The Journal of Chemical Physics

Molecular point groups and symmetry in external magnetic fields

Cite as: J. Chem. Phys. **155**, 201101 (2021); https://doi.org/10.1063/5.0069859
Submitted: 02 September 2021 • Accepted: 07 November 2021 • Published Online: 23 November 2021

Ansgar Pausch, Melanie Gebele and Wim Klopper

View Online Export Citation CrossMark

ARTICLES YOU MAY BE INTERESTED IN

Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and interoperability among computational chemistry programs
The Journal of Chemical Physics **155**, 204801 (2021); https://doi.org/10.1063/5.0059356

OrbNet Denali: A machine learning potential for biological and organic chemistry with semi-empirical cost and DFT accuracy
The Journal of Chemical Physics **155**, 204103 (2021); https://doi.org/10.1063/5.0061990

The momentum of models
The Journal of Chemical Physics **155**, 170902 (2021); https://doi.org/10.1063/5.0023891

Challenge us.
What are your needs for periodic signal detection?
Watch
Zurich Instruments

AIP Publishing

© 2021 Author(s).

The Journal of Chemical Physics COMMUNICATION scitation.org/journal/jcp

Molecular point groups and symmetry in external magnetic fields

Cite as: J. Chem. Phys. 155, 201101 (2021); doi: 10.1063/5.0069859
Submitted: 2 September 2021 • Accepted: 7 November 2021 •
Published Online: 23 November 2021

View Online Export Citation CrossMark

Ansgar Pausch,[1] Melanie Gebele,[1] and Wim Klopper[1,2,a)]

AFFILIATIONS

[1] Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany
[2] Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

[a)] **Author to whom correspondence should be addressed:** klopper@kit.edu

ABSTRACT

As quantum-chemical calculations of molecules in static external magnetic fields are becoming increasingly popular, the description of molecular symmetry under such conditions is also becoming more and more relevant. Using group theory, a general scheme of identifying the molecular point group in an external magnetic field is constructed. For both point groups that are non-existent in the absence of a field (C_∞ and $C_{\infty h}$) and their double groups, the character tables are presented. General properties of all possible point groups are discussed, and it is mathematically proven that they are all Abelian.

© 2021 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/). https://doi.org/10.1063/5.0069859

The concept of molecular symmetry can be adequately described using the mathematical framework of group theory. For quantum-chemical calculations, in particular, this approach is advantageous as the non-relativistic molecular Hamiltonian is of the same symmetry as the molecule itself and thus its eigenfunctions can be classified as belonging to the irreducible representations of the molecular point group. In general, the molecular point group of a system can be identified by examining the symmetry operations (rotations, reflections, and combinations thereof), which map the molecule onto itself. All such operations form a group, and by extension, their matrix representations form a group homomorphic to it.[1]

In recent years, the investigation of molecular properties in external magnetic fields has become increasingly popular.[2–9] Early works in this field were mostly concerned with the quantum-mechanical description of atoms and linear molecules in strong magnetic fields, whereas more recent applications include calculations on larger molecules as well.[10–14] While the symmetry of linear molecules in external magnetic fields has been thoroughly examined by Schmelcher and Cederbaum,[15] a more general group-theoretical description of molecules in external magnetic fields is presented by Ceulemans.[16] In this work, we aim at presenting an easily accessible scheme for the identification of molecular point groups in external magnetic fields in the form of the usually widespread flow charts for point group identification. Furthermore, we further investigate the properties of point groups in magnetic fields presented by Ceulemans,[16] thereby proposing thorough mathematical proofs for the existence of all relevant properties.

If atoms are considered to be points, they belong to the three-dimensional rotation group (K_h).[17] Since molecules can be interpreted as a set of arbitrarily placed atoms in three-dimensional space, it must follow that all possible molecular point groups can be identified as K_h and its subgroups. The symmetry operations from which the molecular point group is formed are rotations about an n-fold axis (C_n), reflections (σ), rotation and reflections about an n-fold axis ($S_n = C_n\sigma_\perp$), the inversion ($I = S_2$), and the identity ($E = C_1$).[1,17] Let M be an arbitrary symmetry operation and $\mathbf{M}$ be its matrix representation in $\mathbb{R}^3$. Any valid symmetry operation of the system will act on the position vector of an atom ($\mathbf{x}$) in such a way that

$$\mathbf{M}\mathbf{x} = \mathbf{x}', \tag{1}$$

where $\mathbf{x}'$ is the position vector belonging to an atom of the same type. This is true because any position vector is a polar vector. A static homogeneous magnetic field, however, is represented by an axial vector ($\mathbf{B} = \nabla \times \mathbf{A}$), and as such, the following relation holds true:

© Author(s) 2021

$$\det(\mathbf{M})\mathbf{MB} = \mathbf{B}. \tag{2}$$

This implies that any improper rotation (σ, I, or S_n) maps the magnetic field onto its inverse, while proper rotations (C_n, E) map the magnetic field onto itself. This has a number of far-reaching implications for molecular symmetry in external magnetic fields, as only those symmetry operations that map $\mathbf{B}$ onto itself according to Eq. (2) can belong to the point group. Upon further investigation, only the following symmetry operations fulfill this requirement:

- the identity (E),
- the inversion (I),
- the rotation about an axis parallel to the field ($C_n \parallel \mathbf{B} := C_n^{\parallel}$),
- the reflection at a mirror plane perpendicular to the field ($\sigma \perp \mathbf{B} := \sigma^{\perp}$), and
- the rotation and reflection about an axis parallel to the field ($S_n \parallel \mathbf{B} := S_n^{\parallel}$).

The point group consisting of all possible combinations of these elements is $C_{\infty h}$, which is thus the point group of an atom in an external magnetic field. Since a molecule in an external magnetic field is simply composed of individual atoms in the field, it must follow that all possible molecular point groups in external magnetic fields can be identified as $C_{\infty h}$ and its subgroups. This fact is later proven in this work (Lemma 2).

Having classified all possible molecular point groups in external magnetic fields, the next step is establishing a standardized procedure of identifying the point group for an arbitrary molecular system. For this, we first prove that the point group of a molecule in an external magnetic field is a subgroup of the molecular point group in the absence of a field. This theorem was previously stated by Ceulemans[16] as it can be used in order to identify point groups in an external magnetic field. Ceulemans's theorem can be proven as follows.

Definition 1. Given a set G and an operation $* : G \times G \to G$, the tuple $(G, *)$ is called a group if for all elements $g_i, g_j, g_k \in G$, the following properties hold:[18]

- Closure: $g_i * g_j \in G$.
- Associativity: $g_i * (g_j * g_k) = (g_i * g_j) * g_k$.
- Identity: There exists an element $E \in G$ such that $g_i * E = E * g_i = g_i \forall g_i \in G$.
- Inverse element: There exists an element $g_i^{-1} \in G$ for all $g_i \in G$ such that $g_i * g_i^{-1} = g_i^{-1} * g_i = E$.

We often denote a group $(G, *)$ simply by G. The operation sign $*$ is often omitted ($g_i * g_j = g_i g_j$) and only explicitly stated if needed for the sake of clarity. If the set G is finite, we denote its order by $n_g = |G|$ and the number by the group elements $\{g_1, g_2, \ldots, g_{n_g}\}$. The set of matrices $\mathbf{G} := \{\mathbf{G}_i | i = 1, 2, \ldots, n_g\}$ contains the matrix representations of G in $\mathbb{R}^3$, which form an isomorphic group.

Theorem 1. If G is the molecular point group of a system in the absence of an external field and H is the point group of the same system in an external magnetic field, then H is a subgroup of G.

Proof. Let G be the molecular point group of a system in the absence of a field; then, $\mathbf{G}$ is the complete set of matrix representations in $\mathbb{R}^3$ corresponding to symmetry operations, which satisfy Eq. (1). Furthermore, let H be the set of all symmetry operations of the same system with an external magnetic field, where $\mathbf{H} := \{\mathbf{H}_i | i = 1, 2, \ldots, n_h\}$ with $n_h = |H|$ being the complete set of symmetry operation matrices in $\mathbb{R}^3$, which fulfill both Eqs. (1) and (2). In order to prove Theorem 1, it must be shown that H is a subset of G and that H is a group.

First, we show that $H \subseteq G$. Any matrix representation of a symmetry element in $\mathbb{R}^3$ is an element of $\mathbf{G}$ if Eq. (1) is fulfilled. Since all matrix representations in $\mathbf{H}$ fulfill both Eqs. (1) and (2), they automatically fulfill the requirement to be contained in $\mathbf{G}$. Therefore, $\mathbf{H} \subseteq \mathbf{G}$, and since these are isomorphic representations of H and G, this implies that $H \subseteq G$.

Second, we have to show that H is a group, that is, all postulates of group theory are fulfilled by H. Associativity automatically transfers to a subset of elements since $H \subseteq G$. The identity element automatically fulfills both Eqs. (1) and (2) and thus lies in H. Furthermore, we need to show that $h_i * h_j$ lies in H for all h_i, h_j. Let $\mathbf{H}_i$ and $\mathbf{H}_j$ be the matrix representations of any two elements of H, which implies that they satisfy the condition in Eq. (2). Then, their combination $\mathbf{H}_k = \mathbf{H}_i\mathbf{H}_j$ fulfills this condition as well,

$$\begin{aligned}\det(\mathbf{H}_k)\mathbf{H}_k\mathbf{B} &= \det(\mathbf{H}_i\mathbf{H}_j)\mathbf{H}_i\mathbf{H}_j\mathbf{B}\\ &= \det(\mathbf{H}_i)\det(\mathbf{H}_j)\mathbf{H}_i\det(\mathbf{H}_j)^{-1}\mathbf{B}\\ &= \det(\mathbf{H}_i)\mathbf{H}_i\mathbf{B} = \mathbf{B}.\end{aligned} \tag{3}$$

Here, we used that the determinant is multiplicative, that is, $\det(\mathbf{MN}) = \det(\mathbf{M})\det(\mathbf{N})$, and we reinserted Eq. (2) twice into itself. Hence, the group operation on G restricts to an operation $* : H \times H \to H$. Finally, we have to show the existence of inverse elements for all elements in H,

$$\begin{aligned}\det\left(\mathbf{H}_i^{-1}\right)\mathbf{H}_i^{-1}\mathbf{B} &= \det\left(\mathbf{H}_i^{-1}\right)\mathbf{H}_i^{-1}\det(\mathbf{H}_i)\mathbf{H}_i\mathbf{B}\\ &= \det\left(\mathbf{H}_i^{-1}\right)\det(\mathbf{H}_i)\mathbf{H}_i^{-1}\mathbf{H}_i\mathbf{B} = \mathbf{B}.\end{aligned} \tag{4}$$

For this, we have inserted Eq. (2) as $\mathbf{B} = \det(\mathbf{H}_i)\mathbf{H}_i\mathbf{B}$ since we know that $\mathbf{H}_i$ must satisfy this condition. ∎

Consequently, the molecular point group in an external magnetic field can easily be identified if the point group of the system in the absence of a field is already known by simply verifying for which symmetry operations Eq. (2) is fulfilled. From this information, a procedure equivalent to the one presented in the commonly used flow charts[1] can be constructed for molecules in external magnetic fields (see Fig. 1). In this flow chart, two molecular point groups are present, which do not appear in the absence of a magnetic field: $C_{\infty h}$ and C_{∞}. For these two point groups, the character tables are presented here in the same fashion as presented by Altmann and Herzig.[18] We have provided these character tables for the double groups of $C_{\infty h}$ and C_{∞} as spin-noncollinear approaches such as the generalized Hartree–Fock (GHF) method[19] are not uncommon for quantum-chemical calculations in strong external magnetic fields.[13,14] By ignoring the characters with non-integer subscripts, the character tables for $C_{\infty h}$ and C_{∞} are obtained (Tables I and II).

Having established all possible molecular point groups in static external magnetic fields and how to identify them, the last part of this

© Author(s) 2021

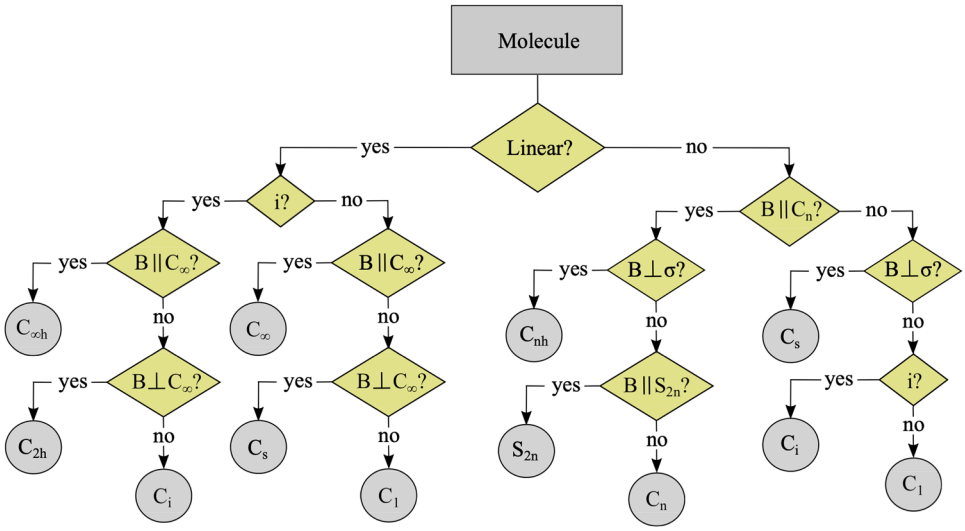

FIG. 1. Flow chart to identify the Schoenflies symbols of molecular point groups in static external magnetic fields.

work is concerned with the general properties of these point groups. More specifically, it can be proven that all molecular point groups in external magnetic fields are Abelian. This theorem was stated by Ceulemans[16] and is further examined and formally proven here.

Definition 2. A group is Abelian if for all $g_i, g_j \in G$, we have $g_i g_j = g_j g_i$.

TABLE I. Character table of the double group C_∞.

C_∞	E	$C_\infty(\phi)$
$A = \Sigma$	+1	+1
$E_1 = \Pi$	+1	$+\varepsilon_1^*$
	+1	$+\varepsilon_1$
$E_2 = \Delta$	+1	$+\varepsilon_2^*$
	+1	$+\varepsilon_2$
$E_3 = \Phi$	+1	$+\varepsilon_3^*$
	+1	$+\varepsilon_3$
E_n	+1	$+\varepsilon_n^*$
	+1	$+\varepsilon_n$
$E_{1/2}$	+1	$+\varepsilon_{1/2}$
	+1	$+\varepsilon_{1/2}^*$
$E_{3/2}$	+1	$+\varepsilon_{3/2}$
	+1	$+\varepsilon_{3/2}^*$
$E_{5/2}$	+1	$+\varepsilon_{5/2}$
	+1	$+\varepsilon_{5/2}^*$
$E_{7/2}$	+1	$+\varepsilon_{7/2}$
	+1	$+\varepsilon_{7/2}^*$
$E_{n+1/2}$	+1	$+\varepsilon_{n+1/2}$
	+1	$+\varepsilon_{n+1/2}^*$
$\varepsilon_k = \exp(ik\phi)$,	$0 < \phi < 2\pi$,	$n = 4, 5, 6, \ldots$

Lemma 1. $C_{\infty h}$ is Abelian.

Proof. Let $G = C_{\infty h}$ be the point group of an atom in a static external magnetic field, that is, the axial point group containing all symmetry operations fulfilling Eqs. (1) and (2). G is a countably infinite set, i.e., $n_g := |G| = \infty$ and $G = \{E, I, \sigma^\perp, C_2^\parallel, C_3^\parallel, \ldots, C_\infty^\parallel, S_4^\parallel, S_6^\parallel, \ldots, S_\infty^\parallel\}$.

For the identity element, this directly follows from its definition: $g_i E = E g_i = g_i$.[18] For the sake of simplicity, we use $I = S_2^\parallel$. The reflection is self-inverse: $\sigma^\perp \sigma^\perp = E$. The combination of proper rotations oriented along the same rotational axis is also commutative since $C_i^\parallel C_j^\parallel = C_{i\cdot j}^{i+j\parallel} = C_{j\cdot i}^{j+i\parallel} = C_j^\parallel C_i^\parallel$. The same is true for improper rotations: $S_i^\parallel S_j^\parallel = C_{i\cdot j}^{i+j\parallel} = C_{j\cdot i}^{j+i\parallel} = S_j^\parallel S_i^\parallel$. The combination of the reflection with any other symmetry operation is commutative: $\sigma^\perp C_i^\parallel = S_i^\parallel = C_i^\parallel \sigma^\perp$ and $\sigma^\perp S_i^\parallel = C_i^\parallel = S_i^\parallel \sigma^\perp$. Finally, proper and improper rotations about the same axis commute: $C_i^\parallel S_j^\parallel = S_{i\cdot j}^{i+j\parallel} = S_{j\cdot i}^{j+i\parallel} = S_j^\parallel C_i^\parallel$. We have thus shown that for all $g_i, g_j \in G$, we have $g_i g_j = g_j g_i$. ∎

Lemma 2. Each molecular point group in a static external magnetic field is a subgroup of $C_{\infty h}$.

Proof. $C_{\infty h}$ is defined to be the point group containing all valid symmetry operations in a static external magnetic field (see Lemma 1). Any symmetry reduction such as the inclusion of other atoms will induce additional constraints in the form of Eq. (1). H is therefore the group consisting of all $\{h_i | i = 1, 2, \ldots, n_h\}$ with $n_h = |H|$ for which their matrix representations $\{\mathbf{H}_i | i = 1, 2, \ldots, n_h\}$ in $\mathbb{R}^3$ fulfill Eq. (1). This cannot introduce any element $\mathbf{H}_i$, which does not satisfy Eq. (2), since H is defined to be a molecular point group in a static external magnetic field (see Theorem 1). Therefore, each element of H is also contained in $C_{\infty h}$. ∎

© Author(s) 2021

TABLE II. Character table of the double group $C_{\infty h}$.

$C_{\infty h}$	E	$C_\infty(\phi)$	I	σ_h	$S_\infty(\phi)$
$A_g = \Sigma_g$	+1	+1	+1	+1	+1
$E_{1g} = \Pi_g$	+1	$+\varepsilon_1^*$	+1	−1	$-\varepsilon_1^*$
	+1	$+\varepsilon_1$	+1	−1	$-\varepsilon_1$
$E_{2g} = \Delta_g$	+1	$+\varepsilon_2^*$	+1	+1	$+\varepsilon_2^*$
	+1	$+\varepsilon_2$	+1	+1	$+\varepsilon_2$
$E_{3g} = \Phi_g$	+1	$+\varepsilon_3^*$	+1	−1	$-\varepsilon_3^*$
	+1	$+\varepsilon_3$	+1	−1	$-\varepsilon_3$
E_{ng}	+1	$+\varepsilon_n^*$	+1	$(-1)^n$	$(-1)^n\varepsilon_n^*$
	+1	$+\varepsilon_n$	+1	$(-1)^n$	$(-1)^n\varepsilon_n$
$A_u = \Sigma_u$	+1	+1	−1	−1	−1
$E_{1u} = \Pi_u$	+1	$+\varepsilon_1^*$	−1	+1	$+\varepsilon_1^*$
	+1	$+\varepsilon_1$	−1	+1	$+\varepsilon_1$
$E_{2u} = \Delta_u$	+1	$+\varepsilon_2^*$	−1	−1	$-\varepsilon_2^*$
	+1	$+\varepsilon_2$	−1	−1	$-\varepsilon_2$
$E_{3u} = \Phi_u$	+1	$+\varepsilon_3^*$	−1	+1	$+\varepsilon_3^*$
	+1	$+\varepsilon_3$	−1	+1	$+\varepsilon_3$
E_{nu}	+1	$+\varepsilon_n^*$	−1	$(-1)^{n+1}$	$(-1)^{n+1}\varepsilon_n^*$
	+1	$+\varepsilon_n$	−1	$(-1)^{n+1}$	$(-1)^{n+1}\varepsilon_n$
$E_{1/2,g}$	+1	$+\varepsilon_{1/2}$	+1	+i	$-\mathrm{i}\varepsilon_{1/2}$
	+1	$+\varepsilon_{1/2}^*$	+1	−i	$+\mathrm{i}\,\varepsilon_{1/2}^*$
$E_{3/2,g}$	+1	$+\varepsilon_{3/2}$	+1	+i	$-\mathrm{i}\varepsilon_{3/2}$
	+1	$+\varepsilon_{3/2}^*$	+1	−i	$+\mathrm{i}\,\varepsilon_{3/2}^*$
$E_{5/2,g}$	+1	$+\varepsilon_{5/2}$	+1	+i	$-\mathrm{i}\varepsilon_{5/2}$
	+1	$+\varepsilon_{5/2}^*$	+1	−i	$+\mathrm{i}\,\varepsilon_{5/2}^*$
$E_{7/2,g}$	+1	$+\varepsilon_{7/2}$	+1	+i	$-\mathrm{i}\varepsilon_{7/2}$
	+1	$+\varepsilon_{7/2}^*$	+1	−i	$+\mathrm{i}\,\varepsilon_{7/2}^*$
$E_{n+1/2,g}$	+1	$+\varepsilon_{n+1/2}$	+1	+i	$-\mathrm{i}\varepsilon_{n+1/2}$
	+1	$+\varepsilon_{n+1/2}^*$	+1	−i	$+\mathrm{i}\,\varepsilon_{n+1/2}^*$
$E_{1/2,u}$	+1	$+\varepsilon_{1/2}$	−1	−i	$+\mathrm{i}\varepsilon_{1/2}$
	+1	$+\varepsilon_{1/2}^*$	−1	+i	$-\mathrm{i}\,\varepsilon_{1/2}^*$
$E_{3/2,u}$	+1	$+\varepsilon_{3/2}$	−1	−i	$+\mathrm{i}\varepsilon_{3/2}$
	+1	$+\varepsilon_{3/2}^*$	−1	+i	$-\mathrm{i}\,\varepsilon_{3/2}^*$
$E_{5/2,u}$	+1	$+\varepsilon_{5/2}$	−1	−i	$+\mathrm{i}\varepsilon_{5/2}$
	+1	$+\varepsilon_{5/2}^*$	−1	+i	$-\mathrm{i}\,\varepsilon_{5/2}^*$
$E_{7/2,u}$	+1	$+\varepsilon_{7/2}$	−1	−i	$+\mathrm{i}\varepsilon_{7/2}$
	+1	$+\varepsilon_{7/2}^*$	−1	+i	$-\mathrm{i}\,\varepsilon_{7/2}^*$
$E_{n+1/2,u}$	+1	$+\varepsilon_{n+1/2}$	−1	−i	$+\mathrm{i}\varepsilon_{n+1/2}$
	+1	$+\varepsilon_{n+1/2}^*$	−1	+i	$-\mathrm{i}\,\varepsilon_{n+1/2}^*$

$\varepsilon_k = \exp(\mathrm{i}k\phi)$, $\quad 0 < \phi < 2\pi$, $\quad n = 4, 5, 6, \ldots$

Theorem 2. All molecular point groups in static external magnetic fields are Abelian.

Proof. This follows directly from Theorem 1 and Lemmas 1 and 2 if we additionally consider that if a group is Abelian, all its subgroups are also Abelian.[20] ■

This property has some implications about the implementation of molecular point groups in finite magnetic fields into quantum chemistry software as Abelian point groups are typically easier to implement than their non-Abelian counterparts. For Abelian groups, the order of the group is equal to the number of conjugation classes and to the number of irreducible representations. It should be noted that separable degenerate irreducible representations with complex characters are still possible, such as those contained in the point group C_3. However, since complex algebra is typically used for calculations of molecular properties in finite external magnetic fields in any case, the resulting complex algebra is much less of a problem than it is for quantum-chemical calculations in the absence of a field.

Using the results of this work, an implementation of a group-theoretical description for arbitrary molecules in external magnetic fields into existing quantum chemistry software appears to be

© Author(s) 2021

feasible. Since all point groups for molecules in magnetic fields are subgroups of their zero-field counterparts, such an implementation should be straightforward if carried out in a program already capable of handling group theory without external fields. The fact that all point groups in external magnetic fields are Abelian further simplifies such an implementation as conjugation classes and degenerate irreducible representations can be disregarded. However, programs using spin-noncollinear approaches such as the GHF method must employ double groups in their implementation to account for the rotational symmetry of the spinors.

The authors would like to thank Andrea Thevis for helpful discussions concerning the mathematical proofs. A.P. acknowledges financial support from Fonds der chemischen Industrie and Studienstiftung des deutschen Volkes.

AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

DATA AVAILABILITY

The data that support the findings of this study are available within the article.

REFERENCES

[1] D. M. Bishop, *Group Theory and Chemistry* (Dover Publications, Inc., New York, 1993).
[2] E. I. Tellgren, A. Soncini, and T. Helgaker, "Nonperturbative *ab initio* calculations in strong magnetic fields using London orbitals," J. Chem. Phys. **129**, 154114 (2008).
[3] E. I. Tellgren, T. Helgaker, and A. Soncini, "Non-perturbative magnetic phenomena in closed-shell paramagnetic molecules," Phys. Chem. Chem. Phys. **11**, 5489–5498 (2009).
[4] K. K. Lange, E. I. Tellgren, M. R. Hoffmann, and T. Helgaker, "A paramagnetic bonding mechanism for diatomics in strong magnetic fields," Science **337**, 327–331 (2012).
[5] S. Stopkowicz, J. Gauss, K. K. Lange, E. I. Tellgren, and T. Helgaker, "Coupled-cluster theory for atoms and molecules in strong magnetic fields," J. Chem. Phys. **143**, 074110 (2015).
[6] T. F. Stetina, S. Sun, D. B. Williams-Young, and X. Li, "Modeling magneto-photoabsorption using time-dependent complex generalized Hartree-Fock," ChemPhotoChem **3**, 739–746 (2019).
[7] S. Sen, K. K. Lange, and E. I. Tellgren, "Excited states of molecules in strong uniform and nonuniform magnetic fields," J. Chem. Theory Comput. **15**, 3974–3990 (2019).
[8] T. J. P. Irons, G. David, and A. M. Teale, "Optimizing molecular geometries in strong magnetic fields," J. Chem. Theory Comput. **17**, 2166–2185 (2021).
[9] M. Wibowo, T. J. P. Irons, and A. M. Teale, "Modeling ultrafast electron dynamics in strong magnetic fields using real-time time-dependent electronic structure methods," J. Chem. Theory Comput. **17**, 2137–2165 (2021).
[10] P. Schmelcher and L. S. Cederbaum, "Two-body effects of the hydrogen atom in crossed electric and magnetic fields," Chem. Phys. Lett. **208**, 548–554 (1993).
[11] T. Detmer, P. Schmelcher, and L. S. Cederbaum, "Hydrogen molecule in a magnetic field: The lowest states of the Π manifold and the global ground state of the parallel configuration," Phys. Rev. A **57**, 1767–1777 (1998).
[12] E. I. Tellgren, S. S. Reine, and T. Helgaker, "Analytical GIAO and hybrid-basis integral derivatives: Application to geometry optimization of molecules in strong magnetic fields," Phys. Chem. Chem. Phys. **14**, 9492–9499 (2012).
[13] S. Sun, D. B. Williams-Young, T. F. Stetina, and X. Li, "Generalized Hartree–Fock with nonperturbative treatment of strong magnetic fields: Application to molecular spin phase transitions," J. Chem. Theory Comput. **15**, 348–356 (2019).
[14] A. Pausch and W. Klopper, "Efficient evaluation of three-centre two-electron integrals over London orbitals," Mol. Phys. **118**, e1736675 (2020).
[15] P. Schmelcher and L. S. Cederbaum, "Crossings of potential-energy surfaces in a magnetic field," Phys. Rev. A **41**, 4936–4943 (1990).
[16] A. J. Ceulemans, *Group Theory Applied to Chemistry* (Springer, Dordrecht, Heidelberg, New York, London, 2013).
[17] L. D. Landau and E. M. Lifschitz, *Lehrbuch der Theoretischen Physik III: Quantenmechanik* (Akademie-Verlag GmbH, Berlin, 1965).
[18] S. L. Altmann and P. Herzig, *Point-Group Theory Tables* (Wien, 2011).
[19] J. J. Goings, F. Egidi, and X. Li, "Current development of noncollinear electronic structure theory," Int. J. Quantum Chem. **118**, e25398 (2018).
[20] J. A. Green, *Sets and Groups: A First Course in Algebra* (Routledge and Kegan Paul, London; New York, 1988).

© Author(s) 2021