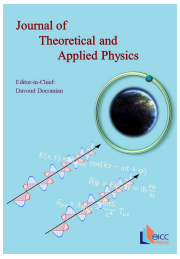

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Magnetic susceptibility and magnetocaloric effect of Frost-Musulin potential subjected to magnetic and Aharonov-Bohm (Flux) fields for CO and NO diatomic molecules

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Abstract:
In this paper, we perform a nonrelativistic study of Frost-Musulin potential (FMP) impacted by the external magnetic and AB flux fields for the CO and NO diatomic molecules using the Nikiforov-Uvarov method with the Greene-Aldrich approximation to the centrifugal barrier. The numerical computation of the proposed potential reveals that the combined impact of the magnetic and AB flux fields completely removes the degeneracy of the energy spectra and controls the behavior of the magnetocaloric effect (MCE) by acting as a regulating factor to cool or heat the MCE. Also, the thermomagnetic plots obtained for the analyzed dimer molecules agreed perfectly with previous work. This research has the potential to be applied in molecular physics and MCE studies for a variety of molecules.

Keywords: Magnetocaloric effect; Thermomagnetic properties; Nikiforov-Uvarov method; Frost-Musulin Potential; Diatomic molecules

1. Introduction

The exact and approximate solutions of various quantum systems have become a fascinating concept due to the remodeled nature of wave equations in relativistic and nonrelativistic realms and have continuously piqued the interest of researchers in various branches of quantum mechanics [1, 2]. Several authors [3–10] have obtained these solutions by employing various potential models and methods. Diatomic molecular potentials are essential for describing intramolecular and intermolecular interactions and atomic pair correlations [3]. Morse's prediction of a three-parameter empirical potential in 1929 [11] paved the way for research on diatomic molecules (DMs) using various interaction potential models. This advancement has contributed significantly to our knowledge of quantum mechanics, which is utilized in molecular spectroscopy and dynamics. This is because the potential energy function incorporates valuable insights that can be used to describe a

molecule [12]. Since then, authors have investigated some of these potentials in their deformed and improved versions [13]. For instance, Maireche [14], carried out a study on the improved modified Mobius square potential model using Bopp's shift and standard perturbation theory methods. Also, Desai et al. [15] discovered that the modified Morse potential function fits the RKR potential energy curve better than the Morse and the Hulbert-Hirschfelder potential functions, particularly near the dissociation limit. Furthermore, an enhanced version of the deformed exponential-type potential's dissociation energy and equilibrium bond length for some selected DMs was studied by Okorie et al. [12]. Sun et al. [16] demonstrated that the deformed modified Rosen-Morse potential and the familiar Tietz potential have the same potential function for DMs. Ikot et al. [17] used the NUFA method to obtain the relativistic equation for the recently developed generalized Morse potential. Oluwadare and Oyewumi [18] studied energy spectra and expectation values of DMs confined by the shifted Deng-Fan potential. Eyube et al. [19] developed analytical solutions for an improved Scarf II potential energy function, which they applied to the selected DMs. Okorie et al. [20] investigated the analytical solutions of the SE with the improved deformed exponential-type potential for H_2, CO, N_2, and LiH molecules. Oluwadare et al. [21] investigated the analytical solutions of an isotropic oscillator plus an inverse quadratic potential for some DMs.

A diatomic molecular potential of interest is the Frost-Musulin potential (FMP) that was proposed by Frost and Musulin [22]. Idiodi and Onate [23] investigated the Shannon and Renyi information entropies in position and momentum space and the Fisher information in the position-dependent mass SE with the FMP. Adepoju and Eweh [24], obtained the solutions of FMP using the functional analysis method. Onate and Onyeaju [25] obtained analytical solutions of the Dirac equation for the FMP via the parametric Nikiforov-Uvarov method and supersymmetric approach. The Frost-Musulin potential function is of the form [23–25]

$$V(r) = -\mathrm{D}_e \alpha r_e e^{-\alpha x} + \frac{\mathrm{D}_e \alpha r_e^2 e^{-\alpha x}}{r}, \; x = r - r_e \qquad (1)$$

where D_e denotes dissociation energy, α and r_e are the screening parameter and the equilibrium bond length.

The Aharonov-Bohm (AB) effects, discovered by Aharonov and Bohm [26], take place when a charge in motion is transformed by scalar and vector potentials even when no external EM fields are present [27]. External fields play a crucial part in changing the behavior of a system's energy spectra, primarily by stripping away degeneracy [28]. Several researchers have studied the effect of external magnetic fields and Aharonov-Bohm flux on certain potentials. For instance, within the framework of quantum theory, Shahin et al. [29] investigated the atomic and molecular properties of a pair of homoatomic and heteroatomic molecules under profound electric fields and discovered that atomic features interact linearly with field strengths, but molecular properties display nonlinear reactions to the applied fields. Horchani et al. [30] investigated the analytical solutions of inversely quadratic Yukawa potential within the framework of external magnetic and AB fields using the NUFA method.

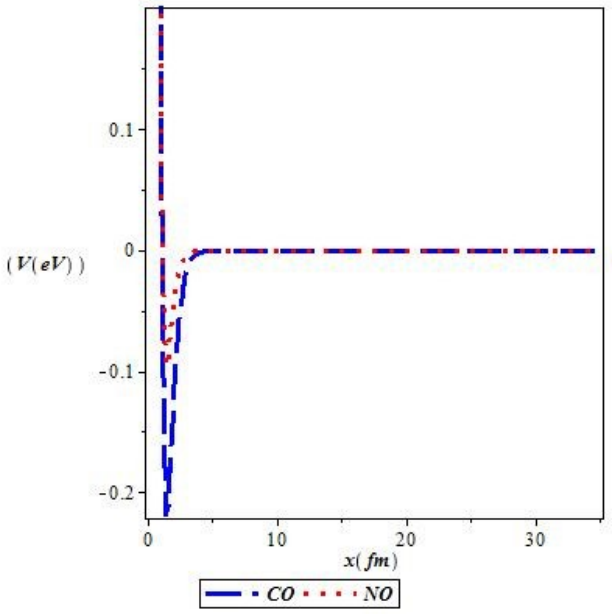

Figure 1. Shape of the Frost-Musulin potential for CO and NO diatomic molecules.

Ikhdair et al. [31] obtain analytical solutions of SE under the influence of magnetic and AB fields using the ansatz analytical procedure.

Another intriguing phenomenon known as magnetocaloric effects (MCE) is an inherent characteristic of a magnetic material identified by the temperature change caused by applying a magnetic field [32]. It is defined as a magnetothermodynamic phenomenon where the adiabatic variation in temperature is identified as the heating or the cooling of magnetic materials caused by changing magnetic fields [33, 34]. Warburg [35] reported this effect in iron. Subsequently, a significant development in magnetocaloric studies and the practical application of magnetic refrigeration technology from room temperature to hydrogen and helium temperatures, magnetic sensors, and so on [36, 37] have been conducted. The MCE is now an efficient tool than traditional gas compression (CGC). It reduces the release of some hazardous gases such as chlorofluorocarbons (CFCs) and hydrofluoric carbons compared (HFCs) to CGC. As a result, a reduction in ozone depletion and environmental health is protected [38]. Recently, William et al. [39] studied quantum description of magnetocaloric effect, thermo-magnetic properties and energy spectra of LiH, TiH, and ScH diatomic molecules under the influence of magnetic and Aharonov-Bohm (AB) flux fields with Deng-Fan-Screened Coulomb potential model. Other studies on MCE materials have been executed in rare earth metals, alloys, and transition metal-based compounds [40–42].

Over the years, numerous authors have studied the thermomagnetic properties of DMs with magnetic and AB fields [43–47].

Motivated by the works on the effect of external magnetic and AB flux fields, we attempt to study the bound state solutions of the FMP function via the Nikiforov-Uvarov approach with the effect of external magnetic and Aharonov-

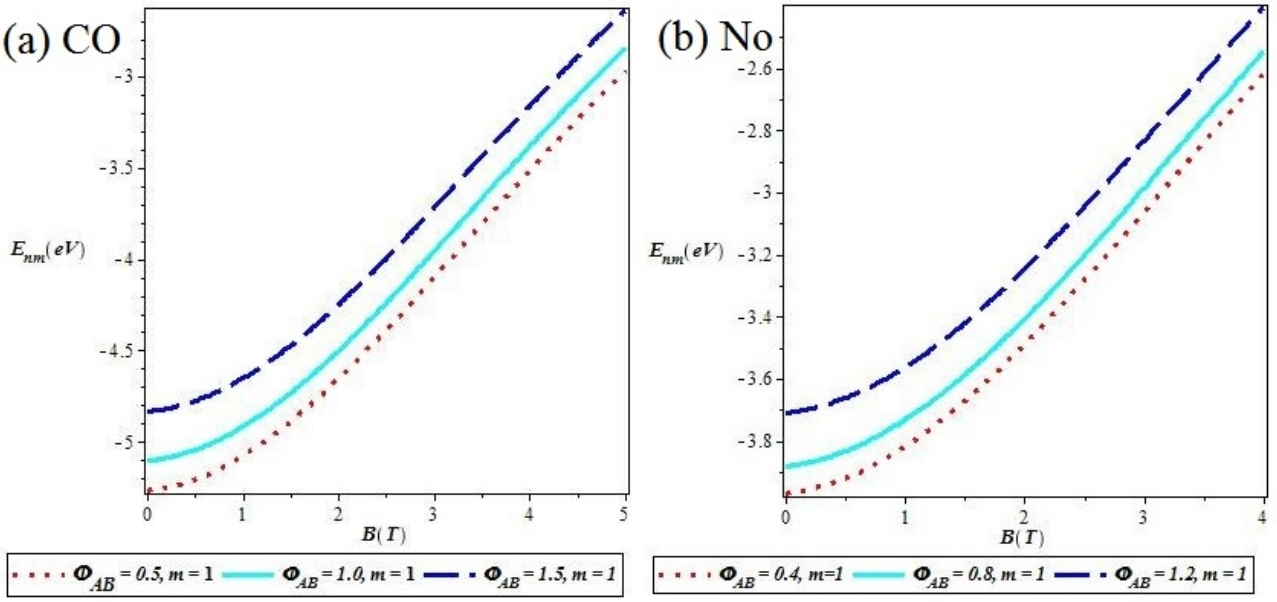

Figure 2. Variation of the energy eigenvalues of CO and NO diatomic molecules with Φ_{AB} for various **B** at $m = n = 1$.

Bohm flux fields, which appears to be lacking in the literature.

2. Nonrelativistic analytical solutions with FMP in external fields

The nonrelativistic analytical solutions with FMP exposed to external fields will be studied using the Nikiforov-Uvarov (NU) method. A detail of the method can be found in Ref. [48]. In 2D, the SE is of the form [49]:

$$\left[\frac{1}{2\mu}\left(i\hbar\nabla-\frac{e}{c}\mathbf{A}\right)^2-\left(-\mathrm{D}_e\alpha r_e e^{-\alpha x}+\frac{\mathrm{D}_e\alpha r_e^2 e^{-\alpha x}}{r}\right)\right]\times R_{nm}(r,\varphi)=E_{nm}R_{nm}(r,\varphi) \tag{2}$$

where the system's energy is E_{nm}, its effective mass is μ, and the vector potential is **A**, designated as

$$\mathbf{A}=\left(0,\frac{\mathbf{B}e^{-\alpha r}}{1-e^{-\alpha r}}\hat{\varphi}+\frac{\Phi_{\mathrm{AB}}}{2\pi r}\hat{\varphi},0\right) \tag{3}$$

where **B** and Φ_{AB} denotes magnetic and AB fields effect, respectively, [29]. The wave function in cylindrical coordinates is designated as

$$\psi(r,\varphi)=\frac{1}{2\pi r}e^{im\varphi}R_{nm}(r) \tag{4}$$

In Eq. (4), the magnetic quantum number is represented as m. Substitute Eqs. (3) and (4) into Eq. (2), yield the

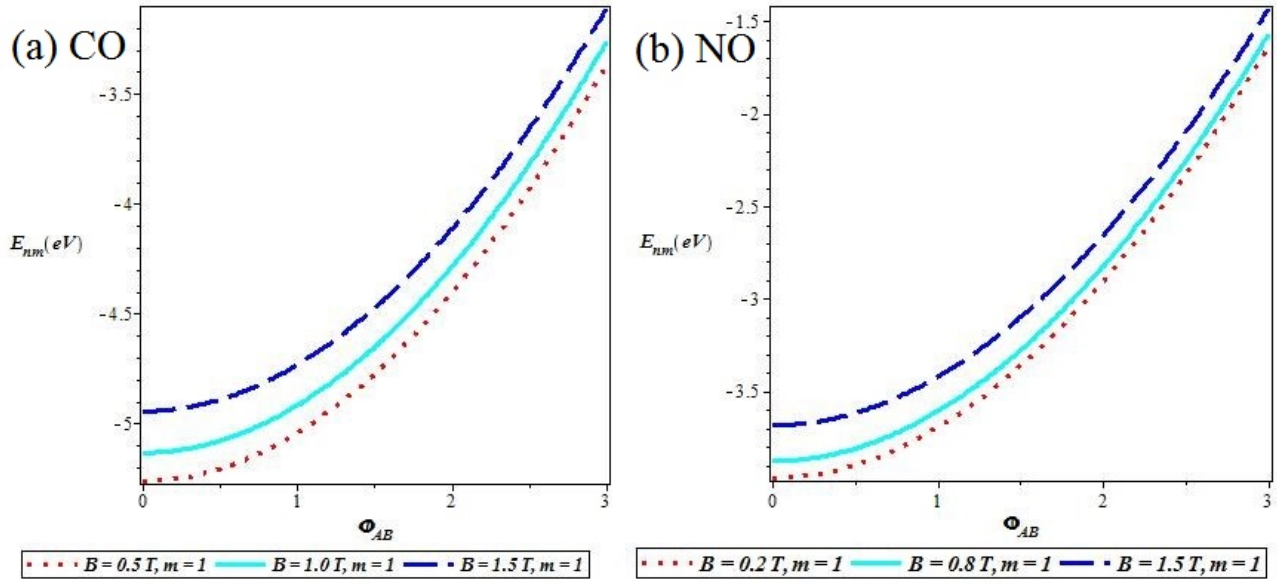

Figure 3. Variation of the energy eigenvalues of CO and NO diatomic molecules with Φ_{AB} for various **B** at $m = n = 1$.

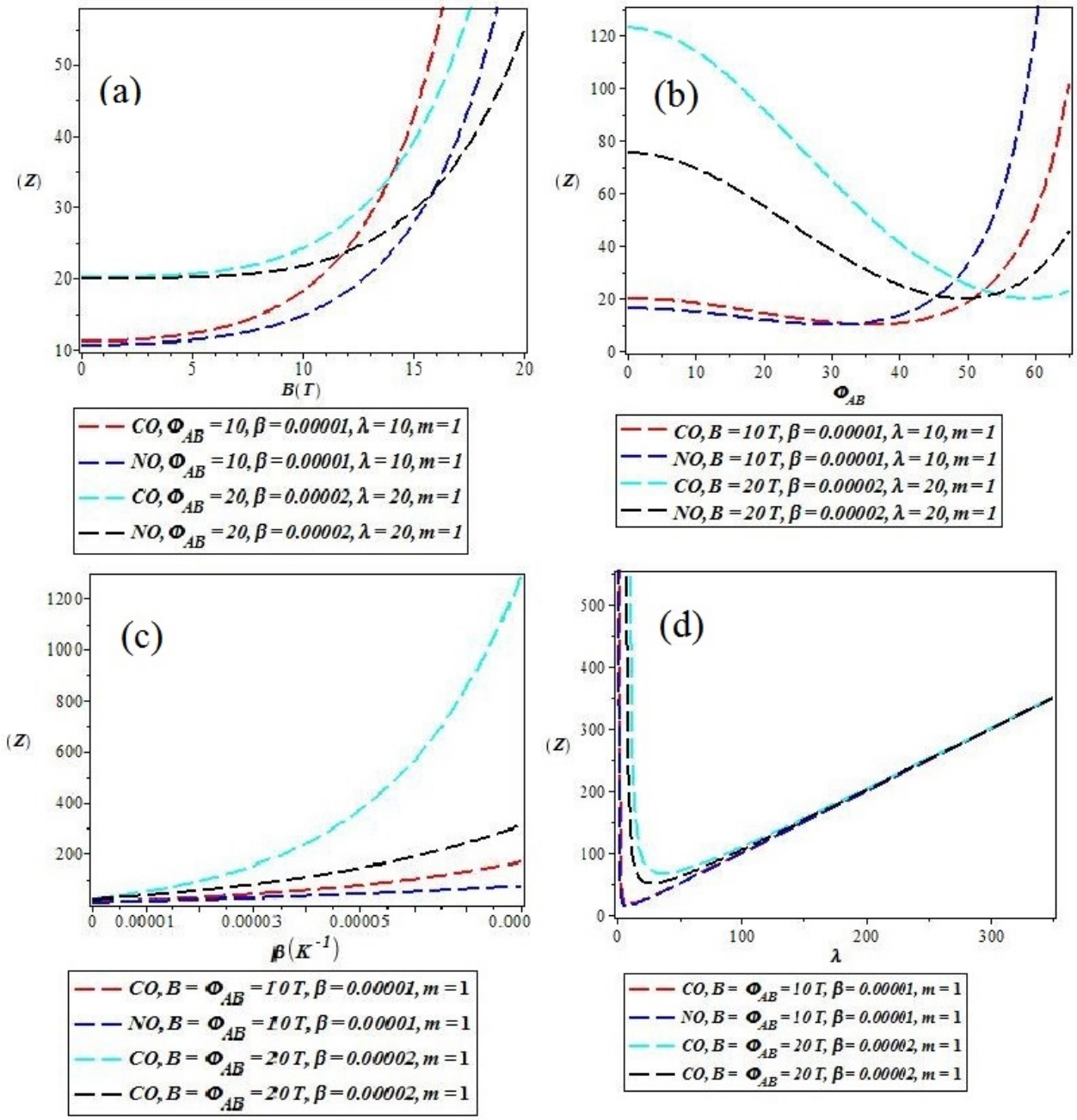

Figure 4. Variation of the partition function against: (a) magnetic flux $\mathbf{B}(T)$ for CO and NO molecules. (b) AB flux (Φ_{AB}) for CO and NO molecules. (c) Inverse temperature parameter (β) for CO and NO molecules (d) λ for CO and NO molecules.

differential equation of the form:

$$\acute{\psi}_{nm}(r)+\frac{2\mu}{\hbar^2}\left[\begin{array}{c} E_{nm}+\mathrm{D}_e\alpha r_e e^{-\alpha x} \\ +\frac{\mathrm{D}_e\alpha^2 r_e^2 e^{-\alpha x}}{(1-e^{-\alpha x})}-\frac{\hbar\omega_c(m+\zeta)\alpha e^{-\alpha x}}{(1-e^{-\alpha x})^2} \\ -\frac{\mu\omega_c^2 e^{-2\alpha x}}{2(1-e^{-\alpha x})^2}-\frac{\hbar^2}{2\mu}\left(\frac{(m+\zeta)^2-\frac{1}{4}}{r^2}\right)\end{array}\right]\psi_{nm}=0 \tag{5}$$

where $\zeta=\Phi_{\mathrm{AB}}/\phi_0$, $\phi_0=hc/e$ and $\omega_c=e\mathbf{B}/\mu c$ designates an integer containing AB field, the flux quantum, and cyclotron frequency, respectively. Equation (5) is not analytically solvable in its current form because of the centrifugal term. As a result, we employ the Greene and Aldrich approximation [50], which is valid only when the screening parameter is small enough and is given as

$$\frac{1}{r^2}\approx\frac{\alpha^2}{(1-e^{-\alpha x})^2} \tag{6}$$

By using Eq. (6) and a new parameter,

$$z=e^{-\alpha x} \tag{7}$$

Equation (2) can be expressed as follows:

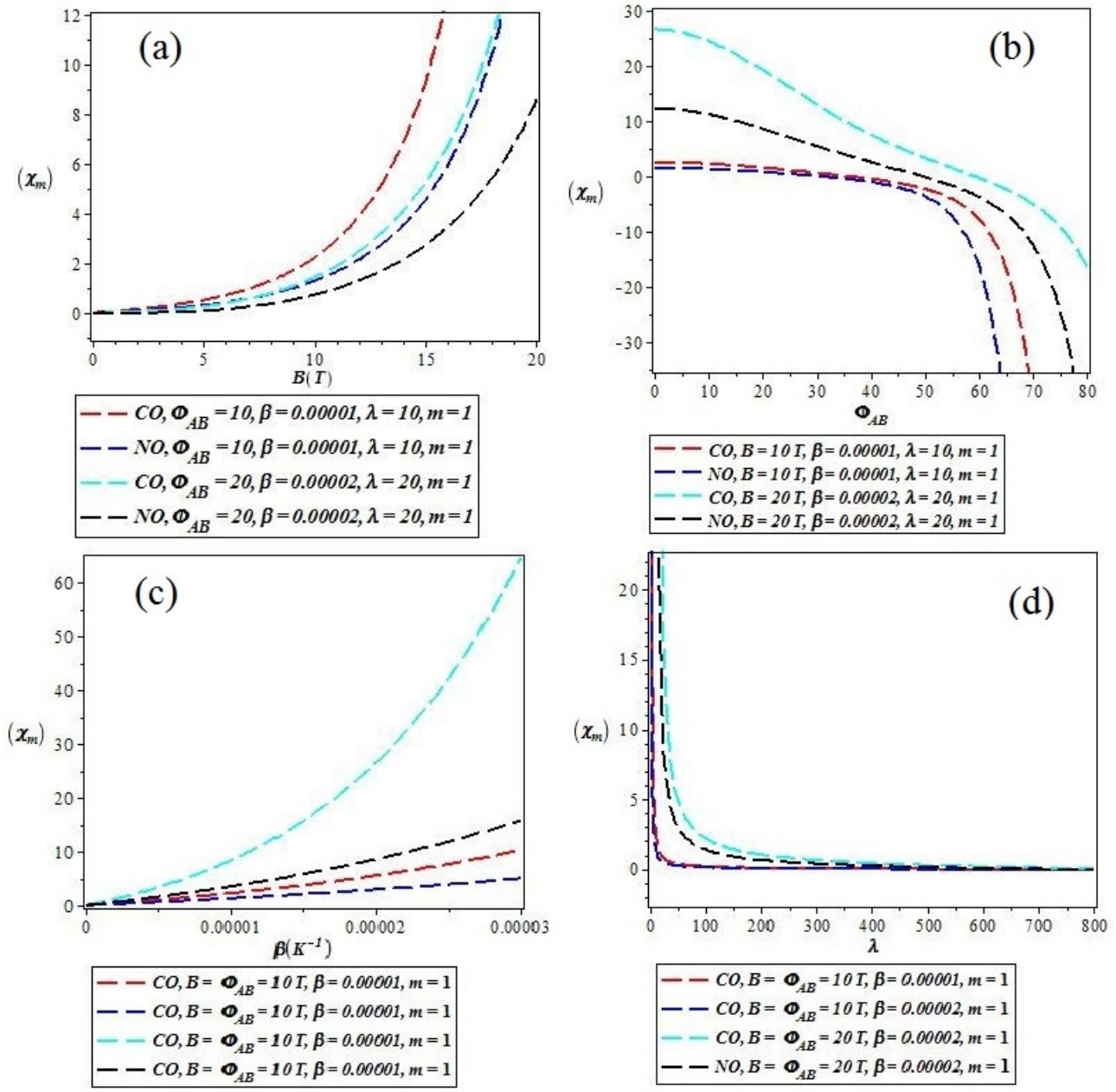

Figure 5. Variation of magnetic susceptibility against: (a) Magnetic flux for CO and NO molecules. (b) AB flux for CO and NO molecules. (c) Inverse temperature parameter (β) for CO and NO molecules (d) λ for CO and NO molecules.

$$\acute{R}_{nm}(z)+\frac{1-z}{z(1-z)}\acute{R}_{nm}(z)$$

$$+\left[\frac{\begin{pmatrix}-(\varepsilon_{nm}+2\Upsilon_0-\Upsilon_1+\Upsilon_3)z^2\\+(2\varepsilon_{nm}+\Upsilon_0-\Upsilon_1-\Upsilon_2)z\\-(\varepsilon_{nm}+\rho_{nm})\end{pmatrix}}{z^2(1-z)^2}\right]R_{nm}(z)=0 \qquad (8)$$

where

$$-\varepsilon_{nm}=\frac{2\mu E_{nm}}{\hbar^2\alpha^2},\ \Upsilon_0=\frac{2\mu \mathrm{D}_e r_e}{\hbar^2\alpha},\ \Upsilon_1=\frac{2\mu r_e^2}{\hbar^2},$$

$$\Upsilon_2=\frac{2\mu w_c}{\hbar\alpha},\ \Upsilon_3=\frac{\mu^2\omega_c^2}{\hbar^2\alpha^2},\ \rho_{nm}=(m+\zeta)^2-\frac{1}{4} \qquad (9)$$

Because Eq. (8) and Eq. (1) of Ref. [48] are the same, we obtain the following parameters:

$$\tilde{\tau}(z)=1-z,\ \sigma(z)=z(1-z),\ \tilde{\sigma}(z)=-(\varepsilon_{nm}-2\Upsilon_0-\Upsilon_1+\Upsilon_3)$$
$$\times z^2+(2\varepsilon_{nm}+\Upsilon_0-\Upsilon_1-\Upsilon_2)z-(\varepsilon_{nm}+\rho_{nm}). \qquad (10)$$

We get $\pi(z)$ by plugging Eq. (10) into Eq. (11) of Ref. [48] as

$$\pi(z)=-\frac{z}{2}\pm\sqrt{(\mathrm{A}_1-k)z^2+(k+\mathrm{A}_2)z+\mathrm{A}_3} \qquad (11)$$

where

$$\mathrm{A}_1=\frac{1}{4}+\varepsilon_{nm}-2\Upsilon_0-\Upsilon_1+\Upsilon_3,$$
$$\mathrm{A}_2=-(2\varepsilon_{nm}+\Upsilon_0-\Upsilon_1-\Upsilon_2),$$

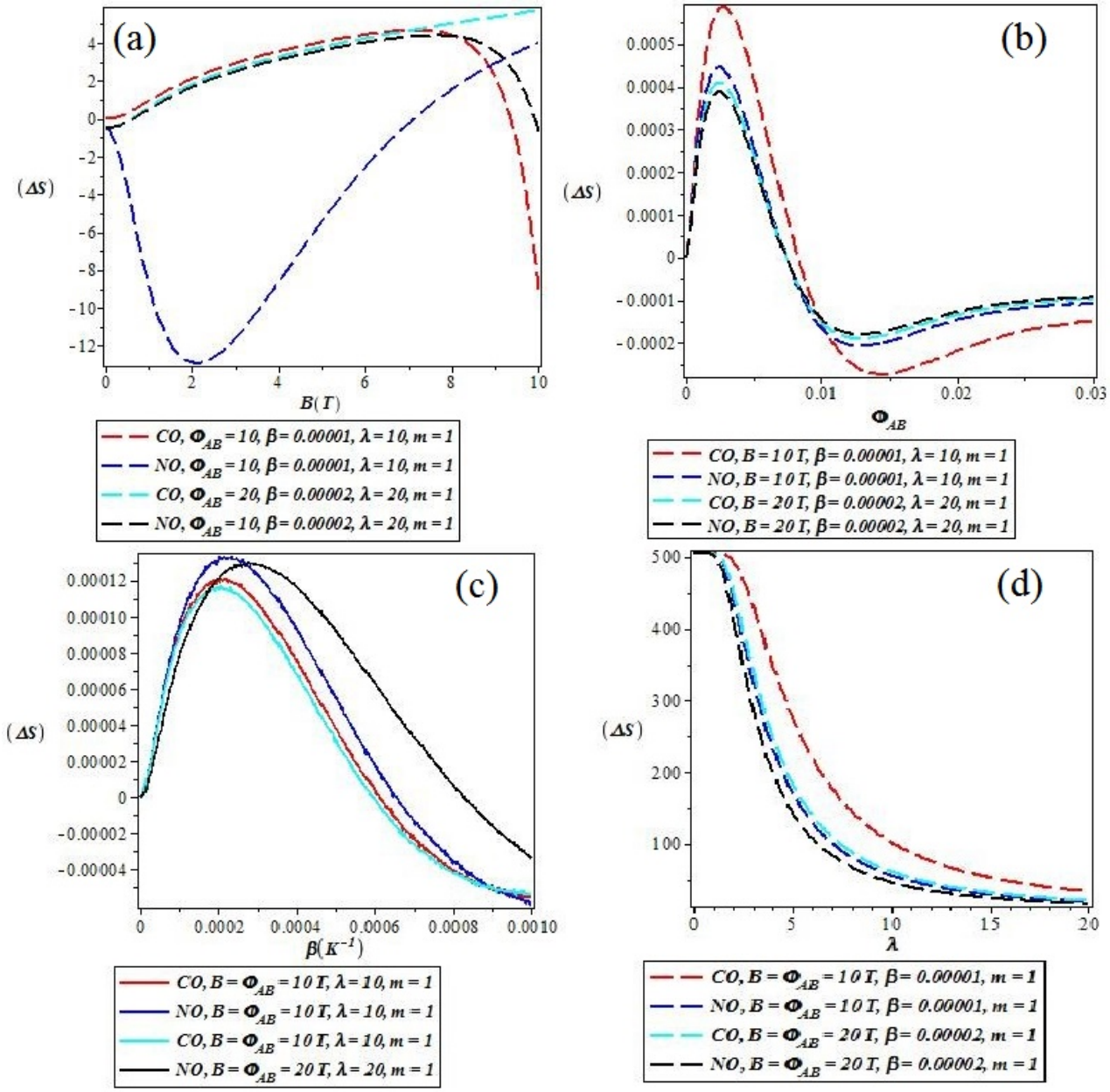

Figure 6. Variation of isothermal magnetocaloric entropy against: (a) Magnetic flux $\mathbf{B}(T)$ for CO and NO molecules. (b) AB flux (Φ_{AB}) for CO and NO molecules. (c) Inverse temperature parameter (β) for CO and NO molecules (d) λ for CO and NO molecules.

$$\mathrm{A}_3 = \varepsilon_{nm} + \rho_{nm}. \tag{12}$$

To calculate k, we set the discriminant in Eq. (11) to zero. As a result, we now have

$$k = -(\mathrm{A}_2 + 2\mathrm{A}_3) \pm 2\sqrt{\mathrm{A}_3}\sqrt{\mathrm{A}_3 + \mathrm{A}_2 + \mathrm{A}_1}. \tag{13}$$

When Eq. (13) is substituted in Eq. (11), $\pi(z)$ is obtained as

$$\pi(z) = -\frac{z}{2} \pm [(\sqrt{\mathrm{A}_3} + \sqrt{\mathrm{A}_3 + \mathrm{A}_2 + \mathrm{A}_1})z - \sqrt{\mathrm{A}_3}], \tag{14}$$

and $\tau(z)$ can be written as

$$\tau(z) = 1 - 2z - 2\sqrt{\mathrm{A}_3}z - 2\sqrt{\mathrm{A}_3 + \mathrm{A}_2 + \mathrm{A}_1}z + 2\sqrt{\mathrm{A}_3}. \tag{15}$$

Also,

$$\acute{\tau}(z) = -2 - 2\sqrt{\mathrm{A}_3} - 2\sqrt{\mathrm{A}_3 + \mathrm{A}_2 + \mathrm{A}_1}. \tag{16}$$

We determine λ by using Eq. (10) from Ref. [48] as

$$\lambda = -\frac{1}{2} - \sqrt{\mathrm{A}_3} - \sqrt{\mathrm{A}_3 + \mathrm{A}_2 + \mathrm{A}_1} - (\mathrm{A}_2 + 2\mathrm{A}_3) - 2\sqrt{\mathrm{A}_3}\sqrt{\mathrm{A}_3 + \mathrm{A}_2 + \mathrm{A}_1}. \tag{17}$$

Equation (10) yields $\acute{\sigma}(z)$ as

$$\acute{\sigma}(z) = -2. \tag{18}$$

We calculate λ_n by substituting Eqs. (15) and (18) into Eq. (13) of Ref. [48] as follows:

Table 1. Diatomic molecular data for this study [2].

Molecule	D_e (eV)	r_e (Å)	α (1/Å)	μ (amu)
CO	10.8451	1.1283	2.2994	6.8607
NO	8.0437	1.1508	2.7534	7.4684

$$\lambda_n = n^2+n+2n\sqrt{\mathrm{A}_3}+2n\sqrt{\mathrm{A}_3+\mathrm{A}_2+\mathrm{A}_1}. \tag{19}$$

We performed arithmetic operations on Eqs. (17) and (19) using Eq.(9), and the resulting equation yields

$$\varepsilon_{nm} = -\rho_{nm}+\frac{1}{4}\left[\frac{\left(n+\frac{1}{2}\right)^2+2\left(n+\frac{1}{2}\right)\varpi}{n+\frac{1}{2}+\sqrt{\frac{1}{4}+\rho_{nm}+\Upsilon_0+\Upsilon_2+\Upsilon_3}}\right] \tag{20}$$

where

$$\varpi = \sqrt{\frac{1}{4}+\rho_{nm}+\Upsilon_0+\Upsilon_2+\Upsilon_3}-\Upsilon_0+\Upsilon_1+\Upsilon_2+\frac{1}{4}+2\rho_{nm}$$

The nonrelativistic analytical solutions of FMP under the influence of external fields can be expressed in the form:

$$E_{nm} = \frac{\alpha^2\hbar^2\rho_{nm}}{2\mu}-\frac{\alpha^2\hbar^2}{8\mu}\left[\frac{\mathfrak{Q}1+\mathfrak{Q}2}{\mathfrak{Q}3}\right]^2 \tag{21}$$

where

$$\mathfrak{Q}1 = \left(n+\frac{1}{2}+\sqrt{\frac{\mu^2\omega_c^2}{\alpha^2\hbar^2}+\frac{2\mu\omega_c}{\alpha\hbar}+\frac{2\mu D_e r_e}{\alpha\hbar^2}+(m+\zeta)^2}\right)^2$$

$$\mathfrak{Q}2 = \frac{-4\mu D_e r_e}{\alpha\hbar^2}+\frac{2\mu r_e^2}{\hbar^2}-\frac{\mu^2\omega_c^2}{\alpha^2\hbar^2}+\rho_{nm}$$

$$\mathfrak{Q}3 = n+\frac{1}{2}+\sqrt{\frac{\mu^2\omega_c^2}{\alpha^2\hbar^2}+\frac{2\mu\omega_c}{\alpha\hbar}+\frac{2\mu D_e r_e}{\alpha\hbar^2}+(m+\zeta)^2}$$

When there is no field, Eq. (21) generates a 3D SE of FMP using the boundary condition $m = l+1/2$,where l is the orbital momentum quantum number

$$E_{nl} = \frac{\alpha^2\hbar^2 l(l+1)}{2\mu}-\frac{\alpha^2\hbar^2}{8\mu}\left[\frac{\mathfrak{Q}4+\mathfrak{Q}5}{\mathfrak{Q}6}\right]^2 \tag{22}$$

where

$$\mathfrak{Q}4 = \left(n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)+\frac{2\mu D_e r_e}{\hbar^2\alpha}}\right)^2$$

$$\mathfrak{Q}5 = -\frac{4\mu D_e r_e}{\hbar^2\alpha}+\frac{2\mu r_e^2}{\hbar^2}+l(l+1)$$

$$\mathfrak{Q}6 = n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)+\frac{2\mu D_e r_e}{\hbar^2\alpha}}$$

We can obtain $\phi(z)$ and $\rho(z)$ by substituting Eqs. (10) and (11) into Eqs. (3) of foundations of special functions and Eq. (3) of basic properties of the hypergeometric type of Ref. [48]:

$$\phi(z) = z^{\sqrt{\varepsilon+\gamma}}(1-z)^{\frac{1}{2}+\sqrt{\frac{1}{4}+\gamma}} \tag{23}$$

$$\rho(z) = z^{2\sqrt{\varepsilon+\gamma}}(1-z)^{2\sqrt{\frac{1}{4}+\gamma}}. \tag{24}$$

To derive the Rodrigues equation, Eqs. (10) and (24) are substituted into Eq (2) of Ref. [48]

$$y(z) = N_{nm}z^{-2\sqrt{\varepsilon+\gamma}}(1-z)^{-2\sqrt{\frac{1}{4}+\gamma}} \times \frac{d^n}{dz^n}\left[z^{n+2\sqrt{\varepsilon+\gamma}}(1-z)^{n+2\sqrt{\frac{1}{4}+\gamma}}\right] \tag{25}$$

where the normalization constant is denoted as N_{nm}. We can express Eq. (25) as

$$P_n^{\left(2\sqrt{\varepsilon+\gamma},2\sqrt{\frac{1}{4}+\gamma}\right)}(1-2z) \tag{26}$$

where Jacobi Polynomials is denoted as $P_n^{(\alpha,\beta)}$.likewise, $\psi_{nm}(z)$ can be expressed as

$$\psi_{nm}(z) = N_{nm}z^{\sqrt{\varepsilon+\gamma}}(1-z)^{\frac{1}{2}+\sqrt{\frac{1}{4}+\gamma}}P_n^{\left(2\sqrt{\varepsilon+\gamma},2\sqrt{\frac{1}{4}+\gamma}\right)}(1-zs). \tag{27}$$

3. Thermomagnetic properties and magnetocaloric effect of FMP

The thermomagnetic properties of CO and NO dimer molecules selected for this study can be calculated using the exact partition function (PF) expressed as [51].

$$Z(\beta,\lambda) = \sum_{n=0}^{\lambda} e^{-\beta E_n},\ \beta = (KT)^{-1}, \tag{28}$$

where λ is an upper bound of the vibrational quantum number calculated by summing the available energy levels. $\beta = 1/KT$, where k and T are Boltzmann constant and absolute temperature, respectively. To account for the PF, the energy eigenvalue of Eq. (21) can be expressed as follows:

$$E_{nm} = Q_1-Q_2\left((n+\delta)+\frac{Q_3}{(n+\delta)}\right)^2 \tag{29}$$

where

$$\begin{cases} Q_1 = \frac{\alpha^2\hbar^2\rho_{nm}}{2\mu},\ Q_2 = \frac{\alpha^2\hbar^2}{8\mu}, \\ \delta = \frac{1}{2}+\sqrt{\frac{\mu^2\omega_c^2}{\alpha^2\hbar^2}+\frac{2\mu\omega_c}{\alpha\hbar}+\frac{2\mu D_e r_e}{\alpha\hbar^2}+(m+\zeta)^2}, \\ Q_3 = -\frac{4\mu D_e r_e}{\alpha\hbar^2}+\frac{2\mu r_e^2}{\hbar^2}-\frac{\mu^2\omega_c^2}{\alpha^2\hbar^2}+\rho_{nm}. \end{cases} \tag{30}$$

Substituting $\rho = n+\delta$ into Eq. (29), we get

$$E_{nm} = -2Q_2Q_3+Q_1-(Q_2\rho^2+\frac{Q_2Q_3^2}{\rho^2}) \tag{31}$$

Table 2. Eigenvalues (eV) of the FMP for CO dimer molecule with **B** and Φ_{AB} flux fields.

m	n	$\mathbf{B} = \Phi_{AB}$=0	**B**=3T, Φ_{AB}=0	**B**=0, Φ_{AB}=3T	$\mathbf{B} = \Phi_{AB}$=3T
0	0	-5.318837025	-4.150194745	-3.417196138	-2.473739598
	1	-5.058113683	-3.934667322	-3.188666520	-2.283097356
	2	-4.806362727	-3.726604934	-2.968313140	-2.099377814
	3	-4.563344245	-3.525832593	-2.755922950	-1.922422312
-1	0	-5.315525135	-4.147294597	-3.565478636	-2.605276128
	1	-5.054858606	-3.931810690	-3.334469566	-2.412701182
	2	-4.803163035	-3.723790861	-3.111697356	-2.227090652
	3	-4.560198567	-3.523060159	-2.896946940	-2.048284648
1	0	-5.315525135	-4.147294597	-3.263528448	-2.337279848
	1	-5.054858606	-3.931810690	-3.037562766	-2.148639064
	2	-4.803163035	-3.723790861	-2.819710760	-1.966877834
	3	-4.560198567	-3.523060159	-2.609761467	-1.791838807

Now, the substitution of Eq. (31) into Eq. (28) yields:

$$z(\beta,\lambda) = \sum_{n=0}^{\lambda} e^{-\beta(-2Q_1Q_2+Q_1)-(Q_2\rho^2+\frac{Q_2Q_3^2}{\rho^2})} \qquad (32)$$

The summation in Eq. (28) is changed into an integral of the form

$$z(\beta,\lambda) = e^{\beta(2Q_2Q_3-Q_1)} \int_0^{\lambda} e^{Q_2\rho^2+\frac{Q_2Q_3^2}{\rho^2}} d\rho \qquad (33)$$

The PF can be evaluated using Maple software as follows:

$$z(\beta) = e^{2\beta Q_2Q_3-\beta Q_1}\sqrt{\pi}\left(\frac{\mathfrak{Q}7+\mathfrak{Q}8}{4\sqrt{-\beta Q_2}}\right) \qquad (34)$$

where

$$\mathfrak{Q}7 = e^{2\sqrt{-Q_2Q_3^2\beta}\sqrt{-\beta Q_2}}$$

$$\times\left(erf\left(\sqrt{-\beta Q_2}\lambda + \frac{\sqrt{-Q_2Q_3^2\beta}}{\lambda}\right) - 1\right)$$

$$\mathfrak{Q}8 = \frac{1+erf\left(\sqrt{-\beta Q_2}\lambda - \frac{\sqrt{-Q_2Q_3^2\beta}}{\lambda}\right)}{e^{2\sqrt{-Q_2Q_3^2\beta}\sqrt{-\beta Q_2}}}$$

Using Eq. (34), the thermo-magnetic properties [28] and magnetocaloric effect [40] of FMP under influence of magnetic and AB flux fields of CO and NO dimer molecules can be calculated as follows:

(a) The magnetization at finite temperature is given as

$$M(\beta,B,\Phi_{AB}) = \frac{1}{\beta}\left(\frac{1}{Z(\beta,B,\Phi_{AB})}\right)\frac{\partial}{\partial B}Z(\beta,B,\Phi_{AB}) \qquad (35)$$

Table 3. Eigenvalues (eV) of the FMP for NO dimer molecule with **B** and Φ_{AB} flux fields.

m	n	$\mathbf{B} = \Phi_{AB}$=0	**B**=3T, Φ_{AB}=0	**B**=0, Φ_{AB}=3T	$\mathbf{B} = \Phi_{AB}$=3T
0	0	-3.980303243	-3.073281966	-1.646856516	-0.998343797
	1	-3.729780426	-2.866744062	-1.443134820	-0.828281092
	2	-3.490118686	-2.669309679	-1.248902712	-0.666380549
	3	-3.260972966	-2.480725840	-1.063870249	-0.512422934
-1	0	-3.976179138	-3.069650430	-1.826354134	-1.159405211
	1	-3.725740642	-2.863177390	-1.619097369	-0.986553256
	2	-3.486160706	-2.665806154	-1.421432044	-0.821934442
	3	-3.257094366	-2.477283842	-1.233064198	-0.665327029
1	0	-3.976179138	-3.069650430	-1.461271281	-0.831563395
	1	-3.725740642	-2.863177390	-1.261192996	-0.664381461
	2	-3.486160706	-2.665806154	-1.070499628	-0.505288545
	3	-3.257094366	-2.477283842	-0.888905372	-0.354068001

(b) Magnetic susceptibility at finite temperature is given as

$$\chi_m(\beta, \mathrm{B}, \Phi_{\mathrm{AB}}) = \frac{\partial M(\beta, \mathrm{B}, \Phi_{\mathrm{AB}})}{\partial \mathrm{B}} \tag{36}$$

(c) The entropy of the thermo-magnetic system is given as

$$\ln Z(\beta, \mathrm{B}, \Phi_{\mathrm{AB}}) - \beta \frac{\partial}{\partial \beta} \ln Z(\beta, \mathrm{B}, \Phi_{\mathrm{AB}}) \tag{37}$$

(d) Isothermal magnetocaloric entropy

$$\Delta s = S(B \neq 0, T) - S(B = 0, T) \tag{38}$$

4. Numerical results

In this study, we obtain analytical solutions of the SE with FMP for the CO and NO dimer molecules in the presence of external magnetic and AB flux fields. We use Eq. (21) to calculate the energy spectra of FMP for the selected diatomic molecules based on the spectroscopic data obtained from [2]. The heterogeneous DMs are selected because of the purposes which they serve in various aspects of molecular and chemical physics. The spectroscopic parameters adopted for this study are shown in Table 1. Here, we have implemented the conversions: 1 amu=931.494028 MeV/c^2 and $\hbar c$=1973.29eV$\mathring{A}$ [2]. The calculated explicit bound state energies for the selected DMs, both with and without the **B** and Φ_{AB} fields with various quantum states are presented in Tables 2 and 3. When both fields are switched off, i.e.$\mathbf{B} = \Phi_{\mathrm{AB}}$, there exists degeneracy in the energy spectra as the energy increase with the increase in quantum states. Subjecting the diatomic molecule system to a magnetic field only cannot eradicates the degeneracy but increases the energy spectra as the quantum states are increased. Hence, for a fixed m, as the quantum number n increases, the individual diatomic molecule becomes attractive. By switching on only the Φ_{AB} field, the degeneracy is gradually removed as the energy spectra of the individual molecule increase with increased quantum states. However, when both fields are activated, the combined effects of the two fields outweigh the individual effects; thereby removing degeneracy completely from the system and leading to a significant shift in the energy spectra as the quantum state increases.

The shape of the potential for the selected molecules is presented in Fig. 1. Figure 2 represents a plot of energy spectra for various values of the Φ_{AB} field of the selected DMs. The plots show that the energy spectra increase gradually and uniformly as **B** is increased. Figure 3 depicts a plot of the FMP energy spectra against the Φ_{AB} flux field. For the diatomic molecule systems considered, the energy spectra followed a similar trend and increased as the Φ_{AB} flux field increased.

Figures 4 (a) and (c) show that the PF increases as the magnetic field strength **B** and inverse temperature parameter (β) increase, whereas the PF remains invariant at lower maximum energy (λ) and begins to increase as λ increases as shown in Fig 4 (d) for the selected DMs. Figure 4 (b) shows that the PF decreases slowly in a uniform manner to a point where the Φ_{AB} is between 45 T and 55 T depending on the molecule parameter and begins to increase.

The magnetic susceptibility in Fig. 5 (a) and (c) increases as the magnetic field and temperature-dependent term are increased. In Fig 5 (b), the magnetic susceptibility decreases slowly to the origin and begins to rapidly decrease from the origin as the AB is increased. The magnetic susceptibility shows a concave shape from the origin and remains invariant as the maximum energy increases.

In Figure 6 (a), the isothermal magnetocaloric entropy increases from the origin to a maximum turning point and begins to decrease as the **B** increases for various magnitudes of the AB field, temperature-dependent term, and maximum energy term for CO and NO molecules. At a lower magnitude of the varying parameter, the NO molecule decreases to 2 T and begins to increase as the magnetic field strength is increased. This implies that the introduction of the magnetic field into the system causes the isothermal entropy to change in a direction depending on the magnitude of the magnetic field strength and other varying parameters. In Figure 6 (b), the isothermal entropy displayed parabolic concave curves with varying degrees of minimum and maximum turning points. The isothermal magnetocaloric entropy peaked from the origin and increased to various maximum turning points as the AB field increased for the CO and NO molecules before decreasing exponentially to various minimum turning points and continuing to increase slowly. The variation of the magnetic entropy shows a complete waveform pattern with the external magnetic field and a sinusoidal waveform showing an increasing and decreasing trend with the AB field, implying that an external field can be used to control the behavior of the magnetocaloric molecules. In Figure 6 (c), the isothermal magnetocaloric entropy peaked from the origin and increased to various maximum turning points and begins to decrease exponentially as the temperature-dependent term increases for the selected DMs. This shows that at a higher temperature, the increases and decreases at a lower temperature, indicating that the variation of temperature with a varying magnitude of magnetic and AB fields operate as a controlling factor for the cooling or heating of the MCE. Figure 6(d) shows that the isothermal magnetocaloric entropy decreases exponentially as the maximum energy term is increased.

5. Conclusion

This research focused on the magnetocaloric effect, thermomagnetic properties, and energy spectra of CO and NO diatomic molecules subjected to varying magnitudes of magnetic and AB flux fields. The SE with FMP is solved using the NU technique under the influence of magnetic and AB flux fields to obtain the energy equation and wave function. The derived energy eigenvalue is used to calculate the numerical energy spectra and thermomagnetic properties of the selected diatomic molecules. The results show that the cumulative impacts of the magnetic and AB flux fields completely remove the degeneracy on the energy spectra of the dimer molecules. Also, the net effect of the combined field with temperature acts as a controlling factor for the cooling or heating of the magnetocaloric effect. This research has the potential to be applied in molecular physics and studies on MCE for several molecules.

Data Availability Statement
Data sharing does not apply to this article as datasets were generated during the current study.

Conflict of interest statement:
The authors declare that they have no conflict of interest.

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