}$	0	0	$-\sqrt{6}B$
													$11B+7C$	$4B+C$	$-\frac{1}{\sqrt{2}}$	0	0	$-10\sqrt{\frac{3}{2}}B$	0	0	0	0	0	0	0	$\frac{1}{\sqrt{2}}$	0
														$-9B+7C$	0	$-\frac{1}{\sqrt{2}}$	0	$-10\sqrt{\frac{3}{2}}B$	0	0	0	0	0	0	$-\sqrt{\frac{3}{2}}$	0	0
															$-10B+5C-\frac{1}{2}$	$4B+C$	0	0	0	0	$5\sqrt{\frac{3}{2}}B$	$-\sqrt{\frac{3}{2}}B$	$\sqrt{3}B$	0	0	$3B+1$	0
																$5C-\frac{1}{2}$	0	0	0	0	$5\sqrt{\frac{3}{2}}B$	$\sqrt{\frac{3}{2}}B$	$-\sqrt{3}B$	0	$-3\sqrt{3}B$	0	$\sqrt{\frac{3}{2}}$
																	$7C$	$\sqrt{2}(3B+C)$	0	0	1	0	0	0	0	0	1
																		$3B+8C$	0	1	$\frac{1}{\sqrt{2}}$	0	0	0	$-\frac{1}{2}$	$\frac{\sqrt{3}}{2}$	0
																			$-13B+4C$	$2\sqrt{2}B$	0	$\frac{1}{2}$	$-\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	0	$6B$
																				$-9B-4C$	$\frac{1}{\sqrt{2}}$	0	0	0	$-\frac{1}{2}$	$-\frac{\sqrt{3}}{2}$	$\frac{6}{\sqrt{2}}B$
																					$-3B+4C+\frac{1}{8}$	$3B$	$\sqrt{2}B$	0	$-\frac{3}{\sqrt{2}}B+\frac{1}{\sqrt{2}}$	$3\sqrt{\frac{3}{2}}B$	$-\frac{1}{2}$
																						$-11B+4C$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{3}{\sqrt{2}}B+\frac{1}{\sqrt{2}}$	$\sqrt{\frac{3}{2}}B$	$\frac{1}{2}$
																							$-13B+4C+\frac{1}{4}$	$-\frac{1}{4}$	$3B$	$3\sqrt{3}B$	0
																								$-21B+\frac{1}{4}$	1	0	$\frac{1}{\sqrt{2}}$
																									$-14B+5C+\frac{1}{2}$	$2\sqrt{3}B$	$\frac{1}{\sqrt{2}}$
																										$-10B+5C-\frac{1}{2}$	0
																											$-8B+5C$

TABELLA II. – *Elementi di matrice di interazione elettrostatica ed interazione* spin–*orbita. Rappresentazione* B_2.

e^3b_2	$e^2b_2^2$	$e^2b_2a_1$			e^3a_1	e^3b_1	$eb_1^2a_1$	$eb_2^2b_1$	$e^2b_2b_1$			$e^2a_1^2$	$e^2b_1^2$	$eb_2a_1^2$	$eb_2b_1^2$	$b_2^2a_1b_1$	$e^2a_1b_1$			$eb_2a_1b_1$				$eb_1^2a_1$	$ea_1^2b_1$	$b_2b_1^2a_1$
^3E	$^1B_2$	$^3B_1$	$^3B_1$	$^1B_2$	^3E	^3E	^3E	^3E	$^5A_1$	$^3B_1$	$^1B_2$	$^1B_2$	$^1B_2$	^3E	^3E	$^3B_1$	$^1B_2$	$^5B_2$	$^3B_1$	^3E	^3E	^3E	^5E	^3E	^3E	$^1B_2$
$-15B+5c+\frac{1}{2}$	$\frac{1}{\sqrt{2}}$	0	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$-2\sqrt{3}B$	-1	$-\sqrt{3}B$	$3B$	$-\frac{1}{\sqrt{2}}$	$\frac{1}{2}$	$\frac{1}{2}$	0	0	$-B-c$	$-3B-c$	0	0	0	0	$-\sqrt{6}B$	0	0	0	0	0	0
	$-9B+7c$	0	0	$-5\sqrt{6}B$	0	0	$-\sqrt{\frac{3}{2}}$	$-\frac{1}{\sqrt{2}}$	0	$-\sqrt{2}$	$3\sqrt{2}B$	$4B+c$	c	0	0	0	0	0	0	0	0	0	0	0	0	0
		$-13B+4c$	$2\sqrt{2}B$	0	0	0	0	0	0	$-\sqrt{6}B$	0	0	0	0	0	$6B$	$-\sqrt{\frac{2}{3}}$	$\frac{1}{\sqrt{3}}$	$\frac{6}{\sqrt{2}}B$	0	$\frac{1}{2}$	$-\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	0	0
			$-9B+4c$	1	$-\frac{1}{2}$	0	$-\frac{1}{2}$	0	0	$\sqrt{3}B$	0	0	0	$-\frac{\sqrt{3}}{2}$	0	$\frac{6}{\sqrt{2}}B$	$\frac{1}{\sqrt{3}}$	$\sqrt{\frac{2}{3}}$	$3B$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2}$	0	0	0	0
				$3B+8c$	$\frac{1}{2}$	0	$-\frac{1}{2}$	0	0	0	$-5\sqrt{3}B$	$-5\sqrt{6}B$	0	$\frac{\sqrt{3}}{2}$	0	0	$-3\sqrt{3}B$	0	-1	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2}$	0	0	0	$\sqrt{2}(3B+c)$
					$B+\frac{1}{2}5c$	$2\sqrt{3}B$	$3B+c$	0	0	0	0	$\sqrt{\frac{3}{2}}$	0	$\sqrt{3}B$	0	0	$\frac{1}{2\sqrt{3}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{2}$	$-\frac{3}{\sqrt{2}}B$	$-\frac{9}{\sqrt{2}}B$	$3B$	0	$3B+c$	$\sqrt{3}B$	0
						$-15B+5c+\frac{1}{2}$	0	$3B+c$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2}$	$-\frac{1}{2}$	0	$\frac{1}{\sqrt{2}}$	0	$-3B$	0	$-\frac{1}{2}$	$-\frac{1}{\sqrt{2}}$	$\frac{\sqrt{3}}{2}$	$\sqrt{\frac{3}{2}}B$	$\sqrt{\frac{3}{2}}B$	$\sqrt{3}B$	0	$\sqrt{3}B$	$B+c$	0
							$-14B+5c+\frac{1}{2}$	$-3\sqrt{3}B$	0	0	0	0	0	$2\sqrt{3}B$	0	$\frac{1}{\sqrt{2}}$	0	0	0	$\frac{1}{\sqrt{2}}$	$-\frac{6}{\sqrt{2}}B+\frac{1}{\sqrt{2}}$	0	1	c	0	0
								$5c-\frac{1}{2}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2}$	$-\frac{1}{2}$	0	0	0	-1	$\sqrt{\frac{3}{2}}$	0	0	0	$\sqrt{6}B$	$4\sqrt{\frac{3}{2}}B$	$2\sqrt{3}B$	0	0	$4B+c$	0
									$-21B$	0	0	0	0	0	$\frac{1}{\sqrt{2}}$	0	0	0	0	$-\frac{\sqrt{3}}{2}$	0	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	0	0	0
										$-9B+4c$	0	0	$-\sqrt{2}$	0	$-\frac{1}{2}$	$-\sqrt{6}B$	0	0	$-5\sqrt{3}B$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	0	$\frac{\sqrt{3}}{2}$	0	0	0
											$-9B+6c$	0	$-\frac{6}{\sqrt{2}}B$	0	$-\frac{1}{2}$	0	$3B$	0	0	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2}$	0	0	0	$-\sqrt{6}B$
												$11B+7c$	$4B+c$	$\frac{1}{\sqrt{2}}$	0	0	$3\sqrt{2}B$	0	0	0	0	0	0	0	$-\frac{1}{\sqrt{2}}$	0
													$-9B+7c$	0	$\frac{1}{\sqrt{2}}$	0	$-3\sqrt{2}B$	0	0	0	0	0	0	$-\sqrt{\frac{3}{2}}$	0	$2\sqrt{3}B$
														$-10B+5c-\frac{1}{2}$	$4B+c$	0	0	0	0	$5\sqrt{\frac{3}{2}}B$	$-\sqrt{\frac{3}{2}}B$	$\sqrt{3}B$	0	0	$3B+1$	0
															$5c-\frac{1}{2}$	0	0	0	0	$5\sqrt{\frac{3}{2}}B$	$\sqrt{\frac{3}{2}}B$	$-\sqrt{3}B$	0	$-3\sqrt{3}B$	0	$-\sqrt{\frac{3}{2}}$
																$-8B+5c$	0	0	$\sqrt{2}(3B+c)$	0	0	$-\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{2}}$	0	0	1
																	$-9B+6c$	0	$-\frac{1}{\sqrt{3}}$	0	$-\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{3}}$	0	$+\frac{1}{2\sqrt{3}}$	$-\frac{1}{2}$	$-3\sqrt{6}B$
																		$-21B$	$-\sqrt{\frac{2}{3}}$	0	$\frac{1}{2\sqrt{3}}$	$\frac{1}{2\sqrt{6}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{2}}$	0
																			$-5B+6c$	0	0	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{\sqrt{3}}{2}$	0
																				$-5B+4c+\frac{1}{2}$	$3B$	$\sqrt{2}B$	0	$-\frac{3}{\sqrt{2}}B+\frac{1}{\sqrt{2}}$	$3\sqrt{\frac{3}{2}}B$	$\frac{1}{2}$
																					$-11B+4c$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{3}{\sqrt{2}}B+\frac{1}{\sqrt{2}}$	$\sqrt{\frac{3}{2}}B$	$\frac{1}{2}$
																						$-13B+4c+\frac{1}{4}$	$-\frac{1}{4}$	$3B$	$3\sqrt{3}B$	$\frac{1}{\sqrt{2}}$
																							$-21B+\frac{1}{4}$	1	0	0
																								$-14B+5c+\frac{1}{2}$	$2\sqrt{3}B$	$\frac{1}{\sqrt{2}}$
																									$-10B+5c-\frac{1}{2}$	0
																										$7c$

TABELLA III. – *Elementi di matrice di interazione elettrostatica ed interazione* spin–*orbita. Rappresentazione* A_2.

$e^3 b_2$	$e^2 b_2 a_1$			$e^3 a_1$	$e^3 b_1$	$e b_2^2 a_1$	$e b_2^2 b_1$	$e^2 b_2 b_1$			$e b_2 a_1^2$	$e b_2 b_1^2$	$e^2 a_1 b_1$			$e b_2 a_1 b_1$				$e b_1^2 a_1$	$e a_1^2 b_1$	$b_2 a_1^2 b_1$
^3E	$^5B_1$	$^3A_1$	$^1A_2$	^3E	^3E	^3E	^3E	$^3A_1$	$^3A_1$	$^1A_2$	^3E	^3E	$^1A_2$	$^5B_2$	$^3A_1$	^3E	^3E	^3E	^5E	^3E	^3E	$^1A_2$
$-15B+5C-\frac{1}{2}$	$-\sqrt{\frac{3}{2}}$	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	$-2\sqrt{3}B$	1	$-\sqrt{3}B$	$3B$	0	$\frac{1}{2}$	$-\frac{1}{2}$	$-B-C$	$-3B-C$	0	0	0	$-\sqrt{6}B$	0	0	0	0	0	0
	$-21B$	0	0	$-\frac{1}{\sqrt{2}}$	0	$-\frac{1}{\sqrt{2}}$	0	0	0	0	$\sqrt{\frac{3}{2}}$	0	0	1	0	$-\frac{1}{2}$	0	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	0	0
		$-11B+4C$	0	$-\frac{1}{2}$	0	$-\frac{1}{2}$	0	$\sqrt{6}B$	$\sqrt{3}B$	0	$-\frac{\sqrt{3}}{2}$	0	-1	0	$-3B$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	$-\frac{1}{2}$	0	0	0
			$-3B+6C$	$\frac{1}{2}$	0	$\frac{1}{2}$	0	0	0	$-5\sqrt{3}B$	$\frac{\sqrt{3}}{2}$	0	$-3B$	0	-1	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2}$	0	0	0	$-\sqrt{6}B$
				$B+5C+\frac{1}{2}$	$2\sqrt{3}B$	$3B+C$	0	0	0	0	$\sqrt{3}B$	0	$-\frac{1}{2}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2}$	$-\frac{3}{\sqrt{2}}B$	$-\frac{9}{\sqrt{2}}B$	$3B$	0	$3B+C$	$\sqrt{3}B$	0
					$-15B+5C-\frac{1}{2}$	0	$3B+C$	0	$\frac{1}{2}$	$-\frac{1}{2}$	0	$-3B$	$-\frac{\sqrt{3}}{2}$	$-\sqrt{\frac{3}{2}}$	$\frac{\sqrt{3}}{2}$	$\sqrt{\frac{3}{2}}B$	$\sqrt{\frac{3}{2}}B$	$\sqrt{3}B$	0	$\sqrt{3}B$	$B+C$	0
						$-14B+5C-\frac{1}{2}$	$-3\sqrt{3}B$	0	0	0	$2\sqrt{3}B$	0	0	0	0	$-\frac{1}{\sqrt{2}}$	$-\frac{6}{\sqrt{2}}B-\frac{1}{\sqrt{2}}$	0	-1	C	0	0
							$5C+\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{1}{2}$	0	1	0	0	0	$\sqrt{6}B$	$4\sqrt{\frac{3}{2}}B$	$2\sqrt{3}B$	0	0	$4B+C$	0
								$-9B+4C$	0	0	0	0	0	0	$\sqrt{6}B$	0	$-\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	0	$3B$	0
									$-15B+4C$	1	0	$-\frac{1}{2}$	0	0	$\sqrt{3}B$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2}$	0	0	0	0
										$-3B+8C$	0	$-\frac{1}{2}$	$-5\sqrt{3}B$	0	0	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2}$	0	0	0	$\sqrt{2}(B+C)$
											$-10B+5C+\frac{1}{2}$	$4B+C$	0	0	0	$5\sqrt{\frac{3}{2}}B$	$-\sqrt{\frac{3}{2}}B$	$\sqrt{3}B$	0	0	$3B-1$	$\frac{1}{\sqrt{2}}$
												$5C+\frac{1}{2}$	0	0	0	$5\sqrt{\frac{3}{2}}B$	$\sqrt{\frac{3}{2}}B$	$-\sqrt{3}B$	0	$-3\sqrt{3}B$	0	0
													$-3B+6C$	0	0	$-\frac{1}{\sqrt{2}}$	0	0	0	$-\frac{1}{2}$	$-\frac{\sqrt{3}}{2}$	$-\sqrt{6}B$
														$-21B$	0	0	$\frac{1}{2}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	$-\sqrt{\frac{3}{2}}$	0
															$-11B+4C$	0	0	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{\sqrt{3}}{2}$	0
																$-3B+4C-\frac{1}{2}$	$3B$	$\sqrt{2}B$	0	$-\frac{3}{\sqrt{2}}B-\frac{1}{\sqrt{2}}$	$3\sqrt{\frac{3}{2}}B$	$-\frac{\sqrt{3}}{2}$
																	$-11B+4C$	$-\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$-\frac{3}{\sqrt{2}}B-\frac{1}{\sqrt{2}}$	$\sqrt{\frac{3}{2}}B$	$\frac{\sqrt{3}}{2}$
																		$-13B+4C-\frac{1}{4}$	$\frac{1}{4}$	$3B$	$3\sqrt{3}B$	$\sqrt{\frac{3}{2}}$
																			$-21B-\frac{1}{4}$	-1	0	0
																				$-14B+5C-\frac{1}{2}$	$2\sqrt{3}B$	0
																					$-10B+5C+\frac{1}{2}$	$-\frac{1}{\sqrt{2}}$
																						$-16B+7C$

TABELLA IV. – *Elementi di matrice di interazione elettrostatica ed interazione* spin–*orbita. Rappresentazione* A_1.

e^4	$e^3 b_2$	$e^2 b_2^2$		$e^2 b_2 a_1$			$e^3 a_1$	$e^3 b_1$	$e b_2^2 a_1$	$e b_2^2 b_1$	$e^2 b_2 b_1$			$e^2 a_1^2$		$b_2^2 a_1^2$	$b_2^2 b_1^2$	$e^2 b_1^2$		$e b_2 a_1^2$	$e b_2 b_1^2$	$e^2 a_1 b_1$			$e b_2 a_1 b_1$		
$^1A_1$	^3E	$^1A_1$	$^3A_2$	$^5B_1$	$^1A_1$	$^3A_2$	^3E	^3E	^3E	^3E	$^5A_1$	$^1A_1$	$^3A_2$	$^1A_1$	$^3A_2$	$^1A_1$	$^1A_1$	$^1A_1$	$^3A_2$	^3E	^3E	$^1A_1$	$^3A_2$	$^5B_2$	^3E	^3E	^3E
$-6B+8C$	1	$-\sqrt{2}(3B+C)$	0	0	$2\sqrt{3}B$	0	$\sqrt{3}$	-1	0	0	0	$-6\sqrt{3}B$	0	$-\sqrt{2}(B+C)$	0	0	0	$-\sqrt{2}(3B+C)$	0	0	0	$2\sqrt{3}B$	0	0	0	0	0
	$-15B+5C-\frac{1}{2}$	$-\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	$\sqrt{\frac{3}{2}}$	$-\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	$-2\sqrt{3}B$	1	$-\sqrt{3}B$	$3B$	$-\frac{1}{\sqrt{6}}$	$\frac{1}{2\sqrt{3}}$	$-\frac{1}{2}$	0	0	0	0	0	0	$-B-C$	$-3B-C$	0	0	0	$-\sqrt{6}B$	0	0
		$-3B+9C$	1	0	$-5\sqrt{6}B$	0	0	0	$-\sqrt{\frac{3}{2}}$	$\frac{1}{\sqrt{2}}$	0	$3\sqrt{6}B$	$-\sqrt{2}$	$4B+C$	0	$\sqrt{2}(B+C)$	$\sqrt{2}(3B+C)$	C	0	0	0	0	0	0	0	0	0
			$-15B+5C$	0	0	$-\sqrt{6}B$	0	0	$\sqrt{\frac{3}{2}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{\sqrt{3}}$	$-\sqrt{\frac{2}{3}}$	$3\sqrt{2}B$	0	$4B+C$	0	0	0	C	0	0	0	0	0	0	0	0
				$-21B$	0	0	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$	0	0	0	0	0	0	0	0	0	0	$-\sqrt{\frac{3}{2}}$	0	0	0	-1	$\frac{1}{2}$	0	$-\frac{1}{2\sqrt{2}}$
					$-3B+6C$	0	$-\frac{1}{2}$	0	$-\frac{1}{2}$	0	0	$-3B$	0	$-10\sqrt{\frac{3}{2}}B$	0	$-2\sqrt{3}B$	0	0	0	$\frac{\sqrt{3}}{2}$	0	$3B$	-1	0	$-\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$-\frac{1}{2}$
						$-11B+4C$	$-\frac{1}{2}$	0	$-\frac{1}{2}$	0	0	0	$-5\sqrt{3}B$	0	$\sqrt{6}B$	0	0	0	0	$\frac{\sqrt{3}}{2}$	0	-1	$3B$	0	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0
							$B+5C+\frac{1}{2}$	$2\sqrt{3}B$	$3B+C$	0	0	0	0	$-\sqrt{\frac{3}{2}}$	$-\sqrt{\frac{3}{2}}$	0	0	0	0	$\sqrt{3}B$	0	$-\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{\sqrt{2}}$	$-\frac{3}{\sqrt{2}}B$	$-\frac{3}{\sqrt{2}}B$	$3B$
								$-15B+5C-\frac{1}{2}$	0	$3B+C$	$\frac{1}{\sqrt{6}}$	$-\frac{1}{2\sqrt{3}}$	$\frac{1}{2}$	0	0	0	0	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$	0	$-3B$	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$-\sqrt{\frac{3}{2}}$	$\sqrt{\frac{3}{2}}B$	$\sqrt{\frac{3}{2}}B$	$\sqrt{3}B$
									$-14B+5C-\frac{1}{2}$	$-3\sqrt{3}B$	0	0	0	0	0	$-\sqrt{3}$	0	0	0	$2\sqrt{3}B$	0	0	0	0	$-\frac{1}{\sqrt{2}}$	$-\frac{6}{\sqrt{2}}B-\frac{1}{\sqrt{2}}$	0
										$5C+\frac{1}{2}$	$\frac{1}{\sqrt{6}}$	$-\frac{1}{2\sqrt{3}}$	$-\frac{1}{2}$	0	0	0	1	0	0	0	1	0	0	0	$\sqrt{6}B$	$4\sqrt{\frac{3}{2}}B$	$2\sqrt{3}B$
											$-21B$	0	$-\frac{2}{\sqrt{6}}$	0	0	0	0	0	$\frac{2}{\sqrt{3}}$	0	$\frac{1}{\sqrt{6}}$	0	0	0	$-\frac{1}{2}$	0	$-\frac{1}{2\sqrt{2}}$
												$-3B+6C$	$\frac{1}{\sqrt{3}}$	0	0	0	$6\sqrt{3}B$	$3\sqrt{6}B$	$-\sqrt{\frac{2}{3}}$	0	$-\frac{1}{2\sqrt{3}}$	$-3B$	0	0	$\frac{1}{2\sqrt{2}}$	$\frac{3}{2\sqrt{2}}$	$-\frac{1}{2}$
													$-3B+6C$	0	0	0	0	$-\sqrt{2}$	$\frac{6}{\sqrt{2}}B$	0	$-\frac{1}{2}$	0	$-5\sqrt{3}B$	0	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	0
														$17B+3C$	1	$\sqrt{2}(3B+C)$	0	$4B+C$	0	$\frac{1}{\sqrt{2}}$	0	$-10\sqrt{\frac{3}{2}}B$	0	0	0	0	0
															$5B+5C$	0	0	0	$4B+C$	$\frac{1}{\sqrt{2}}$	0	0	$\sqrt{6}B$	0	0	0	0
																$16B+8C$	$4B+C$	0	0	1	0	0	0	0	0	0	0
																	$24B+8C$	$\sqrt{2}(3B+C)$	0	0	1	0	0	0	0	0	0
																		$-3B+9C$	1	0	$\frac{1}{\sqrt{2}}$	$-10\sqrt{\frac{3}{2}}B$	0	0	0	0	0
																			$-15B+5C$	0	$\frac{1}{\sqrt{2}}$	0	$-\sqrt{6}B$	0	0	0	0
																				$-10B+5C+\frac{1}{2}$	$4B+C$	0	0	0	$5\sqrt{\frac{3}{2}}B$	$-\sqrt{\frac{3}{2}}B$	$\sqrt{3}B$
																					$5C+\frac{1}{2}$	0	0	0	$5\sqrt{\frac{3}{2}}B$	$\sqrt{\frac{3}{2}}B$	$-\sqrt{3}B$
																						$-3B+6C$	0	0	$-\frac{1}{\sqrt{2}}$	0	0
																							$-11B+4C$	0	0	0	$\frac{1}{2}$
																								$-21B$	0	$\frac{1}{2}$	$\frac{1}{2\sqrt{2}}$
																									$-9B+4C-\frac{1}{2}$	$3B$	$\sqrt{2}B$
																										$-11B+4C$	$-\frac{1}{2\sqrt{2}}$
																											$13B+4C-\frac{1}{2}$

Segue: TABLE IV.

$eb_2a_1b_1$	$eb_1^2a_1$	$ea_1^2b_1$	$b_2a_1b_1$	$a_1^2b_1^2$
^5E	^3E	^3E	$^3A_2$	$^1A_1$
$-21B-\frac{1}{4}$	-1	0	$-\sqrt{\frac{3}{2}}$	0
	$-14B+5C-\frac{1}{2}$	$2\sqrt{3}B$	0	$-\sqrt{3}$
		$-10B+5C+\frac{1}{2}$	$\frac{1}{\sqrt{2}}$	1
			$-16B+5C$	$-\sqrt{2}$
				$-16B+8C$

$eb_2a_1b_1$	$eb_1^2a_1$	$ea_1^2b_1$	$b_2a_1b_1$	$a_1^2b_1^2$	
^5E	^3E	^3E	$^3A_2$	$^1A_1$	
0	0	0	0	0	$^1A_1$
0	0	0	0	0	^3E
0	0	0	0	0	$^1A_1$
0	0	0	0	0	$^3A_2$
$\frac{1}{2\sqrt{2}}$	0	0	0	0	$^5B_1$
0	0	0	0	0	$^1A_1$
$-\frac{1}{2}$	0	0	$-\sqrt{6}B$	0	$^3A_2$
0	$3B+C$	$\sqrt{3}B$	0	0	^3E
0	$\sqrt{3}B$	$B+C$	0	0	^3E
-1	C	0	0	0	^3E
0	0	$4B+C$	0	0	^3E
$-\frac{3}{2\sqrt{2}}$	0	0	0	0	$^5A_1$
0	0	0	0	0	$^1A_1$
$-\frac{\sqrt{3}}{2}$	0	0	$\sqrt{2}(B+C)$	0	$^3A_2$
0	0	$\frac{1}{\sqrt{2}}$	0	$\sqrt{2}(3B+C)$	$^1A_1$
0	0	$\frac{1}{\sqrt{2}}$	$-6B$	0	$^3A_2$
0	0	0	$-\sqrt{2}$	C	$^1A_1$
0	0	0	0	$4B+C$	$^1A_1$
0	$-\sqrt{\frac{3}{2}}$	0	0	$\sqrt{2}(B+C)$	$^1A_1$
0	$\sqrt{\frac{3}{2}}$	0	0	0	$^3A_2$
0	0	$3B-1$	$\frac{1}{\sqrt{2}}$	0	^3E
0	$-3\sqrt{3}B$	0	0	0	^3E
0	$-\frac{1}{2}$	$\frac{\sqrt{3}}{2}$	0	$-2\sqrt{3}B$	$^1A_1$
$-\frac{1}{2}$	$-\frac{1}{2}$	$\frac{\sqrt{3}}{2}$	$-\sqrt{6}B$	0	$^3A_2$
$\frac{1}{2\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	$-\sqrt{\frac{3}{2}}$	0	0	$^5B_2$
0	$-\frac{3}{\sqrt{2}}B-\frac{1}{\sqrt{2}}$	$3\sqrt{\frac{3}{2}}B$	$-\frac{\sqrt{3}}{2}$	0	^3E
$-\frac{1}{2\sqrt{2}}$	$-\frac{3}{\sqrt{2}}B-\frac{1}{\sqrt{2}}$	$\sqrt{\frac{3}{2}}B$	$-\frac{\sqrt{3}}{2}$	0	^3E
$\frac{1}{4}$	$3B$	$3\sqrt{3}B$	0	0	^3E

TABELLA V. – *Elementi di matrice di interazione elettrostatica ed interazione* spin–*orbita. Rappresentazione* E.

$e^3 b_2$		$e^2 b_2^2$	$e^2 b_2 a_1$						$e^3 a_1$		$e^3 b_1$		$e b_2^2 a_1$		$e b_2^2 b_1$		$e^2 b_2 b_1$						$e^2 a_1^2$	$e^2 b_1^2$	$e b_2 a_1^2$	$e b_2 b_1^2$
^3E	^1E	$^3A_2$	$^5B_1$	$^3B_1$	$^3B_1$	$^3A_1$	$^3A_2$	$^3B_2$	^3E	^1E	^3E	^1E	^3E	^1E	^3E	^1E	$^5A_1$	$^3B_1$	$^3A_1$	$^3A_1$	$^3A_2$	$^3B_2$	$^3A_2$	$^3A_2$	^1E	^3E	^1E
$-15B+5C$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{\sqrt{3}}{2}$	0	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$-2\sqrt{3}B$	0	0	1	$-\sqrt{3}B$	0	$3B$	0	$-\frac{1}{2}$	$-\frac{1}{2\sqrt{2}}$	0	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	0	0	$-B-C$	0
	$-9B+7C$	$\frac{1}{2}$	0	$-\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	0	$-4\sqrt{3}B$	1	$-6B$	0	$-\sqrt{3}B$	0	$-9B$	0	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	0	$B+C$	0	$-3B-C$
		$-15B+5C$	0	0	0	0	$-\sqrt{6}B$	0	0	0	0	0	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1	0	-1	0	$3\sqrt{2}B$	0	$4B+C$	C	0	0	0
			$-21B$	0	0	0	0	$-\frac{1}{\sqrt{2}}$	$\frac{1}{2}$	0	0	0	$\frac{1}{2}$	0	0	0	0	0	0	0	0	0	0	0	0	$-\frac{\sqrt{3}}{2}$	0
				$-13B+4C$	$2\sqrt{2}B$	0	0	$-\frac{1}{\sqrt{2}}$	0	$\frac{1}{2}$	0	0	0	$\frac{1}{2}$	0	0	0	$-\sqrt{6}B$	0	0	0	0	0	0	$\frac{\sqrt{3}}{2}$	0	0
					$-9B+4C$	0	0	0	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	0	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	0	0	$\sqrt{3}B$	0	0	0	0	0	0	$\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	0
						$-11B+4C$	0	0	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	0	0	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	0	0	0	0	$-\sqrt{6}B$	$\sqrt{3}B$	0	0	0	0	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	0
							$-11B+4C$	0	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	0	0	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	0	0	0	0	0	0	$-5\sqrt{3}B$	0	$\sqrt{6}B$	0	$\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	0
								$-5B+6C$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	0	0	$-\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	0	0	0	0	0	0	$-5\sqrt{3}B$	0	0	$\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	0
									$B+5C$	$-\frac{1}{2}$	$2\sqrt{3}B$	0	$3B+C$	0	0	0	0	0	0	0	0	0	$-\frac{\sqrt{3}}{2}$	0	0	$\sqrt{3}B$	0
										$3B+7C$	0	$4\sqrt{3}B$	0	$3B+C$	0	0	0	0	0	0	0	0	$-\frac{\sqrt{3}}{2}$	0	$-\sqrt{3}B$	0	0
											$-15B+5C$	$\frac{1}{2}$	0	0	$3B+C$	0	$\frac{1}{2}$	$-\frac{1}{2\sqrt{2}}$	0	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	$-\frac{1}{2}$	0	0	0
												$-9B+7C$	0	0	0	$3B+C$	0	$-\frac{1}{2\sqrt{2}}$	$-\frac{1}{2}$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	$-\frac{1}{2}$	0	0	$9B$
													$-14B+5C$	$\frac{1}{2}$	$-3\sqrt{3}B$	0	0	0	0	0	0	0	0	0	0	$2\sqrt{3}B$	0
														$-12B+7C$	0	$-\sqrt{3}B$	0	0	0	0	0	0	0	0	$-4\sqrt{3}B$	0	0
															$5C$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2\sqrt{2}}$	0	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	0	0	0	1
																$6B+7C$	0	$-\frac{1}{2\sqrt{2}}$	$-\frac{1}{2}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	0	0	0	$6B$
																	$-21B$	0	0	0	$-\frac{1}{\sqrt{2}}$	0	0	1	0	0	0
																		$-9B+4C$	0	0	0	0	0	0	0	0	$\frac{1}{2\sqrt{2}}$
																			$-9B+4C$	0	$-\frac{1}{\sqrt{2}}$	0	0	-1	0	0	$-\frac{1}{2}$
																				$-15B+4C$	0	0	0	0	0	0	$-\frac{1}{2\sqrt{2}}$
																					$-3B+6C$	0	0	$\frac{6}{\sqrt{2}}B$	0	0	$\frac{1}{2\sqrt{2}}$
																						$-9B+4C$	0	0	0	0	$\frac{1}{2\sqrt{2}}$
																							$5B+5C$	$4B+C$	$-\frac{1}{2}$	$\frac{1}{2}$	0
																								$-15B+5C$	0	0	$\frac{1}{2}$
																									$-4B+7C$	$\frac{1}{2}$	$-4B-C$
																										$-10B+5C$	0
																											$6B+7C$

Segue: TABELLA V.

$e b_2 b_1^2$	$b_2^2 b_1 a_1$	$e^2 a_1 b_1$							$e b_2 a_1 b_1$								$e b_1^2 a_1$		$e a_1^2 b_1$		$b_2 b_1^2 a_1$	$b_2 a_1^2 b_1$
^3E	$^3B_1$	$^3B_2$	$^3B_2$	$^3A_2$	$^5B_2$	$^3A_1$	$^3B_1$	^3E	^3E	^3E	^1E	^1E	^5E	^5E	^5E	^3E	^1E	^3E	^1E	$^3B_2$	$^3A_2$
$-3B-C$	0	0	0	0	0	0	0	$-\sqrt{6}B$	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	$\sqrt{6}B$	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	$\frac{1}{2}$	$\frac{1}{\sqrt{2}}$	0	$-\frac{1}{2}$	0	0	$\frac{1}{2\sqrt{2}}$	0	$-\frac{1}{4}$	0	0	$-\frac{\sqrt{3}}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	0	0	0	0	0	0
0	$6B$	$\frac{1}{2}$	$-\frac{1}{\sqrt{2}}$	0	$-\frac{1}{2}$	0	$\frac{6}{\sqrt{2}}B$	0	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{4}$	$-\frac{1}{2\sqrt{6}}$	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{4\sqrt{3}}$	$-\frac{1}{4}$	$\frac{1}{4}$	0	0	0	0	0	0
0	$\frac{6}{\sqrt{2}}B$	$-\frac{1}{\sqrt{2}}$	0	0	$-\frac{1}{\sqrt{2}}$	0	$3B$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{2\sqrt{2}}$	$\frac{\sqrt{3}}{4}$	$-\frac{1}{4}$	0	0	0	0	0	0	0	0	0
0	0	0	0	-1	0	$-3B$	0	$\frac{1}{4}$	$-\frac{1}{4}$	0	$\frac{1}{4\sqrt{3}}$	$\frac{1}{4}$	$\frac{1}{2\sqrt{6}}$	$-\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	0	0	0	0	0
0	0	0	0	$3B$	0	1	0	$\frac{1}{4}$	$-\frac{1}{4}$	0	$\frac{1}{4\sqrt{3}}$	$\frac{1}{4}$	$\frac{1}{2\sqrt{6}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	0	0	0	0	0	$-\sqrt{6}B$
0	0	$\frac{6}{\sqrt{2}}B$	$3B$	0	0	0	1	$-\frac{1}{4}$	$\frac{1}{4}$	0	$\frac{1}{4\sqrt{3}}$	$\frac{1}{4}$	$\frac{1}{2\sqrt{6}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	0	0	0	$\sqrt{2}(3B+C)$	0
0	0	0	$-\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2}$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$-\frac{3}{\sqrt{2}}B$	$-\frac{3}{\sqrt{2}}B$	$3B$	0	0	0	0	0	$3B+C$	0	$\sqrt{3}B$	0	0	0
0	0	$-\frac{1}{2}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	0	$-\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	0	0	$3\sqrt{\frac{3}{2}}B$	$-\frac{9}{\sqrt{2}}B$	0	0	0	0	$3B+C$	0	$\sqrt{3}B$	0	0
$-3B$	0	0	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$\sqrt{\frac{3}{2}}B$	$\sqrt{\frac{3}{2}}B$	$\sqrt{3}B$	0	0	0	0	0	$\sqrt{3}B$	0	$B+C$	0	0	0
0	0	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	0	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	0	0	0	$\frac{3}{\sqrt{2}}B$	$-\sqrt{\frac{3}{2}}B$	0	0	0	0	$\sqrt{3}B$	0	$B+C$	0	0
0	$-\frac{1}{2}$	0	0	0	0	0	0	0	$-3\sqrt{2}B$	0	$-\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{\sqrt{3}}$	0	0	C	0	0	0	0	0
0	$-\frac{1}{2}$	0	0	0	0	0	0	$-\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	-1	0	$-3\sqrt{2}B$	0	0	0	0	C	0	0	0	0
0	$-\frac{\sqrt{3}}{2}$	0	0	0	0	0	0	$\sqrt{6}B$	$4\sqrt{\frac{3}{2}}B$	$2\sqrt{\frac{3}{2}}B$	0	0	0	0	0	0	0	$4B+C$	0	0	0
1	$-\frac{\sqrt{3}}{2}$	0	0	0	0	0	0	0	0	0	$3\sqrt{2}B$	$-4\sqrt{\frac{3}{2}}B$	0	0	0	0	0	0	$4B+C$	0	0
$\frac{1}{2}$	0	0	0	0	0	0	0	$-\frac{\sqrt{3}}{2\sqrt{2}}$	0	$-\frac{\sqrt{3}}{4}$	0	0	$\frac{3}{4}$	$\frac{\sqrt{3}}{4}$	$\frac{\sqrt{3}}{4}$	0	0	0	0	0	0
$\frac{1}{2\sqrt{2}}$	$-\sqrt{6}B$	0	0	0	0	0	$-5\sqrt{3}B$	$-\frac{\sqrt{3}}{4}$	$-\frac{\sqrt{3}}{4}$	0	$-\frac{1}{4}$	$\frac{\sqrt{3}}{4}$	$-\frac{1}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	0	0	0	0	0	0
0	0	0	0	0	0	$\sqrt{6}B$	0	0	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{4}$	$\frac{1}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{1}{4}$	$\frac{\sqrt{3}}{4}$	$\frac{\sqrt{3}}{4}$	0	0	0	0	0	0
$-\frac{1}{2\sqrt{2}}$	0	0	0	0	0	$\sqrt{3}B$	0	$\frac{\sqrt{3}}{4}$	$-\frac{\sqrt{3}}{4}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{3}{4}$	$-\frac{\sqrt{3}}{4}$	0	0	0	0	0	0	0	0	0
$-\frac{1}{2\sqrt{2}}$	0	0	0	$-5\sqrt{3}B$	0	0	0	$-\frac{\sqrt{3}}{4}$	$-\frac{\sqrt{3}}{4}$	0	$\frac{1}{4}$	$-\frac{\sqrt{3}}{4}$	$\frac{1}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	0	0	0	0	0	$\sqrt{2}(B+C)$
$\frac{1}{2\sqrt{2}}$	0	$-\sqrt{6}B$	$\sqrt{3}B$	0	0	0	0	$\frac{\sqrt{3}}{4}$	$\frac{\sqrt{3}}{4}$	0	$\frac{1}{4}$	$-\frac{\sqrt{3}}{4}$	$\frac{1}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	0	0	0	0	$-\sqrt{6}B$	0
0	0	0	0	$\sqrt{6}B$	0	0	0	0	0	0	0	0	0	0	0	0	0	$\frac{1}{2}$	$\frac{1}{2}$	0	$-6B$
$\frac{1}{2}$	0	0	0	$-\sqrt{6}B$	0	0	0	0	0	0	0	0	0	0	0	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	$\frac{3}{\sqrt{2}}B$	$5\sqrt{\frac{3}{2}}B$	0	0	0	0	0	1	$3B$	0	$\frac{1}{2}$
$4B+C$	0	0	0	0	0	0	0	$5\sqrt{\frac{3}{2}}B$	$-\sqrt{\frac{3}{2}}B$	$\sqrt{3}B$	0	0	0	0	0	0	0	$3B$	-1	0	$\frac{1}{2}$
$-\frac{1}{2}$	0	0	0	0	0	0	0	0	0	0	$\frac{3}{\sqrt{2}}B$	$-5\sqrt{\frac{3}{2}}B$	0	0	0	0	$-\sqrt{3}B$	0	0	$\frac{\sqrt{3}}{2}$	0

Segue: TABELLA V.

$e b_2 b_1^2$	$b_2^2 b_1 a_1$	$e^2 a_1 b_1$						$e b_2 a_1 b_1$								$e b_1^2 a_1$		$e a_1^2 b_1$		$b_2 b_1^2 a_1$	$b_2 a_1^2 b_1$
^3E	$^3B_1$	$^3B_2$	$^3B_2$	$^3A_2$	$^5B_2$	$^3A_1$	$^3B_1$	^3E	^3E	^3E	^1E	^1E	^5E	^5E	^5E	^3E	^1E	^3E	^1E	$^3B_2$	$^3A_2$
$5C$	0	0	0	0	0	0	0	$5\sqrt{\frac{3}{2}}B$	$\sqrt{\frac{3}{2}}B$	$-\sqrt{3}B$	0	0	0	0	0	$-3\sqrt{3}B$	0	0	0	$\frac{\sqrt{3}}{2}$	0
	$-8B+5C$	0	0	0	0	0	$\sqrt{2}(3B+C)$	0	0	$\frac{1}{2}$	$\frac{1}{\sqrt{6}}$	0	$-\frac{1}{2\sqrt{3}}$	$\frac{1}{2}$	$-\frac{1}{2}$	0	0	0	0	-1	0
		$-13B+4C$	$2\sqrt{2}B$	0	0	0	$-\frac{1}{\sqrt{2}}$	0	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{4}$	$-\frac{1}{\sqrt{6}}$	0	$-\frac{1}{4\sqrt{3}}$	$-\frac{1}{4}$	$+\frac{1}{4}$	0	$-\frac{1}{2}$	0	$\frac{\sqrt{3}}{2}$	$6B$	0
			$-9B+4C$	0	0	0	0	$\frac{1}{2}$	0	0	0	$\frac{1}{2}$	0	0	0	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{6}{\sqrt{2}}B$	0
				$-11B+4C$	0	0	0	0	0	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{3}}$	0	$\frac{1}{2\sqrt{6}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	0	$-\sqrt{6}B$
					$-21B$	0	$-\frac{1}{\sqrt{2}}$	0	$\frac{1}{2\sqrt{2}}$	$\frac{1}{4}$	0	0	$-\frac{\sqrt{3}}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{2}$	0	$-\frac{\sqrt{3}}{2}$	0	0	0
						$-11B+4C$	0	0	0	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{3}}$	0	$-\frac{1}{2\sqrt{6}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	0	0
							$-5B+6C$	0	0	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{3}}$	0	$-\frac{1}{2\sqrt{6}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	0	0
								$-9B+4C$	$3B$	$\sqrt{2}B$	0	$-\frac{1}{2}$	0	0	0	$-\frac{3}{\sqrt{2}}B$	$-\frac{1}{\sqrt{2}}$	$3\sqrt{\frac{3}{2}}B$	0	$-\frac{1}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$
									$-11B+4C$	0	$\frac{1}{2\sqrt{3}}$	0	$\frac{1}{\sqrt{6}}$	0	0	$-\frac{3}{\sqrt{2}}B$	$\frac{1}{\sqrt{2}}$	$\sqrt{\frac{3}{2}}B$	0	$\frac{1}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$
										$-13B+4C$	$\frac{1}{\sqrt{6}}$	0	$-\frac{1}{2\sqrt{3}}$	0	0	$3B$	-1	$3\sqrt{3}B$	0	0	0
											$-9B+6C$	$-3\sqrt{3}B$	0	0	0	$-\frac{1}{\sqrt{6}}$	$3\sqrt{\frac{3}{2}}B$	0	$\frac{9}{\sqrt{2}}B$	$\frac{1}{2\sqrt{6}}$	$\frac{1}{2\sqrt{2}}$
												$-3B+6C$	0	0	0	$\frac{1}{\sqrt{2}}$	$-\frac{3}{\sqrt{2}}B$	0	$-\sqrt{\frac{3}{2}}B$	$\frac{1}{2\sqrt{2}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$
													$-21B$	0	0	$\frac{2}{\sqrt{3}}$	0	0	0	$\frac{1}{2\sqrt{3}}$	$\frac{1}{2}$
														$-21B$	$-\frac{1}{2}$	0	0	0	0	$\frac{1}{2}$	$\frac{\sqrt{3}}{2}$
															$-21B$	0	0	0	0	$-\frac{1}{2}$	$\frac{\sqrt{3}}{2}$
																$-14B+5C$	$\frac{1}{2}$	$2\sqrt{3}B$	0	$\frac{1}{2}$	0
																	$-12B+7C$	0	$4\sqrt{3}B$	$\frac{1}{2}$	0
																		$-10B+5C$	$-\frac{1}{2}$	0	$\frac{1}{2}$
																			$-4B+7C$	0	$-\frac{1}{2}$
																				$-8B+5C$	0
																					$-16B+5C$

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