# Generalized *CP* symmetries in three-Higgs-doublet models

Iris Bree,[*] Duarte D. Correia,[†] and João P. Silva[‡]

*CFTP, Departamento de Física, Instituto Superior Técnico, Universidade de Lisboa, Avenida Rovisco Pais 1, 1049 Lisboa, Portugal*

(Received 19 July 2024; accepted 30 July 2024; published 26 August 2024)

We study the scalar and Yukawa sectors of three Higgs doublets models with a generalized *CP* symmetry. Imposing the symmetry on the quadratic and quartic couplings of the scalar potential, we show that there are only four classes of scalar potentials, merely one more than in two-Higgs-doublet models (2HDM). Two 3HDM cases are analogs of two 2HDM cases, while the other 2HDM case splits here into two distinct potentials. In 2HDM with generalized *CP* symmetries extended to the Yukawa sector, there are only two possible cases: the usual *CP*, with 18 real Yukawa couplings; and a minimal generalized *CP* model, with 12 real Yukawa parameters. In contrast, with three Higgs there is a rich variety of allowed models. We classify all possible Yukawa textures, showing that there are 40 possibilities, several of which have only 10 real Yukawa couplings.

DOI: 10.1103/PhysRevD.110.035028

## I. INTRODUCTION

The scalar sector responsible for electroweak symmetry breaking is currently being incisively probed. Since there is no conclusive theoretical argument constraining the number of Higgs doublets, ultimately it should be determined experimentally.

However, models with more than one Higgs introduce many new parameters, both in the scalar potential and in the Yukawa couplings. These can be reduced with the introduction of extra symmetries of the type

$$\Phi_a \to S_{ab}\Phi_b, \tag{1}$$

or

$$\Phi_a \to X_{ab}\Phi_b^*, \tag{2}$$

where $S$ and $X$ belong to $SU(n_H)$, $n_H$ is the number of Higgs doublets in the theory, and, unless stated otherwise, summation of repeated indices will always be implied. The former are known as family symmetries. The latter combine unitary transformations with the usual charge-parity ($CP$) conjugation and were named generalized $CP$ ($GCP$) transformations, first analyzed by Lee [1]. Their use in the scalar sector was first developed by the Vienna group [2–4] and their explicit use for quarks first appeared in [5].

It has been shown that applying the $GCP$ symmetry to the 2HDM scalar potential with any possible choice of $X$ leads only to three classes of scalar potentials [6,7]. In a basis where $X$ is written as a usual rotation matrix with angle $\theta$, the three 2HDM cases correspond to $\theta = 0$, $\theta = \pi/2$, and $\theta \notin \{0, \pi/2\}$. Extending that symmetry to the Yukawa sector involves many new parameters and one might expect a bonanza of possibilities. As shown by Ferreira and Silva [8], quite the contrary happens; besides the usual $CP$ conserving 2HDM, there is only one single $GCP$ symmetric 2HDM with both scalar and Yukawa interactions which is consistent with nonzero quark masses. It turns out that model exhibits a new type of spontaneous $CP$ violation [8]; one where the scalar potential by itself is $CP$ conserving (even after spontaneous electroweak symmetry breaking), but where the relative phase of the vacua induces $CP$-violating phases in the coupling to fermions and in the CKM matrix. It is thus interesting to see which of these features are characteristic of 2HDM and which survive when there are extra Higgs doublets. To this end we study the scalar sector and the Yukawa sector of three-Higgs-doublet models (3HDM) with a generalized $CP$ symmetry.

The implications of family symmetries to the three Higgs scalar potential were studied in [9], for the case of symmetry groups with only one generator. Still regarding the scalar potential, the set of all symmetry/constrained 3HDM was mapped in [10],[1] their identification in a basis

[*]Contact author: iris.bree.silva@tecnico.ulisboa.pt
[†]Contact author: duarte.d.correia@tecnico.ulisboa.pt
[‡]Contact author: jpsilva@cftp.ist.utl.pt



[1]One of us (I. B.) proved later that there are a few groups that should be added to the list; such as $U(1) \times U(1) \rtimes \mathbb{Z}_3$ and $O(2) \times U(1)$ [11].

invariant fashion proposed in [12,13], a detailed description of their symmetry breaking patterns discussed in [14], and their decoupling limit properties established in [15]. As for the impact of flavor symmetries on the combined Higgs and Yukawa sector of the 3HDM, it was first tackled for the case of symmetry groups with only one generator in [16], and later generalized into other groups in [17,18].

Here, we concentrate exclusively on $GCP$ symmetries. In Sec. II we introduce the conditions for $GCP$ invariance of the 3HDM scalar potential. When $X$ is written as a rotation matrix, two 3HDM cases correspond to $\theta = 0$ and $\theta = \pi/2$ (in complete analogy with the 2HDM), while two other 3HDM cases correspond to $\theta = \pi/3$ and $\theta \notin \{0, \pi/2, \pi/3\}$ (which can be seen as a branch out of the $\theta \notin \{0, \pi/2\}$ 2HDM case). In Sec. III we propose a much faster and more elegant method to ascertain symmetry constraints, and we analyze the scalar potential, in full detail. The new method is crucial when we extend $GCP$ into the Yukawa sector in Sec. IV. We show explicitly all possible Yukawa textures in Sec. V. It turns out that there are many textures with fewer parameters than present in the $GCP$-symmetric 2HDM. We present our conclusions in Sec. VI. In each section we include only simple examples of the type of analysis required, so that the reasoning leading to the conclusions stated is clear. We relegate some details to the appendixes. In Appendix A we show how one reaches the conclusion that there are only four $GCP$-symmetric 3HDM scalar potentials using a standard (inefficient) analysis. In Appendix B we state a mathematical result which greatly simplifies the analysis, whose detailed proof we supply as Supplemental Material [19].

## II. THE SCALAR POTENTIAL

### A. Notation

Let us consider a three-Higgs-doublet model with 3 Higgs-doublets $\Phi_i$, of the same hypercharge $1/2$, and with vacuum expectation values (vevs)

$$\langle \Phi_i \rangle = \begin{pmatrix} \langle \phi_i^+ \rangle \\ \langle \phi_i^0 \rangle \end{pmatrix} = \begin{pmatrix} 0 \\ v_i/\sqrt{2} \end{pmatrix}. \tag{3}$$

The index $i$ runs from 1 to 3, and we use the standard definition for the electric charge, whereby the upper components of the $SU(2)$ doublets ($\phi_i^+$) are charged and the lower components ($\phi_i^0$) are neutral.

The most general 3HDM scalar potential which is renormalizable and compatible with the gauge symmetries of the Standard Model (SM), can be written as [20–22]

$$V_H = Y_{ij}(\Phi_i^\dagger \Phi_j) + Z_{ij,kl}(\Phi_i^\dagger \Phi_j)(\Phi_k^\dagger \Phi_l), \tag{4}$$

where $Y$ ($Z$) is a rank-2 (rank-4) tensor in three dimensions and $Z_{ij,kl} \equiv Z_{kl,ij}$. Hermiticity implies that

$$\begin{aligned} Y_{ij} &= Y_{ji}^*, \\ Z_{ij,kl} &\equiv Z_{kl,ij} = Z_{ji,lk}^*. \end{aligned} \tag{5}$$

This means that there are only 3 real (and 3 complex) parameters in $Y$ and 9 real (and 18 complex) parameters in $Z$.

### B. $GCP$ symmetries

The scalar potential in Eq. (4) is invariant under the $GCP$ transformation in Eq. (2) if and only if

$$\begin{aligned} Y_{ab}^* &= X_{\alpha a}^* Y_{\alpha\beta} X_{\beta b} = (X^\dagger Y X)_{ab}, \\ Z_{ab,cd}^* &= X_{\alpha a}^* X_{\gamma c}^* Z_{\alpha\beta,\gamma\delta} X_{\beta b} X_{\delta d}. \end{aligned} \tag{6}$$

Solving these equations for every (independent) parameter in $Y$ and $Z$ is a daunting task if we use a general $3\times 3$ unitary matrix in Eq. (2). Fortunately, Ecker, Grimus, and Neufeld [23] proved that there is always a basis of scalar fields, for which the $GCP$ transformation matrix $X$ may be brought to the form

$$X_\theta = \begin{bmatrix} c_\theta & s_\theta & 0 \\ -s_\theta & c_\theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \equiv R_\theta \oplus 1, \tag{7}$$

where the $\oplus$ symbol stands for direct sum, and $0 \le \theta \le \pi/2$. Notice the restricted range for $\theta$. Henceforth,

$$R = \begin{pmatrix} c & s \\ -s & c \end{pmatrix}, \tag{8}$$

where $c = \cos$, $s = \sin$ and the Greek subindices indicate the angle. Next, we will study Eqs. (6) in the basis where Eq. (7) holds.

## III. A NEW STRATEGY FOR $GCP$ CONSTRAINTS

### A. A simple example

Consider a vector of complex entries $(a, b)^\top$, and a system of two equations

$$\begin{pmatrix} a \\ b \end{pmatrix}^* = R_\theta^\top \begin{pmatrix} a \\ b \end{pmatrix}, \tag{9}$$

which may be written alternatively as $(a, b)^\dagger = R_\theta^\top (a, b)^\top$. The system has only 3 distinct solutions:

*i*) if $\theta = 2k\pi$, for integer $k$, then $a, b \in \mathbb{R}$;

*ii*) if $\theta = (2k+1)\pi$, for integer $k$, then $a, b \in \mathbb{I}$;

*iii*) otherwise, $a = b = 0$. (10)

This will be the source of the subsequent analysis, provided one can turn problems into two-dimensional blocks.

Imagine now that there is a 4-vector subject to the constraint

$$\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}^* = R_\alpha^\top \otimes R_\beta^\top \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} c_\alpha c_\beta & -c_\alpha s_\beta & -c_\beta s_\alpha & s_\alpha s_\beta \\ c_\alpha s_\beta & c_\alpha c_\beta & -s_\alpha s_\beta & -c_\beta s_\alpha \\ c_\beta s_\alpha & -s_\alpha s_\beta & c_\alpha c_\beta & -c_\alpha s_\beta \\ s_\alpha s_\beta & c_\beta s_\alpha & c_\alpha s_\beta & c_\alpha c_\beta \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}, \quad (11)$$

where $\otimes$ denotes the Kronecker product of two matrices. One interesting way to solve Eq. (11) is the following. Consider the orthogonal matrix

$$C_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 \end{pmatrix}. \quad (12)$$

It is easy to show that

$$C_2 R_\alpha^\top \otimes R_\beta^\top C_2^\top = R_{\alpha+\beta}^\top \oplus R_{\beta-\alpha}^\top. \quad (13)$$

Again, the $\oplus$ symbol stands for direct sum and, here, it means that a $4 \times 4$ block-diagonal matrix has been built, such that the $2 \times 2$ upper-left corner has the matrix $R_{\alpha+\beta}^\top$, the $2 \times 2$ lower-right corner has the matrix $R_{\beta-\alpha}^\top$, and all other entries vanish. Left multiplying Eq. (11) by $C_2$ and inserting $C_2^\top C_2$ in between $R_\beta^\top$ and $C_2^\top$ on the left-hand side (LHS) of Eq. (13), one finds

$$\begin{pmatrix} a-d \\ b+c \\ a+d \\ b-c \end{pmatrix}^* = \begin{pmatrix} R_{\alpha+\beta}^\top & O \\ O & R_{\beta-\alpha}^\top \end{pmatrix} \begin{pmatrix} a-d \\ b+c \\ a+d \\ b-c \end{pmatrix}, \quad (14)$$

effectively decoupling the problem into much simpler two two-dimensional problems. But now one can use Eq. (10) for immediate conclusions. This is generalized to higher dimensions in Appendix B.

It will prove useful to use the vec(·) operator, which vectorizes by rows.[2] It can be shown that

$$\mathrm{vec}(C_{ck}\bar{Y}_{kl}D_{ld}) = C \otimes D^\top \mathrm{vec}(\bar{Y}_{kl}), \quad (15)$$

$$\mathrm{vec}(A_{ai}C_{ck}\bar{K}_{i,kl}D_{ld}) = A \otimes C \otimes D^\top \mathrm{vec}(\bar{K}_{i,kl}), \quad (16)$$

$$\mathrm{vec}(A_{ai}C_{ck}\bar{Z}_{ij,kl}B_{jb}D_{ld}) = A \otimes B^\top \otimes C \otimes D^\top \mathrm{vec}(\bar{Z}_{ij,kl}), \quad (17)$$

where $A$, $B$, $C$, and $D$ are appropriately sized matrices, whereas $\bar{Y}$, $\bar{K}$, and $\bar{Z}$ are tensors of rank 2, 3, and 4, respectively.

### B. *GCP* constraints on *Y*

Here, we apply the technique of the previous section in order to solve Eqs. (6) and derive the *GCP* constraints on $Y$. We include the study of the *GCP* symmetry conditions on the scalar potential using a different strategy, which mimics [8], in Appendix A. Employing the strategy in Appendix A to the Yukawa sector, however, becomes greatly error prone.

Due to the simple form of Eq. (7), the tensor is divided into 4 regions: $mn$, $m3$, $3n$, and 33 $(m, n = 1, 2)$. But, thanks to Hermiticity, we need not solve the system for $3n$. For 33, we have that $Y_{33}^* = Y_{33} \Leftrightarrow Y_{33} \in \mathbb{R}$, which we already knew.

Henceforth, we will be using the notation

$$\begin{aligned} Y_{\{m3\}} &= (Y_{13}, Y_{23})^\top, \\ Y_{\{3n\}} &= (Y_{31}, Y_{32})^\top, \\ Y_{\{mn\}} &= (Y_{11}, Y_{12}, Y_{21}, Y_{22})^\top. \end{aligned} \quad (18)$$

For $m3$ and $3n$, we have

$$Y_{\{m3\}}^* = R_\theta^\top Y_{\{m3\}}, \qquad Y_{\{3n\}}^* = R_\theta^\top Y_{\{3n\}}. \quad (19)$$

As seen in Eqs. (10) and given the restricted range for $\theta$, we find that

| | | |
|---|---|---|
| i. | $\theta = 0$ | $(Y)_{13} = (Y)_{31}$, $(Y)_{23} = (Y)_{32} \in \mathbb{R}$, |
| ii. | $\theta \neq 0$ | $(Y)_{13} = (Y)_{31} = (Y)_{23} = (Y)_{32} = 0$. |

For $mn$, we use Eq. (15), in order to rewrite Eq. (6) as

$$Y_{\{mn\}}^* = R_\theta^\top \otimes R_\theta^\top Y_{\{mn\}}. \quad (20)$$

To solve this system we use Eq. (13). The $mn$ sector then simplifies to

[2]The usual vec(·) operator vectorizes by columns [24]. Here, we vectorize by rows.

$$\begin{pmatrix} Y_{11}-Y_{22} \\ 2\mathrm{Re}(Y_{12}) \end{pmatrix}^* = R_{2\theta}^\top \begin{pmatrix} Y_{11}-Y_{22} \\ 2\mathrm{Re}(Y_{12}) \end{pmatrix}, \quad \mathrm{Im}(Y_{12}) = 0, \tag{21}$$

and solving it results in the following two options:

| | | |
|---|---|---|
| i. | $\theta = 0$ | $(Y)_{11}$, $(Y)_{22}$, $(Y)_{12} = (Y)_{21} \in \mathbb{R}$, |
| ii. | $\theta \neq 0$ | $(Y)_{11} = (Y)_{22}$, $(Y)_{12} = (Y)_{21} = 0$. |

In conclusion: for $\theta = 0$, all of $Y$'s entries are real, otherwise $Y = \mathrm{diag}(\mu_1, \mu_1, \mu_3)$.

### C. Summary of *GCP* constraints on *Z*

The full simplifying power of the new method comes to light when we deal with the quartic $Z$ couplings.[3] As before, our choice of basis decouples the third entries from the rest, but now we have a total of 16 separate regions, those being $ijkl$, $ijk3$, $ij3l$, $i3kl$, $3jkl$, $ij33$, $i3k3$, $i33l$, $3jk3$, $3j3l$, $33kl$, $i333$, $3j33$, $33k3$, $333l$, and 3333 (here $i$, $j$, $k$, $l = 1, 2$). And thanks once again to Hermiticity, we need not solve all of them. We just need to solve 7: $ijkl$, $ij33$, $i3kl$, $i3k3$, $i33l$, $i333$, and 3333, since these contain all independent entries for $Z$.

The case for 3333 just tells us that $Z_{3333}$ is a real entry, which we already knew. For $i333$, we will have the same as Eqs. (19), and so these entries are always real, and equal to 0 if $\theta \neq 0$. The sectors $ij33$, $i33l$ and $i3k3$ will be the same as Eq. (20). Although the first two cases are identical to Eq. (21), the latter is a bit more interesting, as we discover a new region of interest when $\theta = \pi/2$.

Finally, we have[4] $Z^*_{\{i3kl\}} = R_\theta^{\top\otimes 3} Z_{\{i3kl\}}$ and $Z^*_{\{ijkl\}} = R_\theta^{\top\otimes 4} Z_{\{ijkl\}}$, with a definition analogous to Eq. (18). As before, there are orthogonal matrices $C_3$ and $C_4$ such that

$$C_3 R_\theta^{\top\otimes 3} C_3^\top = R_{3\theta}^\top \oplus R_\theta^\top \oplus R_\theta^\top \oplus R_\theta, \tag{22}$$

and

$$C_4 R_\theta^{\top\otimes 4} C_4^\top = R_{4\theta}^\top \oplus R_{2\theta}^\top \oplus R_{2\theta}^\top \oplus I_2 \oplus R_{2\theta}^\top \oplus I_2 \oplus I_2 \oplus R_{2\theta}. \tag{23}$$

This technique is quite useful since it turns an $R_\theta^{\otimes n}$ matrix, a $2^n \times 2^n$ system, into $2^{n-1}$ $2 \times 2$ systems, which are trivial to solve. The $i3kl$ system provides us with the final region of interest, that being when $\theta = \pi/3$.

At last, we have our four regions of interest: $\theta = 0$, $\theta = \pi/2$, $\theta = \pi/3$ and $\theta \in (0, \pi/2)\backslash\{\pi/3\}$, which we will denote as $CPa$, $CPb$, $CPc$, and $CPd$, respectively.[5] Let us compare this result with what one has in the 2HDM. In the scalar potential of the 2HDM there are 2 real and 1 complex parameters in the quadratic couplings and 4 real and 3 complex parameters in the quartic couplings. Imposing $GCP$ we find only three classes of 2HDM potentials, corresponding to $\theta = 0$, $\theta = \pi/2$, and $\theta \in (0, \pi/2)$. In the 3HDM there are 3 real and 3 complex parameters in the quadratic couplings and 9 real and 18 complex parameters in the quartic couplings. Despite the enormous increase in the number of parameters, there is only one more class of $GCP$-symmetric potentials: corresponding to the singling out of the $\theta = \pi/3$ case.

### D. Proof of *GCP* constraints on *Z*

Using Eq. (17), we can write

$$Z^*_{3333} = Z_{3333}, \tag{24}$$

$$Z^*_{\{i333\}} = R_\theta^\top Z_{\{i333\}}, \qquad Z_{\{i333\}} = (Z_{1333}, Z_{2333})^\top, \tag{25}$$

$$\begin{aligned} Z^*_{\{ij33\}} &= R_\theta^{\top\otimes 2} Z_{\{ij33\}}, \qquad Z_{\{ij33\}} = (Z_{1133}, Z_{1233}, Z_{2133}, Z_{2233})^\top, \\ Z^*_{\{i33l\}} &= R_\theta^{\top\otimes 2} Z_{\{i33l\}}, \qquad Z_{\{i33l\}} = (Z_{1331}, Z_{1332}, Z_{2331}, Z_{2332})^\top, \\ Z^*_{\{i3k3\}} &= R_\theta^{\top\otimes 2} Z_{\{i3k3\}}, \qquad Z_{\{i3k3\}} = (Z_{1313}, Z_{1323}, Z_{2313}, Z_{2323})^\top, \end{aligned} \tag{26}$$

$$Z^*_{\{i3kl\}} = R_\theta^{\top\otimes 3} Z_{\{i3kl\}}, \qquad Z_{\{i3kl\}} = (Z_{1311}, Z_{1312}, Z_{1321}, Z_{1322}, Z_{2311}, Z_{2312}, Z_{2321}, Z_{2322})^\top, \tag{27}$$

$$\begin{aligned} Z^*_{\{ijkl\}} = R_\theta^{\top\otimes 4} Z_{\{ijkl\}}, \qquad Z_{\{ijkl\}} = (&Z_{1111}, Z_{1112}, Z_{1121}, Z_{1122}, Z_{1211}, Z_{1212}, Z_{1221}, Z_{1222}, \\ &Z_{2111}, Z_{2112}, Z_{2121}, Z_{2122}, Z_{2211}, Z_{2212}, Z_{2221}, Z_{2222})^\top. \end{aligned} \tag{28}$$

[3] We included the messier alternative in Appendix A for comparison.
[4] Henceforth, we use the notation $R_\theta^{\otimes 2} \equiv R_\theta \otimes R_\theta$, and similarly for higher powers.
[5] In the notation of the 2HDM case in [8], these would be written as, respectively, $CP1$, $CP2$, with both $c$ and $d$ corresponding there to $CP3$.

Equation (24) tells us that $Z_{3333}$ is real which we already knew. In Eq. (25), due to the restricted range for $\theta$, we have

| | | |
|---|---|---|
| i. | $\theta = 0$ | $Z_{1333},\ Z_{2333} \in \mathbb{R}$, |
| ii. | $\theta \neq 0$ | $Z_{1333} = Z_{2333} = 0$. |

For Eqs. (26), we shall use the result in Eq. (B1) for $n = 2$, along with the following relations: $Z_{1233} = Z^*_{2133}$; $Z_{1332} = Z^*_{2331}$; $Z_{1323} = Z_{2313}$; $Z_{1133}, Z_{2233}, Z_{1331}, Z_{2332} \in \mathbb{R}$. We find

$$\begin{pmatrix} Z_{1133} - Z_{2233} \\ 2\mathrm{Re}(Z_{1233}) \end{pmatrix}^* = R^\top_{2\theta} \begin{pmatrix} Z_{1133} - Z_{2233} \\ 2\mathrm{Re}(Z_{1233}) \end{pmatrix},$$
$$\begin{pmatrix} Z_{1331} - Z_{2332} \\ 2\mathrm{Re}(Z_{1332}) \end{pmatrix}^* = R^\top_{2\theta} \begin{pmatrix} Z_{1331} - Z_{2332} \\ 2\mathrm{Re}(Z_{1332}) \end{pmatrix},$$
$$\mathrm{Im}(Z_{1233}) = \mathrm{Im}(Z_{1332}) = 0, \tag{29}$$

$$\begin{pmatrix} Z_{1313} - Z_{2323} \\ 2Z_{1323} \end{pmatrix}^* = R^\top_{2\theta} \begin{pmatrix} Z_{1313} - Z_{2323} \\ 2Z_{1323} \end{pmatrix},$$
$$Z_{1313} + Z_{2323} \in \mathbb{R}. \tag{30}$$

For Eqs. (29) we find

| | | |
|---|---|---|
| i. | $\theta = 0$ | $Z_{\{ij33\}},\ Z_{\{i33l\}} \in \mathbb{R}$, |
| ii. | $\theta \neq 0$ | $Z_{1133} = Z_{2233},\ Z_{1331} = Z_{2332}$, $Z_{1233} = Z_{2133} = Z_{1332} = Z_{2331} = 0$, |

and, similarly, for Eqs. (30),

| | | |
|---|---|---|
| i. | $\theta = 0$ | $Z_{\{i3k3\}} \in \mathbb{R}$, |
| ii. | $\theta = \pi/2$ | $Z_{1323} = Z_{2313} \in \mathbb{I},\ Z_{1313} = Z^*_{2323}$, |
| iii. | $\theta \neq \{0, \pi/2\}$ | $Z_{1313} = Z_{2323} \in \mathbb{R},\ Z_{1323} = Z_{2313} = 0$. |

For Eqs. (27), we shall use the result in Eq. (B1) for $n = 3$. We find

$$\begin{pmatrix} (Z_{1311} - Z_{1322}) - (Z_{2312} + Z_{2321}) \\ (Z_{1312} + Z_{1321}) + (Z_{2311} - Z_{2322}) \end{pmatrix}^* = R^\top_{3\theta} \begin{pmatrix} (Z_{1311} - Z_{1322}) - (Z_{2312} + Z_{2321}) \\ (Z_{1312} + Z_{1321}) + (Z_{2311} - Z_{2322}) \end{pmatrix},$$
$$\begin{pmatrix} (Z_{1311} - Z_{1322}) + (Z_{2312} + Z_{2321}) \\ (Z_{1312} + Z_{1321}) - (Z_{2311} - Z_{2322}) \end{pmatrix}^* = R^\top_{\theta} \begin{pmatrix} (Z_{1311} - Z_{1322}) + (Z_{2312} + Z_{2321}) \\ (Z_{1312} + Z_{1321}) - (Z_{2311} - Z_{2322}) \end{pmatrix},$$
$$\begin{pmatrix} (Z_{1311} + Z_{1322}) - (Z_{2312} - Z_{2321}) \\ (Z_{1312} - Z_{1321}) + (Z_{2311} + Z_{2322}) \end{pmatrix}^* = R^\top_{\theta} \begin{pmatrix} (Z_{1311} + Z_{1322}) - (Z_{2312} - Z_{2321}) \\ (Z_{1312} - Z_{1321}) + (Z_{2311} + Z_{2322}) \end{pmatrix},$$
$$\begin{pmatrix} (Z_{1311} + Z_{1322}) + (Z_{2312} - Z_{2321}) \\ (Z_{1312} - Z_{1321}) - (Z_{2311} + Z_{2322}) \end{pmatrix}^* = R_{\theta} \begin{pmatrix} (Z_{1311} + Z_{1322}) + (Z_{2312} - Z_{2321}) \\ (Z_{1312} - Z_{1321}) - (Z_{2311} + Z_{2322}) \end{pmatrix}. \tag{31}$$

The solution to these equations is

| | | | |
|---|---|---|---|
| i. | $\theta = 0$ | $Z_{\{i3kl\}} \in \mathbb{R}$, | |
| ii. | $\theta = \pi/3$ | $Z_{\{i3kl\}} \in \mathbb{I}$, | $Z_{1311} = -Z_{1322} = -Z_{2312} = -Z_{2321},\ Z_{1312} = Z_{1321} = Z_{2311} = -Z_{2322}$, |
| iii. | $\theta \neq \{0, \pi/3\}$ | $Z_{\{i3kl\}} = 0$. | |

For Eqs. (28), we shall use the result in Eq. (B1) for $n = 4$ along with the following relations: $Z_{1122} = Z_{2211}$; $Z_{1221} = Z_{2112}$; $Z_{1112} = Z_{1211} = Z^*_{1121} = Z^*_{2111}$; $Z_{1222} = Z_{2212} = Z^*_{2122} = Z^*_{2221}$; $Z_{1212} = Z^*_{2121}$; $Z_{1111}, Z_{2222}, Z_{1122}, Z_{2211}, Z_{1221}, Z_{2112} \in \mathbb{R}$. We find

$$\begin{pmatrix} (Z_{1111} + Z_{2222}) - 2(Z_{1122} + Z_{1221} + \mathrm{Re}(Z_{1212})) \\ 4(\mathrm{Re}(Z_{1112}) - \mathrm{Re}(Z_{1222})) \end{pmatrix}^* = R^\top_{4\theta} \begin{pmatrix} (Z_{1111} + Z_{2222}) - 2(Z_{1122} + Z_{1221} + \mathrm{Re}(Z_{1212})) \\ 4(\mathrm{Re}(Z_{1112}) - \mathrm{Re}(Z_{1222})) \end{pmatrix}, \tag{32}$$

$$\begin{pmatrix} (Z_{1111} - Z_{2222}) - 2i\,\mathrm{Im}(Z_{1212}) \\ 2(Z_{1112} + Z^*_{1222}) \end{pmatrix}^* = R^\top_{2\theta} \begin{pmatrix} (Z_{1111} - Z_{2222}) - 2i\,\mathrm{Im}(Z_{1212}) \\ 2(Z_{1112} + Z^*_{1222}) \end{pmatrix},$$
$$\begin{pmatrix} (Z_{1111} - Z_{2222}) + 2i\,\mathrm{Im}(Z_{1212}) \\ 2(Z^*_{1112} + Z_{1222}) \end{pmatrix}^* = R^\top_{2\theta} \begin{pmatrix} (Z_{1111} - Z_{2222}) + 2i\,\mathrm{Im}(Z_{1212}) \\ 2(Z^*_{1112} + Z_{1222}) \end{pmatrix},$$
$$\mathrm{Im}(Z_{1112}) = -\mathrm{Im}(Z_{1222}). \tag{33}$$

Finally, the conditions that solve these equations are

| | | | |
|---|---|---|---|
| i. | $\theta = 0$ | $Z_{\{ijkl\}} \in \mathbb{R}$, | |
| ii. | $\theta = \pi/2$ | $Z_{\{ijkl\}} \in \mathbb{C}$, | $Z_{1112} = Z_{1211} = Z^*_{1121} = Z^*_{2111} = -Z_{1222} = -Z_{2212} = -Z^*_{2122} = -Z^*_{2221},\ Z_{1111} = Z_{2222}$, |
| iii. | $\theta \neq \{0, \pi/2\}$ | $Z_{\{ijkl\}} \in \mathbb{C}$. | $Z_{1112} = Z_{1211} = Z_{1121} = Z_{2111} = Z_{1222} = Z_{2212} = Z_{2122} = Z_{2221} = 0$, $Z_{1212} = Z_{1111} - Z_{1122} - Z_{1221},\ Z_{1111} = Z_{2222}$. |

This concludes the analysis for the scalar sector. If one were to try to do these calculations in models with more doublets, the trick would remain much the same; but, then, one would have to decouple the entries with 1 and 2 from the ones with 3 and 4, 5 and 6, etc. Since it always involves a rank-2 tensor and a rank-4 tensor, there is no need in N-Higgs-doublet models (NHDM) to go further than $C_4$, which we write explicitly in Eq. (B9) below.

### E. The four *GCP*-constrained 3HDM potentials

We now write the scalar potential for the several classes of models in the basis of Eq. (7). The $CPa$ ($\theta = 0$) scalar potential, corresponding to the usual $CP$, is of the general form of Eq. (4), except all the coefficients are real.

The $CPb$ ($\theta = \pi/2$) scalar potential has the form

$$\begin{aligned} V_H =& \mu_1[(\Phi_1^\dagger\Phi_1)+(\Phi_2^\dagger\Phi_2)]+\mu_3(\Phi_3^\dagger\Phi_3)+r_1[(\Phi_1^\dagger\Phi_1)^2+(\Phi_2^\dagger\Phi_2)^2]+r_3(\Phi_3^\dagger\Phi_3)^2 \\ &+2r_4(\Phi_1^\dagger\Phi_1)(\Phi_2^\dagger\Phi_2)+2r_5[(\Phi_1^\dagger\Phi_1)+(\Phi_2^\dagger\Phi_2)](\Phi_3^\dagger\Phi_3)+2r_7|\Phi_1^\dagger\Phi_2|^2+2r_8[|\Phi_1^\dagger\Phi_3|^2+|\Phi_2^\dagger\Phi_3|^2] \\ &+2c_1[(\Phi_1^\dagger\Phi_1)-(\Phi_2^\dagger\Phi_2)](\Phi_1^\dagger\Phi_2)+c_3(\Phi_1^\dagger\Phi_2)^2+c_5[(\Phi_1^\dagger\Phi_3)^2+(\Phi_3^\dagger\Phi_2)^2]+2iy_{11}(\Phi_1^\dagger\Phi_3)(\Phi_2^\dagger\Phi_3)+\text{H.c.}, \end{aligned} \tag{34}$$

where H.c. stands for Hermitian conjugation. We follow the notation of Ref. [9]: the coefficients $c_k = x_k + iy_k$ are complex, while $r_k$, $x_k$, and $y_k$ are real.

The $CPc$ ($\theta = \pi/3$) scalar potential has the form

$$\begin{aligned} V_H =& \mu_1[(\Phi_1^\dagger\Phi_1)+(\Phi_2^\dagger\Phi_2)]+\mu_3(\Phi_3^\dagger\Phi_3)+r_1[(\Phi_1^\dagger\Phi_1)^2+(\Phi_2^\dagger\Phi_2)^2]+r_3(\Phi_3^\dagger\Phi_3)^2 \\ &+2r_4(\Phi_1^\dagger\Phi_1)(\Phi_2^\dagger\Phi_2)+2r_5[(\Phi_1^\dagger\Phi_1)+(\Phi_2^\dagger\Phi_2)](\Phi_3^\dagger\Phi_3)+2r_7|\Phi_1^\dagger\Phi_2|^2+2r_8[|\Phi_1^\dagger\Phi_3|^2+|\Phi_2^\dagger\Phi_3|^2] \\ &+r_{147}[(\Phi_1^\dagger\Phi_2)^2+(\Phi_2^\dagger\Phi_1)^2]+x_5[(\Phi_1^\dagger\Phi_3)^2+(\Phi_2^\dagger\Phi_3)^2+\text{H.c.}] \\ &+2iy_2[[(\Phi_1^\dagger\Phi_2)+(\Phi_2^\dagger\Phi_1)](\Phi_3^\dagger\Phi_2)+(\Phi_1^\dagger\Phi_1)(\Phi_1^\dagger\Phi_3)+(\Phi_2^\dagger\Phi_2)(\Phi_3^\dagger\Phi_1)]+\text{H.c.}, \\ &+2iy_4[[(\Phi_1^\dagger\Phi_2)+(\Phi_2^\dagger\Phi_1)](\Phi_1^\dagger\Phi_3)+(\Phi_1^\dagger\Phi_1)(\Phi_2^\dagger\Phi_3)+(\Phi_2^\dagger\Phi_2)(\Phi_3^\dagger\Phi_2)]+\text{H.c.}, \end{aligned} \tag{35}$$

where $r_{147} = r_1 - r_4 - r_7$.

Finally, the $CPd$ potential ($\theta \neq 0,\ \pi/2,\ \pi/3$) has the form

$$\begin{aligned} V_H =& \mu_1[(\Phi_1^\dagger\Phi_1)+(\Phi_2^\dagger\Phi_2)]+\mu_3(\Phi_3^\dagger\Phi_3)+r_1[(\Phi_1^\dagger\Phi_1)^2+(\Phi_2^\dagger\Phi_2)^2]+r_3(\Phi_3^\dagger\Phi_3)^2 \\ &+2r_4(\Phi_1^\dagger\Phi_1)(\Phi_2^\dagger\Phi_2)+2r_5[(\Phi_1^\dagger\Phi_1)+(\Phi_2^\dagger\Phi_2)](\Phi_3^\dagger\Phi_3)+2r_7|\Phi_1^\dagger\Phi_2|^2+2r_8[|\Phi_1^\dagger\Phi_3|^2+|\Phi_2^\dagger\Phi_3|^2] \\ &+r_{147}[(\Phi_1^\dagger\Phi_2)^2+(\Phi_2^\dagger\Phi_1)^2]+x_5[(\Phi_1^\dagger\Phi_3)^2+(\Phi_2^\dagger\Phi_3)^2+\text{H.c.}]. \end{aligned} \tag{36}$$

We have built a *Mathematica* program implementing the basis-invariant techniques of Refs. [12,13], and checked that our $CPa$, $CPb$, $CPc$, and $CPd$ potentials obey basis invariant conditions, allowing them to be identified, respectively, as[6] $CP2$, $CP4$, $S_3 \times GCP_{\theta=\pi}$, and $O(2) \times CP$.

Notice that, by construction, all potentials are explicitly $CP$ conserving. One may wonder whether they may lead to spontaneous $CP$ violation. We do not address here the issue of the possible global minima when the symmetry is exact. Aspects of spontaneous symmetry breaking in 3HDM with an exact symmetry have been discussed in [14]. When accessing a model's parametric viability, we take the view that one may wish to add soft-symmetry breaking terms to the potential, thus allowing for general $v_i$. This allows us to map all possibilities, even in that more general context.

## IV. THE YUKAWA COUPLINGS

### A. Yukawa Lagrangian and mass basis

The scalar-quark Yukawa interactions of the 3HDM may be written as

$$-\mathcal{L}_Y = \bar{q}_L(\Gamma_1\Phi_1+\Gamma_2\Phi_2+\Gamma_3\Phi_3)n_R+\bar{q}_L(\Delta_1\tilde{\Phi}_1+\Delta_2\tilde{\Phi}_2+\Delta_3\tilde{\Phi}_3)p_R+\text{H.c.}, \tag{37}$$

[6]We are very grateful to Igor Ivanov for several discussions on this issue, especially pertaining to the identification of $S_3 \times GCP_{\theta=\pi}$.

where $q_L = (p_L, n_L)^\top$ ($n_R$ and $p_R$) is a vector in the 3-dimensional generation space of left-handed doublets (right-handed charge $-1/3$ and $+2/3$) quarks, and $\tilde{\Phi}_k = i\sigma_2\Phi_k^*$, with $\sigma_2$ the second Pauli matrix. $\Gamma_k$ and $\Delta_k$ ($k = 1,\ 2,\ 3$) are completely general $3\times 3$ complex matrices.

After spontaneous symmetry breaking, the Lagrangian's quadratic terms in the quark fields include

$$-\mathcal{L}_Y \supseteq \frac{v}{\sqrt{2}}(\bar{n}_L \Gamma n_R + \bar{p}_L \Delta p_R) + \text{H.c.}, \tag{38}$$

where $v = \sqrt{v_i v_i{}^*} = (\sqrt{2}G_F)^{-1/2}$, $\Gamma = \frac{v_i}{v}\Gamma_i$ and $\Delta = \frac{v_i{}^*}{v}\Delta_i$. We can define

$$M_d \equiv \frac{v}{\sqrt{2}}\Gamma, \qquad M_u \equiv \frac{v}{\sqrt{2}}\Delta, \tag{39}$$

as the mass matrices for the down-type and up-type quarks, respectively. Since the fields we are working with are not mass eigenstates, these matrices will not be diagonal. But we can always perform a unitary change of basis

$$\begin{aligned} \bar{n}_L &= \bar{d}_L U_{d_L}^\dagger, & \bar{p}_L &= \bar{u}_L U_{u_L}^\dagger, \\ n_R &= U_{d_R} d_R, & p_R &= U_{u_R} u_R, \end{aligned} \tag{40}$$

which leaves the kinetic terms unchanged in the Lagrangian, to bidiagonalize the mass matrices. The mass matrices then become

$$\begin{aligned} U_{d_L}^\dagger M_d U_{d_R} &= D_d \equiv \mathrm{diag}(m_d, m_s, m_b), \\ U_{u_L}^\dagger M_u U_{u_R} &= D_u \equiv \mathrm{diag}(m_u, m_c, m_t). \end{aligned} \tag{41}$$

Writing the interaction terms of the physical fields with the $W^+$ boson,

$$\mathcal{L}_W \supset \frac{ig}{\sqrt{2}} \bar{u}_L (U_{u_L}^\dagger U_{d_L}) \gamma^\mu d_L W_\mu^+, \tag{42}$$

one notices the emergence of the $3\times 3$ unitary matrix Cabibbo-Kobayashi-Maskawa (CKM) matrix [25,26], $V \equiv U_{u_L}^\dagger U_{d_L}$. It reflects the fact that the interaction basis is distinct from the physical mass basis. And it describes the quark mixing, responsible also for all *CP*-violating phenomena in theSM.

We can also define

$$\begin{aligned} H_d &\equiv M_d M_d^\dagger = \frac{v^2}{2}\Gamma\Gamma^\dagger = U_{d_L} D_d^2 U_{d_L}^\dagger, \\ H_u &\equiv M_u M_u^\dagger = \frac{v^2}{2}\Delta\Delta^\dagger = U_{u_L} D_u^2 U_{u_L}^\dagger, \end{aligned} \tag{43}$$

showing that the left-handed transformations are the matrices that diagonalize $H_d$ and $H_u$.

### B. *GCP* symmetries for the Yukawa Lagrangian

For the quark fields, the *GCP* transformations take the form

$$\begin{aligned} q_L &\to X_\alpha \gamma^0 C q_L^*, \\ n_R &\to X_\beta \gamma^0 C n_R^*, \\ p_R &\to X_\gamma \gamma^0 C p_R^*, \end{aligned} \tag{44}$$

where $\gamma^0$ ($C$) is the Dirac (charge-conjugation) matrix, and $X_\alpha$, $X_\beta$, and $X_\gamma$ belong to $SU(3)$. With a suitable basis choice, these can be changed into the simplified form [23]

$$X_\alpha = \begin{bmatrix} c_\alpha & s_\alpha & 0 \\ -s_\alpha & c_\alpha & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{45}$$

where $0 \leq \alpha \leq \pi/2$, with similar expressions for $X_\beta$ and $X_\gamma$.

Under the transformations in Eqs. (44), the Yukawa Lagrangian becomes

$$\begin{aligned} -\mathcal{L}_Y \to\ & \bar{n}_R [X_\alpha^\dagger (\Gamma_a)(X_\theta)_{ab} \Phi_b^* X_\beta] q_L \\ & + \bar{p}_R [X_\alpha^\dagger (\Delta_a)(X_\theta)_{ab}^* \tilde{\Phi}_b^* X_\gamma] q_L + \text{H.c.} \end{aligned} \tag{46}$$

Hence, in order for the Lagrangian in Eq. (37) to be symmetric under *GCP*, we must compare each of these terms with their respective Hermitian conjugate

$$\begin{aligned} -\mathcal{L}_Y \supset\ & \bar{n}_R^j [(\Gamma_k)_{ji}\Phi_k]^\dagger q_L^i + \bar{p}_R^j [(\Delta_k)_{ji}\tilde{\Phi}_k]^\dagger q_L^i \\ & = \bar{n}_R^j (\Gamma_k)_{ij}^* \Phi_k^* q_L^i + \bar{p}_R^j (\Delta_k)_{ij}^* \tilde{\Phi}_k^* q_L^i. \end{aligned} \tag{47}$$

Thus, the Yukawa Lagrangian in Eq. (37) is invariant under the *GCP* transformations in Eqs. (44) if and only if

$$\begin{aligned} \Gamma_b^* &= X_\alpha^\dagger (X_\theta)_{ab} (\Gamma_a) X_\beta, \\ \Delta_b^* &= X_\alpha^\dagger (X_\theta)_{ab}^* (\Delta_a) X_\gamma. \end{aligned} \tag{48}$$

Since we are taking all $X$ matrices to be real, the condition for the charged $+2/3$ quark matrices $\Delta$ will yield the same equations as the charged $-1/3$ quark matrices $\Gamma$, under the substitution $\beta \longrightarrow \gamma$. Therefore, we will focus on the down-type quarks, and subsequently compute the results for the up-type quarks.

We may write conditions (48) as

$$\begin{aligned} X_\alpha \Gamma_1^* - (c_\theta \Gamma_1 - s_\theta \Gamma_2) X_\beta &= 0, \\ X_\alpha \Gamma_2^* - (s_\theta \Gamma_1 + c_\theta \Gamma_2) X_\beta &= 0, \end{aligned} \tag{49}$$

and

$$X_\alpha \Gamma_3^* - \Gamma_3 X_\beta = 0, \tag{50}$$

where the basis choices of Eqs. (7) and (45) are implied.[7]

Equations (49) give us 36 equations in the 36 unknown real and imaginary parts of the various entries of the $\Gamma_1$ and $\Gamma_2$ matrices. In each block we have a system of homogeneous linear equations; the parameters are zero unless the determinant of the system vanishes. Recall that our choice of basis decouples the third entry from the other two, like we did for the scalar potential, except that now we may think of $\Gamma_k$ as one rank-3 tensor. It is for the analysis of the Yukawa matrices that we see the full power of the new strategy discussed in Sec. III and Appendix B. Next, we turn to a detailed view of this analysis.

### C. *GCP* constraints on Yukawas for down-type quarks

As mentioned, our choice of basis for the $X$ matrices decouples the system for $\Gamma_1$ and $\Gamma_2$ from that of $\Gamma_3$, and in each we will have 4 distinct regions $mn$, $m3$, $3n$. and 33. Thenceforth, we will use the notation $\Gamma_{\bar{k}}$ ($\bar{k} = 1, 2$) when we wish to refer collectively to $\Gamma_1$ and $\Gamma_2$. If we vectorize each block, we can turn Eq. (48) into

$$\Gamma^*_{\{1,2\}} = [(R_\theta^\top \otimes R_\alpha^\top \otimes R_\beta^\top) \oplus (R_\theta^\top \otimes R_\alpha^\top) \oplus (R_\theta^\top \otimes R_\beta^\top) \oplus R_\theta^\top]\Gamma_{\{1,2\}}, \Gamma^*_{\{3\}} = [(R_\alpha^\top \otimes R_\beta^\top) \oplus (R_\alpha^\top) \oplus (R_\beta^\top) \oplus 1]\Gamma_{\{3\}}, \tag{51}$$

where

$$\begin{aligned} \Gamma_{\{1,2\}} &= ((\Gamma_1)_{\{mn\}}, (\Gamma_2)_{\{mn\}}, (\Gamma_1)_{\{m3\}}, (\Gamma_2)_{\{m3\}}, (\Gamma_1)_{\{3n\}}, (\Gamma_2)_{\{n3\}}, (\Gamma_1)_{33}, (\Gamma_2)_{33})^\top, \\ \Gamma_{\{3\}} &= ((\Gamma_3)_{\{mn\}}, (\Gamma_3)_{\{m3\}}, (\Gamma_3)_{\{3n\}}, (\Gamma_3)_{33})^\top, \end{aligned} \tag{52}$$

using the notation in Eq. (18). To be specific, in $(\Gamma_i)_{ab}$, "$i$" refers to the Higgs-family index of Eq. (37), while "$a$, $b$" refers to the entries of this matrix in down-type quark generation space.

Let us start by looking at the 33 regions. Immediately, we see that

$$(\Gamma_3)^*_{33} = (\Gamma_3)_{33}, \tag{53}$$

and, thus, $(\Gamma_3)_{33}$ is always real. As for $(\Gamma_{\bar{k}})_{33}$, we have

$$(\Gamma_{\bar{k}})^*_{33} = R_\theta^\top (\Gamma_{\bar{k}})^*_{33}, \quad (\Gamma_{\bar{k}})_{33} = ((\Gamma_1)_{33}, (\Gamma_2)_{33})^\top. \tag{54}$$

These equations are the analog of Eqs. (19), applied here to the Yukawa couplings. Using Eq. (10) and the restricted range for $\theta$, we conclude that either $\theta = 0$, in which case $(\Gamma_1)_{33}$ and $(\Gamma_2)_{33}$ are also real, or, else, $\theta \neq 0$, in which case $(\Gamma_1)_{33} = (\Gamma_2)_{33} = 0$. This constitutes conditions i and ii, respectively, for the $(\Gamma_{\bar{k}})_{33}$ region:

| | | |
|---|---|---|
| i. | $\theta = 0$ | $(\Gamma_1)_{33}, (\Gamma_2)_{33} \in \mathbb{R}$, |
| ii. | $\theta \neq 0$ | $(\Gamma_1)_{33} = (\Gamma_2)_{33} = 0$. |

The $m3$ ($3n$) region in $\Gamma_3$ is similar under the substitution $\theta \to \alpha$ ($\theta \to \beta$). Indeed,

$$\begin{aligned} (\Gamma_3)^*_{\{m3\}} &= R_\alpha^\top (\Gamma_3)_{\{m3\}}, \qquad (\Gamma_3)_{\{m3\}} = ((\Gamma_3)_{13}, (\Gamma_3)_{23})^\top, \\ (\Gamma_3)^*_{\{3n\}} &= R_\beta^\top (\Gamma_3)_{\{3n\}}, \qquad (\Gamma_3)_{\{3n\}} = ((\Gamma_3)_{31}, (\Gamma_3)_{32})^\top. \end{aligned} \tag{55}$$

The conditions for the $(\Gamma_3)_{m3}$ region, then, become

| | | |
|---|---|---|
| i. | $\alpha = 0$ | $(\Gamma_3)_{13}, (\Gamma_3)_{23} \in \mathbb{R}$, |
| ii. | $\alpha \neq 0$ | $(\Gamma_3)_{13} = (\Gamma_3)_{23} = 0$, |

whereas, in the $(\Gamma_3)_{3n}$ region, we find

| | | |
|---|---|---|
| i. | $\beta = 0$ | $(\Gamma_3)_{31}, (\Gamma_3)_{32} \in \mathbb{R}$, |
| ii. | $\beta \neq 0$ | $(\Gamma_3)_{31} = (\Gamma_3)_{32} = 0$. |

Now looking at systems involving two angles, we have

$$\begin{aligned} (\Gamma_{\bar{k}})^*_{\{m3\}} &= R_\theta^\top \otimes R_\alpha^\top (\Gamma_{\bar{k}})^*_{\{m3\}}, \qquad (\Gamma_{\bar{k}})_{\{m3\}} = ((\Gamma_1)_{13}, (\Gamma_1)_{23}, (\Gamma_2)_{13}, (\Gamma_2)_{23})^\top, \\ (\Gamma_{\bar{k}})^*_{\{3n\}} &= R_\theta^\top \otimes R_\beta^\top (\Gamma_{\bar{k}})^*_{\{3n\}}, \qquad (\Gamma_{\bar{k}})_{\{3n\}} = ((\Gamma_1)_{31}, (\Gamma_1)_{32}, (\Gamma_2)_{31}, (\Gamma_2)_{32})^\top, \\ (\Gamma_3)^*_{\{mn\}} &= R_\alpha^\top \otimes R_\beta^\top (\Gamma_3)_{\{mn\}}, \qquad (\Gamma_3)_{\{mn\}} = ((\Gamma_3)_{11}, (\Gamma_3)_{12}, (\Gamma_3)_{21}, (\Gamma_3)_{22})^\top. \end{aligned} \tag{56}$$

[7]Notice that Eq. (50) is identical to Eqs. (49) in the limit of $\theta = 0$.

For Eqs. (56), we shall use the result in Eq. (B1) for $n = 2$, which simplifies the equations to

$$\begin{pmatrix} (\Gamma_1)_{13} - (\Gamma_2)_{23} \\ (\Gamma_1)_{23} + (\Gamma_2)_{13} \end{pmatrix}^* = R^\top_{\theta+\alpha} \begin{pmatrix} (\Gamma_1)_{13} - (\Gamma_2)_{23} \\ (\Gamma_1)_{23} + (\Gamma_2)_{13} \end{pmatrix},$$
$$\begin{pmatrix} (\Gamma_1)_{13} + (\Gamma_2)_{23} \\ (\Gamma_1)_{23} - (\Gamma_2)_{13} \end{pmatrix}^* = R^\top_{\alpha-\theta} \begin{pmatrix} (\Gamma_1)_{13} + (\Gamma_2)_{23} \\ (\Gamma_1)_{23} - (\Gamma_2)_{13} \end{pmatrix}, \tag{57}$$

$$\begin{pmatrix} (\Gamma_1)_{31} - (\Gamma_2)_{32} \\ (\Gamma_1)_{32} + (\Gamma_2)_{31} \end{pmatrix}^* = R^\top_{\theta+\beta} \begin{pmatrix} (\Gamma_1)_{31} - (\Gamma_2)_{32} \\ (\Gamma_1)_{32} + (\Gamma_2)_{31} \end{pmatrix},$$
$$\begin{pmatrix} (\Gamma_1)_{31} + (\Gamma_2)_{32} \\ (\Gamma_1)_{32} - (\Gamma_2)_{31} \end{pmatrix}^* = R^\top_{\beta-\theta} \begin{pmatrix} (\Gamma_1)_{31} + (\Gamma_2)_{32} \\ (\Gamma_1)_{32} - (\Gamma_2)_{31} \end{pmatrix}, \tag{58}$$

$$\begin{pmatrix} (\Gamma_3)_{11} - (\Gamma_3)_{22} \\ (\Gamma_3)_{12} + (\Gamma_3)_{21} \end{pmatrix}^* = R^\top_{\alpha+\beta} \begin{pmatrix} (\Gamma_3)_{11} - (\Gamma_3)_{22} \\ (\Gamma_3)_{12} + (\Gamma_3)_{21} \end{pmatrix},$$
$$\begin{pmatrix} (\Gamma_3)_{11} + (\Gamma_3)_{22} \\ (\Gamma_3)_{12} - (\Gamma_3)_{21} \end{pmatrix}^* = R^\top_{\beta-\alpha} \begin{pmatrix} (\Gamma_3)_{11} + (\Gamma_3)_{22} \\ (\Gamma_3)_{12} - (\Gamma_3)_{21} \end{pmatrix}. \tag{59}$$

These systems of equations lead to different textures in the cases where the respective rotation angle is either zero, $\pi$ or any different value. In Eqs. (57), if $\theta + \alpha$ equals zero, the only possibility is that they are both zero, which means that $\alpha - \theta$ is also equal to zero in this case. If instead $\theta + \alpha$ equals $\pi$, the only possibility is that they both equal $\pi/2$, which again means $\alpha - \theta$ equals zero. In fact, $\alpha - \theta$ can only be either zero, if $\alpha = \theta$, or different than zero, if $\alpha \neq \theta$, but never actually $\pi$. This means that this region has only 4 possible textures: $\theta = \alpha = 0$; $\theta = \alpha = \pi/2$; $\theta = \alpha \neq \{0, \pi/2\}$; $\theta \neq \alpha$. Equations (58) and (59) are solved in identical fashion. For the former we have $\theta = \beta = 0$; $\theta = \beta = \pi/2$; $\theta = \beta \neq \{0, \pi/2\}$; $\theta \neq \beta$. For the latter we have $\alpha = \beta = 0$; $\alpha = \beta = \pi/2$; $\alpha = \beta \neq \{0, \pi/2\}$; $\alpha \neq \beta$.

Each condition fully determines the amount of free parameters in each region. For the $m3$ region in $\Gamma_{\bar{k}}$, we have

| | | | |
|---|---|---|---|
| i. | $\theta = \alpha = 0$ | $(\Gamma_{\bar{k}})_{\{m3\}} \in \mathbb{R}$, | |
| ii. | $\theta = \alpha = \pi/2$ | $(\Gamma_{\bar{k}})_{\{m3\}} \in \mathbb{C}$, | $(\Gamma_1)_{13} = (\Gamma_2)^*_{23}, (\Gamma_1)_{23} = -(\Gamma_2)^*_{13}$, |
| iii. | $\theta = \alpha \neq \{0, \pi/2\}$ | $(\Gamma_{\bar{k}})_{\{m3\}} \in \mathbb{R}$, | $(\Gamma_1)_{13} = (\Gamma_2)_{23}, (\Gamma_1)_{23} = -(\Gamma_2)_{13}$, |
| iv. | $\theta \neq \alpha$ | $(\Gamma_{\bar{k}})_{\{m3\}} = \mathbf{0}$. | |

Likewise, for the $3n$ region in $\Gamma_{\bar{k}}$,

| | | | |
|---|---|---|---|
| i. | $\theta = \beta = 0$ | $(\Gamma_{\bar{k}})_{\{3n\}} \in \mathbb{R}$, | |
| ii. | $\theta = \beta = \pi/2$ | $(\Gamma_{\bar{k}})_{\{3n\}} \in \mathbb{C}$, | $(\Gamma_1)_{31} = (\Gamma_2)^*_{32}, (\Gamma_1)_{32} = -(\Gamma_2)^*_{31}$, |
| iii. | $\theta = \beta \neq \{0, \pi/2\}$ | $(\Gamma_{\bar{k}})_{\{3n\}} \in \mathbb{R}$, | $(\Gamma_1)_{31} = (\Gamma_2)_{32}, (\Gamma_1)_{32} = -(\Gamma_2)_{31}$, |
| iv. | $\theta \neq \beta$ | $(\Gamma_{\bar{k}})_{\{3n\}} = \mathbf{0}$. | |

And, the conditions for the $mn$ block in $\Gamma_3$ are

| | | | |
|---|---|---|---|
| i. | $\alpha = \beta = 0$ | $(\Gamma_3)_{\{mn\}} \in \mathbb{R}$, | |
| ii. | $\alpha = \beta = \pi/2$ | $(\Gamma_3)_{\{mn\}} \in \mathbb{C}$, | $(\Gamma_3)_{11} = (\Gamma_3)^*_{22}, (\Gamma_3)_{12} = -(\Gamma_3)^*_{21}$, |
| iii. | $\alpha = \beta \neq \{0, \pi/2\}$ | $(\Gamma_3)_{\{mn\}} \in \mathbb{R}$, | $(\Gamma_3)_{11} = (\Gamma_3)_{22}, (\Gamma_3)_{12} = -(\Gamma_3)_{21}$, |
| iv. | $\alpha \neq \beta$ | $(\Gamma_3)_{\{mn\}} = \mathbf{0}$. | |

Finally, we turn to the $mn$ sector of $\Gamma_{\bar{k}}$, $\bar{k} = 1, 2$. We find

$$(\Gamma_{\bar{k}})^*_{\{mn\}} = R^\top_\theta \otimes R^\top_\alpha \otimes R^\top_\beta (\Gamma_{\bar{k}})_{\{mn\}},$$
$$(\Gamma_{\bar{k}})_{\{mn\}} \equiv ((\Gamma_1)_{11}, (\Gamma_1)_{12}, (\Gamma_1)_{21}, (\Gamma_1)_{22}, (\Gamma_2)_{11}, (\Gamma_2)_{12}, (\Gamma_2)_{21}, (\Gamma_2)_{22})^\top. \tag{60}$$

For Eqs. (60), we shall use the result in Eq. (B1) for $n = 3$, which simplifies the equations to

$$\begin{aligned}
\begin{pmatrix} [(\Gamma_1)_{11} - (\Gamma_1)_{22}] - [(\Gamma_2)_{12} + (\Gamma_2)_{21}] \\ [(\Gamma_1)_{12} + (\Gamma_1)_{21}] + [(\Gamma_2)_{11} - (\Gamma_2)_{22}] \end{pmatrix}^* &= R^\top_{\theta+\alpha+\beta} \begin{pmatrix} [(\Gamma_1)_{11} - (\Gamma_1)_{22}] - [(\Gamma_2)_{12} + (\Gamma_2)_{21}] \\ [(\Gamma_1)_{12} + (\Gamma_1)_{21}] + [(\Gamma_2)_{11} - (\Gamma_2)_{22}] \end{pmatrix}, \\
\begin{pmatrix} [(\Gamma_1)_{11} - (\Gamma_1)_{22}] + [(\Gamma_2)_{12} + (\Gamma_2)_{21}] \\ [(\Gamma_1)_{12} + (\Gamma_1)_{21}] - [(\Gamma_2)_{11} - (\Gamma_2)_{22}] \end{pmatrix}^* &= R^\top_{\alpha+\beta-\theta} \begin{pmatrix} [(\Gamma_1)_{11} - (\Gamma_1)_{22}] + [(\Gamma_2)_{12} + (\Gamma_2)_{21}] \\ [(\Gamma_1)_{12} + (\Gamma_1)_{21}] - [(\Gamma_2)_{11} - (\Gamma_2)_{22}] \end{pmatrix}, \\
\begin{pmatrix} [(\Gamma_1)_{11} + (\Gamma_1)_{22}] - [(\Gamma_2)_{12} - (\Gamma_2)_{21}] \\ [(\Gamma_1)_{12} - (\Gamma_1)_{21}] + [(\Gamma_2)_{11} + (\Gamma_2)_{22}] \end{pmatrix}^* &= R^\top_{\theta+\beta-\alpha} \begin{pmatrix} [(\Gamma_1)_{11} + (\Gamma_1)_{22}] - [(\Gamma_2)_{12} - (\Gamma_2)_{21}] \\ [(\Gamma_1)_{12} - (\Gamma_1)_{21}] + [(\Gamma_2)_{11} + (\Gamma_2)_{22}] \end{pmatrix}, \\
\begin{pmatrix} [(\Gamma_1)_{11} + (\Gamma_1)_{22}] + [(\Gamma_2)_{12} - (\Gamma_2)_{21}] \\ [(\Gamma_1)_{12} - (\Gamma_1)_{21}] - [(\Gamma_2)_{11} + (\Gamma_2)_{22}] \end{pmatrix}^* &= R_{\theta+\alpha-\beta} \begin{pmatrix} [(\Gamma_1)_{11} + (\Gamma_1)_{22}] + [(\Gamma_2)_{12} - (\Gamma_2)_{21}] \\ [(\Gamma_1)_{12} - (\Gamma_1)_{21}] - [(\Gamma_2)_{11} + (\Gamma_2)_{22}] \end{pmatrix}.
\end{aligned} \tag{61}$$

As before, each angle can either be $0, \pi$, or some other value in order to give a unique texture in the Yukawa matrices. Naively, there would be a total of $3 \times 3 \times 3 \times 3 = 81$ different combinations. But, like before, if for example $\theta + \alpha + \beta = 0$, the only possibility is that $\theta = \alpha = \beta = 0$ and therefore all the angle combinations would also give zero. The conditions that the other combinations equal zero are, respectively, $\alpha + \beta = \theta$, $\theta + \beta = \alpha$, and $\theta + \alpha = \beta$. These conditions make the real part of the respective entries in the Yukawa matrices nonzero. The conditions for non-zero imaginary parts are, respectively, $\theta + \alpha + \beta = \pi$, $\alpha + \beta = \theta + \pi$, $\theta + \beta = \alpha + \pi$, and $\alpha + \theta = \beta + \pi$. However, the last three can only be achieved if the two angles on the left-hand side equal $\pi/2$ and the other one equals zero, which means that $\theta + \alpha + \beta$ also equals $\pi$. Performing all valid combinations results in just 15 different textures for the $mn$ system in $\Gamma_1$ and $\Gamma_2$:

| | | | |
|---|---|---|---|
| i. | $\theta = \alpha = \beta = 0$ | $(\Gamma_{\bar{k}})_{\{mn\}} \in \mathbb{R}$, | |
| ii. | $\beta = 0,\ \theta = \alpha = \pi/2$ | $(\Gamma_{\bar{k}})_{\{mn\}} \in \mathbb{C}$, | $(\Gamma_1)_{11} = (\Gamma_2)^*_{21}, (\Gamma_1)_{12} = (\Gamma_2)^*_{22},\ (\Gamma_1)_{21} = -(\Gamma_2)^*_{11}, (\Gamma_1)_{22} = -(\Gamma_2)^*_{12}$ |
| iii. | $\beta = 0,\ \theta = \alpha \neq \{0, \pi/2\}$ | $(\Gamma_{\bar{k}})_{\{mn\}} \in \mathbb{R}$, | $(\Gamma_1)_{11} = (\Gamma_2)_{21}, (\Gamma_1)_{12} = (\Gamma_2)_{22},\ (\Gamma_1)_{21} = -(\Gamma_2)_{11}, (\Gamma_1)_{22} = -(\Gamma_2)_{12}$ |
| iv. | $\alpha = 0,\ \theta = \beta = \pi/2$ | $(\Gamma_{\bar{k}})_{\{mn\}} \in \mathbb{C}$, | $(\Gamma_1)_{11} = (\Gamma_2)^*_{12}, (\Gamma_1)_{12} = -(\Gamma_2)^*_{11},\ (\Gamma_1)_{21} = (\Gamma_2)^*_{22}, (\Gamma_1)_{22} = -(\Gamma_2)^*_{21}$ |
| v. | $\alpha = 0,\ \theta = \beta \neq \{0, \pi/2\}$ | $(\Gamma_{\bar{k}})_{\{mn\}} \in \mathbb{R}$, | $(\Gamma_1)_{11} = (\Gamma_2)_{12}, (\Gamma_1)_{12} = -(\Gamma_2)_{11},\ (\Gamma_1)_{21} = (\Gamma_2)_{22}, (\Gamma_1)_{22} = -(\Gamma_2)_{21}$, |
| vi. | $\theta = 0,\ \alpha = \beta = \pi/2$ | $(\Gamma_{\bar{k}})_{\{mn\}} \in \mathbb{C}$, | $(\Gamma_1)_{11} = (\Gamma_1)^*_{22}, (\Gamma_1)_{12} = -(\Gamma_1)^*_{21},\ (\Gamma_2)_{11} = (\Gamma_2)^*_{22}, (\Gamma_2)_{12} = -(\Gamma_2)^*_{21}$, |
| vii. | $\theta = 0,\ \alpha = \beta \neq \{0, \pi/2\}$ | $(\Gamma_{\bar{k}})_{\{mn\}} \in \mathbb{R}$, | $(\Gamma_1)_{11} = (\Gamma_1)_{22}, (\Gamma_1)_{12} = -(\Gamma_1)_{21},\ (\Gamma_2)_{11} = (\Gamma_2)_{22}, (\Gamma_2)_{12} = -(\Gamma_2)_{21}$, |
| viii. | $\theta = \pi/2,\ \alpha + \beta = \pi/2,$ $\alpha, \beta \neq \{0, \pi/2\}$ | $(\Gamma_{\bar{k}})_{\{mn\}} \in \mathbb{C}$, | $(\Gamma_1)_{11} = -(\Gamma_1)_{22} = (\Gamma_2)^*_{12} = (\Gamma_2)^*_{21},\ (\Gamma_1)_{12} = (\Gamma_1)_{21} = -(\Gamma_2)^*_{11} = (\Gamma_2)^*_{22}$, |
| ix. | $\alpha = \pi/2,\ \theta + \beta = \pi/2,$ $\theta, \beta \neq \{0, \pi/2\}$ | $(\Gamma_{\bar{k}})_{\{mn\}} \in \mathbb{C}$, | $(\Gamma_1)_{11} = -(\Gamma_2)_{12} = (\Gamma_1)^*_{22} = (\Gamma_2)^*_{21},\ (\Gamma_1)_{12} = (\Gamma_2)_{11} = -(\Gamma_1)^*_{21} = (\Gamma_2)^*_{22}$, |
| x. | $\beta = \pi/2,\ \theta + \alpha = \pi/2,$ $\theta, \alpha \neq \{0, \pi/2\}$ | $(\Gamma_{\bar{k}})_{\{mn\}} \in \mathbb{C}$, | $(\Gamma_1)_{11} = -(\Gamma_2)_{21} = (\Gamma_1)^*_{22} = (\Gamma_2)^*_{12},\ -(\Gamma_1)_{12} = (\Gamma_2)_{22} = (\Gamma_1)^*_{21} = (\Gamma_2)^*_{11}$, |
| xi. | $\alpha + \beta = \theta,\ \theta \neq \{\alpha, \beta, \pi/2\}$ | $(\Gamma_{\bar{k}})_{\{mn\}} \in \mathbb{R}$, | $(\Gamma_1)_{11} = -(\Gamma_1)_{22} = (\Gamma_2)_{12} = (\Gamma_2)_{21},\ (\Gamma_1)_{12} = (\Gamma_1)_{21} = -(\Gamma_2)_{11} = (\Gamma_2)_{22}$, |
| xii. | $\theta + \beta = \alpha,\ \alpha \neq \{\theta, \beta, \pi/2\}$ | $(\Gamma_{\bar{k}})_{\{mn\}} \in \mathbb{R}$, | $(\Gamma_1)_{11} = (\Gamma_1)_{22} = -(\Gamma_2)_{12} = (\Gamma_2)_{21},\ (\Gamma_1)_{12} = -(\Gamma_1)_{21} = (\Gamma_2)_{11} = (\Gamma_2)_{22}$, |
| xiii. | $\theta + \alpha = \beta,\ \beta \neq \{\theta, \alpha, \pi/2\}$ | $(\Gamma_{\bar{k}})_{\{mn\}} \in \mathbb{R}$, | $(\Gamma_1)_{11} = (\Gamma_1)_{22} = (\Gamma_2)_{12} = -(\Gamma_2)_{21},\ -(\Gamma_1)_{12} = (\Gamma_1)_{21} = (\Gamma_2)_{11} = (\Gamma_2)_{22}$, |
| xiv. | $\theta + \alpha + \beta = \pi,\ \theta, \alpha, \beta \neq \pi/2$ | $(\Gamma_{\bar{k}})_{\{mn\}} \in \mathbb{I}$, | $-(\Gamma_1)_{11} = (\Gamma_1)_{22} = (\Gamma_2)_{12} = (\Gamma_2)_{21},\ (\Gamma_1)_{12} = (\Gamma_1)_{21} = (\Gamma_2)_{11} = -(\Gamma_2)_{22}$, |
| xv. | $\alpha + \beta \neq \theta,\ \theta + \beta \neq \alpha,\ \theta + \alpha \neq \beta,$ $\theta + \alpha + \beta \neq \pi$ | $(\Gamma_{\bar{k}})_{\{mn\}} = \mathbf{0}$. | |

The next step is to combine these 15 conditions with the 18 from the other blocks and then we should have all different combinations of angles $\theta$, $\alpha$, and $\beta$ that produce unique textures on $\Gamma_k$, and thus on $M_d$. Recall that, in the spirit that adding to the scalar potential soft breaking terms might be useful for some model building, we are using the most general vevs $v_i$.

Excluding combinations that lead either to null or degenerate eigenvalues, using the notation $(\theta, \alpha, \beta)$, we have the results in Table I.

An asterisk here means that the third quark decouples, i.e., $M_d$ is block diagonal. A diamond here means that the quarks couple only to $\Phi_3$, i.e., $\Gamma_1 = \Gamma_2 = \mathbf{0}$.

### D. *GCP* constraints on the whole Yukawa sector

Now, we must combine the cases from the down-type $\Gamma_k$ matrices with the ones from the up-type $\Delta_k$ matrices, which, for our choice of basis, are the same under the replacement $\beta \to \gamma$. The final cases $(\theta, \alpha, \beta, \gamma)$ must have the same value of $\theta$ and $\alpha$ for the up and down matrices simultaneously, and we must not combine two cases bearing an asterisk, as that would lead

TABLE I. Combinations of $(\theta,\alpha,\beta)$ and respective conditions for the 33, m3, 3n, and mn blocks of $\Gamma_{\bar{k}}$ and $\Gamma_3$.

| | | $(\Gamma_{\bar{k}})_{33}$ | $(\Gamma_3)_{m3}$ | $(\Gamma_3)_{3n}$ | $(\Gamma_{\bar{k}})_{m3}$ | $(\Gamma_{\bar{k}})_{3n}$ | $(\Gamma_3)_{mn}$ | $(\Gamma_{\bar{k}})_{mn}$ |
|---|---|---|---|---|---|---|---|---|
| 1. | (0,0,0) | i | i | i | i | i | i | i |
| 2. | $(\pi/2,\pi/2,0)$ | ii | ii | i | ii | iv | iv | ii |
| 3. | $(\theta,\theta,0)$ | ii | ii | i | iii | iv | iv | iii |
| 4. | $(\pi/2,0,\pi/2)$ | ii | i | ii | iv | ii | iv | iv |
| 5. | $(\theta,0,\theta)$ | ii | i | ii | iv | iii | iv | v |
| 6. | $(0,\pi/2,\pi/2)^*$ | i | ii | ii | iv | iv | ii | vi |
| 7. | $(0,\alpha,\alpha)^*$ | i | ii | ii | iv | iv | iii | vii |
| 8. | $(\pi/2,\pi/4,\pi/4)^*$ | ii | ii | ii | iv | iv | iii | viii |
| 9. | $(\pi/2,\alpha,\pi/2-\alpha)^*$ | ii | ii | ii | iv | iv | iv | viii |
| 10. | $(\pi/4,\pi/2,\pi/4)$ | ii | ii | ii | iv | iii | iv | ix |
| 11. | $(\theta,\pi/2,\pi/2-\theta)^*$ | ii | ii | ii | iv | iv | iv | ix |
| 12. | $(\pi/4,\pi/4,\pi/2)$ | ii | ii | ii | iii | iv | iv | x |
| 13. | $(\theta,\pi/2-\theta,\pi/2)^*$ | ii | ii | ii | iv | iv | iv | x |
| 14. | $(\theta,\theta/2,\theta/2)^*$ | ii | ii | ii | iv | iv | iii | xi |
| 15. | $(\theta,\alpha,\theta-\alpha)^*$ | ii | ii | ii | iv | iv | iv | xi |
| 16. | $(\theta,2\theta,\theta)$ | ii | ii | ii | iv | iii | iv | xii |
| 17. | $(\theta,\alpha,\alpha-\theta)^*$ | ii | ii | ii | iv | iv | iv | xii |
| 18. | $(\theta,\theta,2\theta)$ | ii | ii | ii | iii | iv | iv | xiii |
| 19. | $(\theta,\alpha,\theta+\alpha)^*$ | ii | ii | ii | iv | iv | iv | xiii |
| 20. | $(\pi/3,\pi/3,\pi/3)$ | ii | ii | ii | iii | iii | iii | xiv |
| 21. | $(\theta,\theta,\pi-2\theta)$ | ii | ii | ii | iii | iv | iv | xiv |
| 22. | $(\theta,\pi-2\theta,\theta)$ | ii | ii | ii | iv | iii | iv | xiv |
| 23. | $(\theta,(\pi-\theta)/2,(\pi-\theta)/2)^*$ | ii | ii | ii | iv | iv | iii | xiv |
| 24. | $(\theta,\alpha,\pi-\theta-\alpha)^*$ | ii | ii | ii | iv | iv | iv | xiv |
| 25. | $(\theta,0,0)^\diamond$ | ii | i | i | iv | iv | i | xv |
| 26. | $(\pi/2,\pi/2,\pi/2)$ | ii | ii | ii | ii | ii | ii | xv |
| 27. | $(\theta,\theta,\theta)$ | ii | ii | ii | iii | iii | iii | xv |

to a block-diagonal CKM matrix, which is ruled out experimentally. We exclude those textures leading to a massless quark or to a block-diagonal CKM matrix. Thus, we have the results in Table II.

These 51 combinations of angles $(\theta,\alpha,\beta,\gamma)$ for the *GCP* transformations are all the combinations that lead to unique textures on the mass matrices $M_u$ and $M_d$, consistent with nonzero and nondegenerate quark masses and a CKM matrix which is not block-diagonal.

But there is one further simple constraint, regarding *CP* violation. Experiments in *B* decays prompt the conclusion that there must be *CP* violation in the CKM matrix, which is related to a physical quantity called the Jarlskog invariant $J_{CP}$ [27,28]. In terms of the CKM matrix elements this invariant is given by [29]

$$J_{CP}=\mathrm{Im}(V_{us}V_{cb}V_{ub}^*V_{cs}^*)=(3.08^{+0.15}_{-0.13})\times10^{-5}. \quad (62)$$

One can construct another related *CP*-violating, basis invariant, quantity [5,27,28]

$$J=\mathrm{Tr}[H_u,H_d]^3=6i(m_t^2-m_c^2)(m_t^2-m_u^2)(m_c^2-m_u^2)\times(m_b^2-m_s^2)(m_b^2-m_d^2)(m_s^2-m_d^2)J_{CP}. \quad (63)$$

We have already excluded models with quarks bearing zero mass or equal mass among each other. Therefore, $J=0$ if and only if the CKM matrix conserves *CP*, i.e., $J_{CP}=0$, which is ruled out experimentally.

If we compute $H_u$, $H_d$, and $J$ for each of our 51 models, we find that for $(\pi/6,\pi/3,\pi/2,\pi/6)$, $(\theta,\pi-2\theta,3\theta-\pi,\theta)$, $(\pi/6,\pi/3,\pi/6,\pi/2)$, $(\theta,2\theta,\theta,3\theta)$, $(\theta,2\theta,\theta,\pi-3\theta)$, $(\theta,\pi-2\theta,\pi-3\theta,\theta)$, $(\theta,2\theta,3\theta,\theta)$, $(\theta,\pi-2\theta,\theta,3\theta-\pi)$, $(\theta,\pi-2\theta,\theta,\pi-3\theta)$, $(\theta,2\theta,\pi-3\theta,\theta)$ and $(\theta,0,0,0)$, $J$ is always zero. Therefore, we can eliminate these models from our list, leaving us with just 40 models.

Finally, we can list every *GCP* symmetry that can be imposed on the 3HDM consistent with nonzero and nondegenerate quark masses and with nondiagonal and *CP*-violating CKM matrix. For each model we note the allowed values for $\theta$, from which we can deduce the form of the scalar potential (*CPa*, *CPb*, *CPc*, or *CPd*), along with the amount of real independent parameters in the down-type and up-type Yukawa matrices. This is shown in Table III. An asterisk means that, for that Yukawa matrix, the third quark decouples from the first two and a diamond means that the quarks couple only to $\Phi_3$. [Recall that we are always considering the basis of Eq. (7) for the *GCP* transformation *X* of Eq. (2).]

Table III is one main result from our work. Notice the dramatic reduction in the number of unknowns. Indeed, in each charge sector we would generally have 3 matrices, with 9 complex entries for a total of 54 (real) parameters.

TABLE II. Combinations of $(\theta,\alpha,\beta,\gamma)$ and respective constraints on the up and down Yukawa sectors.

| $(\theta,\alpha,\beta,\gamma)$ | $(\theta,\alpha,\beta)$ | $(\theta,\alpha,\gamma)$ |
|---|---|---|
| (0, 0, 0, 0) | 1 | 1 |
| $(\pi/2,\pi/2,0,0)$ | 2 | 2 |
| $(\pi/2,\pi/2,0,\pi/2)$ | 2 | 26 |
| $(\theta,\theta,0,0)$ | 3 | 3 |
| $(\pi/4,\pi/4,0,\pi/2)$ | 3 | 12 |
| $(\theta,\theta,0,2\theta)$ | 3 | 18 |
| $(\pi/3,\pi/3,0,\pi/3)$ | 3 | 20 |
| $(\theta,\theta,0,\pi-2\theta)$ | 3 | 21 |
| $(\theta,\theta,0,\theta)$ | 3 | 27 |
| $(\pi/2,0,\pi/2,\pi/2)$ | 4 | 4 |
| $(\pi/2,0,\pi/2,0)$ | 4 | 25 |
| $(\theta,0,\theta,\theta)$ | 5 | 5 |
| $(\theta,0,\theta,0)$ | 5 | 25 |
| $(\pi/4,\pi/2,\pi/4,\pi/4)$ | 10 | 10 |
| $(\pi/4,\pi/4,\pi/2,0)$ | 12 | 3 |
| $(\pi/4,\pi/4,\pi/2,\pi/2)$ | 12 | 12 |
| $(\pi/4,\pi/4,\pi/2,\pi/4)$ | 12 | 27 |
| $(\pi/6,\pi/3,\pi/2,\pi/6)$ | 13 | 16 |
| $(\frac{2\pi}{5},\pi/5,\pi/5,\frac{2\pi}{5})$ | 14 | 22 |
| $(\theta,\pi-2\theta,3\theta-\pi,\theta)$ | 15 | 22 |
| $(\pi/6,\pi/3,\pi/6,\pi/2)$ | 16 | 13 |
| $(\theta,2\theta,\theta,\theta)$ | 16 | 16 |
| $(\theta,2\theta,\theta,3\theta)$ | 16 | 19 |
| $(\pi/5,\frac{2\pi}{5},\pi/5,\frac{2\pi}{5})$ | 16 | 23 |
| $(\theta,2\theta,\theta,\pi-3\theta)$ | 16 | 24 |
| $(\theta,\pi-2\theta,\pi-3\theta,\theta)$ | 17 | 22 |
| $(\theta,\theta,2\theta,0)$ | 18 | 3 |
| $(\theta,\theta,2\theta,2\theta)$ | 18 | 18 |
| $(\theta,\theta,2\theta,\theta)$ | 18 | 27 |
| $(\theta,2\theta,3\theta,\theta)$ | 19 | 16 |
| $(\pi/3,\pi/3,\pi/3,0)$ | 20 | 3 |
| $(\pi/3,\pi/3,\pi/3,\pi/3)$ | 20 | 20 |
| $(\theta,\theta,\pi-2\theta,0)$ | 21 | 3 |
| $(\theta,\theta,\pi-2\theta,\pi-2\theta)$ | 21 | 21 |
| $(\theta,\theta,\pi-2\theta,\theta)$ | 21 | 27 |
| $(\frac{2\pi}{5},\pi/5,\frac{2\pi}{5},\pi/5)$ | 22 | 14 |
| $(\theta,\pi-2\theta,\theta,3\theta-\pi)$ | 22 | 15 |
| $(\theta,\pi-2\theta,\theta,\pi-3\theta)$ | 22 | 17 |
| $(\theta,\pi-2\theta,\theta,\theta)$ | 22 | 22 |
| $(\pi/5,\frac{2\pi}{5},\frac{2\pi}{5},\pi/5)$ | 23 | 16 |
| $(\theta,2\theta,\pi-3\theta,\theta)$ | 24 | 16 |
| $(\pi/2,0,0,\pi/2)$ | 25 | 4 |
| $(\theta,0,0,\theta)$ | 25 | 5 |
| $(\theta,0,0,0)$ | 25 | 25 |
| $(\pi/2,\pi/2,\pi/2,0)$ | 26 | 2 |
| $(\pi/2,\pi/2,\pi/2,\pi/2)$ | 26 | 26 |
| $(\theta,\theta,\theta,0)$ | 27 | 3 |
| $(\pi/4,\pi/4,\pi/4,\pi/2)$ | 27 | 12 |
| $(\theta,\theta,\theta,2\theta)$ | 27 | 18 |
| $(\theta,\theta,\theta,\pi-2\theta)$ | 27 | 21 |
| $(\theta,\theta,\theta,\theta)$ | 27 | 27 |

Imposing the various *GCP* symmetries reduces these numbers to those shown in Table III.

TABLE III. All 40 *GCP*-symmetric 3HDM compatible with nonzero and nondegenerate quark masses as well as a nonvanishing Jarlskog invariant.

| $(\theta,\alpha,\beta,\gamma)$ | Range for $\theta$ | Number of real parameters in down-type Yukawa | Number of real parameters in up-type Yukawa |
|---|---|---|---|
| (0,0,0,0) | 0 | 27 | 27 |
| $(\frac{\pi}{2},0,0,\frac{\pi}{2})$ | $\frac{\pi}{2}$ | $9^\diamond$ | 15 |
| $(\frac{\pi}{2},0,\frac{\pi}{2},0)$ | | 15 | $9^\diamond$ |
| $(\frac{\pi}{2},0,\frac{\pi}{2},\frac{\pi}{2})$ | | 15 | 15 |
| $(\frac{\pi}{2},\frac{\pi}{2},0,0)$ | | 15 | 15 |
| $(\frac{\pi}{2},\frac{\pi}{2},0,\frac{\pi}{2})$ | | 15 | 13 |
| $(\frac{\pi}{2},\frac{\pi}{2},\frac{\pi}{2},0)$ | | 13 | 15 |
| $(\frac{\pi}{2},\frac{\pi}{2},\frac{\pi}{2},\frac{\pi}{2})$ | | 13 | 13 |
| $(\frac{\pi}{3},\frac{\pi}{3},0,\frac{\pi}{3})$ | $\frac{\pi}{3}$ | 9 | 9 |
| $(\frac{\pi}{3},\frac{\pi}{3},\frac{\pi}{3},0)$ | | 9 | 9 |
| $(\frac{\pi}{3},\frac{\pi}{3},\frac{\pi}{3},\frac{\pi}{3})$ | | 9 | 9 |
| $(\frac{\pi}{4},\frac{\pi}{4},0,\frac{\pi}{2})$ | $\frac{\pi}{4}$ | 9 | 7 |
| $(\frac{\pi}{4},\frac{\pi}{4},\frac{\pi}{2},0)$ | | 7 | 9 |
| $(\frac{\pi}{4},\frac{\pi}{4},\frac{\pi}{4},\frac{\pi}{2})$ | | 7 | 7 |
| $(\frac{\pi}{4},\frac{\pi}{4},\frac{\pi}{2},\frac{\pi}{4})$ | | 7 | 7 |
| $(\frac{\pi}{4},\frac{\pi}{4},\frac{\pi}{2},\frac{\pi}{2})$ | | 7 | 7 |
| $(\frac{\pi}{4},\frac{\pi}{2},\frac{\pi}{4},\frac{\pi}{4})$ | | 7 | 7 |
| $(\frac{\pi}{5},\frac{2\pi}{5},\frac{\pi}{5},\frac{2\pi}{5})$ | $\frac{\pi}{5}$ | 5 | $5^*$ |
| $(\frac{\pi}{5},\frac{2\pi}{5},\frac{2\pi}{5},\frac{\pi}{5})$ | | $5^*$ | 5 |
| $(\frac{2\pi}{5},\frac{\pi}{5},\frac{2\pi}{5},\frac{\pi}{5})$ | $\frac{2\pi}{5}$ | 5 | $5^*$ |
| $(\frac{2\pi}{5},\frac{\pi}{5},\frac{\pi}{5},\frac{2\pi}{5})$ | | $5^*$ | 5 |
| $(\theta,0,0,\theta)$ | $(0,\frac{\pi}{2})$ | $9^\diamond$ | 9 |
| $(\theta,0,\theta,0)$ | | 9 | $9^\diamond$ |
| $(\theta,0,\theta,\theta)$ | | 9 | 9 |
| $(\theta,\theta,0,0)$ | | 9 | 9 |
| $(\theta,\theta,0,\theta)$ | $(0,\frac{\pi}{2})\backslash\{\frac{\pi}{3}\}$ | 9 | 7 |
| $(\theta,\theta,\theta,0)$ | | 7 | 9 |
| $(\theta,\theta,\theta,\theta)$ | | 7 | 7 |
| $(\theta,\theta,0,2\theta)$ | $(0,\frac{\pi}{4})$ | 9 | 5 |
| $(\theta,\theta,2\theta,0)$ | | 5 | 9 |
| $(\theta,\theta,\theta,2\theta)$ | | 7 | 5 |
| $(\theta,\theta,2\theta,\theta)$ | | 5 | 7 |
| $(\theta,\theta,2\theta,2\theta)$ | | 5 | 5 |
| $(\theta,2\theta,\theta,\theta)$ | | 5 | 5 |
| $(\theta,\theta,0,\pi-2\theta)$ | $(\frac{\pi}{4},\frac{\pi}{2})\backslash\{\frac{\pi}{3}\}$ | 9 | 5 |
| $(\theta,\theta,\pi-2\theta,0)$ | | 5 | 9 |
| $(\theta,\theta,\theta,\pi-2\theta)$ | | 7 | 5 |
| $(\theta,\theta,\pi-2\theta,\theta)$ | | 5 | 7 |
| $(\theta,\theta,\pi-2\theta,\pi-2\theta)$ | | 5 | 5 |
| $(\theta,\pi-2\theta,\theta,\theta)$ | | 5 | 5 |

## V. YUKAWA TEXTURES CONSISTENT WITH EACH *GCP* IMPLEMENTATION

In this section we list the Yukawa textures for all possible *GCP* implementations in the scalar and down-type quark Yukawa sectors of the 3HDM. (As mentioned, for the up-type quark Yukawa matrices one simply makes the replacement $\beta \to \gamma$). This has been performed in two independent ways. The first used the method described in the previous section. For the second, we have developed an extensive *Mathematica* program that automatically tests all possible *GCP* assignments. This is done by solving Eqs. (49) and (50) through the method described in Appendix A. Through this strategy, we can obtain, for each aforementioned block, a homogeneous system of equations $\mathbf{M}(\theta,\alpha,\beta)\Gamma' = \mathbf{0}$, where $\mathbf{M}$ is a matrix which depends on the angles of the *GCP* symmetry assignment and $\Gamma'$ is a vector containing the real (imaginary) part of the entries of $\Gamma_{\bar{k}}$ and $\Gamma_3$ for each block. To find the solutions for the system, the program evaluates which sets of $(\theta,\alpha,\beta)$ nullify the determinant of $\mathbf{M}$ and subsequently calculates $\Gamma'$ such that it is in the null space of $\mathbf{M}$. It then performs all possible logical combinations of these solutions, as well as the trivial solution, and simplifies the result excluding redundant and impossible cases. Finally, it computes de eigenvalues of $H_d$ and $H_u$ as well as the Jarlskog invariant for each possible case, and excludes nonphysical results.

We have confirmed that Table III is correct and complete. Moreover, the program also identifies automatically all relevant Yukawa matrices; they are shown explicitly in this section.

### A. *CPa*: Consistent Yukawa textures

*CPa* (the usual type of *CP*) implies simply that all parameters are real:

$$\Gamma_1 = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}, \qquad \Gamma_2 = \begin{pmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{pmatrix}, \qquad \Gamma_3 = \begin{pmatrix} e_{11} & e_{12} & e_{13} \\ e_{21} & e_{22} & e_{23} \\ e_{31} & e_{32} & e_{33} \end{pmatrix}. \tag{64}$$

Here and in the following subsections, the parameters $a_{ij}$, $b_{ij}$, $c_{ij}$, $d_{ij}$, $e_{ij}$, and $f_{ij}$ are all real. Imaginary numbers will be shown explicitly.

### B. *CPb*: Consistent Yukawa textures

#### *1.* $(\theta,\ \alpha,\ \beta) = (\pi/2,\ 0,\ 0)$

Here,

$$\Gamma_1 = \Gamma_2 = 0, \qquad \Gamma_3 = \begin{pmatrix} e_{11} & e_{12} & e_{13} \\ e_{21} & e_{22} & e_{23} \\ e_{31} & e_{32} & e_{33} \end{pmatrix}. \tag{65}$$

#### *2.* $(\theta,\ \alpha,\ \beta) = (\pi/2,\ 0,\ \pi/2)$

$$\Gamma_1 = \begin{pmatrix} a_{11}+ib_{11} & a_{12}+ib_{12} & 0 \\ a_{21}+ib_{21} & a_{22}+ib_{22} & 0 \\ a_{31}+ib_{31} & a_{32}+ib_{32} & 0 \end{pmatrix}, \quad \Gamma_2 = \begin{pmatrix} -a_{12}+ib_{12} & a_{11}-ib_{11} & 0 \\ -a_{22}+ib_{22} & a_{21}-ib_{21} & 0 \\ -a_{32}+ib_{32} & a_{31}-ib_{31} & 0 \end{pmatrix}, \quad \Gamma_3 = \begin{pmatrix} 0 & 0 & e_{13} \\ 0 & 0 & e_{23} \\ 0 & 0 & e_{33} \end{pmatrix}. \tag{66}$$

#### *3.* $(\theta,\alpha,\beta) = (\pi/2,\pi/2,0)$

$$\Gamma_1 = \begin{pmatrix} a_{11}+ib_{11} & a_{12}+ib_{12} & a_{13}+ib_{13} \\ a_{21}+ib_{21} & a_{22}+ib_{22} & a_{23}+ib_{23} \\ 0 & 0 & 0 \end{pmatrix}, \quad \Gamma_2 = \begin{pmatrix} -a_{21}+ib_{21} & -a_{22}+ib_{22} & -a_{23}+ib_{23} \\ a_{11}-ib_{11} & a_{12}-ib_{12} & a_{13}-ib_{13} \\ 0 & 0 & 0 \end{pmatrix}, \quad \Gamma_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ e_{31} & e_{32} & e_{33} \end{pmatrix}. \tag{67}$$

#### *4.* $(\theta,\alpha,\beta) = (\pi/2,\pi/2,\pi/2)$

$$\Gamma_1 = \begin{pmatrix} 0 & 0 & a_{13}+ib_{13} \\ 0 & 0 & a_{23}+ib_{23} \\ a_{31}+ib_{31} & a_{32}+ib_{32} & 0 \end{pmatrix}, \quad \Gamma_2 = \begin{pmatrix} 0 & 0 & -a_{23}+ib_{23} \\ 0 & 0 & a_{13}-ib_{13} \\ -a_{32}+ib_{32} & a_{31}-ib_{31} & 0 \end{pmatrix}, \quad \Gamma_3 = \begin{pmatrix} e_{11}+if_{11} & e_{12}+if_{12} & 0 \\ -e_{12}+if_{12} & e_{11}-if_{11} & 0 \\ 0 & 0 & e_{33} \end{pmatrix}. \tag{68}$$

### C. *CPc*: Consistent Yukawa textures

#### *1.* $(\theta,\alpha,\beta) = (\pi/3,0,0)$

$$\Gamma_1 = \Gamma_2 = 0, \qquad \Gamma_3 = \begin{pmatrix} e_{11} & e_{12} & e_{13} \\ e_{21} & e_{22} & e_{23} \\ e_{31} & e_{32} & e_{33} \end{pmatrix}. \tag{69}$$

#### 2. $(\theta, \alpha, \beta) = (\pi/3, 0, \pi/3)$

$$\Gamma_1 = \begin{pmatrix} a_{11} & a_{12} & 0 \\ a_{21} & a_{22} & 0 \\ a_{31} & a_{32} & 0 \end{pmatrix}, \qquad \Gamma_2 = \begin{pmatrix} -a_{12} & a_{11} & 0 \\ -a_{22} & a_{21} & 0 \\ -a_{32} & a_{31} & 0 \end{pmatrix}, \qquad \Gamma_3 = \begin{pmatrix} 0 & 0 & e_{13} \\ 0 & 0 & e_{23} \\ 0 & 0 & e_{33} \end{pmatrix}. \tag{70}$$

#### 3. $(\theta, \alpha, \beta) = (\pi/3, \pi/3, 0)$

$$\Gamma_1 = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ 0 & 0 & 0 \end{pmatrix}, \qquad \Gamma_2 = \begin{pmatrix} -a_{21} & -a_{22} & -a_{23} \\ a_{11} & a_{12} & a_{13} \\ 0 & 0 & 0 \end{pmatrix}, \qquad \Gamma_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ e_{31} & e_{32} & e_{33} \end{pmatrix}. \tag{71}$$

#### 4. $(\theta, \alpha, \beta) = (\pi/3, \pi/3, \pi/3)$

$$\Gamma_1 = \begin{pmatrix} ib_{11} & ib_{12} & a_{13} \\ ib_{12} & -ib_{11} & a_{23} \\ a_{31} & a_{32} & 0 \end{pmatrix}, \qquad \Gamma_2 = \begin{pmatrix} ib_{12} & -ib_{11} & -a_{23} \\ -ib_{11} & -ib_{12} & a_{13} \\ -a_{32} & a_{31} & 0 \end{pmatrix}, \qquad \Gamma_3 = \begin{pmatrix} e_{11} & e_{12} & 0 \\ -e_{12} & e_{11} & 0 \\ 0 & 0 & e_{33} \end{pmatrix}. \tag{72}$$

### D. *CPd*: Consistent Yukawa textures

#### 1. $(\theta, \alpha, \beta) = (\pi/4, \pi/4, \pi/2)$

$$\begin{aligned} \Gamma_1 &= \begin{pmatrix} a_{11} + ib_{11} & a_{12} + ib_{12} & a_{13} \\ -a_{12} + ib_{12} & a_{11} - ib_{11} & a_{23} \\ 0 & 0 & 0 \end{pmatrix}, \\ \Gamma_2 &= \begin{pmatrix} -a_{12} + ib_{12} & a_{11} - ib_{11} & -a_{23} \\ -a_{11} - ib_{11} & -a_{12} - ib_{12} & a_{13} \\ 0 & 0 & 0 \end{pmatrix}, \qquad \Gamma_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & e_{33} \end{pmatrix}. \end{aligned} \tag{73}$$

#### 2. $(\theta, \alpha, \beta) = (\pi/4, \pi/2, \pi/4)$

$$\begin{aligned} \Gamma_1 &= \begin{pmatrix} a_{11} + ib_{11} & a_{12} + ib_{12} & 0 \\ -a_{12} + ib_{12} & a_{11} - ib_{11} & 0 \\ a_{31} & a_{32} & 0 \end{pmatrix}, \\ \Gamma_2 &= \begin{pmatrix} a_{12} + ib_{12} & -a_{11} - ib_{11} & 0 \\ a_{11} - ib_{11} & a_{12} - ib_{12} & 0 \\ -a_{32} & a_{31} & 0 \end{pmatrix}, \qquad \Gamma_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & e_{33} \end{pmatrix}. \end{aligned} \tag{74}$$

#### 3. $(\theta, \alpha, \beta) = (\pi/5, 2\pi/5, 2\pi/5)$

$$\Gamma_1 = \begin{pmatrix} ib_{11} & ib_{12} & 0 \\ ib_{12} & -ib_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \Gamma_2 = \begin{pmatrix} ib_{12} & -ib_{11} & 0 \\ -ib_{11} & -ib_{12} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \Gamma_3 = \begin{pmatrix} e_{11} & e_{12} & 0 \\ -e_{12} & e_{11} & 0 \\ 0 & 0 & e_{33} \end{pmatrix}. \tag{75}$$

#### 4. $(\theta, \alpha, \beta) = (2\pi/5, \pi/5, \pi/5)$

$$\Gamma_1 = \begin{pmatrix} a_{11} & a_{12} & 0 \\ a_{12} & -a_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \Gamma_2 = \begin{pmatrix} -a_{12} & a_{11} & 0 \\ a_{11} & a_{12} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \Gamma_3 = \begin{pmatrix} e_{11} & e_{12} & 0 \\ -e_{12} & e_{11} & 0 \\ 0 & 0 & e_{33} \end{pmatrix}. \tag{76}$$

#### 5. $\theta \notin \{0, \pi/3, \pi/2\}$ and $(\alpha, \beta) = (0, 0)$

$$\Gamma_1 = \Gamma_2 = 0, \qquad \Gamma_3 = \begin{pmatrix} e_{11} & e_{12} & e_{13} \\ e_{21} & e_{22} & e_{23} \\ e_{31} & e_{32} & e_{33} \end{pmatrix}. \tag{77}$$

#### 6. $\theta \notin \{0, \pi/3, \pi/2\}$ and $(\alpha, \beta) = (0, \theta)$

$$\Gamma_1 = \begin{pmatrix} a_{11} & a_{12} & 0 \\ a_{21} & a_{22} & 0 \\ a_{31} & a_{32} & 0 \end{pmatrix}, \qquad \Gamma_2 = \begin{pmatrix} -a_{12} & a_{11} & 0 \\ -a_{22} & a_{21} & 0 \\ -a_{32} & a_{31} & 0 \end{pmatrix}, \qquad \Gamma_3 = \begin{pmatrix} 0 & 0 & e_{13} \\ 0 & 0 & e_{23} \\ 0 & 0 & e_{33} \end{pmatrix}. \tag{78}$$

#### 7. $\theta \notin \{0, \pi/3, \pi/2\}$ and $(\alpha, \beta) = (\theta, 0)$

$$\Gamma_1 = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ 0 & 0 & 0 \end{pmatrix}, \qquad \Gamma_2 = \begin{pmatrix} -a_{21} & -a_{22} & -a_{23} \\ a_{11} & a_{12} & a_{13} \\ 0 & 0 & 0 \end{pmatrix}, \qquad \Gamma_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ e_{31} & e_{32} & e_{33} \end{pmatrix}. \tag{79}$$

#### 8. $\theta \in \{0, \pi/3, \pi/2\}$ and $(\alpha, \beta) = (\theta, \theta)$

$$\Gamma_1 = \begin{pmatrix} 0 & 0 & a_{13} \\ 0 & 0 & a_{23} \\ a_{31} & a_{32} & 0 \end{pmatrix}, \qquad \Gamma_2 = \begin{pmatrix} 0 & 0 & -a_{23} \\ 0 & 0 & a_{13} \\ -a_{32} & a_{31} & 0 \end{pmatrix}, \qquad \Gamma_3 = \begin{pmatrix} e_{11} & e_{12} & 0 \\ -e_{12} & e_{11} & 0 \\ 0 & 0 & e_{33} \end{pmatrix}. \tag{80}$$

#### 9. $\theta \in (0, \pi/4)$ and $(\alpha, \beta) = (\theta, 2\theta)$

$$\Gamma_1 = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ -a_{12} & a_{11} & a_{23} \\ 0 & 0 & 0 \end{pmatrix}, \qquad \Gamma_2 = \begin{pmatrix} -a_{12} & a_{11} & -a_{23} \\ -a_{11} & -a_{12} & a_{13} \\ 0 & 0 & 0 \end{pmatrix}, \qquad \Gamma_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & e_{33} \end{pmatrix}. \tag{81}$$

#### 10. $\theta \in (0, \pi/4)$ and $(\alpha, \beta) = (2\theta, \theta)$

$$\Gamma_1 = \begin{pmatrix} a_{11} & a_{12} & 0 \\ -a_{12} & a_{11} & 0 \\ a_{31} & a_{32} & 0 \end{pmatrix}, \qquad \Gamma_2 = \begin{pmatrix} a_{12} & -a_{11} & 0 \\ a_{11} & a_{12} & 0 \\ -a_{32} & a_{31} & 0 \end{pmatrix}, \qquad \Gamma_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & e_{33} \end{pmatrix}. \tag{82}$$

### 11. $\theta \in (\pi/4, \pi/2) \backslash \{\pi/3\}$ and $(\alpha, \beta) = (\theta, \pi - 2\theta)$

$$\Gamma_1 = \begin{pmatrix} ib_{11} & ib_{12} & a_{13} \\ ib_{12} & -ib_{11} & a_{23} \\ 0 & 0 & 0 \end{pmatrix}, \qquad \Gamma_2 = \begin{pmatrix} ib_{12} & -ib_{11} & -a_{23} \\ -ib_{11} & -ib_{12} & a_{13} \\ 0 & 0 & 0 \end{pmatrix}, \qquad \Gamma_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & e_{33} \end{pmatrix}. \tag{83}$$

### 12. $\theta \in (\pi/4, \pi/2) \backslash \{\pi/3\}$ and $(\alpha, \beta) = (\pi - 2\theta, \theta)$

$$\Gamma_1 = \begin{pmatrix} ib_{11} & ib_{12} & 0 \\ ib_{12} & -ib_{11} & 0 \\ a_{31} & a_{32} & 0 \end{pmatrix}, \qquad \Gamma_2 = \begin{pmatrix} ib_{12} & -ib_{11} & 0 \\ -ib_{11} & -ib_{12} & 0 \\ -a_{32} & a_{31} & 0 \end{pmatrix}, \qquad \Gamma_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & e_{33} \end{pmatrix}. \tag{84}$$

## VI. CONCLUSIONS

We have studied the implementation of a generalized $CP$ symmetry on the scalar and Yukawa sectors of the 3HDM. By introducing a key mathematical result, we simplify the analysis, especially in the Yukawa sector.

In the scalar sector, we identified four classes of potentials, just one more than the two Higgs doublet models. We were also able to identify that these four potentials are classified as $CP2$, $CP4$, $S_3 \times GCP_{\theta=\pi}$, and $O(2) \times CP$ in a notation close to [13].

Additionally, we categorize all possible Yukawa textures, excluding those that result in null or degenerate quark masses, or a null Jarlskog invariant. We found that there are 40 different possible implementations of $GCP$ symmetry in the Yukawa sector. This is in contrast with the 2HDM case with generalized $CP$ symmetries extended to the Yukawa sector, where only two scenarios exist. While many of these cases have a large number of parameters in the Yukawa sector, there are 8 models which entail only 10 parameters and, therefore, may be more easily tested against experimental constraints.

## ACKNOWLEDGMENTS

We are grateful to I. P. Ivanov for important discussions and to J. C. Romão for help with running the project. J. P. S. acknowledges discussions with L. Lavoura and P. M. Ferreira in very early stages. This work is supported in part by FCT (Fundação para a Ciência e Tecnologia) under Contracts CERN/FIS-PAR/0002/2021, CERN/FIS-PAR/0008/2019, UIDB/00777/2020, and UIDP/00777/2020; these projects are partially funded through POCTI (FEDER), COMPETE, QREN, and the EU.

## APPENDIX A: *GCP* CONSTRAINTS ON THE SCALAR POTENTIAL

In this appendix we discuss how one would show that there are four classes of $GCP$-symmetric scalar potentials in the 3HDM, using the classical method already used in [8]. We show the result in the special basis in which $X$ has the form in Eq. (7). This is to be contrasted with the much simpler and elegant method we establish in Appendix B and use in Sec. III.

Introducing [7]

$$\begin{aligned} \Delta Y_{ab} &= Y_{ab} - X_{\alpha a} Y^*_{\alpha\beta} X^*_{\beta b} = [Y - (X^\dagger Y X)^*]_{ab}, \\ \Delta Z_{ab,cd} &= Z_{ab,cd} - X_{\alpha a} X_{\gamma c} Z^*_{\alpha\beta,\gamma\delta} X^*_{\beta b} X^*_{\delta d}, \end{aligned} \tag{A1}$$

we may write the conditions for invariance under $GCP$ as

$$\Delta Y_{ab} = 0, \tag{A2}$$

$$\Delta Z_{ab,cd} = 0. \tag{A3}$$

Given Eqs. (5), it is easy to show that

$$\begin{aligned} \Delta Y_{ab} &= \Delta Y^*_{ba}, \\ \Delta Z_{ab,cd} \equiv \Delta Z_{cd,ab} &= \Delta Z^*_{ba,dc}. \end{aligned} \tag{A4}$$

The task of solving Eqs. (6) or, what is the same, Eqs. (A2)–(A3) becomes tedious but systematic. Let us look at the quadratic terms. We find

$$\begin{aligned} & 0 = \mathrm{Im}(\Delta Y_{12}) = 2\mathrm{Im}(Y_{12}), \\ & \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \Delta Y_{11} = -\Delta Y_{22} \\ \mathrm{Re}(\Delta Y_{12}) \end{bmatrix} = s_\theta \begin{bmatrix} s_\theta & c_\theta \\ -c_\theta & s_\theta \end{bmatrix} \begin{bmatrix} Y_{11} - Y_{22} \\ 2\mathrm{Re}(Y_{12}) \end{bmatrix}, \\ & \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \mathrm{Re}(\Delta Y_{13}) \\ \mathrm{Re}(\Delta Y_{23}) \end{bmatrix} = \begin{bmatrix} 1 - c_\theta & s_\theta \\ -s_\theta & 1 - c_\theta \end{bmatrix} \begin{bmatrix} \mathrm{Re}(Y_{13}) \\ \mathrm{Re}(Y_{23}) \end{bmatrix}, \\ & \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \mathrm{Im}(\Delta Y_{13}) \\ \mathrm{Im}(\Delta Y_{23}) \end{bmatrix} = \begin{bmatrix} 1 + c_\theta & -s_\theta \\ s_\theta & 1 + c_\theta \end{bmatrix} \begin{bmatrix} \mathrm{Im}(Y_{13}) \\ \mathrm{Im}(Y_{23}) \end{bmatrix}. \end{aligned} \tag{A5}$$

The determinants of the three systems are $s_\theta^2$, $2(1 - c_\theta)$, and $2(1 + c_\theta)$, respectively. Given the restricted range $0 \le \theta \le \pi/2$, the first two are zero if and only if $\theta = 0$, while the third never vanishes. As a result, we conclude that there are two possibilities: either $\theta = 0$ (corresponding to the usual definition of *CP*, denoted here by CPa), and all quadratic coefficients are real; or $\theta \neq 0$, and $Y = \mathrm{diag}(\mu_1, \mu_1, \mu_3)$, with $\mu_1$ and $\mu_3$ real. The first case corresponds to 6 real parameters; the second case corresponds to 2 real parameters.

The study of the *GCP* symmetry conditions on the quartic couplings using this strategy is more involved. To see the impact on the quartic potential, we follow Ref. [9] and organize the $Z_{ij,kl}$ tensor into a matrix of matrices. The uppermost-leftmost matrix corresponds to the phases affecting $Z_{11,kl}$. The next matrix along the same line corresponds to the phases affecting $Z_{12,kl}$, and so on... We use the following notation for the various entries [9]

$$\begin{bmatrix} \begin{bmatrix} r_1 & c_1 & c_2 \\ c_1^* & r_4 & c_6 \\ c_2^* & c_6^* & r_5 \end{bmatrix} & \begin{bmatrix} c_1 & c_3 & c_4 \\ r_7 & c_7 & c_8 \\ c_9^* & c_{12} & c_{13} \end{bmatrix} & \begin{bmatrix} c_2 & c_4 & c_5 \\ c_9 & c_{10} & c_{11} \\ r_8 & c_{14} & c_{15} \end{bmatrix} \\ \begin{bmatrix} c_1^* & r_7 & c_9 \\ c_3^* & c_7^* & c_{12}^* \\ c_4^* & c_8^* & c_{13}^* \end{bmatrix} & \begin{bmatrix} r_4 & c_7 & c_{10} \\ c_7^* & r_2 & c_{16} \\ c_{10}^* & c_{16}^* & r_6 \end{bmatrix} & \begin{bmatrix} c_6 & c_8 & c_{11} \\ c_{12}^* & c_{16} & c_{17} \\ c_{14}^* & r_9 & c_{18} \end{bmatrix} \\ \begin{bmatrix} c_2^* & c_9^* & r_8 \\ c_4^* & c_{10}^* & c_{14}^* \\ c_5^* & c_{11}^* & c_{15}^* \end{bmatrix} & \begin{bmatrix} c_6^* & c_{12} & c_{14} \\ c_8^* & c_{16}^* & r_9 \\ c_{11}^* & c_{17}^* & c_{18}^* \end{bmatrix} & \begin{bmatrix} r_5 & c_{13} & c_{15} \\ c_{13}^* & r_6 & c_{18} \\ c_{15}^* & c_{18}^* & r_3 \end{bmatrix} \end{bmatrix}, \tag{A6}$$

where $r_k$ $(k = 1\ldots9)$ are real and $c_k$ $(k = 1\ldots18)$ are complex. We will write $c_k = x_k + iy_k$, with $x_k$ and $y_k$ real.

We now wish to study Eqs. (A3). Due to Eqs. (A4), we only need the 9 real coefficients $\Delta Z_{11,11}$, $\Delta Z_{22,22}$, $\Delta Z_{33,33}$, $\Delta Z_{11,22}$, $\Delta Z_{11,33}$, $\Delta Z_{22,33}$, $\Delta Z_{12,21}$, $\Delta Z_{13,31}$, $\Delta Z_{23,32}$, and the 18 complex coefficients $\Delta Z_{11,12}$, $\Delta Z_{11,13}$, $\Delta Z_{11,23}$, $\Delta Z_{22,12}$, $\Delta Z_{22,13}$, $\Delta Z_{22,23}$, $\Delta Z_{33,12}$, $\Delta Z_{33,13}$, $\Delta Z_{33,23}$, $\Delta Z_{12,12}$, $\Delta Z_{12,13}$, $\Delta Z_{12,23}$, $\Delta Z_{12,31}$, $\Delta Z_{12,32}$, $\Delta Z_{13,13}$, $\Delta Z_{13,23}$, $\Delta Z_{13,32}$, and $\Delta Z_{23,23}$. However,

$$\begin{aligned} -2\Delta Z_{11,22} &= \Delta Z_{11,11} + \Delta Z_{22,22} \\ \Delta Z_{22,33} &= -\Delta Z_{11,33}, \\ \Delta Z_{33,33} &= 0, \\ \Delta Z_{12,21} &= \Delta Z_{11,22}, \\ \Delta Z_{23,32} &= -\Delta Z_{13,31}, \\ \mathrm{Re}(\Delta Z_{12,12}) &= \mathrm{Re}(\Delta Z_{11,22}), \\ \mathrm{Re}(\Delta Z_{23,23}) &= -\mathrm{Re}(\Delta Z_{13,13}), \end{aligned} \tag{A7}$$

simplifying the analysis. One then proceeds as for the quadratic terms finding systems such as, for example,

$$\begin{aligned} \begin{bmatrix} 0 \\ 0 \end{bmatrix} &= \begin{bmatrix} \mathrm{Im}(\Delta Z_{12,13} - \Delta Z_{11,23}) \\ \mathrm{Im}(\Delta Z_{22,13} + \Delta Z_{12,32}) \end{bmatrix} = \begin{bmatrix} 1 + c_\theta & -s_\theta \\ s_\theta & 1 + c_\theta \end{bmatrix} \begin{bmatrix} y_4 - y_6 \\ y_{10} + y_{12} \end{bmatrix}, \\ \begin{bmatrix} 0 \\ 0 \end{bmatrix} &= \begin{bmatrix} \mathrm{Im}(\Delta Z_{11,23} + \Delta Z_{12,31}) \\ \mathrm{Im}(\Delta Z_{12,23} - \Delta Z_{22,13}) \end{bmatrix} = \begin{bmatrix} 1 + c_\theta & -s_\theta \\ s_\theta & 1 + c_\theta \end{bmatrix} \begin{bmatrix} y_6 - y_9 \\ y_8 - y_{10} \end{bmatrix}, \\ \begin{bmatrix} 0 \\ 0 \end{bmatrix} &= \begin{bmatrix} \mathrm{Im}(\Delta Z_{33,13}) \\ \mathrm{Im}(\Delta Z_{33,23}) \end{bmatrix} = \begin{bmatrix} 1 + c_\theta & -s_\theta \\ s_\theta & 1 + c_\theta \end{bmatrix} \begin{bmatrix} y_{15} \\ y_{18} \end{bmatrix} \end{aligned} \tag{A8}$$

These systems have determinant $2(1 + c_\theta)$, which never vanishes due to the restricted range $0 \leq \theta \leq \pi/2$. As a result, any *GCP* symmetry will force $y_{15} = y_{18} = 0$, $y_4 = y_6 = y_9$, and $y_8 = y_{10} = -y_{12}$.

A more challenging example is

$$\begin{aligned} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} &= \begin{bmatrix} \mathrm{Im}(\Delta Z_{11,13}) \\ 4\mathrm{Im}(\Delta Z_{12,13} + \Delta Z_{11,23} - \Delta Z_{12,31}) \\ 4\mathrm{Im}(\Delta Z_{12,23} + \Delta Z_{22,13} - \Delta Z_{12,32}) \\ \mathrm{Im}(\Delta Z_{22,23}) \end{bmatrix} \\ &= \begin{bmatrix} 1 + c_\theta^3 & -c_\theta^2 s_\theta & c_\theta s_\theta^2 & -s_\theta^3 \\ 12 c_\theta^2 s_\theta & 4 + c_\theta + 3c_{3\theta} & s_\theta - 3s_{3\theta} & 12 c_\theta s_\theta^2 \\ 12 c_\theta s_\theta^2 & 3s_{3\theta} - s_\theta & 4 + c_\theta + 3c_{3\theta} & -12 c_\theta^2 s_\theta \\ s_\theta^3 & c_\theta s_\theta^2 & c_\theta^2 s_\theta & 1 + c_\theta^3 \end{bmatrix} \begin{bmatrix} y_2 \\ y_4 + y_6 + y_9 \\ y_8 + y_{10} - y_{12} \\ y_{16} \end{bmatrix}, \end{aligned} \tag{A9}$$

with determinant $64(1+c_\theta)^2(1-2c_\theta)^2$. Given the restricted range $0 \le \theta \le \pi/2$, this determinant can only vanish if $c_\theta = 1/2$, that is, $\theta = \pi/3$.

We have checked explicitly that this procedure does reproduce the results for the scalar potential obtained in the main text, although in a much more tedious way.

## APPENDIX B: A MATHEMATICAL RESULT ON KROENECKER PRODUCTS OF ROTATIONS

In this appendix we state and use a result that greatly simplifies systems of equations involving tensors and rotation matrices. If we work in the scalar field basis where the *GCP* transformation matrix is of the form in Eq. (7), with $\oplus$ denoting the direct sum operation, we can use this result to solve the equations regarding *GCP* invariance in both the scalar and Yukawa sectors of the SM Lagrangian with great ease.

### 1. Result

Suppose we have a $2^n \times 2^n$ matrix, with $n \in \mathbb{N}$, defined as

$$\mathbf{R}^n_\Theta \equiv \bigotimes_{q=1}^{n} R_{\theta_q} = R_{\theta_1} \otimes R_{\theta_2} \otimes \cdots \otimes R_{\theta_n}. \tag{B1}$$

Then, $\forall\ n \ge 1\, \exists\, C_n \in M_{2^n\times 2^n}:\ C_n C_n^\top = I_{2^n}$, and

$$C_n \mathbf{R}^n_\Theta C_n^\top = \bigoplus_{p=0}^{2^{n-1}-1} R_{\omega^n_p} = R_{\omega^n_0} \oplus R_{\omega^n_1} \oplus \cdots \oplus R_{\omega^n_{2^{n-1}-1}}, \tag{B2}$$

where

$$\omega^n_p = \sum_{q=1}^{n} (-1)^{\mathrm{Mod}(\lfloor \frac{p}{2^{q-1}} \rfloor, 2)} \theta_q, \tag{B3}$$

$I_{2^n}$ is the identity $2^n \times 2^n$ matrix, and $\lfloor\rfloor$ is the floor function, which yields the previous largest integer. For example, for $n=3$ we have $\omega^3_0 = \theta_1 + \theta_2 + \theta_3$, $\omega^3_1 = -\theta_1 + \theta_2 + \theta_3$, $\omega^3_2 = \theta_1 - \theta_2 + \theta_3$, and $\omega^3_3 = -\theta_1 - \theta_2 + \theta_3$.

The $C_n$ matrices are defined as follows:

$$C_n = \left(\bigoplus_{p=1}^{2^n} U^{-1}\right)(P_n)\left(\bigotimes_{p=1}^{n} U\right), \tag{B4}$$

where

$$(P_n)_{pq} = 1, \quad \text{if} \begin{cases} p \text{ is odd} & \text{and} \quad q = \frac{p+1}{2} \\ p \text{ is even} & \text{and} \quad q = 2^n - \frac{p}{2} + 1 \end{cases},$$
$$(P_n)_{pq} = 0, \quad \text{otherwise}, \tag{B5}$$

and

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}. \tag{B6}$$

We include in the Supplemental Material [19] a proof of Eqs. (B3)–(B4). In addition, using the first few $C_n$ matrices,

$$C_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 \end{pmatrix} \tag{B7}$$

$$C_3 = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & -1 & 0 & -1 & -1 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & -1 \\ 1 & 0 & 0 & -1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & -1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 & -1 & 0 \\ 0 & 1 & -1 & 0 & -1 & 0 & 0 & -1 \end{pmatrix} \tag{B8}$$

$$C_4 = \frac{1}{\sqrt{8}} \begin{pmatrix} 1 & 0 & 0 & -1 & 0 & -1 & -1 & 0 & 0 & -1 & -1 & 0 & -1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & -1 & 1 & 0 & 0 & -1 & 0 & -1 & -1 & 0 \\ 1 & 0 & 0 & -1 & 0 & -1 & -1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & -1 & -1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & -1 & 0 & 1 & 1 & 0 & 0 & -1 & -1 & 0 & 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 & -1 & 0 & 0 & 1 & 1 & 0 & 0 & -1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & -1 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & -1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & -1 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & 0 & -1 & -1 & 0 \\ 1 & 0 & 0 & 1 & 0 & -1 & 1 & 0 & 0 & -1 & 1 & 0 & -1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & -1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & -1 & 1 & 0 & 0 & 1 & -1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 & 1 & 0 & 0 & 1 & -1 & 0 & 0 & -1 & 0 & 1 & -1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & -1 & 0 & 0 & -1 & 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 & -1 & 0 & 0 & -1 & 1 & 0 & 0 & 1 & 0 & 1 & -1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & 0 & -1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 & -1 & 0 & 0 & -1 & -1 & 0 & 0 & -1 & 0 & -1 & 1 & 0 \end{pmatrix}, \tag{B9}$$

we have confirmed by explicit construction of the corresponding matrices that Eqs. (B2)–(B4) hold up to the highest $n = 4$ case needed for our article.


[1] T. D. Lee and G. C. Wick, Space inversion, time reversal, and other discrete symmetries in local field theories, Phys. Rev. **148**, 1385 (1966).

[2] G. Ecker, W. Grimus, and W. Konetschny, Quark mass matrices in left-right symmetric gauge theories, Nucl. Phys. **B191**, 465 (1981).

[3] G. Ecker, W. Grimus, and H. Neufeld, Spontaneous *CP* violation in left-right symmetric gauge theories, Nucl. Phys. **B247**, 70 (1984).

[4] H. Neufeld, W. Grimus, and G. Ecker, Generalized *CP* invariance, neutral flavor conservation and the structure of the mixing matrix, Int. J. Mod. Phys. A **03**, 603 (1988).

[5] J. Bernabeu, G. C. Branco, and M. Gronau, *CP* restrictions on quark mass matrices, Phys. Lett. **169B**, 243 (1986).

[6] I. P. Ivanov, Minkowski space structure of the Higgs potential in 2HDM. II. Minima, symmetries, and topology, Phys. Rev. D **77**, 015017 (2008).

[7] P. M. Ferreira, H. E. Haber, and J. P. Silva, Generalized *CP* symmetries and special regions of parameter space in the two-Higgs-doublet model, Phys. Rev. D **79**, 116004 (2009).

[8] P. M. Ferreira and J. P. Silva, A two-Higgs doublet model with remarkable *CP* properties, Eur. Phys. J. C **69**, 45 (2010).

[9] P. M. Ferreira and J. P. Silva, Discrete and continuous symmetries in multi-Higgs-doublet models, Phys. Rev. D **78**, 116007 (2008).

[10] I. P. Ivanov and E. Vdovin, Classification of finite reparametrization symmetry groups in the three-Higgs-doublet model, Eur. Phys. J. C **73**, 2309 (2013).

[11] I. Brée, Some aspects of symmetry constrained multi-Higgs models, Master's thesis, IST, University of Lisbon, 2023, https://fenix.tecnico.ulisboa.pt/cursos/meft21/dissertacao/1972678479055825.

[12] I. P. Ivanov, C. C. Nishi, J. P. Silva, and A. Trautner, Basis-invariant conditions for *CP* symmetry of order four, Phys. Rev. D **99**, 015039 (2019).

[13] I. de Medeiros Varzielas and I. P. Ivanov, Recognizing symmetries in a 3HDM in a basis-independent way, Phys. Rev. D **100**, 015008 (2019).

[14] I. P. Ivanov and C. C. Nishi, Symmetry breaking patterns in 3HDM, J. High Energy Phys. 01 (2015) 021.

[15] S. Carrolo, J. C. Romão, J. P. Silva, and F. Vazão, Symmetry and decoupling in multi-Higgs boson models, Phys. Rev. D **103**, 075026 (2021).

[16] P. M. Ferreira and J. P. Silva, Abelian symmetries in the two-Higgs-doublet model with fermions, Phys. Rev. D **83**, 065026 (2011).

[17] H. Serôdio, Yukawa sector of multi Higgs doublet models in the presence of Abelian symmetries, Phys. Rev. D **88**, 056015 (2013).

[18] I. P. Ivanov and C. C. Nishi, Abelian symmetries of the N-Higgs-doublet model with Yukawa interactions, J. High Energy Phys. 11 (2013) 069.

[19] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevD.110.035028 for proof of a result relating tensor products of $2 \times 2$ rotation matrices with direct sums of (related) $2 \times 2$ rotation matrices.
[20] F. J. Botella and J. P. Silva, Jarlskog-like invariants for theories with scalars and fermions, Phys. Rev. D **51**, 3870 (1995).
[21] G. C. Branco, L. Lavoura, and J. P. Silva, *CP* violation, Int. Ser. Monogr. Phys. **103**, 1 (1999).
[22] S. Davidson and H. E. Haber, Basis-independent methods for the two-Higgs-doublet model, Phys. Rev. D **72**, 035004 (2005); Phys. Rev. D **72**, 099902(E) (2005).
[23] G. Ecker, W. Grimus, and H. Neufeld, A standard form for generalized *CP* transformations, J. Phys. A **20**, L807 (1987).
[24] K. M. Abadir and J. R. Magnus, *Matrix Algebra* (Cambridge University Press, Cambridge, England, 2005), 10.1017/CBO9780511810800.
[25] N. Cabibbo, Unitary symmetry and leptonic decays, Phys. Rev. Lett. **10**, 531 (1963).
[26] M. Kobayashi and T. Maskawa, *CP* violation in the renormalizable theory of weak interaction, Prog. Theor. Phys. **49**, 652 (1973).
[27] C. Jarlskog, Commutator of the quark mass matrices in the standard electroweak model and a measure of maximal *CP* nonconservation, Phys. Rev. Lett. **55**, 1039 (1985).
[28] C. Jarlskog, A basis independent formulation of the connection between quark mass matrices, *CP* violation and experiment, Z. Phys. C **29**, 491 (1985).
[29] R. L. Workman *et al.* (Particle Data Group), Review of particle physics, Prog. Theor. Exp. Phys. **2022**, 083C01 (2022).