

Classifying accidental symmetries in multi-Higgs doublet models

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The potential of n -Higgs doublet models (n HDMs) contains a large number of $SU(2)_L$ -preserving accidental symmetries as subgroups of the symplectic group $Sp(2n)$. To classify these, we introduce prime invariants and irreducible representations in bilinear field space that enable us to explicitly construct accidentally symmetric n HDM potentials. We showcase the classifications of symmetries and present the relationship among the theoretical parameters of the scalar potential for the following: (i) the two Higgs doublet model (2HDM), and (ii) the three Higgs doublet model (3HDM). We recover the maximum number of 13 accidental symmetries for the 2HDM potential, and *for the first time*, we present the complete list of 40 accidental symmetries for the 3HDM potential.

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I. INTRODUCTION

The discovery of the Higgs particle at the CERN Large Hadron Collider (LHC) [1,2], which was previously predicted by the Standard Model (SM) of particle physics [3–7], generated renewed interest in beyond the SM (BSM) Higgs physics. This is corroborated by the fact that the SM fails to address several key questions, such as the origin of the observed matter-antimatter asymmetry and the dark matter relic abundance in the Universe.

There is a plethora of well-motivated new physics models with additional Higgs scalars that have been introduced to solve these problems [8–13]. To distinguish such models, one usually employs symmetry transformations that leave the particular model invariant. These symmetries impose constraints over the theoretical parameters of the models and thus enhance their predictability to be probed in future experiments.

In this paper we construct potentials of multi-Higgs doublet models (n HDMs) with n scalar doublets based on $SU(2)_L$ -preserving accidental symmetries. These symmetries can be realized in two sets: (i) as continuous symmetries, and (ii) as discrete symmetries (Abelian and non-Abelian symmetry groups). To find continuous symmetries, we present an algorithmic method that provides the full list of proper, improper, and semisimple subgroups for

any given integer n . We also include all known discrete symmetries in n HDM potentials [14–24]. Previous analyses led to a maximum of 13 accidental symmetries for the two Higgs doublet model (2HDM) potential, where the maximal symmetry group is $G_{2\text{HDM}}^\Phi = Sp(4)/Z_2 \otimes SU(2)_L$ [25]. Here, we extend this theoretical framework to n HDM potentials based on the maximal symmetric group $Sp(2n)/Z_2 \otimes SU(2)_L$ [26,27]. The maximally symmetric n HDM (MS- n HDM) can provide natural SM alignment that exhibits quartic coupling unification up to the Planck scale [26–29].

Identifying the symplectic group $Sp(2n)$ as the maximal symmetry group allows us to classify all $SU(2)_L$ -preserving accidental symmetries in n HDM potentials. We introduce *prime invariants* to construct accidentally symmetric potentials in terms of fundamental building blocks that respect the symmetries. In the same context, we use irreducible representations to derive all potentials that are invariant under non-Abelian discrete symmetries.

The layout of this paper is as follows. In Sec. II, we define the n HDMs in the bilinear scalar field formalism. Given that $Sp(2n)$ is the maximal symmetry of the n HDM potential, we adopt the biadjoint representation of this group which becomes relevant to this bilinear formalism. In Sec. III, we start with classifying continuous symmetries for n HDM potentials. As illustrative examples, we classify all accidentally symmetric potentials for the 2HDM and the three Higgs doublet model (3HDM). Then, we introduce prime invariants to build potentials that are invariant under $SU(2)_L$ -preserving continuous symmetries. In Sec. IV, we discuss possible and known discrete symmetries for n HDM potentials and recover the discrete symmetries for the 2HDM and the 3HDM cases [21,23,24]. This section also includes our approach to building 3HDM potentials with

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the help of irreducible representations of discrete symmetries. Having discussed the classifications of symmetries, we provide the list of all $SU(2)_L$ -preserving accidental symmetries for the 2HDM and the 3HDM potentials including the relationships among the theoretical parameters of the scalar potentials. Section V contains our conclusions. Finally, technical details are delegated to Appendixes A, B, C, and D.

II. BILINEAR FORMALISM AND THE MAXIMAL SYMMETRY $SP(2n)$

The n HDMs contain n scalar doublet fields, $\phi_i (i = 1, 2, \dots, n)$, which all share the same $U(1)_Y$ -hypercharge quantum number, i.e., $Y_{\phi_i} = 1/2$. The most general form of the n HDM potential may conventionally be expressed as follows [30]:

$$V_n = \sum_{i,j=1}^n m_{ij}^2 (\phi_i^\dagger \phi_j) + \sum_{i,j,k,l=1}^n \lambda_{ijkl} (\phi_i^\dagger \phi_j) (\phi_k^\dagger \phi_l), \quad (2.1)$$

with $\lambda_{ijkl} = \lambda_{klji}$. In general, the $SU(2)_L \times U(1)_Y$ invariant n HDM potential contains n^2 physical mass terms along with $n^2(n^2 + 1)/2$ physical quartic couplings.

An equivalent way to write the n HDM potential is based on the so-called bilinear field formalism [53,31–34]. To this end, we first define a $4n$ -dimensional ($4n$ -D) complex Φ_n multiplet as

$$\Phi_2 = \begin{pmatrix} \phi_1 \\ \phi_2 \\ i\sigma^2 \phi_1^* \\ i\sigma^2 \phi_2^* \end{pmatrix}, \quad \Phi_3 = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ i\sigma^2 \phi_1^* \\ i\sigma^2 \phi_2^* \\ i\sigma^2 \phi_3^* \end{pmatrix}, \dots, \Phi_n = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \cdot \\ \cdot \\ \cdot \\ i\sigma^2 \phi_1^* \\ i\sigma^2 \phi_2^* \\ i\sigma^2 \phi_3^* \\ \cdot \\ \cdot \\ \cdot \end{pmatrix}, \quad (2.2)$$

where $\sigma^{1,2,3}$ are the Pauli matrices and $i\sigma^2 \phi_i^*$ (with $i = 1, 2, \dots, n$) are the $U(1)_Y$ hypercharge conjugate of ϕ_i . Observe that the Φ_n multiplet transforms covariantly under an $SU(2)_L$ gauge transformation as

$$\Phi_n \rightarrow U_L \Phi_n, \quad U_L \in SU(2)_L. \quad (2.3)$$

Note that U_L is the 2×2 unitary matrix that may also be represented as $\sigma^0 \otimes \mathbf{1}_n \otimes U_L$ in the Φ_n space.

Additionally, the Φ_n multiplet satisfies the Majorana-type property [34],

$$\Phi_n = C \Phi_n^*, \quad (2.4)$$

where $C = \sigma^2 \otimes \mathbf{1}_n \otimes \sigma^2$ ($C = C^{-1} = C^*$) is the charge conjugation operator and $\mathbf{1}_n$ is the $n \times n$ identity matrix.

With the help of the Φ_n multiplet, we may now define the bilinear field vector [25,33,34],

$$R_n^A \equiv \Phi_n^\dagger \Sigma_n^A \Phi_n, \quad (2.5)$$

with $A = 0, 1, 2, \dots, n(2n - 1) - 1$. Notice that $n(2n - 1)$ -vector R_n^A is invariant under $SU(2)_L$ transformations thanks to (2.3).

The matrices Σ_n^A have $4n \times 4n$ elements and can be expressed in terms of double tensor products as

$$\Sigma_n^A = (\sigma^0 \otimes t_S^a \otimes \sigma^0, \quad \sigma^i \otimes t_A^b \otimes \sigma^0), \quad (2.6)$$

where t_S^a and t_A^b are the symmetric and antisymmetric matrices of the $SU(n)$ symmetry generators, respectively. Specifically, for the case of the 2HDM, the following six matrices may be defined:

$$\begin{aligned} \Sigma_2^{0,1,3} &= \frac{1}{2} \sigma^0 \otimes \sigma^{0,1,3} \otimes \sigma^0, & \Sigma_2^2 &= \frac{1}{2} \sigma^3 \otimes \sigma^2 \otimes \sigma^0, \\ \Sigma_2^4 &= -\frac{1}{2} \sigma^2 \otimes \sigma^2 \otimes \sigma^0, & \Sigma_2^5 &= -\frac{1}{2} \sigma^1 \otimes \sigma^2 \otimes \sigma^0. \end{aligned} \quad (2.7)$$

Correspondingly, for the 3HDM, we have the following 15 matrices:

$$\begin{aligned} \Sigma_3^{0,1,2,3,7,8} &= \frac{1}{2} \sigma^0 \otimes G^{0,1,4,6,3,8} \otimes \sigma^0, \\ \Sigma_3^{4,5,6} &= \frac{1}{2} \sigma^3 \otimes G^{2,5,7} \otimes \sigma^0, \\ \Sigma_3^{9,10,11} &= \frac{1}{2} \sigma^2 \otimes G^{2,5,7} \otimes \sigma^0, \\ \Sigma_3^{12,13,14} &= \frac{1}{2} \sigma^1 \otimes G^{2,5,7} \otimes \sigma^0, \end{aligned} \quad (2.8)$$

where G^i are the standard Gell-Mann matrices of $SU(3)$ [35]. Note that the Σ_n^A matrices satisfy the property

$$C^{-1} \Sigma_n^A C = (\Sigma_n^A)^T, \quad (2.9)$$

which means that Σ_n^A are C even.

Consequently, the vectors R_2^A and R_3^A for the 2HDM and the 3HDM cases are given by

$$R_2^A = \begin{pmatrix} \phi_1^\dagger \phi_1 + \phi_2^\dagger \phi_2 \\ \phi_1^\dagger \phi_2 + \phi_2^\dagger \phi_1 \\ -i[\phi_1^\dagger \phi_2 - \phi_2^\dagger \phi_1] \\ \phi_1^\dagger \phi_1 - \phi_2^\dagger \phi_2 \\ -[\phi_1^\dagger i\sigma^2 \phi_2 - \phi_2^\dagger i\sigma^2 \phi_1^*] \\ i[\phi_1^\dagger i\sigma^2 \phi_2 + \phi_2^\dagger i\sigma^2 \phi_1^*] \end{pmatrix},$$

$$R_3^A = \begin{pmatrix} \phi_1^\dagger \phi_1 + \phi_2^\dagger \phi_2 + \phi_3^\dagger \phi_3 \\ \phi_1^\dagger \phi_2 + \phi_2^\dagger \phi_1 \\ \phi_1^\dagger \phi_3 + \phi_3^\dagger \phi_1 \\ \phi_2^\dagger \phi_3 + \phi_3^\dagger \phi_2 \\ -i[\phi_1^\dagger \phi_2 - \phi_2^\dagger \phi_1] \\ -i[\phi_1^\dagger \phi_3 - \phi_3^\dagger \phi_1] \\ -i[\phi_2^\dagger \phi_3 - \phi_3^\dagger \phi_2] \\ \phi_1^\dagger \phi_1 - \phi_2^\dagger \phi_2 \\ \frac{1}{\sqrt{3}}[\phi_1^\dagger \phi_1 + \phi_2^\dagger \phi_2 - 2\phi_3^\dagger \phi_3] \\ -[\phi_1^\dagger i\sigma^2 \phi_2 - \phi_2^\dagger i\sigma^2 \phi_1^*] \\ -[\phi_1^\dagger i\sigma^2 \phi_3 - \phi_3^\dagger i\sigma^2 \phi_1^*] \\ -[\phi_2^\dagger i\sigma^2 \phi_3 - \phi_3^\dagger i\sigma^2 \phi_2^*] \\ i[\phi_1^\dagger i\sigma^2 \phi_2 + \phi_2^\dagger i\sigma^2 \phi_1^*] \\ i[\phi_1^\dagger i\sigma^2 \phi_3 + \phi_3^\dagger i\sigma^2 \phi_1^*] \\ i[\phi_2^\dagger i\sigma^2 \phi_3 + \phi_3^\dagger i\sigma^2 \phi_2^*] \end{pmatrix}. \quad (2.10)$$

With the aid of the $n(2n-1)$ -dimensional vectors R_n^A , the potential V_n for an n HDM can be written in the quadratic form as

$$V_n = -\frac{1}{2} M_A^n R_n^A + \frac{1}{4} L_{AA'}^n R_n^A R_n^{A'}, \quad (2.11)$$

where M_A^n is the $1 \times n(2n-1)$ -dimensional mass matrix and $L_{AA'}^n$ is a quartic coupling matrix with $n(2n-1) \times n(2n-1)$ entries. Evidently, for a $U(1)_Y$ -invariant n HDM potential, the first n^2 elements of M_A^n and $n^2 \times n^2$ elements of $L_{AA'}^n$ are only relevant, since the other $U(1)_Y$ -violating components vanish. The general 2HDM and 3HDM potentials with their corresponding M_A^n and $L_{AA'}^n$ are presented in Appendix A.

The gauge-kinetic term of the Φ_n multiplet is given by

$$T_n = \frac{1}{2} (D_\mu \Phi_n)^\dagger (D^\mu \Phi_n), \quad (2.12)$$

where the covariant derivative in the Φ_n space is

$$D_\mu = \sigma^0 \otimes \mathbf{1}_n \otimes (\sigma^0 \partial_\mu^0 + ig_w W_\mu^i \sigma^i / 2) + \sigma^3 \otimes \mathbf{1}_n \otimes i \frac{g_Y}{2} B_\mu \sigma^0. \quad (2.13)$$

In the limit $g_Y \rightarrow 0$, the gauge-kinetic term T_n is invariant under $Sp(2n)/Z_2 \otimes SU(2)_L$ transformations of the Φ_n multiplet. In general, the maximal symmetry group acting on the Φ_n space in the n HDM potentials is

$$G_{n\text{-HDM}}^{\Phi_n} = Sp(2n)/Z_2 \otimes SU(2)_L,$$

which leaves the local $SU(2)_L$ gauge kinetic term of Φ_n canonical. The local $SU(2)_L$ group generators can be represented as $\sigma^0 \otimes \mathbf{1}_n \otimes (\sigma^{1,2,3}/2)$, which commute with all generators of the $Sp(2n)$ group.

Let us turn our attention to the $Sp(2n)$ generators K_n^B , with $B = 0, 1, \dots, n(2n+1) - 1$. They satisfy the important relation [25]

$$C^{-1} K_n^B C = -K_n^{B*} = -(K_n^B)^T, \quad (2.14)$$

which implies that K_n^B are C odd. The $Sp(2n)$ generators may conveniently be expressed in terms of double tensor products as [36]

$$K_n^B = (\sigma^0 \otimes t_A^b \otimes \sigma^0, \sigma^i \otimes t_S^a \otimes \sigma^0), \quad (2.15)$$

where t_S^a (t_A^b) are the symmetric (antisymmetric) generators of the $SU(n)$ symmetry group. For instance, the ten generators of $Sp(4)$ are [25]

$$K_2^{0,1,3} = \frac{1}{2} \sigma^3 \otimes \sigma^{0,1,3} \otimes \sigma^0, \quad K_2^2 = \frac{1}{2} \sigma^0 \otimes \sigma^2 \otimes \sigma^0, \\
 K_2^{4,5,8} = \frac{1}{2} \sigma^1 \otimes \sigma^{0,3,1} \otimes \sigma^0, \quad K_2^{6,7,9} = \frac{1}{2} \sigma^2 \otimes \sigma^{0,3,1} \otimes \sigma^0. \quad (2.16)$$

Likewise, the $Sp(6)$ group has 21 generators, which are

$$K_3^{0,1,2,3,4,5} = \frac{1}{2} \sigma^3 \otimes G^{0,1,3,4,6,8} \otimes \sigma^0, \\
 K_3^{6,7,8} = \frac{1}{2} \sigma^0 \otimes G^{2,5,7} \otimes \sigma^0, \\
 K_3^{9,10,11,12,13,14} = \frac{1}{2} \sigma^1 \otimes G^{0,1,3,4,6,8} \otimes \sigma^0, \\
 K_3^{15,16,17,18,19,20} = \frac{1}{2} \sigma^2 \otimes G^{0,1,3,4,6,8} \otimes \sigma^0. \quad (2.17)$$

It is interesting to state the Lie commutators between the Σ_n^A and K_n^B generators,

$$[K_n^B, \Sigma_n^I] = 2if_n^{BIJ} \Sigma_n^J, \quad (2.18)$$

where $I, J = 1, \dots, n(2n-1) - 1$ and f_n^{BIJ} is a subset of the structure constants of the $SU(2n)$ group. Employing (2.18), we may define the $Sp(2n)$ generators in the

biadjoint representation (i.e., the adjoint representation in the bilinear formalism) as

$$(T_n^B)_{IJ} = -if_n^{BIJ} = \text{Tr}([\Sigma_n^I, K_n^B]\Sigma_n^J). \quad (2.19)$$

Note that the dimensionality of the biadjoint representation differs from the standard adjoint representation. The former representation has $(2n^2 - n - 1) \times (2n^2 - n - 1)$ dimensions, whereas the latter has $n(2n + 1) \times n(2n + 1)$ dimensions [37–40]. The generators of T_n^B for Sp(4) and Sp(6) corresponding to the 2HDM and 3HDM are presented in Appendix B.

Knowing that Sp($2n$) is the maximal symmetry group allows us to classify all SU(2)_L-preserving accidental symmetries of n HDM potentials. These symmetries can be grouped into two categories: (i) continuous symmetries, and (ii) discrete symmetries (Abelian and non-Abelian symmetry groups). In the next section, we demonstrate the structure of continuous symmetries and prime invariants for building n HDM potentials.

III. CONTINUOUS SYMMETRIES AND PRIME INVARIANTS

The symplectic group Sp($2n$) acts on the Φ_n space, such that the bilinear vector R_n^A transforms in the biadjoint representation of Sp($2n$) defined in (2.18) and (2.19). It is therefore essential to consider the maximal subgroups of Sp($2n$). Then, the accidental maximal subgroups would be the combinations of smaller symplectic groups, such as [41]

$$\text{Sp}(2n) \supset \text{Sp}(2p) \otimes \text{Sp}(2q), \quad (3.1)$$

where $p + q = n$. The other maximal subgroup is

$$\text{Sp}(2n) \supset \text{SU}(n) \otimes \text{U}(1). \quad (3.2)$$

The breaking pattern of SU(n) in the maximal subgroups are

$$\text{SU}(n) \supset \text{SU}(p) \otimes \text{SU}(q) \otimes \text{U}(1) \quad (3.3)$$

$$\supset \text{Sp}(2k) \quad (3.4)$$

$$\supset \text{SO}(n), \quad (3.5)$$

with $p + q + 1 = n$ and $n \leq 2k$. The breaking pattern for SO(n) is

$$\text{SO}(n) \supset \text{SO}(p) \otimes \text{SO}(q), \quad (3.6)$$

where $p + q = n$. Note that local isomorphisms should also be taken into account, such as

$$\text{SO}(3) \cong \text{SU}(2) \cong \text{Sp}(2),$$

$$\text{SO}(4) \cong \text{SU}(2) \otimes \text{SU}(2),$$

$$\text{SO}(5) \cong \text{Sp}(4),$$

$$\text{SO}(6) \cong \text{SU}(4).$$

Following this procedure, it is straightforward to identify all accidental continuous symmetries for n HDM potentials. For the simplest case, i.e., that of the 2HDM, the above breaking chain gives rise to the following continuous symmetries [25]:

$$(a) \text{Sp}(4) \cong \text{SO}(5),$$

$$(b) \text{Sp}(2) \otimes \text{Sp}(2) \cong \text{SO}(4),$$

$$(c) \text{Sp}(2) \cong \text{SO}(3),$$

$$(d) \text{SU}(2)_{\text{HF}} \cong \text{O}(3) \otimes \text{O}(2),$$

$$(e) \text{SO}(2)_{\text{HF}} \cong \text{Z}_2 \otimes [\text{O}(2)]^2,$$

$$(f) \text{U}(1)_{\text{PQ}} \otimes \text{Sp}(2) \cong \text{O}(2) \otimes \text{O}(3),$$

$$(g) \text{U}(1)_{\text{PQ}} \otimes \text{U}(1)_Y \cong \text{O}(2) \otimes \text{O}(2), \quad (3.7)$$

where HF indicates Higgs family symmetries that only involve the elements of $\Phi = (\phi_1, \phi_2, \dots, \phi_n)^T$ and not their complex conjugates. In the case of 3HDM, the maximal symmetry is Sp(6), so in addition to all symmetries in (3.7) we find

$$(h) \text{Sp}(6),$$

$$(i) \text{Sp}(4) \otimes \text{Sp}(2),$$

$$(j) \text{Sp}(2) \otimes \text{Sp}(2) \otimes \text{Sp}(2),$$

$$(k) \text{SU}(3) \otimes \text{U}(1),$$

$$(l) \text{SO}(3). \quad (3.8)$$

We may now construct accidentally symmetric n HDM potentials in terms of fundamental building blocks that respect the symmetries. To this end, we introduce the invariants S_n , D_n^2 , and T_n^2 . In detail, S_n is defined as

$$S_n = \Phi_n^\dagger \Phi_n, \quad (3.9)$$

which is invariant under both the SU(n)_L ⊗ U(1)_Y gauge group and Sp($2n$). Moreover, we define the SU(2)_L-covariant quantity D_n^a in the HF space as

$$D_n^a = \Phi^\dagger \sigma^a \Phi. \quad (3.10)$$

Under an SU(2)_L gauge transformation, $D_n^a \rightarrow D_n'^a = O^{ab} D_n^b$, where $O \in \text{SO}(3)$. Hence, the quadratic quantity $D_n^2 \equiv D_n^a D_n^a$ is both gauge and SU(n) invariant. Finally, we define the auxiliary quantity T_n in the HF space as

$$T_n = \Phi \Phi^T, \quad (3.11)$$

which transforms as a triplet under $SU(2)_L$, i.e., $T_n \rightarrow T'_n = U_L T_n U_L^\dagger$. As a consequence, a proper prime invariant may be defined as $T_n^2 \equiv \text{Tr}(TT^*)$, which is also both gauge and $SO(n)$ invariant.

In addition to the above maximal prime invariants, it is useful to define minimal invariants. For instance, prime invariants that respect $Sp(2)$ can be derived from the doublets $\begin{pmatrix} \phi_i \\ i\sigma^2 \phi_i^* \end{pmatrix}$ and $\begin{pmatrix} \phi_j \\ i\sigma^2 \phi_j^* \end{pmatrix}$,

$$\begin{aligned} S_{ij} &= (\phi_i^\dagger, -i\phi_i^\dagger \sigma^2) \begin{pmatrix} \phi_j \\ i\sigma^2 \phi_j^* \end{pmatrix} = \phi_i^\dagger \phi_j + \phi_j^\dagger \phi_i, \\ S'_{ij} &= (\phi_i^\dagger, -i\phi_j^\dagger \sigma^2) \begin{pmatrix} \phi_i \\ i\sigma^2 \phi_j^* \end{pmatrix} = \phi_i^\dagger \phi_i + \phi_j^\dagger \phi_j. \end{aligned} \quad (3.12)$$

Likewise, to obtain minimal $SU(2) \otimes U(1)$ invariants from $\begin{pmatrix} \phi_i \\ \phi_j \end{pmatrix}$ and $\begin{pmatrix} \phi_i \\ i\sigma^2 \phi_j^* \end{pmatrix}$, we define

$$\begin{aligned} D_{ij}^a &= (\phi_i^\dagger, \phi_j^\dagger) \sigma^a \begin{pmatrix} \phi_i \\ \phi_j \end{pmatrix} = \phi_i^\dagger \sigma^a \phi_i + \phi_j^\dagger \sigma^a \phi_j = D_{ji}^a, \\ D_{ij}^{\prime a} &= (\phi_i^\dagger, -i\phi_j^\dagger \sigma^2) \sigma^a \begin{pmatrix} \phi_i \\ i\sigma^2 \phi_j^* \end{pmatrix} \\ &= \phi_i^\dagger \sigma^a \phi_i - \phi_j^\dagger \sigma^a \phi_j = -D_{ji}^{\prime a}, \end{aligned} \quad (3.13)$$

where the identity $\sigma^2 \sigma^a \sigma^2 = -(\sigma^a)^\dagger$ has been used.

By analogy, to construct an $SO(2)$ -invariant expression from the doublet $\begin{pmatrix} \phi_i \\ \phi_j \end{pmatrix}$, we may use quantities such as

$$T_{ij} = \phi_i \phi_i^\dagger + \phi_j \phi_j^\dagger = T_{ji}. \quad (3.14)$$

Moreover, extra prime invariants can be constructed from $\begin{pmatrix} \phi_i \\ i\sigma^2 \phi_i^* \end{pmatrix}$ and $\begin{pmatrix} \phi_j \\ i\sigma^2 \phi_j^* \end{pmatrix}$, e.g.,

$$S_{ij} = \phi_i^\dagger \phi_j + \underbrace{(i\sigma^2 \phi_i^*)^\dagger (i\sigma^2 \phi_j^*)}_{\phi_i^\dagger \phi_j^*} = \phi_i^\dagger \phi_j + \phi_j^\dagger \phi_i, \quad (3.15)$$

$$iD_{ij}^{\prime a} = \phi_i^\dagger \sigma^a \phi_j + (i\sigma^2 \phi_i^*)^\dagger \sigma^a (i\sigma^2 \phi_j^*) = \phi_i^\dagger \sigma^a \phi_j - \phi_j^\dagger \sigma^a \phi_i. \quad (3.16)$$

Note that $D_{ij}^{\prime a} D_{ij}^{\prime a}$ depends on S_{ij} and $S_{ii, jj}$, since

$$-D_{ij}^{\prime 2} = S_{ij}^2 - (\phi_i^\dagger \phi_j)(\phi_j^\dagger \phi_i) = S_{ij}^2 - S_{ii} S_{jj}. \quad (3.17)$$

Observe that T_{ij} and S_{ij} are not invariant under phase reparametrizations, $\phi_i \rightarrow e^{i\alpha_i} \phi_i$, and so they need to be appropriately combined with their complex conjugates.

We are now able to build a symmetric scalar potential V_{sym} in terms of prime invariants as follows:

$$V_{\text{sym}} = -\mu^2 S_n + \lambda_S S_n^2 + \lambda_D D_n^2 + \lambda_T T_n^2. \quad (3.18)$$

Obviously, the simplest form of the n HDM potentials obeys the maximal symmetry $Sp(2n)$, which has the same form as the SM potential,

$$V_{\text{SM}} = -\mu^2 (\phi^\dagger \phi) + \lambda (\phi^\dagger \phi)^2,$$

with a single mass term and a single quartic coupling. For example, the 2HDM $Sp(4)$ -invariant potential, the so-called MS-2HDM is given by [29]

$$V_{\text{MS-2HDM}} = -\mu_1^2 (|\phi_1|^2 + |\phi_2|^2) + \lambda_1 (|\phi_1|^2 + |\phi_2|^2)^2, \quad (3.19)$$

with the obvious relations among the parameters,

$$\begin{aligned} \mu_1^2 = \mu_2^2, \quad m_{12}^2 = 0, \quad 2\lambda_2 = 2\lambda_1 = \lambda_3, \\ \lambda_4 = \text{Re}(\lambda_5) = \lambda_6 = \lambda_7 = 0. \end{aligned} \quad (3.20)$$

Note that the functional form of the potential in (3.19) is $V = V[S_2] = V[S_{11} + S_{22}]$.

Similarly, the 3HDM potential invariant under $Sp(6)/Z_2$ will be a function of the symmetric block $S_3 = S_{11} + S_{22} + S_{33}$, i.e.,

$$\begin{aligned} V_{\text{MS-3HDM}} &= -\mu_1^2 (|\phi_1|^2 + |\phi_2|^2 + |\phi_3|^2) \\ &\quad + \lambda_{11} (|\phi_1|^2 + |\phi_2|^2 + |\phi_3|^2)^2, \end{aligned} \quad (3.21)$$

where the nonzero parameters are

$$\mu_1 = \mu_2 = \mu_3, \quad \lambda_{11} = \lambda_{22} = \lambda_{33} = 2\lambda_{1122} = 2\lambda_{1133} = 2\lambda_{2233}.$$

Remarkably, the MS- n HDM potentials obey naturally the SM-alignment constraints, and all quartic couplings of the MS- n HDM potential can vanish simultaneously [27,29].

Another example is the $SU(3) \otimes U(1)$ -invariant 3HDM potential. The corresponding symmetric blocks are $S_3 = S_{11} + S_{22} + S_{33}$ and $D_3^2 = D_{12}^2 + D_{13}^2 + D_{23}^2$, given in (3.9) and (3.10), respectively. Therefore, the $SU(3) \otimes U(1)$ -invariant 3HDM potential takes on the form

$$\begin{aligned} V_{\text{SU}(3) \otimes U(1)} &= -\mu_1^2 (|\phi_1|^2 + |\phi_2|^2 + |\phi_3|^2) \\ &\quad + \lambda_{11} (|\phi_1|^4 + |\phi_2|^4 + |\phi_3|^4) \\ &\quad + \lambda_{1122} (|\phi_1|^2 |\phi_2|^2 + |\phi_1|^2 |\phi_3|^2 + |\phi_2|^2 |\phi_3|^2) \\ &\quad + (2\lambda_{11} - \lambda_{1122}) (|\phi_1^\dagger \phi_2|^2 + |\phi_1^\dagger \phi_3|^2 + |\phi_2^\dagger \phi_3|^2), \end{aligned} \quad (3.22)$$

with the following relations between the parameters:

$$\begin{aligned}
\mu_1 &= \mu_2 = \mu_3, \\
\lambda_{11} &= \lambda_{22} = \lambda_{33}, \\
\lambda_{1122} &= \lambda_{1133} = \lambda_{2233}, \\
\lambda_{1221} &= \lambda_{1331} = \lambda_{2332} = 2\lambda_{11} - \lambda_{1122}.
\end{aligned}$$

This method can be applied to all continuous symmetries of n HDM potentials. We present all explicit symmetric blocks under all continuous symmetries for the 2HDM and the 3HDM potentials in Appendix C. The complete list of accidental symmetries for the 2HDM and 3HDM potentials, along with the relations among the nonzero parameters, are exhibited in Tables I and II.

IV. DISCRETE SYMMETRIES AND IRREDUCIBLE REPRESENTATIONS

As discussed in Sec. II, $\text{Sp}(2n)$ is the maximal symmetry group for n HDM potentials. This will help us to classify all $\text{SU}(2)_L$ -preserving accidental symmetries of such potentials. In addition to continuous symmetries shown in Sec. III, there are also discrete symmetries as subgroups of continuous symmetries. Known examples of this type are the standard charge-parity (CP) symmetry, the cyclic discrete group Z_n , the permutation group S_n , or a product of them possibly combining with continuous symmetries. In general, these discrete symmetries can be grouped into Abelian and non-Abelian symmetry groups. In this section, we discuss all possible and known discrete symmetries for n HDM potentials, including our approach to build n HDM potentials by employing irreducible representations of discrete symmetry groups.

A. Abelian discrete symmetries

To start with, let us first consider the Abelian discrete symmetry groups [42,43]

$$Z_2, Z_3, Z_4, Z_2 \times Z_2, \dots, Z_n, \dots, \quad (4.1)$$

where $Z_n = \{1, \omega, \dots, \omega^{(n-1)}\}$ with $\omega^n = 1$. Note that iff n and m have no common prime factor, the product $Z_n \times Z_m$ is identical to $Z_{n \times m}$. These discrete symmetries can be imposed to restrict the independent theoretical parameters of the model. For example, in the 2HDM, the Z_2 symmetry is invoked to avoid flavor changing neutral currents [44] or to ensure the stability of dark matter [45].

In addition to these discrete symmetries, there are generalized CP (GCP) transformations defined as

$$\text{GCP}[\phi_i] = G_{ij} \phi_j^*, \quad (4.2)$$

with $G_{ij} \in \text{SU}(n) \times \text{U}(1)$, where $\text{U}(1)$ can always be eliminated by $\text{U}(1)_Y$ transformation. The GCP transformations realize different types of CP symmetry. For example, in the

case of the 2HDM (3HDM), there are two types of CP symmetries: (i) standard CP or $CP1$: $\phi_{1,2}(\phi_3) \rightarrow \phi_{1,2}^*(\phi_3^*)$, and (ii) nonstandard CP or $CP2$: $\phi_1 \rightarrow \phi_2^*$, $\phi_2 \rightarrow -\phi_1^*$ ($\phi_3 \rightarrow \phi_3^*$) [46,47].¹ In general, without continuous group factors, the discrete symmetries for the 2HDM are $CP1$, $CP2$, and Z_2 . The generators of these discrete symmetries can be expressed in terms of double tensor products as

$$\Delta_{CP1} = \sigma^2 \otimes \sigma^0 \otimes \sigma^2, \quad (4.3)$$

$$\Delta_{CP2} = i\sigma^2 \otimes \sigma^2 \otimes \sigma^2, \quad (4.4)$$

$$\Delta_{Z_2} = \sigma^0 \otimes \sigma^3 \otimes \sigma^0. \quad (4.5)$$

In the bilinear R_2^A space, the transformation matrices (or the generating group elements) associated with $CP1$, $CP2$, and Z_2 discrete symmetries are given by

$$D_{CP1} = \text{diag}(\mathbf{1}, -\mathbf{1}, \mathbf{1}, 1, -1), \quad (4.6)$$

$$D_{CP2} = \text{diag}(-\mathbf{1}, -\mathbf{1}, -\mathbf{1}, 1, -1), \quad (4.7)$$

$$D_{Z_2} = \text{diag}(-\mathbf{1}, -\mathbf{1}, \mathbf{1}, -1, -1). \quad (4.8)$$

where the $\text{U}(1)_Y$ -conserving elements are denoted in boldface.

Let us turn our attention to the 3HDM potential. In this case, the corresponding $CP1$ discrete symmetry can be represented as

$$\Delta_{CP1} = \sigma^2 \otimes G^0 \otimes \sigma^2, \quad (4.9)$$

resulting in the following transformation matrix in the R_3^A space:

$$D_{CP1} = \text{diag}(\mathbf{1}, \mathbf{1}, \mathbf{1}, -\mathbf{1}, -\mathbf{1}, -\mathbf{1}, \mathbf{1}, \mathbf{1}, 1, 1, 1, -1, -1, -1). \quad (4.10)$$

On the other hand, $CP2$ discrete symmetries may be given by

$$\Delta_{CP2} = \begin{pmatrix} 0 & -i\bar{G}^2 \otimes \sigma^2 \\ i\bar{G}^{2*} \otimes \sigma^2 & 0 \end{pmatrix}, \quad (4.11)$$

with [48]

¹In some of the earlier literature, there has been a third class of CP symmetries called $CP3$ which relies on $\text{SO}(2)_{\text{HF}}$ [or $\text{SO}(3)_{\text{HF}}$ for a 3HDM potential] and the standard CP symmetry. However, continuous $\text{SO}(n)_{\text{HF}}$ symmetries lead automatically to CP -invariant n HDM potentials, without introducing further restrictions on the theoretical parameters. In other words, $CP1$ is an emergent symmetry that results from $\text{SO}(n)_{\text{HF}}$, so $CP3$ should not be regarded as a new CP symmetry.

$$\bar{G}^2 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & e^{i\alpha} \end{pmatrix}, \quad (4.12)$$

where the phase $e^{i\alpha}$ is an arbitrary phase factor. This results in the following transformation matrix in the bilinear R_3^A space (dots stand for zero elements):

$$D_{\text{CP}2} = \begin{pmatrix} -1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & -\cos\alpha & \cdot & \cdot & \sin\alpha & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cos\alpha & \cdot & \cdot & -\sin\alpha & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \sin\alpha & \cdot & \cdot & \cos\alpha & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & -\sin\alpha & \cdot & \cdot & -\cos\alpha & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \mathbf{1} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \mathbf{1} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -\cos\alpha & \cdot & \sin\alpha & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cos\alpha & \cdot & -\sin\alpha & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -\sin\alpha & \cdot & \cdot & \cos\alpha & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \sin\alpha & \cdot & -\cos\alpha & \cdot & \cdot & \cdot & \cdot \end{pmatrix}. \quad (4.13)$$

Note that the CP2 transformation matrix $D_{\text{CP}2}$ in the bilinear R_3^A space is nondiagonal, contrary to the 2HDM case. We must remark here that in the case of 2HDM, $\Delta_{\text{CP}2}^2 = -\mathbf{1}_8 \neq \mathbf{1}_8$ and $\Delta_{\text{CP}2}^4 = \mathbf{1}_8$, and in the bilinear space $D_{\text{CP}2}^2 = \mathbf{1}_6$. However, in the case of the 3HDM, we have $\Delta_{\text{CP}2}^2 \neq -\mathbf{1}_{12}$, $\Delta_{\text{CP}2}^4 = \mathbf{1}_{12}$, and $D_{\text{CP}2}^4 = \mathbf{1}_{14}$, in agreement with a property termed CP4 in [48]. Without loss of generality, we set $\alpha = 0$.

In addition, there are several Abelian discrete symmetries for the 3HDM potential [49], i.e.,

$$Z_2, Z'_2, Z_3, Z_4, Z_2 \times Z_2. \quad (4.14)$$

The generators of these Abelian discrete symmetries are given by

$$\begin{aligned} \Delta_{Z_2} &= \sigma^0 \otimes z_2 \otimes \sigma^0, & \Delta_{Z'_2} &= \sigma^0 \otimes z'_2 \otimes \sigma^0, \\ \Delta_{Z_3} &= \text{diag}[z_3 \otimes \sigma^0, z_3^* \otimes \sigma^0], & \Delta_{Z_4} &= \text{diag}[z_4 \otimes \sigma^0, z_4^* \otimes \sigma^0], \end{aligned} \quad (4.15)$$

where

$$\begin{aligned} z_2 &= \text{diag}[1, -1, 1], & z'_2 &= \text{diag}[1, -1, -1], \\ z_3 &= \text{diag}[\omega^2, \omega, 1], & z_4 &= \text{diag}[i, -i, 1], \end{aligned} \quad (4.16)$$

with $\omega = e^{i2\pi/3}$. In the bilinear R_3^A space, as a result of flipping the sign of the one or two doublets, the following diagonal transformation matrices for the discrete symmetries Z_2 and Z'_2 may be derived:

$$D_{Z_2} = \text{diag}(-1, \mathbf{1}, -\mathbf{1}, -\mathbf{1}, \mathbf{1}, -\mathbf{1}, \mathbf{1}, \mathbf{1}, -1, 1, -1, -1, 1, -1), \quad (4.17)$$

$$D_{Z'_2} = \text{diag}(-1, -\mathbf{1}, \mathbf{1}, -\mathbf{1}, -\mathbf{1}, \mathbf{1}, \mathbf{1}, \mathbf{1}, -1, -1, 1, -1, -1, 1). \quad (4.18)$$

In the same way, the transformation matrices for Z_3 and Z_4 may be represented by the nondiagonal matrices

$$D_{Z_3} = \frac{1}{2} \begin{pmatrix} -1 & . & . & \sqrt{3} & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & -1 & . & -\sqrt{3} & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & -1 & . & . & \sqrt{3} & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ -\sqrt{3} & . & . & -1 & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & \sqrt{3} & . & . & -1 & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & -\sqrt{3} & . & . & -1 & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 2 & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & 2 & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & 2 & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & -1 & . & \sqrt{3} & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & -1 & . & -\sqrt{3} & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . & 2 & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . & . & -\sqrt{3} & . & -1 & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . & . & . & \sqrt{3} & . & . & -1 & . & . & . \end{pmatrix}, \quad (4.19)$$

$$D_{Z_4} = \frac{1}{2} \begin{pmatrix} -1 & . \\ . & . & . & . & 1 & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & -1 & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & -1 & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & -1 & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & 1 & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 1 & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & 1 & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & 1 & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & -1 & . & . & . & . & . & . & . & . & . & . \\ . & 1 \\ . & . \\ . & -1 \\ . & . \end{pmatrix}. \quad (4.20)$$

Now, with the help of the D -transformation matrices, we can construct accidentally symmetric n HDM potentials. For example, in the case of Z_4 symmetry, applying the transformation matrix D_{Z_4} on the $U(1)_Y$ -conserving elements of R_3^A yields

$$\begin{aligned} R_3^1 &\rightarrow -R_3^1, & R_3^5 &\rightarrow -R_3^2, \\ R_3^2 &\rightarrow +R_3^5, & R_3^6 &\rightarrow +R_3^3, \\ R_3^3 &\rightarrow -R_3^6, & R_3^7 &\rightarrow +R_3^7, \\ R_3^4 &\rightarrow -R_3^4, & R_3^8 &\rightarrow +R_3^8. \end{aligned} \quad (4.21)$$

Therefore, all possible combinations $R_3^i R_3^j$ ($i, j = 1, \dots, 8$) that respect the Z_4 symmetry may be obtained as

$$\begin{aligned} &(R_3^1)^2, (R_3^4)^2, R_3^1 R_3^4, (R_3^7)^2, (R_3^8)^2, R_3^7 R_3^8, \\ &R^{1,4}[(R_3^2 \pm R_3^3) - (R_3^5 \mp R_3^6)], (R_3^5 \pm R_3^6)^2 + (R_3^2 \mp R_3^3)^2. \end{aligned} \quad (4.22)$$

These combinations lead to the following Z_4 -invariant 3HDM potential:

$$\begin{aligned} V_{Z_4} &= -\mu_1^2 |\phi_1|^2 - \mu_2^2 |\phi_2|^2 - \mu_3^2 |\phi_3|^2 \\ &\quad + \lambda_{11} |\phi_1|^4 + \lambda_{22} |\phi_2|^4 + \lambda_{33} |\phi_3|^4 \\ &\quad + \lambda_{1122} |\phi_1|^2 |\phi_2|^2 + \lambda_{1133} |\phi_1|^2 |\phi_3|^2 + \lambda_{2233} |\phi_2|^2 |\phi_3|^2 \\ &\quad + \lambda_{1221} |\phi_1^\dagger \phi_2|^2 + \lambda_{1331} |\phi_1^\dagger \phi_3|^2 + \lambda_{2332} |\phi_2^\dagger \phi_3|^2 \\ &\quad + \lambda_{1323} (\phi_1^\dagger \phi_3) (\phi_2^\dagger \phi_3) + \lambda_{1323}^* (\phi_3^\dagger \phi_1) (\phi_3^\dagger \phi_2) \\ &\quad + \frac{\lambda_{1212}}{2} (\phi_1^\dagger \phi_2)^2 + \frac{\lambda_{1212}^*}{2} (\phi_2^\dagger \phi_1)^2, \end{aligned} \quad (4.23)$$

where the complex phase of λ_{1212} can be rotated away by a field redefinition.

In the same fashion, we can use this procedure to construct n HDM potentials invariant under all Abelian discrete symmetries. Tables I and II give the parameter relations of the 2HDM and 3HDM potentials constrained by these symmetries.

B. Non-Abelian discrete symmetries

Non-Abelian discrete symmetries constitute another class of discrete symmetries, which may be thought of as combinations of Abelian discrete symmetries. The most

familiar non-Abelian groups can be summarized as follows [20,50]:

- (i) *Permutation group* S_N . The best known non-Abelian discrete groups are the permutation groups. The order of this group is $N!$. An S_2 group is an Abelian symmetry group and consists of a permutation in the form $(x_1, x_2) \rightarrow (x_2, x_1)$. Thus, the lowest order non-Abelian group is S_3 .
- (ii) *Alternating group* A_N . This group consists of only even permutations of S_N , and thus, its order is $N!/2$. The smallest non-Abelian group of this class is A_4 since $A_3 \cong Z_3$.
- (iii) *Dihedral group* D_N . This group is also denoted as $\Delta(2N)$ and its order is $2N$. The D_N group is isomorphic to $Z_N \rtimes Z_2$ that consists of the cyclic rotation Z_N and its reflections. Note that $D_3 \cong S_3$.
- (iv) *Binary dihedral group* Q_{2N} . This group, which is also called *quaternion group*, is a double cover of D_N symmetry group and its order is $4N$.
- (v) *Tetrahedral group* T_N . This group is of order $3N$ and isomorphic to $Z_N \rtimes Z_3$, where N is any prime number. The smallest non-Abelian discrete symmetry of this type is T_7 . This would imply that a T_N -symmetric n HDM potential will also be symmetric under Z_7 .
- (vi) *Dihedral-like groups*. These generic groups obey the following isomorphisms:

$$\begin{aligned}\Sigma(2N^2) &\cong (Z_N \times Z'_N) \rtimes Z_2, \\ \Delta(3N^2) &\cong (Z_N \times Z'_N) \rtimes Z_3, \\ \Sigma(3N^3) &\cong (Z_N \times Z'_N \times Z''_N) \rtimes Z_3, \\ \Delta(6N^2) &\cong (Z_N \times Z'_N) \rtimes S_3.\end{aligned}\quad (4.24)$$

The simplest groups of this type are $\Sigma(2) \cong Z_2$, $\Delta(6) \cong S_3$, $\Delta(24) \cong S_4$, $\Delta(12) \cong A_4$, and $\Sigma(24) \cong Z_2 \times \Delta(12)$.

- (vii) *Crystal-like groups* $\Sigma(M\phi)$, with $\phi = 1, 2, 3$. These groups are of order M and are given by

$$\begin{aligned}\Sigma(60\phi), & \quad \Sigma(168\phi), & \quad \Sigma(36\phi), \\ \Sigma(72\phi), & \quad \Sigma(216\phi), & \quad \Sigma(360\phi),\end{aligned}\quad (4.25)$$

where $\Sigma(60) \cong A_5$ and $\Sigma(216) \cong A_4$.

The decomposition of tensor products of three-dimensional irreducible representations of these groups are given in Appendix D. Note that imposing many of these symmetry groups lead to identical potentials or to potentials that are invariant under continuous symmetries. These non-Abelian discrete symmetries can be the symmetry of n HDM potentials for sufficiently large n , as discussed in Sec. III.

In the case of the 3HDM, the complete list of non-Abelian discrete symmetries has been reported in [20–24]. There are two non-Abelian discrete symmetries as

subgroups of $SO(3)$, namely D_3 and D_4 . In addition, there are non-Abelian discrete symmetries as subgroups of $SU(3)$,

$$A_4, S_4, \{\Sigma(18), \Delta(27), \Delta(54)\}, \Sigma(36), \quad (4.26)$$

where the symmetry groups stacked in curly brackets produce identical potentials. Here, we discuss the cases D_3 and A_4 , while the description of the rest of these types of symmetries for the 3HDM potential may be found in Appendix D.

Let us start with the smallest non-Abelian discrete group $D_3 \cong S_3$. The irreducible representations of the D_3 symmetry group can be expressed by two singlets, $\mathbf{1}$ and $\mathbf{1}'$, and one doublet $\mathbf{2}$. The $2 \otimes 2$ tensor product of this group decomposes as

$$D_3: \mathbf{2} \otimes \mathbf{2} = \mathbf{1} \oplus \mathbf{1}' \oplus \mathbf{2}. \quad (4.27)$$

Moreover, the generators of D_3 discrete symmetry group should satisfy the conditions: $g_1^3 = 1$, $g_2^2 = 1$, and $g_1 \cdot g_2 = g_2 \cdot (g_1 \cdot g_1)$. Thus, two generators of D_3 in terms of double tensor products are given by

$$\Delta_{D_3}^1 = \text{diag}[g_1 \otimes \sigma^0, g_1^* \otimes \sigma^0], \quad \Delta_{D_3}^2 = \sigma^0 \otimes g_2 \otimes \sigma^0, \quad (4.28)$$

where

$$g_1 = \begin{pmatrix} \omega^2 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad g_2 = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (4.29)$$

Imposing D_3 on the $U(1)$ -conserving part of the R_3^A vector will lead to the following linear decomposition:

$$\begin{aligned}\mathbf{1}: & (R_3^0), & \mathbf{2}: & \begin{pmatrix} R_3^1 \\ R_3^4 \end{pmatrix}, & \mathbf{2}'': & \begin{pmatrix} R_3^2 + R_3^6 \\ R_3^3 + R_3^5 \end{pmatrix}, \\ \mathbf{1}': & (R_3^7), & \mathbf{2}': & \begin{pmatrix} -R_3^2 - R_3^3 \\ R_3^5 - R_3^6 \end{pmatrix}, & \mathbf{2}''': & \begin{pmatrix} R_3^2 - R_3^6 \\ R_3^3 - R_3^5 \end{pmatrix}.\end{aligned}\quad (4.30)$$

Note that in the bilinear space, there are three singlets $\mathbf{1}$, $\mathbf{1}'$, and $\mathbf{1}''$, and two doublets, $\mathbf{2}$ and $\mathbf{2}'$. Thus, given the irreducible representations in (4.30), we may parametrize the D_3 -invariant 3HDM potential as follows:

$$\begin{aligned}V_{D_3} = & -M_1 \mathbf{1} - M_2 \mathbf{1}'' + \Lambda_0 \mathbf{1}^2 + \Lambda_1 \mathbf{1}'^2 + \Lambda_2 \mathbf{1}''^2 \\ & + \Lambda_3 \mathbf{1} \cdot \mathbf{1}'' + \Lambda_4 \mathbf{2}^T \cdot \mathbf{2} + \Lambda_5 \mathbf{2}'^T \cdot \mathbf{2}' \\ & + \Lambda_6 \mathbf{2}^T \cdot \mathbf{2}' + \Lambda_7 \mathbf{2}''^T \cdot \mathbf{2}'' + \Lambda_8 \mathbf{2}''^T \cdot \mathbf{2}''.\end{aligned}\quad (4.31)$$

This can be rewritten as

$$\begin{aligned}
V_{D_3} = & -\mu_1^2(|\phi_1|^2 + |\phi_2|^2) - \mu_3^2|\phi_3|^2 \\
& + \lambda_{11}(|\phi_1|^4 + |\phi_2|^4) + \lambda_{33}|\phi_3|^4 \\
& + \lambda_{1122}|\phi_1|^2|\phi_2|^2 + \lambda_{1133}(|\phi_1|^2|\phi_3|^2 + |\phi_2|^2|\phi_3|^2) \\
& + \lambda_{1221}|\phi_1^\dagger\phi_2|^2 + \lambda_{2332}(|\phi_2^\dagger\phi_3|^2 + |\phi_1^\dagger\phi_3|^2) \\
& + \lambda_{2131}((\phi_2^\dagger\phi_1)(\phi_3^\dagger\phi_1) - (\phi_1^\dagger\phi_2)(\phi_3^\dagger\phi_2)) \\
& + (\phi_1^\dagger\phi_2)(\phi_1^\dagger\phi_3) - (\phi_2^\dagger\phi_1)(\phi_2^\dagger\phi_3) \\
& + \lambda_{1323}(\phi_1^\dagger\phi_3)(\phi_2^\dagger\phi_3) + \lambda_{1323}^*(\phi_3^\dagger\phi_1)(\phi_3^\dagger\phi_2), \quad (4.32)
\end{aligned}$$

where λ_{1323} is complex while all other couplings are real.

Another example of a non-Abelian discrete symmetry for the 3HDM potential is A_4 , which is a subgroup of $SU(3)$. This symmetry group consists of three singlets, $\mathbf{1}$, $\mathbf{1}'$, and $\mathbf{1}''$, and one triplet $\mathbf{3}$. The $\mathbf{3} \otimes \mathbf{3}$ tensor product of A_4 decomposes:

$$A_4: \mathbf{3} \otimes \mathbf{3} = \mathbf{1} \oplus \mathbf{1}' \oplus \mathbf{1}'' \oplus \mathbf{3} \oplus \mathbf{3}'. \quad (4.33)$$

The generators of the A_4 discrete symmetry group in terms of double tensor products are

$$\Delta_{A_4}^1 = \sigma^0 \otimes g_1 \otimes \sigma^0, \quad \Delta_{A_4}^2 = \sigma^0 \otimes g_2 \otimes \sigma^0, \quad (4.34)$$

where

$$g_1 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad g_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad (4.35)$$

satisfy the conditions $g_1^3 = g_2^2 = (g_1 \cdot g_2)^3 = 1$. The A_4 -symmetric blocks in the bilinear space can be represented as

$$\begin{aligned}
\mathbf{1}: & (\phi_1^\dagger\phi_1 + \phi_2^\dagger\phi_2 + \phi_3^\dagger\phi_3), \\
\mathbf{1}': & (\phi_1^\dagger\phi_1 + \omega^2\phi_2^\dagger\phi_2 + \omega\phi_3^\dagger\phi_3), \\
\mathbf{1}'': & (\phi_1^\dagger\phi_1 + \omega\phi_2^\dagger\phi_2 + \omega^2\phi_3^\dagger\phi_3), \\
\mathbf{3}: & \begin{pmatrix} R_3^1 \\ R_3^2 \\ R_3^3 \end{pmatrix}, \quad \mathbf{3}': \begin{pmatrix} R_3^4 \\ -R_3^5 \\ R_3^6 \end{pmatrix}. \quad (4.36)
\end{aligned}$$

Thus, an A_4 -invariant 3HDM potential may be written as

$$\begin{aligned}
V_{A_4} = & -M\mathbf{1} + \Lambda_0\mathbf{1}^2 + \Lambda_1\mathbf{1}^* \cdot \mathbf{1}'' + \Lambda_2\mathbf{3}^\top \cdot \mathbf{3} \\
& + \Lambda_3\mathbf{3}'^\top \cdot \mathbf{3}' + \Lambda_4\mathbf{3}'^\top \cdot \mathbf{3}. \quad (4.37)
\end{aligned}$$

Equivalently, the A_4 -symmetric potential can be rewritten as follows:

$$\begin{aligned}
V_{A_4} = & -\mu_1^2(|\phi_1|^2 + |\phi_2|^2 + |\phi_3|^2) + \lambda_{11}(|\phi_1|^4 + |\phi_2|^4 + |\phi_3|^4) \\
& + \lambda_{1122}(|\phi_1|^2|\phi_2|^2 + |\phi_1|^2|\phi_3|^2 + |\phi_2|^2|\phi_3|^2) \\
& + \lambda_{1221}(|\phi_1^\dagger\phi_2|^2 + |\phi_1^\dagger\phi_3|^2 + |\phi_2^\dagger\phi_3|^2) \\
& + \frac{\lambda_{1212}}{2}((\phi_1^\dagger\phi_2)^2 + (\phi_1^\dagger\phi_3)^2 + (\phi_2^\dagger\phi_3)^2) \\
& + \frac{\lambda_{1212}^*}{2}((\phi_2^\dagger\phi_1)^2 + (\phi_3^\dagger\phi_1)^2 + (\phi_3^\dagger\phi_2)^2). \quad (4.38)
\end{aligned}$$

In a similar way, the remaining 3HDM potentials that are invariant under non-Abelian discrete symmetries may be obtained. These are presented in Appendix D.

In Tables I and II, we present all $SU(2)_L$ -preserving accidental symmetries for the 2HDM and the 3HDM potentials. The 2HDM potential has a total number of 13 accidental symmetries [34], of which 6 preserve $U(1)_Y$ [46,47,51] and 7 are custodially symmetric [25]. Given the isomorphism of the Lie algebras: $SO(5) \sim Sp(4)$, the maximal symmetry group of the 2HDM in the original Φ -field space is $G_{2\text{HDM}}^\Phi = [Sp(4)/Z_2] \otimes SU(2)_L$ [25].

For the case of the 3HDM potential, we find that there exists a total number of 40 $SU(2)_L$ -preserving accidental symmetries, of which 18 preserve $U(1)_Y$ and 22 are custodially symmetric. The maximal symmetry group of the 3HDM potential in the original Φ -field space is $G_{3\text{HDM}}^\Phi = [Sp(6)/Z_2] \otimes SU(2)_L$ [25]. Note that the 40 accidental symmetries are subgroups of $Sp(6)$.

V. CONCLUSIONS

The n HDM potentials may realize a large number of $SU(2)_L$ -preserving accidental symmetries as subgroups of the symplectic group $Sp(2n)$. We have shown that there are *two* sets of symmetries: (i) continuous symmetries and (ii) discrete symmetries (Abelian and non-Abelian symmetry groups). For the continuous symmetries, we have offered an algorithmic method that provides the full list of proper, improper, and semisimple subgroups for any given integer n . We have also included all known discrete symmetries in n HDM potentials.

Having defined the biadjoint representation of the $Sp(2n)$ symmetry group, we introduced prime invariants and irreducible representations in the bilinear field space to construct the scalar sector of n HDM potentials. These quantities have been systematically used to construct accidentally symmetric n HDM potentials by employing fundamental building blocks that respect the symmetries.

Using the method presented in this paper, we have been able to classify all symmetries and the relations among the theoretical parameters of the scalar potential for the following: (i) the 2HDM and (ii) the 3HDM. For the 2HDM potential, we recover the maximum number of 13 accidental symmetries. For the 3HDM potential, we derive *for the first time to our knowledge* the complete list of 40 accidental symmetries.

Our approach can be systematically applied to n HDM potentials, with $n > 3$, once all possible discrete symmetries have been identified.

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APPENDIX A: THE 2HDM AND THE 3HDM POTENTIALS

In Sec. II, we have shown that the potential V_n for an n HDM can be written down in the quadratic form with the help of $n(2n - 1)$ -vector R_n^A as

$$V_n = -\frac{1}{2}M_A^n R_n^A + \frac{1}{4}L_{AA'}^n R_n^A R_n^{A'},$$

where M_A^n is the mass matrix and $L_{AA'}^n$ is a quartic coupling matrix.

In the case of 2HDM, the general potential is given by

$$\begin{aligned} V_{2\text{HDM}} = & -\mu_1^2(\phi_1^\dagger\phi_1) - \mu_2^2(\phi_2^\dagger\phi_2) - [m_{12}^2(\phi_1^\dagger\phi_2) + \text{H.c.}] \\ & + \lambda_1(\phi_1^\dagger\phi_1)^2 + \lambda_2(\phi_2^\dagger\phi_2)^2 + \lambda_3(\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_2) + \lambda_4(\phi_1^\dagger\phi_2)(\phi_2^\dagger\phi_1) \\ & + \left[\frac{1}{2}\lambda_5(\phi_1^\dagger\phi_2)^2 + \lambda_6(\phi_1^\dagger\phi_1)(\phi_1^\dagger\phi_2) + \lambda_7(\phi_1^\dagger\phi_2)(\phi_2^\dagger\phi_2) + \text{H.c.} \right]. \end{aligned} \quad (\text{A1})$$

Thus, in the bilinear formalism, the mass M_A^2 and the quartic couplings $L_{AA'}^2$ matrices for the 2HDM potential assume the following forms [25]:

$$M_A^2 = (\mu_1^2 + \mu_2^2, 2\text{Re}(m_{12}^2), -2\text{Im}(m_{12}^2), \mu_1^2 - \mu_2^2, 0, 0) \quad (\text{A2})$$

and

$$L_{AA'}^2 = \begin{pmatrix} \lambda_1 + \lambda_2 + \lambda_3 & \text{Re}(\lambda_6 + \lambda_7) & -\text{Im}(\lambda_6 + \lambda_7) & \lambda_1 - \lambda_2 & \dots \\ \text{Re}(\lambda_6 + \lambda_7) & \lambda_4 + \text{Re}(\lambda_5) & -\text{Im}(\lambda_5) & \text{Re}(\lambda_6 - \lambda_7) & \dots \\ -\text{Im}(\lambda_6 + \lambda_7) & -\text{Im}(\lambda_5) & \lambda_4 - \text{Re}(\lambda_5) & -\text{Im}(\lambda_6 - \lambda_7) & \dots \\ \lambda_1 - \lambda_2 & \text{Re}(\lambda_6 - \lambda_7) & -\text{Im}(\lambda_6 - \lambda_7) & \lambda_1 + \lambda_2 - \lambda_3 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad (\text{A3})$$

Evidently, for a $U(1)_Y$ -invariant 2HDM potential, not all the elements of M_A^2 and $L_{AA'}^2$ are nonzero, but only those for which $A, A' = 0, 1, 2, 3$.

In the case of 3HDM, the general potential has the following form:

$$\begin{aligned} V_{3\text{HDM}} = & -\mu_1^2(\phi_1^\dagger\phi_1) - \mu_2^2(\phi_2^\dagger\phi_2) - \mu_3^2(\phi_3^\dagger\phi_3) - [m_{12}^2(\phi_1^\dagger\phi_2) + m_{13}^2(\phi_1^\dagger\phi_3) \\ & + m_{23}^2(\phi_2^\dagger\phi_3) + \text{H.c.}] + \lambda_{11}(\phi_1^\dagger\phi_1)^2 + \lambda_{22}(\phi_2^\dagger\phi_2)^2 + \lambda_{33}(\phi_3^\dagger\phi_3)^2 \\ & + \lambda_{1122}(\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_2) + \lambda_{1133}(\phi_1^\dagger\phi_1)(\phi_3^\dagger\phi_3) + \lambda_{2233}(\phi_2^\dagger\phi_2)(\phi_3^\dagger\phi_3) \\ & + \lambda_{1221}(\phi_1^\dagger\phi_2)(\phi_2^\dagger\phi_1) + \lambda_{1331}(\phi_1^\dagger\phi_3)(\phi_3^\dagger\phi_1) + \lambda_{2332}(\phi_2^\dagger\phi_3)(\phi_3^\dagger\phi_2) \\ & + \left[\frac{\lambda_{1212}}{2}(\phi_1^\dagger\phi_2)^2 + \frac{\lambda_{1313}}{2}(\phi_1^\dagger\phi_3)^2 + \frac{\lambda_{2323}}{2}(\phi_2^\dagger\phi_3)^2 \right. \\ & + \lambda_{1213}(\phi_1^\dagger\phi_2)(\phi_1^\dagger\phi_3) + \lambda_{2113}(\phi_2^\dagger\phi_1)(\phi_1^\dagger\phi_3) + \lambda_{1323}(\phi_1^\dagger\phi_3)(\phi_2^\dagger\phi_3) \\ & + \lambda_{1332}(\phi_1^\dagger\phi_3)(\phi_3^\dagger\phi_2) + \lambda_{2123}(\phi_2^\dagger\phi_1)(\phi_2^\dagger\phi_3) + \lambda_{1223}(\phi_1^\dagger\phi_2)(\phi_2^\dagger\phi_3) \\ & + \lambda_{1112}(\phi_1^\dagger\phi_1)(\phi_1^\dagger\phi_2) + \lambda_{2212}(\phi_2^\dagger\phi_2)(\phi_1^\dagger\phi_2) + \lambda_{1113}(\phi_1^\dagger\phi_1)(\phi_1^\dagger\phi_3) \\ & + \lambda_{1123}(\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_3) + \lambda_{2213}(\phi_2^\dagger\phi_2)(\phi_1^\dagger\phi_3) + \lambda_{2223}(\phi_2^\dagger\phi_2)(\phi_2^\dagger\phi_3) \\ & \left. + \lambda_{3312}(\phi_3^\dagger\phi_3)(\phi_1^\dagger\phi_2) + \lambda_{3313}(\phi_3^\dagger\phi_3)(\phi_1^\dagger\phi_3) + \lambda_{3323}(\phi_3^\dagger\phi_3)(\phi_2^\dagger\phi_3) + \text{H.c.} \right]. \end{aligned} \quad (\text{A4})$$

In the bilinear formalism for this model, the mass M_A^3 and the quartic couplings $L_{AA'}^3$ matrices are given by

$$M_A^3 = \left(\mu_1^2 + \mu_2^2 + \mu_3^2, 2\text{Re}(m_{12}^2), 2\text{Re}(m_{13}^2), 2\text{Re}(m_{23}^2), -2\text{Im}(m_{12}^2), -2\text{Im}(m_{13}^2), \right. \\ \left. -2\text{Im}(m_{23}^2), \mu_1^2 - \mu_2^2, \frac{1}{\sqrt{3}}(\mu_1^2 + \mu_2^2 - 2\mu_3^2), 0, 0, 0, 0, 0 \right) \quad (\text{A5})$$

and

$$L_{AA'}^3 = \begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} & a_{04} & a_{05} & a_{06} & a_{07} & a_{08} & \dots & \dots \\ a_{01} & a_{11} & a_{12} & a_{13} & a_{14} & a_{15} & a_{16} & a_{17} & a_{18} & \dots & \dots \\ a_{02} & a_{12} & a_{22} & a_{23} & a_{24} & a_{25} & a_{26} & a_{27} & a_{28} & \dots & \dots \\ a_{03} & a_{13} & a_{23} & a_{33} & a_{34} & a_{35} & a_{36} & a_{37} & a_{38} & \dots & \dots \\ a_{04} & a_{14} & a_{24} & a_{34} & a_{44} & a_{45} & a_{46} & a_{47} & a_{48} & \dots & \dots \\ a_{05} & a_{15} & a_{25} & a_{35} & a_{45} & a_{55} & a_{56} & a_{57} & a_{58} & \dots & \dots \\ a_{06} & a_{16} & a_{26} & a_{36} & a_{46} & a_{56} & a_{66} & a_{67} & a_{68} & \dots & \dots \\ a_{07} & a_{17} & a_{27} & a_{37} & a_{47} & a_{57} & a_{67} & a_{77} & a_{78} & \dots & \dots \\ a_{08} & a_{18} & a_{28} & a_{38} & a_{48} & a_{58} & a_{68} & a_{78} & a_{88} & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}, \quad (\text{A6})$$

with $L_{AA'}^3 = L_{A'A}^3$ and $A, A' = 0, 1, \dots, 14$. The nonzero elements of $L_{AA'}^3$ are

$$\begin{aligned} a_{00} &= \frac{4}{9}(\lambda_{11} + \lambda_{1122} + \lambda_{1133} + \lambda_{22} + \lambda_{2233} + \lambda_{33}), & a_{01} &= \frac{2}{3}\text{Re}(\lambda_{1112} + \lambda_{2212} + \lambda_{3312}), \\ a_{02} &= \frac{2}{3}\text{Re}(\lambda_{1113} + \lambda_{2213} + \lambda_{3313}), & a_{03} &= \frac{2}{3}\text{Re}(\lambda_{1123} + \lambda_{2223} + \lambda_{3323}), \\ a_{04} &= -\frac{2}{3}\text{Im}(\lambda_{1112} + \lambda_{2212} + \lambda_{3312}), & a_{05} &= -\frac{2}{3}\text{Im}(\lambda_{1113} + \lambda_{2213} + \lambda_{3313}), \\ a_{06} &= -\frac{2}{3}\text{Im}(\lambda_{1123} + \lambda_{2223} + \lambda_{3323}), & a_{07} &= \frac{1}{3}(2\lambda_{11} + \lambda_{1133} - 2\lambda_{22} - \lambda_{2233}), \\ a_{08} &= \frac{\sqrt{3}}{9}[2\lambda_{11} + 2\lambda_{1122} - \lambda_{1133} + 2\lambda_{22} - \lambda_{2233} - 4\lambda_{33}], & a_{11} &= \text{Re}(\lambda_{1212}) + \lambda_{1221}, \\ a_{12} &= \text{Re}(\lambda_{1213} + \lambda_{2113}), & a_{13} &= \text{Re}(\lambda_{1223} + \lambda_{2123}), \\ a_{14} &= -\text{Im}(\lambda_{1212}), & a_{15} &= \text{Im}(\lambda_{2113} - \lambda_{1213}), \\ a_{16} &= \text{Im}(\lambda_{2123} - \lambda_{1223}), & a_{17} &= \text{Re}(\lambda_{1112} - \lambda_{2212}), \\ a_{18} &= \frac{1}{\sqrt{3}}\text{Re}(\lambda_{1112} + \lambda_{2212} - 2\lambda_{3312}), & a_{22} &= \text{Re}(\lambda_{1313}) + 2\lambda_{1331}, \\ a_{23} &= 2\text{Re}(\lambda_{1323} + \lambda_{1332}), & a_{24} &= \text{Im}(\lambda_{2113} - \lambda_{1213}), \\ a_{25} &= -\text{Im}(\lambda_{1313}), & a_{26} &= \text{Im}(\lambda_{1332} - \lambda_{1323}), \\ a_{27} &= \text{Re}(\lambda_{1113} - \lambda_{2213}), & a_{28} &= \frac{1}{\sqrt{3}}\text{Re}(\lambda_{1113} + \lambda_{2213} - 2\lambda_{3313}), \\ a_{33} &= \text{Re}(\lambda_{2323} + 2\lambda_{2332}), & a_{34} &= \text{Im}(\lambda_{2123} - \lambda_{1223}), \\ a_{35} &= -\text{Im}(\lambda_{1323} + \lambda_{1332}), & a_{36} &= -\text{Im}(\lambda_{2323}), \\ a_{37} &= \text{Re}(\lambda_{1123} - \lambda_{2223}), & a_{38} &= \frac{1}{\sqrt{3}}\text{Re}(\lambda_{1123} + \lambda_{2223} - 2\lambda_{3323}), \\ a_{44} &= 2\lambda_{1221} - \text{Re}(\lambda_{1212}), & a_{45} &= \text{Re}(\lambda_{2113} - \lambda_{1213}), \\ a_{46} &= \text{Re}(\lambda_{2123} - \lambda_{1223}), & a_{47} &= \text{Im}(\lambda_{2212} - \lambda_{1112}), \\ a_{48} &= \frac{1}{\sqrt{3}}\text{Im}(2\lambda_{3312} - \lambda_{1112} - \lambda_{2212}), & a_{55} &= \lambda_{1331} - \text{Re}(\lambda_{1313}) +, \\ a_{56} &= \text{Re}(\lambda_{1332} - \lambda_{1323}), & a_{57} &= \text{Im}(\lambda_{2213} - \lambda_{1113}), \\ a_{58} &= \frac{1}{\sqrt{3}}\text{Im}(2\lambda_{3313} - \lambda_{1113} - \lambda_{2213}), & a_{66} &= \lambda_{2332} - \text{Re}(\lambda_{2323}), \\ a_{67} &= \text{Im}(\lambda_{2223} - \lambda_{1123}), & a_{68} &= \frac{1}{\sqrt{3}}\text{Im}(2\lambda_{3323} - \lambda_{1123} - \lambda_{2223}), \\ a_{77} &= \lambda_{11} + \lambda_{22} - 2\lambda_{1122}, & a_{78} &= \frac{1}{\sqrt{3}}(\lambda_{11} - \lambda_{22} - 2\lambda_{1133} + 2\lambda_{2233}), \\ a_{88} &= \frac{1}{3}(\lambda_{11} + \lambda_{22} + 4\lambda_{33} + 2\lambda_{1122} - 4\lambda_{1133} - 4\lambda_{2233}). \end{aligned}$$

Note that the remaining elements denoted by dots are zero. Specifically, for a $U(1)_Y$ -invariant 3HDM potential, all elements of M_A^3 and $L_{AA'}^3$ corresponding to $A, A' = 9, 10, \dots, 14$ vanish.

APPENDIX B: THE BIADJOINT REPRESENTATIONS OF $SP(4)$ AND $SP(6)$

In Sec. II, we introduced the $Sp(2n)$ generators in the biadjoint representation as

$$(T_n^B)_{IJ} = -if_n^{BIJ} = \text{Tr}([\Sigma_n^I, K_n^B]\Sigma_n^J).$$

The maximal symmetry of the potential in the case of 2HDM is $Sp(4)$. With the help of the above relation, we may derive the following ten generators in the biadjoint representation of $Sp(4)$:

$$\begin{aligned} T^0 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix}, & T^1 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, & T^2 &= \begin{pmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, & T^3 &= \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \\ T^4 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, & T^5 &= \begin{pmatrix} 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix}, & T^6 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}, & T^7 &= \begin{pmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \\ T^8 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & i & 0 \end{pmatrix}, & T^9 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \end{aligned}$$

Note that these generators are identical to those of the $SO(5)$ group in the fundamental representation [25], thereby establishing the local group isomorphism: $Sp(4) \cong SO(5)$.

For the case of the 3HDM, the maximal symmetry is $Sp(6)$. Similarly, the 21 generators of $Sp(6)$ in the biadjoint representation read

$$T^0 = i \begin{pmatrix} \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}, \quad T^1 = i \begin{pmatrix} \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & -1 & \dots & \dots & \dots \\ \dots & \dots & -1 & \dots & \dots & \dots \\ \dots & \dots & \dots & -2 & \dots & \dots \\ \dots & \dots & \dots & \dots & 1 & \dots \\ \dots & \dots & \dots & \dots & 1 & \dots \\ \dots & \dots & \dots & \dots & \dots & 2 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix},$$

Likewise, we may use maximal and minimal invariants to construct the 3HDM potentials. The symmetry groups and the 3HDM potentials as functions of prime invariants are

- (i) $\text{SO}(2)_{\phi_1, \phi_2}$: $V[S_{11} + S_{22}, D_{12}^2, T_{12}^2, S_{33}, D_{13}^2 + D_{23}^2, T_{13}^2 + T_{23}^2]$.
- (ii) $\text{SO}(2)_{\phi_1, \phi_2} \otimes \text{Sp}(2)_{\phi_3}$: $V[S_{11} + S_{22}, D_{12}^2, T_{12}^2, S_{33}]$.
- (iii) $\text{SU}(2)_{\phi_1, \phi_2}$: $V[S_{11} + S_{22}, D_{12}^2, S_{33}, D_{13}^2 + D_{23}^2]$.
- (iv) $\text{SU}(2)_{\phi_1, \phi_2} \otimes \text{Sp}(2)_{\phi_3}$: $V[S_{11} + S_{22}, D_{12}^2, S_{33}]$.
- (v) $\text{Sp}(2)_{\phi_1 + \phi_2 + \phi_3}$: $V[S_{11}, S_{22}, S_{33}, S_{12}, S_{13}, S_{23}]$.
- (vi) $\text{Sp}(2)_{\phi_1 + \phi_2} \otimes \text{Sp}(2)_{\phi_3}$: $V[S_{11}, S_{22}, S_{33}, S_{12}]$.
- (vii) $\text{Sp}(2)_{\phi_1, \phi_2} \otimes \text{Sp}(2)_{\phi_3}$: $V[S_{11} + S_{22}, D_{12}^2, S_{33}]$.
- (viii) $\text{Sp}(2)_{\phi_1, \phi_2}$: $V[S_{11} + S_{22}, S_{33}, D_{12}^2, D_{13}^2 + D_{23}^2]$.
- (ix) $\text{Sp}(2)_{\phi_1} \otimes \text{Sp}(2)_{\phi_2} \otimes \text{Sp}(2)_{\phi_3}$: $V[S_{11}, S_{22}, S_{33}]$.
- (x) $\text{SO}(3)$: $V[S_{11} + S_{22} + S_{33}, D_{12}^2 + D_{13}^2 + D_{23}^2, T_{12}^2 + T_{13}^2 + T_{23}^2]$.
- (xi) $\text{Sp}(4) \otimes \text{Sp}(2)_{\phi_3}$: $V[S_{11} + S_{22}, S_{33}]$.
- (xii) $\text{SU}(3) \otimes \text{U}(1)$: $V[S_{11} + S_{22} + S_{33}, D_{12}^2 + D_{13}^2 + D_{23}^2]$.
- (xiii) $\text{Sp}(6)$: $V[S_{11} + S_{22} + S_{33}]$.

In the above list, we have used the subscript $\phi_1 + \phi_2 + \phi_3$ to show a transformation that acts simultaneously on $(\phi_1, i\sigma^2\phi_1^*)^\top$, $(\phi_2, i\sigma^2\phi_2^*)^\top$, and $(\phi_3, i\sigma^2\phi_3^*)^\top$. Also, the subscripts $\phi_1\phi_2$, and ϕ_3 denote $\text{Sp}(2)$ transformations that act on $(\phi_1, i\sigma^2\phi_2^*)^\top$ and $(\phi_3, i\sigma^2\phi_3^*)^\top$, respectively. Finally, the subscripts ϕ_1, ϕ_2 denote $\text{SU}(2)$ or $\text{SO}(2)$ transformations acting on $(\phi_1, \phi_2)^\top$.

APPENDIX D: IRREDUCIBLE REPRESENTATIONS OF NON-ABELIAN DISCRETE SYMMETRIES

The most familiar non-Abelian subgroups of $\text{SU}(3)$ are summarized in Sec. IV. The direct sum decomposition of $3 \otimes 3$ tensor products in terms of irreducible representations of these groups are listed below:

- (1) $1 \oplus 1 \oplus 1 \oplus 1 \oplus 1 \oplus 1 \oplus 1 \oplus 1 \oplus 1$: $\Delta(3N^2)$
- (2) $1 \oplus 1 \oplus 1 \oplus 1 \oplus 1 \oplus 1 \oplus 2$: $\Sigma(2N^2)$
- (3) $1 \oplus 1 \oplus 1 \oplus 3 \oplus 3$: A_4
- (4) $1 \oplus 2 \oplus 2 \oplus 2 \oplus 2$: $\Delta(6N^2)$
- (5) $1 \oplus 2 \oplus 3 \oplus 3$: S_4
- (6) $1 \oplus 2 \oplus 6$: $\Delta(6N^2)$
- (7) $1 \oplus 3 \oplus 5$: A_5
- (8) $1 \oplus 4 \oplus 4$: $\Sigma(36\phi)$
- (9) $1 \oplus 8$: $\Sigma(72\phi), \Sigma(168), \Sigma(216\phi), \Sigma(360\phi)$
- (10) $3 \oplus 3 \oplus 3$: $\Sigma(36\phi), \Delta(3N^2), \Delta(6N^2)$
- (11) $3 \oplus 6$: $\Sigma(72\phi), \Sigma(168), \Sigma(216\phi), \Sigma(360\phi), \Delta(6N^2)$
- (12) $4 \oplus 5$: A_5
- (13) 9 : $\Sigma(216\phi), \Sigma(360\phi)$

As can be seen from the above list, only the decompositions (1)–(9) are relevant for building $\text{SU}(2)_L$ -preserving n HDM

invariant potentials, since they contain a singlet. However, only those symmetries for which their prime factor decomposition lead to distinct n HDM potentials can be considered as candidates for a novel symmetry of a model. For example, the A_5 symmetry with Z_n prime factors 2, 3, 5 does not lead to a distinct 3HDM potential. Moreover, in the case of the 3HDM, the decompositions given in (6) and (9) produce potentials invariant under $\text{SU}(3)$. The remaining possibilities (10)–(13) have been checked up to Z_n prime factors of the model, but they do not seem to lead to new forms of symmetric potentials.

For the case of the 3HDM, there are two non-Abelian discrete symmetries as subgroups of $\text{SO}(3)$, namely D_3 and D_4 . In addition, there are non-Abelian discrete symmetries as subgroups of $\text{SU}(3)$ [20–24],

$$A_4, S_4, \{\Sigma(18), \Delta(27), \Delta(54)\}, \Sigma(36). \quad (\text{D1})$$

In Sec. IV, we have shown the procedure for constructing 3HDM potentials invariant under the non-Abelian discrete symmetries D_3 and A_4 . Here, we apply this method for the rest of non-Abelian discrete symmetries of the 3HDM potential [20–24].

The other two-dimensional non-Abelian discrete symmetry of the 3HDM is D_4 . The $2 \otimes 2$ tensor product of D_4 decomposes as

$$D_4: 2 \otimes 2 = 1 \oplus 1' \oplus 1'' \oplus 1'''. \quad (\text{D2})$$

This group is generated by two generators,

$$\begin{aligned} \Delta_{D_4}^1 &= \text{diag}[g_1 \otimes \sigma^0, g_1^* \otimes \sigma^0], \\ \Delta_{D_4}^2 &= \text{diag}[g_2 \otimes \sigma^0, g_2^* \otimes \sigma^0], \end{aligned} \quad (\text{D3})$$

with

$$g_1 = \begin{pmatrix} i & 0 & 0 \\ 0 & -i & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad g_2 = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (\text{D4})$$

that satisfy the conditions $g_1^4 = 1$, $g_2^2 = 1$, and $g_2 \cdot g_1 \cdot g_2 = g_1^{-1}$. The irreducible representations of D_4 in the bilinear space may be given by

TABLE II. Nonzero parameters for the 40 accidental symmetries related to the 3HDM potential. Note that all entries which contain a symplectic group are only custodially symmetric, and so violate $U(1)_Y$.^{a,b}The generators of $U(1)$ and $U(1)'$ are $\text{diag}(e^{i\alpha}, e^{-i\alpha}, 1)$ and $\text{diag}(e^{i\beta/3}, e^{i\beta/3}, e^{-i2\beta/3})$, with $\alpha, \beta \in [0, 2\pi)$, respectively. Moreover, the subscripts ϕ_1, ϕ_2 denote $SU(2)$ or $SO(2)$ transformations acting on $(\phi_1, \phi_2)^T$ and the subscript $\phi_1 + \phi_2 + \phi_3$ shows an $Sp(2)$ transformation acting on all doublets $(\phi_1, i\sigma^2\phi_1^*)^T, (\phi_2, i\sigma^2\phi_2^*)^T$, and $(\phi_3, i\sigma^2\phi_3^*)^T$. Finally, the subscripts $\phi_1\phi_2$ and ϕ_3 indicate an $Sp(2)$ transformation acting on $(\phi_1, i\sigma^2\phi_2^*)^T$ and $(\phi_3, i\sigma^2\phi_3^*)^T$, respectively.

No.	Symmetry	Nonzero parameters for 3HDM potentials
1	CPI	$\mu_1^2, \mu_2^2, \mu_3^2, \text{Re}(m_{12}^2), \text{Re}(m_{13}^2), \text{Re}(m_{23}^2), \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233}, \lambda_{1221}, \lambda_{1331}, \lambda_{2332}, \text{Re}(\lambda_{1212}), \text{Re}(\lambda_{1313}), \text{Re}(\lambda_{2323}), \text{Re}(\lambda_{1213}), \text{Re}(\lambda_{2113}), \text{Re}(\lambda_{1223}), \text{Re}(\lambda_{2123}), \text{Re}(\lambda_{1323}), \text{Re}(\lambda_{1332}), \text{Re}(\lambda_{1112}), \text{Re}(\lambda_{2212}), \text{Re}(\lambda_{3312}), \text{Re}(\lambda_{1113}), \text{Re}(\lambda_{2213}), \text{Re}(\lambda_{3313}), \text{Re}(\lambda_{1123}), \text{Re}(\lambda_{2223}), \text{Re}(\lambda_{3323})$
2	Z_2	$\mu_1^2, \mu_2^2, \mu_3^2, \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233}, \lambda_{1221}, \lambda_{1331}, \lambda_{2332}, \{m_{13}^2, \lambda_{1212}, \lambda_{1313}, \lambda_{2323}, \lambda_{1232}, \lambda_{1113}, \lambda_{2213}, \lambda_{3313} \text{ and H.c.}\}$
2'	Z_2'	$\mu_1^2, \mu_2^2, \mu_3^2, \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233}, \lambda_{1221}, \lambda_{1331}, \lambda_{2332}, \{m_{23}^2, \lambda_{1212}, \lambda_{1313}, \lambda_{2323}, \lambda_{1213}, \lambda_{1123}, \lambda_{2223}, \lambda_{3323} \text{ and H.c.}\}$
3	$Z_2 \otimes Z_2'$	$\mu_1^2, \mu_2^2, \mu_3^2, \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233}, \lambda_{1221}, \lambda_{1331}, \lambda_{2332}, \{\lambda_{1212}, \lambda_{1313}, \lambda_{2323} \text{ and H.c.}\}$
4	Z_3	$\mu_1^2, \mu_2^2, \mu_3^2, \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233}, \lambda_{1221}, \lambda_{1331}, \lambda_{2332}, \{\lambda_{1213}, \lambda_{1323}, \lambda_{2123} \text{ and H.c.}\}$
5	Z_4	$\mu_1^2, \mu_2^2, \mu_3^2, \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233}, \lambda_{1221}, \lambda_{1331}, \lambda_{2332}, \{\lambda_{1212}, \lambda_{1323} \text{ and H.c.}\}$
5'	Z_4'	$\mu_1^2, \mu_2^2, \mu_3^2, \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233}, \lambda_{1221}, \lambda_{1331}, \lambda_{2332}, \{\lambda_{1313}, \lambda_{3212} \text{ and H.c.}\}$
6	^a $U(1)$	$\mu_1^2, \mu_2^2, \mu_3^2, \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233}, \lambda_{1221}, \lambda_{1331}, \lambda_{2332}, \{\lambda_{1323} \text{ and H.c.}\}$
6'	^b $U(1)'$	$\mu_1^2, \mu_2^2, \mu_3^2, \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233}, \lambda_{1221}, \lambda_{1331}, \lambda_{2332}, \{m_{12}^2, \lambda_{1212}, \lambda_{1112}, \lambda_{2212}, \lambda_{3312}, \lambda_{1332} \text{ and H.c.}\}$
7	$U(1) \otimes U(1)'$	$\mu_1^2, \mu_2^2, \mu_3^2, \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233}, \lambda_{1221}, \lambda_{1331}, \lambda_{2332}$
8	$Z_2 \otimes U(1)'$	$\mu_1^2, \mu_2^2, \mu_3^2, \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233}, \lambda_{1221}, \lambda_{1331}, \lambda_{2332}, \{\lambda_{1212} \text{ and H.c.}\}$
9	$CPI \otimes Sp(2)_{\phi_3}$	$\mu_1^2, \mu_2^2, \mu_3^2, \text{Re}(m_{12}^2), \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233}, \lambda_{1221}, \text{Re}(\lambda_{1212}), \text{Re}(\lambda_{1112}), \text{Re}(\lambda_{2212}), \text{Re}(\lambda_{3312})$
10	$CPI \otimes Z_2 \otimes Sp(2)_{\phi_3}$	$\mu_1^2, \mu_2^2, \mu_3^2, \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233}, \lambda_{1221}, \text{Re}(\lambda_{1212})$
11	$U(1) \otimes Sp(2)_{\phi_3}$	$\mu_1^2, \mu_2^2, \mu_3^2, \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233}, \lambda_{1221}$
12	CP2	$\mu_1^2 = \mu_2^2, \mu_3^2, \lambda_{11} = \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1221}, \lambda_{1133} = \lambda_{2233}, \lambda_{1331} = \lambda_{2332}, \text{Re}(\lambda_{1313}) = \text{Re}(\lambda_{2323}), \text{Re}(\lambda_{1212}), \{\lambda_{1112} = -\lambda_{2212} \text{ and H.c.}\}$
13	$CP2 \otimes Sp(2)_{\phi_3}$	$\mu_1^2 = \mu_2^2, \mu_3^2, \lambda_{11} = \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1221}, \lambda_{1133} = \lambda_{2233}, \text{Re}(\lambda_{1212}), \{\lambda_{1112} = -\lambda_{2212} \text{ and H.c.}\}$
14	$SO(2)_{\phi_1, \phi_2}$	$\mu_1^2 = \mu_2^2, \mu_3^2, \lambda_{11} = \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1221}, \lambda_{1133} = \lambda_{2233}, \lambda_{1331} = \lambda_{2332}, \text{Re}(\lambda_{1313}) = \text{Re}(\lambda_{2323}), \text{Re}(\lambda_{1212}) = 2\lambda_{11} - (\lambda_{1122} + \lambda_{1221}),$
15	D_3	$\mu_1^2 = \mu_2^2, \mu_3^2, \lambda_{11} = \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133} = \lambda_{2233}, \lambda_{1221}, \lambda_{1331} = \lambda_{2332}, \{\lambda_{2131} = -\lambda_{1232}, \lambda_{1323} \text{ and H.c.}\}$
16	D_4	$\mu_1^2 = \mu_2^2, \mu_3^2, \lambda_{11} = \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133} = \lambda_{2233}, \lambda_{1221}, \{\lambda_{1212} \text{ and H.c.}\}, \lambda_{1331} = \lambda_{2332} = \text{Re}(\lambda_{3231})$
17	$D_3 \otimes Sp(2)_{\phi_3}$	$\mu_1^2 = \mu_2^2, \mu_3^2, \lambda_{11} = \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133} = \lambda_{2233}, \lambda_{1221}$
18	$D_4 \otimes Sp(2)_{\phi_3}$	$\mu_1^2 = \mu_2^2, \mu_3^2, \lambda_{11} = \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133} = \lambda_{2233}, \lambda_{1221}, \text{Re}(\lambda_{1212})$
19	$SO(2)_{\phi_1, \phi_2} \otimes Sp(2)_{\phi_3}$	$\mu_1^2 = \mu_2^2, \mu_3^2, \lambda_{11} = \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133} = \lambda_{2233}, \lambda_{1221} = \text{Re}(\lambda_{1212}) = \lambda_{11} - \frac{1}{2}\lambda_{1122}$
20	$SU(2)_{\phi_1, \phi_2}$	$\mu_1^2 = \mu_2^2, \mu_3^2, \lambda_{11} = \lambda_{22}, \lambda_{33}, \lambda_{1122} = 2\lambda_{11} - \lambda_{1221}, \lambda_{1221}, \lambda_{1133} = \lambda_{2233}, \lambda_{1331} = \lambda_{2332}$
21	$SU(2)_{\phi_1, \phi_2} \otimes Sp(2)_{\phi_3}$	$\mu_1^2 = \mu_2^2, \mu_3^2, \lambda_{11} = \lambda_{22}, \lambda_{33}, \lambda_{1122} = 2\lambda_{11} - \lambda_{1221}, \lambda_{1133} = \lambda_{2233}, \lambda_{1221}$
22	$Sp(2)_{\phi_1 + \phi_2 + \phi_3}$	$\mu_1^2, \mu_2^2, \mu_3^2, \text{Re}(m_{12}^2), \text{Re}(m_{13}^2), \text{Re}(m_{23}^2), \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233}, \lambda_{1221} = \text{Re}(\lambda_{1212}), \lambda_{1331} = \text{Re}(\lambda_{1313}),$

(Table continued)

TABLE II. (Continued)

No.	Symmetry	Nonzero parameters for 3HDM potentials
23	$Z_2 \otimes \text{Sp}(2)_{\phi_1+\phi_2+\phi_3}$	$\lambda_{2332} = \text{Re}(\lambda_{2323}), \text{Re}(\lambda_{1213}) = \text{Re}(\lambda_{2113}), \text{Re}(\lambda_{1223}) = \text{Re}(\lambda_{2123}),$ $\text{Re}(\lambda_{1323}) = \text{Re}(\lambda_{1332}), \text{Re}(\lambda_{1112}), \text{Re}(\lambda_{2212}), \text{Re}(\lambda_{3312}),$ $\text{Re}(\lambda_{1113}), \text{Re}(\lambda_{2213}), \text{Re}(\lambda_{3313}), \text{Re}(\lambda_{1123}), \text{Re}(\lambda_{2223}), \text{Re}(\lambda_{3323})$ $\mu_1^2, \mu_2^2, \mu_3^2, \text{Re}(m_{13}^2), \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233},$ $\lambda_{1221} = \text{Re}(\lambda_{1212}), \lambda_{1331} = \text{Re}(\lambda_{1313}), \lambda_{2332} = \text{Re}(\lambda_{2323}),$ $\text{Re}(\lambda_{1113}), \text{Re}(\lambda_{2213}), \text{Re}(\lambda_{3313})$
23'	$Z_2' \otimes \text{Sp}(2)_{\phi_1+\phi_2+\phi_3}$	$\mu_1^2, \mu_2^2, \mu_3^2, \text{Re}(m_{23}^2), \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233},$ $\lambda_{1221} = \text{Re}(\lambda_{1212}), \lambda_{1331} = \text{Re}(\lambda_{1313}), \lambda_{2332} = \text{Re}(\lambda_{2323}),$ $\text{Re}(\lambda_{1123}), \text{Re}(\lambda_{2223}), \text{Re}(\lambda_{3323})$
24	$Z_2 \otimes Z_2' \otimes \text{Sp}(2)_{\phi_1+\phi_2+\phi_3}$	$\mu_1^2, \mu_2^2, \mu_3^2, \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233},$ $\lambda_{1221} = \text{Re}(\lambda_{1212}), \lambda_{1331} = \text{Re}(\lambda_{1313}), \lambda_{2332} = \text{Re}(\lambda_{2323})$
25	$Z_4 \otimes \text{Sp}(2)_{\phi_1+\phi_2+\phi_3}$	$\mu_1^2, \mu_2^2, \mu_3^2, \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233}, \lambda_{1221} = \text{Re}(\lambda_{1212})$
26	$(\text{CP1} \rtimes S_2) \otimes \text{Sp}(2)_{\phi_1+\phi_2+\phi_3}$	$\mu_1^2 = \mu_2^2, \mu_3^2, \text{Re}(m_{12}^2), \text{Re}(m_{13}^2) = \text{Re}(m_{23}^2), \lambda_{11} = \lambda_{22}, \lambda_{33},$ $\lambda_{1122}, \lambda_{1133} = \lambda_{2233}, \lambda_{1221} = \text{Re}(\lambda_{1212}),$ $\lambda_{1331} = \lambda_{2332} = \text{Re}(\lambda_{1313}) = \text{Re}(\lambda_{2323}), \text{Re}(\lambda_{1323}) = \text{Re}(\lambda_{1332}),$ $\text{Re}(\lambda_{1223}) = \text{Re}(\lambda_{2123}) = \text{Re}(\lambda_{1213}) = \text{Re}(\lambda_{2113}),$ $\text{Re}(\lambda_{3313}) = \text{Re}(\lambda_{3323}), \text{Re}(\lambda_{1112}) = \text{Re}(\lambda_{2212}),$ $\text{Re}(\lambda_{3312}), \text{Re}(\lambda_{1113}) = \text{Re}(\lambda_{1123}) = \text{Re}(\lambda_{2213}) = \text{Re}(\lambda_{2223})$
27	$D_4 \otimes \text{Sp}(2)_{\phi_1+\phi_2+\phi_3}$	$\mu_1^2 = \mu_2^2, \mu_3^2, \lambda_{11} = \lambda_{22} = \frac{1}{2}\lambda_{1122}, \lambda_{33}, \lambda_{1133} = \lambda_{2233},$ $\lambda_{1221} = \text{Re}(\lambda_{1212})$
28	$\text{Sp}(2)_{\phi_1+\phi_2} \otimes \text{Sp}(2)_{\phi_3}$	$\mu_1^2, \mu_2^2, \mu_3^2, \text{Re}(m_{12}^2), \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233},$ $\lambda_{1221} = \text{Re}(\lambda_{1212}), \text{Re}(\lambda_{1112}), \text{Re}(\lambda_{2212}), \text{Re}(\lambda_{3312})$
29	$\text{Sp}(2)_{\phi_1\phi_2}$	$\mu_1^2 = \mu_2^2, \mu_3^2, \lambda_{11} = \lambda_{22} = \frac{1}{2}\lambda_{1122}, \lambda_{33}, \lambda_{1133} = \lambda_{2233}, \lambda_{1221},$ $\lambda_{1331} = \lambda_{2332}$
30	$\text{Sp}(2)_{\phi_1\phi_2} \otimes \text{Sp}(2)_{\phi_3}$	$\mu_1^2 = \mu_2^2, \mu_3^2, \lambda_{11} = \lambda_{22} = \frac{1}{2}\lambda_{1122}, \lambda_{33}, \lambda_{1133} = \lambda_{2233}, \lambda_{1221}$
31	A_4	$\mu_1^2 = \mu_2^2 = \mu_3^2, \lambda_{11} = \lambda_{22} = \lambda_{33}, \lambda_{1122} = \lambda_{1133} = \lambda_{2233},$ $\lambda_{1221} = \lambda_{1331} = \lambda_{2332}, \{\lambda_{1212} = \lambda_{1313} = \lambda_{2323}, \text{ and H.c.}\}$
32	S_4	$\mu_1^2 = \mu_2^2 = \mu_3^2, \lambda_{11} = \lambda_{22} = \lambda_{33}, \lambda_{1122} = \lambda_{1133} = \lambda_{2233},$ $\lambda_{1221} = \lambda_{1331} = \lambda_{2332}, \text{Re}(\lambda_{1212}) = \text{Re}(\lambda_{1313}) = \text{Re}(\lambda_{2323})$
33	$\text{SO}(3)$	$\mu_1^2 = \mu_2^2 = \mu_3^2, \lambda_{11} = \lambda_{22} = \lambda_{33}, \lambda_{1122} = \lambda_{1133} = \lambda_{2233},$ $\lambda_{1221} = \lambda_{1331} = \lambda_{2332},$ $\text{Re}(\lambda_{1212}) = \text{Re}(\lambda_{1313}) = \text{Re}(\lambda_{2323}) = 2\lambda_{11} - (\lambda_{1122} + \lambda_{1221})$
34	$S_4 \otimes \text{Sp}(2)_{\phi_1+\phi_2+\phi_3}$	$\mu_1^2 = \mu_2^2 = \mu_3^2, \lambda_{11} = \lambda_{22} = \lambda_{33} = \frac{1}{2}\lambda_{1122} = \frac{1}{2}\lambda_{1133} = \frac{1}{2}\lambda_{2233},$ $\lambda_{1221} = \lambda_{1331} = \lambda_{2332} = \text{Re}(\lambda_{1212}) = \text{Re}(\lambda_{1313}) = \text{Re}(\lambda_{2323})$
35	$\Delta(54)$	$\mu_1^2 = \mu_2^2 = \mu_3^2, \lambda_{11} = \lambda_{22} = \lambda_{33}, \lambda_{1122} = \lambda_{1133} = \lambda_{2233},$ $\lambda_{1221} = \lambda_{1331} = \lambda_{2332}, \{\lambda_{1213} = \lambda_{2123} = \lambda_{3231} \text{ and H.c.}\}$
36	$\Sigma(36)$	$\mu_1^2 = \mu_2^2 = \mu_3^2, \lambda_{11} = \lambda_{22} = \lambda_{33}, \lambda_{1122} = \lambda_{1133} = \lambda_{2233},$ $\lambda_{1221} = \lambda_{1331} = \lambda_{2332}, \text{Re}(\lambda_{1213}) = \text{Re}(\lambda_{1323}) = \text{Re}(\lambda_{1232}) =$ $\frac{3}{4}(2\lambda_{11} - \lambda_{1122} - \lambda_{1221})$
37	$\text{Sp}(2)_{\phi_1} \otimes \text{Sp}(2)_{\phi_2} \otimes \text{Sp}(2)_{\phi_3}$	$\mu_1^2, \mu_2^2, \mu_3^2, \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{1122}, \lambda_{1133}, \lambda_{2233}$
38	$\text{Sp}(4) \otimes \text{Sp}(2)_{\phi_3}$	$\mu_1^2 = \mu_2^2, \mu_3^2, \lambda_{11} = \lambda_{22} = \frac{1}{2}\lambda_{1122}, \lambda_{33}, \lambda_{1133} = \lambda_{2233}$
39	$\text{SU}(3) \otimes \text{U}(1)$	$\mu_1^2 = \mu_2^2 = \mu_3^2, \lambda_{11} = \lambda_{22} = \lambda_{33}, \lambda_{1122} = \lambda_{1133} = \lambda_{2233},$ $\lambda_{1221} = \lambda_{1331} = \lambda_{2332} = 2\lambda_{11} - \lambda_{1122}$
40	$\text{Sp}(6)$	$\mu_1^2 = \mu_2^2 = \mu_3^2, \lambda_{11} = \lambda_{22} = \lambda_{33} = \frac{1}{2}\lambda_{1122} = \frac{1}{2}\lambda_{1133} = \frac{1}{2}\lambda_{2233}$

$$\begin{aligned}
\mathbf{1}: & \left(\phi_1^\dagger \phi_1 + \phi_2^\dagger \phi_2 + \phi_3^\dagger \phi_3 \right), \\
\mathbf{1}': & \left(\phi_1^\dagger \phi_1 - \phi_2^\dagger \phi_2 \right), \\
\mathbf{1}'': & \left(\frac{1}{\sqrt{3}} [\phi_1^\dagger \phi_1 + \phi_2^\dagger \phi_2 - 2\phi_3^\dagger \phi_3] \right), \\
\mathbf{1}''': & \left(\phi_1^\dagger \phi_2 + \phi_2^\dagger \phi_1 \right), \\
\mathbf{1}''': & \left(-i[\phi_1^\dagger \phi_2 - \phi_2^\dagger \phi_1] \right), \\
\mathbf{2}: & \left(\begin{array}{c} \phi_1^\dagger \phi_3 + \phi_3^\dagger \phi_1 + \phi_2^\dagger \phi_3 + \phi_3^\dagger \phi_2 \\ -i[\phi_1^\dagger \phi_3 - \phi_3^\dagger \phi_1] + i[\phi_2^\dagger \phi_3 - \phi_3^\dagger \phi_2] \end{array} \right). \quad (\text{D5})
\end{aligned}$$

$$\begin{aligned}
\mathbf{1}: & (\phi_1^\dagger \phi_1 + \phi_2^\dagger \phi_2 + \phi_3^\dagger \phi_3), \\
\mathbf{2}: & \left(\begin{array}{c} \phi_1^\dagger \phi_1 + \omega^2 \phi_2^\dagger \phi_2 + \omega \phi_3^\dagger \phi_3 \\ \phi_1^\dagger \phi_1 + \omega \phi_2^\dagger \phi_2 + \omega^2 \phi_3^\dagger \phi_3 \end{array} \right), \\
\mathbf{3}: & \left(\begin{array}{c} \phi_1^\dagger \phi_2 + \phi_2^\dagger \phi_1 \\ \phi_1^\dagger \phi_3 + \phi_3^\dagger \phi_1 \\ \phi_2^\dagger \phi_3 + \phi_3^\dagger \phi_2 \end{array} \right), \\
\mathbf{3}': & \left(\begin{array}{c} -i[\phi_1^\dagger \phi_2 - \phi_2^\dagger \phi_1] \\ i[\phi_1^\dagger \phi_3 - \phi_3^\dagger \phi_1] \\ -i[\phi_2^\dagger \phi_3 - \phi_3^\dagger \phi_2] \end{array} \right). \quad (\text{D11})
\end{aligned}$$

Therefore, the S_4 -invariant 3HDM potential takes on the following form:

$$V_{S_4} = -M\mathbf{1} + \Lambda_0\mathbf{1}^2 + \Lambda_1\mathbf{2}^\top \cdot \mathbf{2} + \Lambda_2\mathbf{3}^\top \cdot \mathbf{3} + \Lambda_3\mathbf{3}'^\top \cdot \mathbf{3}'. \quad (\text{D12})$$

Hence, the D_4 -invariant 3HDM potential takes on the form

$$V_{D_4} = -M\mathbf{1} - M_2\mathbf{1}'' + \Lambda_0\mathbf{1}^2 + \Lambda_1\mathbf{1}'^2 + \Lambda_2\mathbf{1}''^2 + \Lambda_3\mathbf{1}''''^2 + \Lambda_4\mathbf{1}''''^2 + \Lambda_5\mathbf{1} \cdot \mathbf{1}'' + \Lambda_6\mathbf{2}^\top \cdot \mathbf{2}. \quad (\text{D6})$$

This potential can also be written as

$$\begin{aligned}
V_{D_4} = & -\mu_1^2(|\phi_1|^2 + |\phi_2|^2) - \mu_3^2|\phi_3|^2 + \lambda_{11}(|\phi_1|^4 + |\phi_2|^4) \\
& + \lambda_{33}|\phi_3|^4 + \lambda_{1122}|\phi_1|^2|\phi_2|^2 + \lambda_{1133}(|\phi_1|^2|\phi_3|^2 \\
& + |\phi_2|^2|\phi_3|^2) + \lambda_{1221}|\phi_1^\dagger\phi_2|^2 + \lambda_{1212}(\phi_1^\dagger\phi_2)^2 \\
& + \lambda_{1331}(|\phi_1^\dagger\phi_3|^2 + |\phi_2^\dagger\phi_3|^2 + |\phi_3^\dagger\phi_2|^2 \\
& + (\phi_2^\dagger\phi_3)(\phi_1^\dagger\phi_3) + (\phi_3^\dagger\phi_2)(\phi_3^\dagger\phi_1)), \quad (\text{D7})
\end{aligned}$$

where all parameters are real.

Likewise, we find the S_4 invariant 3HDM potential. The S_4 group can be defined by the two generators [16–18,20],

$$\Delta_{S_4}^1 = \sigma^0 \otimes g_1 \otimes \sigma^0, \quad \Delta_{S_4}^2 = \sigma^0 \otimes g_2 \otimes \sigma^0, \quad (\text{D8})$$

with

$$g_1 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad g_2 = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (\text{D9})$$

which obey the conditions $g_1^4 = g_2^3 = 1$ and $g_1 \cdot g_2 \cdot g_1 = g_2$. The $\mathbf{3} \otimes \mathbf{3}$ tensor product of S_4 consists of one singlet $\mathbf{1}$, one doublet $\mathbf{2}$, and two triplets $\mathbf{3}$ and $\mathbf{3}'$,

$$S_4: \mathbf{3} \otimes \mathbf{3} = \mathbf{1} \oplus \mathbf{2} \oplus \mathbf{3} \oplus \mathbf{3}'. \quad (\text{D10})$$

The S_4 -symmetric blocks $\mathbf{1}$, $\mathbf{2}$, $\mathbf{3}$, and $\mathbf{3}'$ may be obtained as

Note that the S_4 -invariant 3HDM potential has a similar form to the A_4 -invariant 3HDM potential shown in Eq. (4.38). However, in the S_4 -invariant 3HDM potential all parameters are real, due to the absence of $\mathbf{3}'^\top \cdot \mathbf{3}$ and $\mathbf{3}^\top \cdot \mathbf{3}'$ terms which are allowed by the A_4 symmetry. In addition, if $\text{Re}(\lambda_{1212}) = 2\lambda_{11} - (\lambda_{1122} + \lambda_{1221})$, one gets an $SO(3)$ -invariant 3HDM potential.

The next symmetry of the 3HDM potential is the $\Delta(54)$ symmetry group, which can be defined through the three generators:

$$\begin{aligned}
\Delta_{\Delta(54)}^1 &= \text{diag}[g_1 \otimes \sigma^0, g_1^* \otimes \sigma^0], \\
\Delta_{\Delta(54)}^2 &= \sigma^0 \otimes g_2 \otimes \sigma^0, \\
\Delta_{\Delta(54)}^3 &= \sigma^0 \otimes g_3 \otimes \sigma^0, \quad (\text{D13})
\end{aligned}$$

where

$$\begin{aligned}
g_1 &= \begin{pmatrix} \omega^2 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad g_2 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \\
g_3 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (\text{D14})
\end{aligned}$$

These generators satisfy the conditions $g_1^3 = 1$, $g_2^3 = 1$, and $g_3^2 = 1$. The $\mathbf{3} \otimes \mathbf{3}$ tensor product of $\Delta(54)$ can be decomposed in one singlet $\mathbf{1}$ and four doublets $\mathbf{2}$, $\mathbf{2}'$, $\mathbf{2}''$, and $\mathbf{2}'''$ as

$$\Delta(54): \mathbf{3} \otimes \mathbf{3} = \mathbf{1} \oplus \mathbf{2} \oplus \mathbf{2}' \oplus \mathbf{2}'' \oplus \mathbf{2}'''. \quad (\text{D15})$$

The irreducible representations of $\Delta(54)$ in the bilinear space can be represented as [52]

$$\begin{aligned}
\mathbf{1}: & (\phi_1^\dagger \phi_1 + \phi_2^\dagger \phi_2 + \phi_3^\dagger \phi_3), \\
\mathbf{2}: & \begin{pmatrix} \phi_1^\dagger \phi_1 + \omega \phi_2^\dagger \phi_2 + \omega^2 \phi_3^\dagger \phi_3 \\ \phi_1^\dagger \phi_1 + \omega^2 \phi_2^\dagger \phi_2 + \omega \phi_3^\dagger \phi_3 \end{pmatrix}, \\
\mathbf{2}': & \begin{pmatrix} \phi_1^\dagger \phi_2 + \phi_3^\dagger \phi_1 + \phi_2^\dagger \phi_3 \\ \phi_2^\dagger \phi_1 + \phi_1^\dagger \phi_3 + \phi_3^\dagger \phi_2 \end{pmatrix}, \\
\mathbf{2}'': & \begin{pmatrix} \phi_2^\dagger \phi_3 + \omega \phi_3^\dagger \phi_1 + \omega^2 \phi_1^\dagger \phi_2 \\ \omega \phi_2^\dagger \phi_1 + \phi_3^\dagger \phi_2 + \omega^2 \phi_1^\dagger \phi_3 \end{pmatrix}, \\
\mathbf{2}''': & \begin{pmatrix} \omega^2 \phi_2^\dagger \phi_1 + \phi_3^\dagger \phi_2 + \omega \phi_1^\dagger \phi_3 \\ \phi_2^\dagger \phi_3 + \omega^2 \phi_3^\dagger \phi_1 + \omega \phi_1^\dagger \phi_2 \end{pmatrix}.
\end{aligned} \tag{D16}$$

Having obtained the $\Delta(54)$ -symmetric blocks, the $\Delta(54)$ -invariant 3HDM potential is given by

$$\begin{aligned}
V_{\Delta(54)} = & -M\mathbf{1} + \Lambda_0 \mathbf{1}^2 + \Lambda_1 \mathbf{2}^\dagger \cdot \mathbf{2} + \Lambda_2 \mathbf{2}^{\text{T}} \cdot \mathbf{2}' \\
& + \Lambda_3 \mathbf{2}^{\text{H}\dagger} \cdot \mathbf{2}'' + \Lambda_4 \mathbf{2}^{\text{H}\dagger} \cdot \mathbf{2}''',
\end{aligned} \tag{D17}$$

and can be rewritten in the following form:

$$\begin{aligned}
V_{\Delta(54)} = & -\mu_1^2 (|\phi_1|^2 + |\phi_2|^2 + |\phi_3|^2) + \lambda_{11} (|\phi_1|^4 \\
& + |\phi_2|^4 + |\phi_3|^4) + \lambda_{1122} (|\phi_1|^2 |\phi_2|^2 + |\phi_1|^2 |\phi_3|^2 \\
& + |\phi_2|^2 |\phi_3|^2) + \lambda_{1221} (|\phi_1^\dagger \phi_2|^2 + |\phi_1^\dagger \phi_3|^2 \\
& + |\phi_2^\dagger \phi_3|^2) + \lambda_{1213} ((\phi_1^\dagger \phi_2)(\phi_1^\dagger \phi_3) + (\phi_2^\dagger \phi_1)(\phi_2^\dagger \phi_3) \\
& + (\phi_3^\dagger \phi_2)(\phi_3^\dagger \phi_1)) + \lambda_{1213}^* ((\phi_2^\dagger \phi_1)(\phi_3^\dagger \phi_1) \\
& + (\phi_1^\dagger \phi_2)(\phi_3^\dagger \phi_2) + (\phi_2^\dagger \phi_3)(\phi_1^\dagger \phi_3)).
\end{aligned} \tag{D18}$$

The largest non-Abelian discrete symmetry of 3HDM is the $\Sigma(36)$ group [21–24]. The relevant $\mathbf{3} \otimes \mathbf{3}$ tensor product of $\Sigma(36)$ may be decomposed as

$$\Sigma(36) : \mathbf{3} \otimes \mathbf{3} = \mathbf{1} \oplus \mathbf{4} \oplus \mathbf{4}'. \tag{D19}$$

The three generators of this group are

$$\begin{aligned}
\Delta_{\Sigma(36)}^1 &= \text{diag}[g_1 \otimes \sigma^0, g_1^* \otimes \sigma^0], \\
\Delta_{\Sigma(36)}^2 &= \sigma^0 \otimes g_2 \otimes \sigma^0, \\
\Delta_{\Sigma(36)}^3 &= \text{diag}[g_3 \otimes \sigma^0, g_3^* \otimes \sigma^0],
\end{aligned} \tag{D20}$$

with

$$\begin{aligned}
g_1 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega^2 \end{pmatrix}, \quad g_2 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \\
g_3 &= \frac{1}{\omega - \omega^2} \begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega \end{pmatrix},
\end{aligned} \tag{D21}$$

which obey the conditions $g_1^3 = g_2^3 = 1$ and $g_3^4 = 1$. Now, we can define the irreducible representations of $\Sigma(36)$ as [52]

$$\begin{aligned}
\mathbf{1}: & (\phi_1^\dagger \phi_1 + \phi_2^\dagger \phi_2 + \phi_3^\dagger \phi_3), \\
\mathbf{4}: & \begin{pmatrix} \omega^2 \phi_1^\dagger \phi_2 + \phi_2^\dagger \phi_3 + \omega \phi_3^\dagger \phi_1 \\ \omega^2 \phi_1^\dagger \phi_3 + \phi_2^\dagger \phi_1 + \omega \phi_3^\dagger \phi_2 \\ \omega^2 \phi_1^\dagger \phi_2 + \omega \phi_2^\dagger \phi_3 + \phi_3^\dagger \phi_1 \\ \omega^2 \phi_1^\dagger \phi_3 + \omega \phi_2^\dagger \phi_1 + \phi_3^\dagger \phi_2 \end{pmatrix}, \\
\mathbf{4}': & \begin{pmatrix} \omega \phi_1^\dagger \phi_3 + \omega \phi_2^\dagger \phi_1 + \omega \phi_3^\dagger \phi_2 \\ \omega \phi_1^\dagger \phi_1 + \phi_2^\dagger \phi_2 + \omega^2 \phi_3^\dagger \phi_3 \\ \omega^2 \phi_1^\dagger \phi_2 + \omega^2 \phi_2^\dagger \phi_3 + \omega^2 \phi_3^\dagger \phi_1 \\ \omega \phi_1^\dagger \phi_1 + \omega^2 \phi_2^\dagger \phi_2 + \phi_3^\dagger \phi_3 \end{pmatrix}.
\end{aligned} \tag{D22}$$

Finally, the $\Sigma(36)$ -invariant potential then takes on the form

$$V_{\Sigma(36)} = -M\mathbf{1} + \Lambda_0 \mathbf{1}^2 + \Lambda_1 \mathbf{4}^\dagger \cdot \mathbf{4} + \Lambda_2 \mathbf{4}'^\dagger \cdot \mathbf{4}'. \tag{D23}$$

Equivalently, the $\Sigma(36)$ -invariant 3HDM potential can be given by

$$\begin{aligned}
V_{\Sigma(36)} &= -\mu_1^2 (|\phi_1|^2 + |\phi_2|^2 + |\phi_3|^2) + \lambda_{11} (|\phi_1|^4 + |\phi_2|^4 + |\phi_3|^4) \\
&+ \lambda_{1122} (|\phi_1|^2 |\phi_2|^2 + |\phi_1|^2 |\phi_3|^2 + |\phi_2|^2 |\phi_3|^2) \\
&+ \lambda_{1221} (|\phi_1^\dagger \phi_2|^2 + |\phi_1^\dagger \phi_3|^2 + |\phi_2^\dagger \phi_3|^2) \\
&+ \frac{3}{4} (2\lambda_{11} - \lambda_{1122} - \lambda_{1221}) ((\phi_1^\dagger \phi_2)(\phi_1^\dagger \phi_3) \\
&+ (\phi_1^\dagger \phi_3)(\phi_2^\dagger \phi_3) + (\phi_1^\dagger \phi_2)(\phi_3^\dagger \phi_2) + \text{H.c.}),
\end{aligned} \tag{D24}$$

with all real parameters.

These symmetries for the 3HDM potential, along with their nonzero theoretical parameters, are presented in Table II.

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