Two-Higgs-doublet models with a flavored $\mathbb{Z}_2$ symmetry

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Two-Higgs-doublet models usually consider an *ad-hoc* $\mathbb{Z}_2$ discrete symmetry to avoid flavor changing neutral currents. We consider a new class of two-Higgs-doublet models where $\mathbb{Z}_2$ is enlarged to the symmetry group $\mathcal{F} \rtimes \mathbb{Z}_2$, i.e., an inner semidirect product of a discrete symmetry group $\mathcal{F}$ and $\mathbb{Z}_2$. In such a scenario, the symmetry constrains the Yukawa interactions but goes unnoticed by the scalar sector. In the most minimal scenario, $\mathbb{Z}_3 \rtimes \mathbb{Z}_2 = D_3$, flavor changing neutral currents mediated by scalars are absent at tree and one-loop level, while at the same time predictions to quark and lepton mixing are obtained, namely a trivial Cabibbo-Kobayashi-Maskawa matrix and a Pontecorvo-Maki-Nakagawa-Sakata matrix (upon introduction of three heavy right-handed neutrinos) containing maximal atmospheric mixing. Small extensions allow to fully reproduce mixing parameters, including cobimaximal mixing in the lepton sector (maximal atmospheric mixing and a maximal charge-parity violating phase).

I. INTRODUCTION

The discovery of a Higgs boson with a mass of $m_h \simeq 125$ GeV has opened the door to the possibility of having in Nature multiple fundamental scalars. In principle, nothing forbids their proliferation. Nonetheless, the amount of parameters dramatically increases, both in the Yukawa and scalar sector. Here, we consider a simple extension to the standard model (SM) by only introducing a second Higgs doublet (2HDM) with quantum numbers identical to the SM Higgs and three right-handed neutrinos to generate active neutrino masses. Furthermore, we mainly focus on the problem of fermion mixing by first adopting the common 2HDM framework with natural flavor conservation (NFC) [1,2], achieved through a $\mathbb{Z}_2$ reflection symmetry. Then, we add *flavor* to it via the enlargement of the symmetry group in a very particular manner, $\mathcal{F} \rtimes \mathbb{Z}_2$. This denotes an inner semidirect product of a discrete symmetry group $\mathcal{F}$ and a $\mathbb{Z}_2$ symmetry. The non-Abelian nature of the enlarged symmetry group then strongly reduces the number of Yukawa couplings, thus providing a more predictive theory. Moreover, the *ad-hoc* nature of the $\mathbb{Z}_2$ is explained as a part of a larger group.[1]

To understand the need for the $\mathbb{Z}_2$ symmetry, we briefly sketch its impact. In a general setup, one may immediately write the Yukawa Lagrangian for a given fermion,

$$-\mathcal{L}_Y \supset \bar{\psi}_L (\mathbf{Y}_1^\psi \Phi_1 + \mathbf{Y}_2^\psi \Phi_2)\psi_R + \text{H.c.}, \qquad (1)$$

where ψ_R or ψ_L are three-dimensional vectors in flavor space each denoting a weak singlet or a weak doublet, respectively, and ψ representing any of the four fermion types, $\psi = q_u, q_d, \ell, \nu$. Notice that the Higgs doublets must be replaced by their charge-conjugate fields, $\tilde{\Phi}_k = i\sigma_2 \Phi_k^*$, for the up-type quark and neutrino cases.[2] If the neutral components of both scalar doublets acquire a vacuum expectation value (VEV), $\langle \Phi_1^0 \rangle = v_1$ and $\langle \Phi_2^0 \rangle = v_2$, both Yukawa matrices contribute to the fermion masses and mixing. It is clear that diagonalization of the mass matrix,

$$\mathbf{M} = v_1 \mathbf{Y}_1 + v_2 \mathbf{Y}_2, \qquad (2)$$

cannot mean, in general, diagonalization of the individual Yukawa matrices. This brings about dangerous tree-level flavor-changing neutral currents (FCNCs). To avoid them,

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[1]There are other possibilities to explain the *ad-hoc* $\mathbb{Z}_2$, for instance, by linking it to the remnant symmetry of a spontaneously broken $U(1)$; see, e.g., [3–5].

[2]For brevity, we left aside the Majorana option. However, we return to it later.

it is sufficient to assume NFC by introducing a $\mathbb{Z}_2$ symmetry and by assigning a single scalar doublet for a given fermion species such that only one of the two Yukawa matrices contributes to the mass matrix. This is, the scalar fields transform under the discrete symmetry such that

$$\Phi_1 \to -\Phi_1, \qquad \Phi_2 \to +\Phi_2, \tag{3}$$

while the left-handed quarks and leptons transform trivially and the right-handed parts transform appropriately. The different assignment possibilities lead to four nonequivalent types of 2HDMs[3]:

   (i) Type I: all charged fermions couple to Φ_2.
   (ii) Type II: q_d and ℓ couple to Φ_1 and q_u to Φ_2.
   (iii) Type X: q_u and q_d couple to Φ_2 and ℓ to Φ_1.
   (iv) Type Y: q_u and ℓ couple to Φ_2 and q_d to Φ_1.

Other possibilities are the Type III which is the general 2HDM with all couplings permitted and the inert doublet model where Φ_2 couples to all fermions while Φ_1 has no VEV, thus leaving unbroken the $\mathbb{Z}_2$ symmetry and providing a viable dark matter candidate. Although other approaches, such as Yukawa-alignment [6] or singular-alignment [7], may also avoid tree-level FCNC, here we only focus on those 2HDM employing the discrete symmetry $\mathbb{Z}_2$. Attempts to add flavor to 2HDMs have already been made, e.g., [8–10]. However, our approach offers an alternative and novel way to consider the NFC theories as the starting point to build minimal extensions where the patterns in fermion mixing are taken as a guide for new physics. Note that the nonequivalence nature between the four types comes from the fact that each framework ends up having different effective Yukawa couplings of the fermions to the various scalar particles; for a thorough discussion on various phenomenological and theoretical aspects of 2HDMs, see Ref. [11].

On the other hand, a general feature shared by the four different types (I, II, X, and Y) is the $\mathbb{Z}_2$-invariant scalar potential given by

$$
\begin{aligned}
V_{\text{2HDM}}^{\mathbb{Z}_2} = \sum_{x=1,2} & \left[m_{xx}^2 (\Phi_x^\dagger \Phi_x) + \frac{\lambda_x}{2} (\Phi_x^\dagger \Phi_x)^2 \right] \\
& + \lambda_3 (\Phi_1^\dagger \Phi_1)(\Phi_2^\dagger \Phi_2) + \lambda_4 (\Phi_1^\dagger \Phi_2)(\Phi_2^\dagger \Phi_1) \\
& + \frac{1}{2} [\lambda_5 (\Phi_1^\dagger \Phi_2)^2 + \lambda_5^* (\Phi_2^\dagger \Phi_1)^2].
\end{aligned}
\tag{4}
$$

The hermiticity condition of the potential leaves λ_5 as the only complex coefficient while the rest, m_{11}^2, m_{22}^2, and $\lambda_{1,2,3,4}$, are real. There are in total eight real parameters. However, not all of them are physical. A phase redefinition can make λ_5 real and only seven parameters are physical. Note that our potential has explicitly become charge-parity (*CP*)-symmetric.

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[3]The types X and Y are also called the lepton-specific and flipped scenarios, respectively.

No matter the amount of Higgs doublets one employs, the full mass matrix for any given fermion is parametrized by nine complex parameters. The initial arbitrariness may then be reduced via weak-basis transformations (unitary transformations leaving invariant the kinetic terms), but not enough to claim predictivity. In the mass basis, for either quarks or leptons, one has six fermion masses and four (six for Majorana neutrinos) mixing parameters, plus arbitrary Yukawa couplings. The flavor sector thus gives to the SM and its extensions (without symmetries) the highest amount of arbitrariness. It is only when symmetries are introduced that the initial arbitrariness can be drastically reduced. Here, we intend to explore the effect of symmetries in the flavor sector such that we find correlations among the quark and lepton mixing parameters.

The paper is organized as follows: in Sec. II, we discuss the meaning of adding flavor to $\mathbb{Z}_2$. Next, in Sec. III, we provide the most minimal scenario realizing the features of our approach. Also, we highlight the main differences when compared to the four types of 2HDMs. Thereafter, in Sec. IV, we take the incompleteness of fermion mixing in our simple model as a hint to the presence of additional new physics and introduce a flavor doublet of real scalar gauge singlets. Finally, in Sec. V, we conclude. Some technical details are delegated to appendices.

II. ADDING FLAVOR TO $\mathbb{Z}_2$

We are interested in those finite symmetry groups, $\mathcal{G}$, which can be written as an inner semidirect product of an arbitrary group $\mathcal{F}$ and $\mathbb{Z}_2$,

$$\mathcal{G} = \mathcal{F} \rtimes \mathbb{Z}_2. \tag{5}$$

There are in fact many examples of such groups (see Ref. [12] for more details): $D_N = \Delta(2N) \simeq \mathbb{Z}_N \rtimes \mathbb{Z}_2$, $\Sigma(2N^2) \simeq (\mathbb{Z}_N \times \mathbb{Z}'_N) \rtimes \mathbb{Z}_2$, $\Sigma(24) \simeq \mathbb{Z}_2 \times \mathbb{Z}_6 \rtimes \mathbb{Z}_2$, etc.

The main property of this kind of groups is that they contain two one-dimensional irreducible representations (denoted singlets), which behave exactly as if we only had a $\mathbb{Z}_2$ symmetry. Thus, by assigning each Higgs doublet to one of these singlets, we are mimicking in the scalar sector any of the NFC models with a $\mathbb{Z}_2$ symmetry. On the other hand, the non-Abelian nature of the symmetry only impacts the Yukawa interactions, thus providing a way to approach the problem of mixing while simultaneously tackling minimal scalar extensions to the SM.

An additional feature of this approach is the following. Since the number of Higgs doublets in a theory restricts the maximum group order of allowed symmetries ("realizable symmetries") that would otherwise imply massless Goldstone bosons [13], then by implementing symmetry groups as here proposed we avoid these constrictions.

Let us take as a first example the Klein group given by $\mathbb{Z}_2 \rtimes \mathbb{Z}_2$. It is the smallest possibility within this approach. It has four elements and four irreducible representations

(irreps): $\mathbf{1}_{++}$, $\mathbf{1}_{+-}$, $\mathbf{1}_{-+}$, and $\mathbf{1}_{--}$. However, as it is still an Abelian group, its effect on the Yukawa couplings is only of reduction but not of relation. For example, we could assign the Higgs doublets as $\Phi_1 \sim \mathbf{1}_{--}$ and $\Phi_2 \sim \mathbf{1}_{++}$, while the third, second, and first fermion families as $\mathbf{1}_{-+}$, $\mathbf{1}_{+-}$, and $\mathbf{1}_{++}$, respectively. In return, the mass matrix for Dirac fermions would take the generic form

$$\mathbf{M} = \begin{pmatrix} y_1 v_{++} & y_4 v_{--} & 0 \\ y_5 v_{--} & y_2 v_{++} & 0 \\ 0 & 0 & y_3 v_{++} \end{pmatrix}, \qquad (6)$$

where $\langle \Phi_1^0 \rangle = v_{--}$ and $\langle \Phi_2^0 \rangle = v_{++}$. Therefore, although we have reduced the number of complex parameters from nine to five, we yet have no predictions except for the fact that we only expect mixing between the first two generations. Nevertheless, it demonstrates that the combination of the flavor-safe $\mathbb{Z}_2$ with an additional group will simplify the Yukawa sector. Going to the non-Abelian case will result in predictive scenarios, and we will study a very minimal approach in what follows.

III. THE MINIMAL CASE: $\mathbb{Z}_3 \rtimes \mathbb{Z}_2$

The smallest non-Abelian finite group has six elements and is denoted by $D_3 \equiv \mathbb{Z}_3 \rtimes \mathbb{Z}_2$. This dihedral group describes the symmetrical properties of an equilateral triangle.[4] It has three irreducible representations: two singlets $\mathbf{1}_+$, $\mathbf{1}_-$ and one doublet $\mathbf{2}$. The product rules can be found in Appendix A.

Although different assignments between the D_3 irreps and the fermion fields could be done, here we opt to consider

$$Q_{L,3} \sim \mathbf{1}_+, \qquad Q_{L,D} = \begin{pmatrix} Q_{L,1} \\ Q_{L,2} \end{pmatrix} \sim \mathbf{2},$$

$$u_{R,3} \sim \mathbf{1}_+, \qquad u_{R,D} = \begin{pmatrix} u_{R,1} \\ u_{R,2} \end{pmatrix} \sim \mathbf{2},$$

$$d_{R,3} \sim \mathbf{1}_-, \qquad d_{R,D} = \begin{pmatrix} d_{R,1} \\ d_{R,2} \end{pmatrix} \sim \mathbf{2}, \qquad (7)$$

whereas in the lepton sector

$$E_{L,1} \sim \mathbf{1}_+, \qquad E_{L,D} = \begin{pmatrix} E_{L,2} \\ E_{L,3} \end{pmatrix} \sim \mathbf{2},$$

$$e_{R,1} \sim \mathbf{1}_-, \qquad e_{R,D} = \begin{pmatrix} e_{R,2} \\ e_{R,3} \end{pmatrix} \sim \mathbf{2},$$

$$N_{R,1} \sim \mathbf{1}_-, \qquad N_{R,D} = \begin{pmatrix} N_{R,2} \\ N_{R,3} \end{pmatrix} \sim \mathbf{2}. \qquad (8)$$

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[4]D_3 is isomorphic to S_3, the group describing the permutations of three indistinguishable objects.

We are motivated to this choice, as we will see, because the dominant contributions to quark and lepton mixing are the Cabibbo and atmospheric angle, correspondingly.

Recall that the scalar sector should be assigned to

$$\Phi_1 \sim \mathbf{1}_- \quad \text{and} \quad \Phi_2 \sim \mathbf{1}_+. \qquad (9)$$

The neutral component of both Higgs doublets acquires a VEV, spontaneously breaking the electroweak symmetry; we denote them as

$$v_1 \equiv \langle \Phi_1^0 \rangle \quad \text{and} \quad v_2 \equiv \langle \Phi_2^0 \rangle. \qquad (10)$$

Note we are using the convention $v^2 = v_1^2 + v_2^2 = (174 \text{ GeV})^2$.

The $\mathbb{Z}_3 \rtimes \mathbb{Z}_2$-symmetric Yukawa Lagrangian is

$$-\mathcal{L}_Y = \mathcal{L}_Y^Q + \mathcal{L}_Y^E, \qquad (11)$$

with

$$\begin{aligned} \mathcal{L}_Y^Q = {} & y_t \bar{Q}_{L,3} \tilde{\Phi}_2 u_{R,3} + y_b \bar{Q}_{L,3} \Phi_1 d_{R,3} \\ & + y_1^u [\bar{Q}_{L,D} u_{R,D}]_- \tilde{\Phi}_1 + y_2^u [\bar{Q}_{L,D} u_{R,D}]_+ \tilde{\Phi}_2 \\ & + y_1^d [\bar{Q}_{L,D} d_{R,D}]_- \Phi_1 + y_2^d [\bar{Q}_{L,D} d_{R,D}]_+ \Phi_2 \\ & + \text{H.c.} \end{aligned} \qquad (12)$$

and

$$\begin{aligned} \mathcal{L}_Y^E = {} & y_{\nu 1} \bar{E}_{L,1} \tilde{\Phi}_1 N_{R,1} + y_e \bar{E}_{L,1} \Phi_1 e_{R,1} \\ & + y_1^\nu [\bar{E}_{L,D} N_{R,D}]_- \tilde{\Phi}_1 + y_2^\nu [\bar{E}_{L,D} N_{R,D}]_+ \tilde{\Phi}_2 \\ & + y_1^e [\bar{E}_{L,D} e_{R,D}]_- \Phi_1 + y_2^e [\bar{E}_{L,D} e_{R,D}]_+ \Phi_2 \\ & + \frac{1}{2} M_1 \overline{N_{R,1}^c} N_{R,1} + \frac{1}{2} M_2 [\overline{N_{R,D}^c} N_{R,D}]_+ \\ & + \text{H.c.}, \end{aligned} \qquad (13)$$

where $[\,]_k = \{\mathbf{1}_+, \mathbf{1}_-, \mathbf{2}\}$ represents one of the three possible outputs from the D_3 tensorial product. Also, notice that we are now assuming Majorana neutrinos by virtue of a standard seesaw.

In the quark sector, the resulting Yukawa matrices take the form

$$\Delta_1 = \begin{pmatrix} 0 & y_1^u & 0 \\ -y_1^u & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \Delta_2 = \begin{pmatrix} y_2^u e^{i\gamma_u} & 0 & 0 \\ 0 & y_2^u e^{i\gamma_u} & 0 \\ 0 & 0 & y_t \end{pmatrix},$$

$$\Gamma_1 = \begin{pmatrix} 0 & y_1^d & 0 \\ -y_1^d & 0 & 0 \\ 0 & 0 & y_b \end{pmatrix}, \quad \Gamma_2 = \begin{pmatrix} y_2^d e^{i\gamma_d} & 0 & 0 \\ 0 & y_2^d e^{i\gamma_d} & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$(14)$$

while in the lepton sector, we have

$$
\mathbf{\Pi}_1 = \begin{pmatrix} y_e & 0 & 0 \\ 0 & 0 & y_1^e \\ 0 & -y_1^e & 0 \end{pmatrix}, \quad \mathbf{\Pi}_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & y_2^e e^{i\gamma_e} & 0 \\ 0 & 0 & y_2^e e^{i\gamma_e} \end{pmatrix},
$$

$$
\mathbf{\Omega}_1 = \begin{pmatrix} y_{\nu 1} & 0 & 0 \\ 0 & 0 & y_1^\nu \\ 0 & -y_1^\nu & 0 \end{pmatrix}, \quad \mathbf{\Omega}_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & y_2^\nu e^{i\gamma_\nu} & 0 \\ 0 & 0 & y_2^\nu e^{i\gamma_\nu} \end{pmatrix},
$$
(15)

where all the parameters are real and positive and where we have taken $\{y_1^u, y_1^d, y_t, y_b, y_1^e, y_e\} \in \Re^+$ without loss of generality. All Dirac mass matrices satisfy

$$
\mathbf{M} = v_1 \mathbf{\Xi}_1 + v_2 \mathbf{\Xi}_2,
$$
(16)

where $\mathbf{\Xi} = \mathbf{\Gamma}, \mathbf{\Delta}, \mathbf{\Pi}$, and $\mathbf{\Omega}$. Each mass matrix has three complex parameters and possesses the feature of being diagonalizable by the same transformation that brings to diagonal form its individual Yukawa matrices. It is this property that guarantees the absence of FCNC at tree level, and it represents an explicit realization of the singular alignment ansatz [7].

Note how we end up, in the quark sector, with only eight real parameters, six of which correspond to the six quark masses while the other two, being complex phases, are forced to be nearly $\pm\pi/2$ due to the phenomenological observation of hierarchical fermion masses. We return to this point later.

The effective Majorana neutrino mass matrix can be computed from the standard seesaw formula, $\mathcal{M}_\nu = -\mathbf{M}_\nu \mathcal{M}_R^{-1} \mathbf{M}_\nu^T$, and is found to be diagonal,

$$
\mathcal{M}_\nu = - \begin{pmatrix} \frac{(y_{\nu 1} v_1)^2}{M_1} & 0 & 0 \\ 0 & \frac{(y_2^\nu)^2 v_2^2 - (y_1^\nu)^2 v_1^2}{M_2} & 0 \\ 0 & 0 & \frac{(y_2^\nu)^2 v_2^2 - (y_1^\nu)^2 v_1^2}{M_2} \end{pmatrix}.
$$
(17)

Here, $\mathcal{M}_R = \mathrm{diag}(M_1, M_2, M_2)$, which is a consequence of the D_3 flavor symmetry. The mass matrix has a mass degeneracy between the two neutrino states, $\nu_{L,2}$ and $\nu_{L,3}$, while, since it is diagonal, it does not contribute to the mixing.

Toward studying the phenomenology of this scenario, we note that complex matrices of the form

$$
\mathbf{m} = a\mathbb{I} + \begin{pmatrix} 0 & b \\ -b & 0 \end{pmatrix}
$$
(18)

are brought to diagonal shape via a maximal biunitary transformation

$$
\mathbf{u}_L = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \pm i \\ \pm i & 1 \end{pmatrix}, \quad \mathbf{u}_R = \begin{pmatrix} e^{i\gamma_1} & 0 \\ 0 & e^{i\gamma_2} \end{pmatrix} \cdot \mathbf{u}_L,
$$
(19)

that is,

$$
\mathbf{u}_L \cdot \mathbf{m} \cdot \mathbf{u}_R^\dagger = \begin{pmatrix} |a \mp ib| & 0 \\ 0 & |a \pm ib| \end{pmatrix},
$$
(20)

with $\gamma_1 = \arg(a \mp ib)$ and $\gamma_2 = \arg(a \pm ib)$ implying real and positive masses. The choice of the signs will depend on the ordering of the masses. The singular values of such a matrix $\mathbf{m}$ are given by

$$
m_{1,2} = |a \pm ib| = \sqrt{|a|^2 + |b|^2 \mp 2|a||b|\sin\rho},
$$
(21)

where $\rho = \arg(a) - \arg(b)$. Moreover, note that if the parameters a and b are taken to be real ($\rho = 0$), then the masses would be degenerate. In particular, if ρ is in the first quadrant, then $\rho \in [\mathrm{ArcSin}(\frac{m_2^2 - m_1^2}{m_2^2 + m_1^2}), \pi/2]$. The transformations $\rho \to \pm\rho + \pi$ and $\rho \to -\rho$ will lead to the same masses as ρ. Additionally, when the masses are hierarchical, $m_2 \gg m_1$, the allowed interval for ρ shrinks to $\rho \in [\pi/2 - 2m_1/m_2 + \mathcal{O}(m_1^3/m_2^3), \pi/2]$, essentially implying that $\rho \simeq \pm\pi/2$. We have chosen the off-diagonal Yukawas to be real and positive without loss of generality. Therefore, the complex phase of the diagonal Yukawas is found to be $\gamma_f \simeq \pm\pi/2$.

With these results in mind and looking at the form of the mass matrices of the charged fermions shown in Eqs. (14)–(16), we can extract the masses and mixing parameters,

$$
m_t = y_t v_2, \qquad m_b = y_b v_1, \qquad m_e = y_e v_1,
$$
$$
m_{c,u} = |y_2^u v_2 \pm y_1^u v_1|, \qquad m_{s,d} = |y_2^d v_2 \pm y_1^d v_1|,
$$
$$
m_{\tau,\mu} = |y_2^e v_2 \pm y_1^e v_1|,
$$
(22)

with the Majorana neutrino masses as given in Eq. (17). The quark Yukawa couplings can now be generically fixed to (defining $\tan\beta = v_2/v_1$)

$$
y_1^{u(d)} = \frac{m_{c(s)} - m_{u(d)}}{2v\cos\beta} \quad \text{and} \quad y_2^{u(d)} = \frac{m_{c(s)} + m_{u(d)}}{2v\sin\beta}.
$$
(23)

An alternative solution exists when one exchanges $y_1^f \leftrightarrow y_2^f$. Similarly, for the charged leptons,

$$
y_1^e = \frac{m_\tau - m_\mu}{2v\cos\beta} \quad \text{and} \quad y_2^e = \frac{m_\tau + m_\mu}{2v\sin\beta},
$$
(24)

and again it is possible to exchange $y_1^e \leftrightarrow y_2^e$.

Turning to fermion mixing, we can parametrize the relevant diagonalization matrices in terms of the complex rotation matrices $\mathbf{U}_{ij}(\theta, \phi)$, which are defined as

$$\mathbf{U}_{12}(\theta, \phi) = \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} & 0 \\ -\sin\theta e^{i\phi} & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (25)$$

and similarly for U_{13} and U_{23}. Then, the mixing matrices for the up and down quarks and for the charged leptons are simply given by

$$\mathbf{U}_L^u = \mathbf{U}_{12}(\pi/4, \pm\pi/2), \quad (26)$$

$$\mathbf{U}_L^d = \mathbf{U}_{12}(\pi/4, \pm\pi/2), \quad (27)$$

$$\mathbf{U}_L^e = \mathbf{U}_{23}(\pi/4, \pm\pi/2). \quad (28)$$

We obtain for the Cabibbo-Kobayashi-Maskawa (CKM) and Pontecorvo-Maki-Nakagawa-Sakata (PMNS) matrices,

$$\mathbf{V}_{\mathrm{CKM}}^{(0)} = \mathbf{U}_L^u(\mathbf{U}_L^d)^\dagger = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$\mathbf{U}_{\mathrm{PMNS}}^{(0)} = \mathbf{U}_L^e(\mathbf{U}_L^\nu)^\dagger = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \pm\frac{i}{\sqrt{2}} \\ 0 & \pm\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}, \quad (29)$$

where one of the signs of the PMNS matrix is realized when Eq. (24) applies and the opposite when $y_1^e \leftrightarrow y_2^e$.

This is, by enlarging $\mathbb{Z}_2$ to $\mathbb{Z}_3 \rtimes \mathbb{Z}_2$, we are now able to predict trivial mixing in the quark sector and a maximal atmospheric mixing angle in the lepton sector. There is also a maximal CP violation phase, which is unphysical if the angles θ_{12} and θ_{13} remain 0, but it will become important later. These features have to be understood as the dominant characteristics of this model at leading order. Its incompleteness points to further investigation on how the model should be extended; see Sec. IV.

A. FCNC

There are no tree level FCNCs since all Yukawa matrices are simultaneously diagonalizable. However, at the one-loop level, quantum corrections could induce misalignment in the different Yukawa matrices and generate FCNC. To check this effect, we employ the formulas obtained for a theory with N-Higgs doublets [14] and given in Appendix B. It is straightforward to see that for our particular model in all cases the one-loop renormalization group equations may only give place to flavor-conserving terms,[5]

$$16\pi^2 \mu \frac{d}{d\mu}\mathbf{\Xi}_a \propto \mathbf{\Xi}_a, \quad (a = 1, 2), \quad (30)$$

where μ is the renormalization scale and $\mathbf{\Xi} = \mathbf{\Gamma}, \mathbf{\Delta}, \mathbf{\Pi}$, and $\mathbf{\Omega}$. More details can be found in Appendix B.[6]

B. Nonuniversal charged fermion-scalar couplings

In order to find the couplings between the charged fermions and the Higgs scalars, we need to move both of them to their mass basis. In our case, only the latter are still in the symmetry adapted basis. We first introduce their notation,

$$\Phi_1 = \begin{pmatrix} \Phi_1^+ \\ v_1 + \frac{\phi_1^0 + i\varphi_1^0}{\sqrt{2}} \end{pmatrix}, \qquad \Phi_2 = \begin{pmatrix} \Phi_2^+ \\ v_2 + \frac{\phi_2^0 + i\varphi_2^0}{\sqrt{2}} \end{pmatrix}. \quad (31)$$

Since the scalar potential is CP-symmetric, there are states with definite CP-odd and CP-even quantum numbers. This allows one to write two independent mass matrices,

$$\mathbf{M}_{CP\text{-even}}^2 = \begin{pmatrix} 2v_2^2\lambda_2 & 2v_1v_2\lambda_{345} \\ 2v_1v_2\lambda_{345} & 2v_1^2\lambda_1 \end{pmatrix}, \quad (32)$$

where $\lambda_{345} = \lambda_3 + \lambda_4 + \lambda_5$, and

$$\mathbf{M}_{CP\text{-odd}}^2 = \begin{pmatrix} 2v_2^2\lambda_5 & -2v_1v_2\lambda_5 \\ -2v_1v_2\lambda_5 & 2v_1^2\lambda_5 \end{pmatrix}. \quad (33)$$

The first case can be brought to diagonal form by means of the orthogonal transformation

$$\begin{pmatrix} h \\ H \end{pmatrix} = \begin{pmatrix} c_\alpha & s_\alpha \\ -s_\alpha & c_\alpha \end{pmatrix}\begin{pmatrix} \phi_2^0 \\ \phi_1^0 \end{pmatrix}, \quad (34)$$

with $\tan 2\alpha = 2v_1v_2\lambda_{345}/(v_1^2\lambda_1 - v_2^2\lambda_2)$, while the second one by

$$\begin{pmatrix} G^0 \\ A \end{pmatrix} = \begin{pmatrix} c_\beta & s_\beta \\ -s_\beta & c_\beta \end{pmatrix}\begin{pmatrix} \varphi_2^0 \\ \varphi_1^0 \end{pmatrix}. \quad (35)$$

Here the latter angle of rotation satisfies $\tan\beta = v_2/v_1$, and G^0 is the neutral pseudo-Goldstone boson to be "eaten" by the Z mass. Similarly, one has for the charged scalars a mass matrix,

$$\mathbf{M}_{\mathrm{charged}}^2 = \begin{pmatrix} 2v_2^2(\lambda_4 + \lambda_5) & -2v_1v_2(\lambda_4 + \lambda_5) \\ -2v_1v_2(\lambda_4 + \lambda_5) & 2v_1^2(\lambda_4 + \lambda_5) \end{pmatrix}, \quad (36)$$

diagonalized by the same rotation as for the CP-odd neutral scalars,

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[5]As we are only interested in finding flavor-violating structures, we have not considered the quantum corrections to the VEVs.

[6]Due to the fact that we are employing the standard seesaw, FCNC with heavy sterile neutrinos are sufficiently suppressed and are not discussed here.

TABLE I.   Flavor universal Yukawa couplings of the charged fermions to the Higgs bosons h, H, A, and H^+ in the conventional 2HDMs with only $\mathbb{Z}_2$.

	Type			
	I	II	X	Y
$\xi_{q_u}^h$	c_α/s_β	c_α/s_β	c_α/s_β	c_α/s_β
$\xi_{q_d}^h$	c_α/s_β	$-s_\alpha/c_\beta$	c_α/s_β	$-s_\alpha/c_\beta$
ξ_ℓ^h	c_α/s_β	$-s_\alpha/c_\beta$	$-s_\alpha/c_\beta$	c_α/s_β
$\xi_{q_u}^H$	s_α/s_β	s_α/s_β	s_α/s_β	s_α/s_β
$\xi_{q_d}^H$	s_α/s_β	c_α/c_β	s_α/s_β	c_α/c_β
ξ_ℓ^H	s_α/s_β	c_α/c_β	c_α/c_β	s_α/s_β
$\xi_{q_u}^A$	$\cot\beta$	$\cot\beta$	$\cot\beta$	$\cot\beta$
$\xi_{q_d}^A$	$-\cot\beta$	$\tan\beta$	$-\cot\beta$	$\tan\beta$
ξ_ℓ^A	$-\cot\beta$	$\tan\beta$	$\tan\beta$	$-\cot\beta$
$\xi_{q_u}^{H^+}$	$\cot\beta$	$\cot\beta$	$\cot\beta$	$\cot\beta$
$\xi_{q_d}^{H^+}$	$\cot\beta$	$-\tan\beta$	$\cot\beta$	$-\tan\beta$
$\xi_\ell^{H^+}$	$\cot\beta$	$-\tan\beta$	$-\tan\beta$	$\cot\beta$

$$\begin{pmatrix} G^+ \\ H^+ \end{pmatrix} = \begin{pmatrix} c_\beta & s_\beta \\ -s_\beta & c_\beta \end{pmatrix} \begin{pmatrix} \Phi_2^+ \\ \Phi_1^+ \end{pmatrix}. \qquad (37)$$

The Yukawa Lagrangian related to the interactions to the neutral scalars is

$$-\mathcal{L}_Y \supset \sum_f \frac{m_f}{(246 \text{ GeV})} (\xi_h^f \bar{f} f h + \xi_H^f \bar{f} f H - i\xi_A^f \bar{f}\gamma_5 f A), \qquad (38)$$

while the one related to the interactions to the charged scalar is

$$-\mathcal{L}_Y \supset -H^+ \frac{[\mathbf{V}_{\text{CKM}}^{(0)}]_{ij}}{(246 \text{ GeV})} \bar{u}_i(m_i\xi_{q_u}^{H^+}\mathbf{P}_L + m_j\xi_{q_d}^{H^+}\mathbf{P}_R)d_j$$
$$- H^+ \frac{m_\ell}{(246 \text{ GeV})} \xi_\ell^{H^+} \bar{\nu}_{L,i}\ell_{R,j} + \text{H.c.}, \qquad (39)$$

with $\mathbf{P}_{L,R} = (1 \mp \gamma_5)/2$. In order to compare this expression to that appearing in conventional 2HDMs, we have assumed, for the moment, massless neutrinos.

We find that an important distinction between this framework with typical 2HDMs with NFC (see Table I) is that fermion couplings become nonuniversal; see Table II. Furthermore, those fermions which initially talk to both Higgs doublets ($\Phi_{1,2}$) have the following couplings:

$$f_\pm(\alpha, \beta, y_1, y_2) = \frac{y_2 c_\alpha \mp y_1 s_\alpha}{y_2 s_\beta \pm y_1 c_\beta},$$
$$g_\pm(\alpha, \beta, y_1, y_2) = \frac{y_2 s_\alpha \pm y_1 c_\alpha}{y_2 s_\beta \pm y_1 c_\beta}. \qquad (40)$$

TABLE II.   Flavor nonuniversal Yukawa couplings, cf. Eqs. (38) and (39), of the charged fermions to the Higgs bosons h, H, A, and H^+ in the 2HDM with $\mathbb{Z}_3 \times \mathbb{Z}_2$. We have grouped the couplings into different sets with equal or similar characteristics.

$\mathbb{Z}_3 \times \mathbb{Z}_2$ model	
ξ_t^h	c_α/s_β
$\xi_{b,e}^h$	$-s_\alpha/c_\beta$
$\xi_{\tau,s,c}^h$	$f_+(\alpha, \beta, y_1, y_2)$
$\xi_{\mu,d,u}^h$	$f_-(\alpha, \beta, y_1, y_2)$
ξ_t^H	s_α/s_β
$\xi_{b,e}^H$	c_α/c_β
$\xi_{\tau,s,c}^H$	$g_+(\alpha, \beta, y_1, y_2)$
$\xi_{\mu,d,u}^H$	$g_-(\alpha, \beta, y_1, y_2)$
ξ_t^A	$\cot\beta$
$\xi_{b,e}^A$	$\tan\beta$
$\xi_{\tau,s,c}^A$	$f_+(\beta, \beta, y_1, y_2)$
$\xi_{\mu,d,u}^A$	$f_-(\beta, \beta, y_1, y_2)$
$\xi_t^{H^+}$	$\cot\beta$
$\xi_{b,e}^{H^+}$	$-\tan\beta$
$\xi_{\tau,s}^{H^+}$	$-f_+(\beta, \beta, y_1, y_2)$
$\xi_{\mu,d}^{H^+}$	$-f_-(\beta, \beta, y_1, y_2)$
$\xi_c^{H^+}$	$f_+(\beta, \beta, y_1, y_2)$
$\xi_u^{H^+}$	$f_-(\beta, \beta, y_1, y_2)$

Note that cancellations can occur, which could make $f_\pm$ or $g_\pm$ vanish. The observed hierarchy in the fermion masses, $m_3 \gg m_2 \gg m_1$, may be applied to Eq. (40) to obtain the approximate relations

$$f_\pm \approx \frac{m_2}{2m_{2,1}}\left(\frac{c_\alpha}{s_\beta} \mp \frac{s_\alpha}{c_\beta}\right), \qquad g_\pm \approx \frac{m_2}{2m_{2,1}}\left(\frac{s_\alpha}{s_\beta} \pm \frac{c_\alpha}{c_\beta}\right). \qquad (41)$$

For small or large $\tan\beta$, both relations reduce to $f_- \approx \frac{m_2}{m_1} f_+$ and $g_- \approx \frac{m_2}{m_1} g_+$, meaning that the fermion with a lighter mass ($m_1 < m_2$) has an $\mathcal{O}(10-100)$ enhancement in its coupling to the scalars compared to the heavier one. Moreover, for $\alpha \to \beta - \pi/2$, all couplings to the 125 GeV scalar state, h, including the new functions $f_\pm$, are automatically made SM-like, i.e., $\xi_{q_u,q_d,\ell}^h \to 1$, while the other couplings end up only depending on $\tan\beta$. A further implication of the alignment limit is that the coupling of the CP-even state H with the W and Z bosons becomes null.

The resulting couplings have been grouped into different sets corresponding to similar characteristics in Table II. This also holds for couplings which depend on the Yukawa parameters (and therefore, to the different fermion masses), like $\xi_f^H = g_+(\alpha, \beta, y_1^f, y_2^f)$ for $f = \tau, s, c$. As they have the same functional dependence, they are grouped under the category $\xi_{\tau,s,c}^H$.
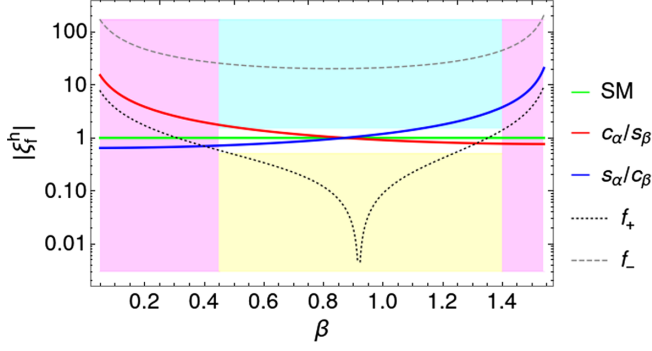
FIG. 1. Effective couplings to the 125 GeV scalar (h), as a function of β, in any of the 2HDM types and the $\mathbb{Z}_3 \rtimes \mathbb{Z}_2$ model. We considered $\alpha = 0.7$. The blue and red continuous lines represent any of the conventional 2HDMs couplings with NFC, whereas the black (dotted) and gray (dashed) lines the new couplings of our model. The left and right (magenta) shaded regions depict the small and large $\tan \beta$ limits, while the upper (cyan) and lower (yellow) regions the philic ($|\xi_f^h| > 1.5$) and phobic ($|\xi_f^h| < 0.5$) limits, respectively. The middle (green) line is the SM limit. Note that the funnel is a consequence of plotting the absolute values of the coupling ξ_f^h.

In general, conventional 2HDMs with NFC have a moderate behavior for moderate values of $\tan \beta$. Their main differences appear in the small (or large) $\tan \beta$ limits. For example, take the couplings to the charged scalar, H^+. In the type-II scenario, its coupling to $t\bar{b}$ is large (philic) at large $\tan \beta$, whereas in the same limit, it is always small (phobic) for the type-I case. In contrast to this typical situation, the $\mathbb{Z}_3 \rtimes \mathbb{Z}_2$ model shows already at moderate values of $\tan \beta$ either phobic or philic behavior; see Figs. 1–3. Also, it can be seen that for a given value of
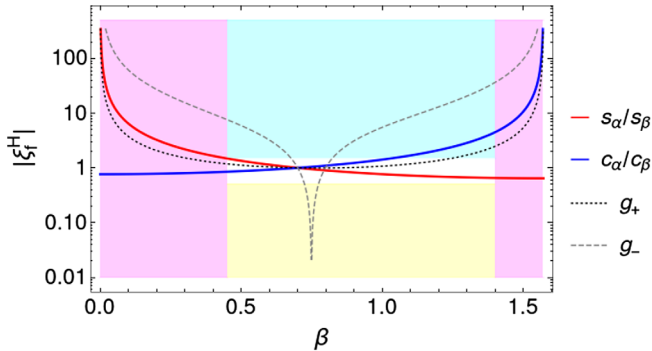

FIG. 2. Effective couplings to the heavy CP-even scalar (H), as a function of β, in any of the 2HDM types and the $\mathbb{Z}_3 \rtimes \mathbb{Z}_2$ model. We considered $\alpha = 0.7$. The blue and red continuous lines represent any of the conventional 2HDMs couplings with NFC, whereas the black (dotted) and gray (dashed) lines the new couplings of our model. The left and right (magenta) shaded regions depict the small and large $\tan \beta$ limits, while the upper (cyan) and lower (yellow) regions the philic ($|\xi_f^H| > 1.5$) and phobic ($|\xi_f^H| < 0.5$) limits, respectively. Note that the funnel is a consequence of plotting the absolute values of the coupling ξ_f^H.
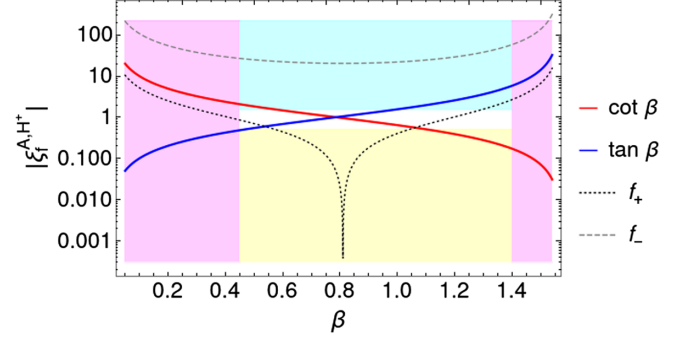

FIG. 3. Effective couplings to the neutral CP-odd (A) and charged (H^+) scalars, as a function of β, in any of the 2HDM types and the $\mathbb{Z}_3 \rtimes \mathbb{Z}_2$ model. The blue and red continuous lines represent any of the conventional 2HDMs couplings with NFC, whereas the black (dotted) and gray (dashed) lines the new couplings of our model. The left and right (magenta) shaded regions depict the small and large $\tan \beta$ limits, while the upper (cyan) and lower (yellow) regions the philic ($|\xi_f^{A,H^+}| > 1.5$) and phobic ($|\xi_f^{A,H^+}| < 0.5$) limits, respectively. Note that the funnel is a consequence of plotting the absolute values of the coupling ξ_f^{A,H^+}.

β, a given fermion may completely decouple from one of the four scalars and accidentally become inert to that scalar.

IV. COMPLETING MIXING AS A GUIDE FOR NEW PHYSICS

While possessing attractive features, the minimal $\mathbb{Z}_3 \rtimes \mathbb{Z}_2$ model presented so far does not fully reproduce the fermion mixing and masses. We take this "incomplete mixing" as a hint pointing toward new physics. In the quark sector, the vanishing mixing points to the introduction of a $\dim > 4$ operator that generates small corrections. In a similar fashion, the Majorana nature of neutrinos could allow dim-4 operators and therefore large contributions to mixing. The simplest possibility is obtained by introducing a real singlet scalar field, which is assumed to transform under D_3 as a doublet,

$$\eta \sim \mathbf{2}. \tag{42}$$

This field acquires a VEV,

$$\langle \eta \rangle = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}. \tag{43}$$

Note that by introducing η and its nonrenormalizable interactions we have allowed at tree level the appearance of FCNC. We may assume a large mass and later decouple it from the theory. While perturbing 2HDMs is typically done to explain anomalies [15,16], here we need it to complete fermion mixing. Note however that our approach uses an explicit model, i.e., the symmetry and field content

of our model determine the type of Yukawa matrices to be added. At last, notice that integrating out the singlet scalar means that our theory has become a 2HDM of type III. We will later demonstrate that the model can be easily made flavor safe. An explicit numerical example will be provided in Sec. IV D.

A. Quark mixing

In the quark sector, the nonrenormalizable dim-5 operators leading to a correct CKM matrix requires a complete UV formulation to be realized. As a simple example that serves as a plausibility argument, consider the following dim-5 effective interactions, invariant under the SM gauge group and the flavor symmetry,

$$
-\Delta\mathcal{L}_Y^Q = \frac{g_1^d}{\Lambda}[\bar{Q}_{L,D}\eta]_- d_{R,3}\Phi_2 + \frac{g_2^d}{\Lambda}[\bar{Q}_{L,D}\eta]_+ d_{R,3}\Phi_1
$$
$$
+ \frac{g_3^d}{\Lambda}\bar{Q}_{L,3}[d_{R,D}\eta]_+\Phi_2 + \frac{g_4^d}{\Lambda}\bar{Q}_{L,3}[d_{R,D}\eta]_-\Phi_1
$$
$$
+ \frac{g_5^d}{\Lambda}[\bar{Q}_{L,D}d_{R,D}\eta]_+\Phi_2 + \frac{g_6^d}{\Lambda}[\bar{Q}_{L,D}d_{R,D}\eta]_-\Phi_1
$$
$$
+ \text{H.c.} \tag{44}
$$

These contributions give rise to small corrections in quark mixing through perturbations to the down quark mass matrix of the form

$$
\Delta\mathbf{M}_d = \begin{pmatrix} \epsilon_1 & \epsilon_2 & \epsilon_3 \\ \epsilon_2 & -\epsilon_1 & \epsilon_4 \\ \epsilon_3' & \epsilon_4' & 0 \end{pmatrix}, \tag{45}
$$

i.e., the six new parameters g_i^d, the scale of the dimension-five operators Λ, and the two new VEVs $\langle\eta_i\rangle = \omega_i$ can be absorbed intofour4 parameters ϵ_i in the down quark mass matrix, which are enough to perturb our initial identity matrix and reproduce the CKM mixing. These effective operators can be realized in a UV-complete model just by adding a vectorlike pair of colored particles with the same gauge quantum numbers as the right-handed down quarks.

In the basis where $\mathbf{M}_u$ and $\mathbf{M}_d$ are diagonal, the perturbation matrix becomes

$$
\Delta\tilde{\mathbf{M}}_d = \begin{pmatrix} 0 & -(\epsilon_1 - i\epsilon_2) & \frac{\epsilon_3 - i\epsilon_4}{\sqrt{2}} \\ \epsilon_1 + i\epsilon_2 & 0 & \frac{-i(\epsilon_3 + i\epsilon_4)}{\sqrt{2}} \\ \frac{i(\epsilon_5 + i\epsilon_6)}{\sqrt{2}} & \frac{-(\epsilon_5 - i\epsilon_6)}{\sqrt{2}} & 0 \end{pmatrix}. \tag{46}
$$

Recall that here we still have trivial quark mixing. In order to obtain a realistic mixing scenario, the perturbations need to be sufficiently small compared to the bottom quark mass but large enough compared to the down and strange quark masses. This implies that the Yukawa parameters $y_{1,2}^d$ are no

longer completely satisfying Eq. (23). Through a qualitative analysis, we find that for

$$
\tilde{\mathbf{M}}_d = \text{diag}(|y_2^d|v_2 - y_1^d v_1, |y_2^d|v_2 + y_1^d v_1, y_b v_1) + \Delta\tilde{\mathbf{M}}_d
$$
$$
\sim \begin{pmatrix} m_d & \lambda m_s & \lambda^3 m_b \\ \lambda m_s & m_s & \lambda^2 m_b \\ - & - & m_b \end{pmatrix}, \tag{47}
$$

where $\lambda \simeq 0.225$, it is possible to fully reproduce quark mixing without introducing unacceptably large amounts of flavor violation at tree level. The (3,1) and (3,2) matrix elements could be taken as zero or of the same order that their transpose counterparts. On the other hand, all entries are given up to $\mathcal{O}(1)$ complex factors. It is interesting to note that Eq. (47) shows an approximate $U(2)$ flavor symmetry for the first two generations, $m_b \gg m_{d,s}$ (analogously for the up-type quarks). The above resulting mass matrix is a similar realization of the "flavorful" 2HDMs investigated in Ref. [10] wherein Yukawa couplings, for all charged fermions, are chosen as to approximately preserve a $U(2)^5$ flavor symmetry acting on the first two generations.

Alternatively, we could have introduced perturbations through the up-type quarks; however, to reproduce the CKM mixing would have required a larger modification of the initial Yukawa parameters, $|y_2^u|$ and y_1^u, by at least 1 order of magnitude. This may be easily appreciated by considering that a perturbation to the 1–2 sector of the size $\sqrt{m_1 m_2}$ is enough in the down quark sector, $\sqrt{m_d m_s} \sim 10$ MeV, to generate Cabibbo mixing, while for the up-type quarks it would still require an additional order of magnitude, $\mathcal{O}(10)\sqrt{m_u m_c} \sim 100$ MeV, plus some extra tuning in the Yukawa parameters to get the correct light quark masses, m_u and m_c.

B. Lepton mixing

In the lepton sector, the dominant perturbation contributions come through the right-handed neutrinos,

$$
-\Delta\mathcal{L}_Y^N = \frac{1}{2}g_1^N \bar{N}_{R,1}^c[\eta N_{R,D}]_- + g_2^N[\eta[\bar{N}_{R,D}^c N_{R,D}]_2]_+ + \text{H.c.}, \tag{48}
$$

producing

$$
\Delta\mathcal{M}_R = \begin{pmatrix} 0 & \delta_{N1} & r\delta_{N1} \\ \delta_{N1} & r\delta_{N2} & \delta_{N2} \\ r\delta_{N1} & \delta_{N2} & -r\delta_{N2} \end{pmatrix}, \tag{49}
$$

where we have defined $r = \omega_1/\omega_2$, $\delta_{N1} = g_1^N\omega_2$ and $\delta_{N2} = g_2^N\omega_1$, i.e., we can rewrite the four new parameters given by g_1^N, g_2^N, ω_1, and ω_2 in terms of only three: r, δ_{N1}, and δ_{N2}.

The charged lepton contribution remains untouched by the addition of the scalar η and is given by Eq. (27). Once we consider the contributions to the mass matrix of the right-handed neutrinos shown in Eq. (49), the initial lepton mixing given by Eq. (29) gets modified. If the Yukawa couplings appearing in the neutrino mass matrix are taken real, then we have

$$\mathbf{U}_L^e = \mathbf{U}_{23}(\pi/4, \pm\pi/2),$$
$$\mathbf{U}_L^\nu = \mathbf{O}_{23}(\theta_{23}^\nu)\mathbf{O}_{13}(\theta_{13}^\nu)\mathbf{O}_{12}(\theta_{12}^\nu), \quad (50)$$

where $\mathbf{O}_{ij}(\theta)$ is the usual rotation matrix in the (i, j) plane. It can be shown that

$$\mathbf{U}_{23}(\pi/4, \pm\pi/2)\mathbf{O}_{23}(\theta_{23}^\nu) = \mathbf{P} \cdot \mathbf{U}_{23}(\pi/4, \mp\pi/2), \quad (51)$$

where $\mathbf{P}$ is a diagonal unitary matrix which is unphysical. Therefore, if the neutrino sector is real, we obtain *cobimaximal mixing* [17] with $\theta_{23} = \pi/4$ and $\delta_{CP} = \pm\pi/2$ in the lepton sector. While the sign of δ_{CP} is not fixed, data seem to favor the negative option [18]. Note that this is a particular case of the general theorem derived in Ref. [19], i.e., if cobimaximal mixing is present in the charged lepton sector and the neutrino sector is real, then the full PMNS matrix is also cobimaximal. In particular, the full lepton mixing parameters are given by

$$\theta_{12} = \theta_{12}^\nu, \quad \theta_{13} = \theta_{13}^\nu, \quad \theta_{23} = \pi/4,$$
$$\delta_{CP} = \pm\pi/2, \quad \phi_{12} = 0, \quad \pi/2 = \phi_{13}, \quad (52)$$

irrespective of θ_{23}^ν. That is, the large hierarchy between the charged lepton masses coupled with the assumption that the neutrino Yukawas are real leads to cobimaximal mixing, i.e., maximal atmospheric mixing angle and $\delta_{CP} = \pm\pi/2$. For the other two mixing angles θ_{12} and θ_{13}, no predictions can be made, but the parameters can be chosen in such a way that they lie inside the experimental constraints. Moreover, the Majorana phases relevant for neutrinoless double beta decay maintain their *CP*-conserving values.

We remark that of course there is no need to assume the neutrino sector to remain real; in the most general scenario with complex parameters, there is enough freedom to fit all the mixing parameters. The assumption that the neutrino Yukawas are real, while the charged lepton Yukawas are forced to be complex due to hierarchical masses, may seem *ad-hoc* but can actually be justified in many different scenarios. For example, in Ref. [20], the author derives a general loop mechanism in which the neutrino mass matrix is complex but diagonalized by a real orthogonal matrix. This same mechanism could be applied here by changing the type I seesaw neutrino mass generation by an inverted loop seesaw mediated by three real scalars. Then, the cobimaximal nature of the PMNS would remain. Another

option would be to explicitly impose a remnant *CP* symmetry in the neutrino sector.

It is worth to note that our scenario is minimal and quite simple, yet it leads to such a restricted scenario. The SM symmetry group is extended by just D_3 while the particle content is enlarged by an extra Higgs gauge doublet and an D_3 doublet η which is a gauge singlet.

C. The scalar potential

The most general scalar potential invariant under $\mathbb{Z}_3 \rtimes \mathbb{Z}_2$ is

$$V = V_{2\text{HDM}}^{\mathbb{Z}_2} + V_\eta^{\mathbb{Z}_3 \rtimes \mathbb{Z}_2} + V_{\Phi\eta}^{\mathbb{Z}_3 \rtimes \mathbb{Z}_2}, \quad (53)$$

with the first term given in Eq. (4) and

$$V_\eta^{\mathbb{Z}_3 \rtimes \mathbb{Z}_2} = \frac{\mu_\eta^2}{2}[\eta\eta]_+ + \frac{\lambda_{\eta 1}}{2}[\eta\eta]_+^2 + \frac{\lambda_{\eta 2}}{2}[[\eta\eta]_2[\eta\eta]_2]_+,$$
$$V_{\Phi\eta}^{\mathbb{Z}_3 \rtimes \mathbb{Z}_2} = [\zeta_1(\Phi_1^\dagger\Phi_1) + \zeta_2(\Phi_2^\dagger\Phi_2)](\eta\eta)_+, \quad (54)$$

where $[\eta\eta]_k$ represents one of the three possible choices ($\mathbf{1}_+$, $\mathbf{1}_-$, $\mathbf{2}$), all couplings are real (due to hermiticity) ensuring a *CP*-conserving potential and we have omitted those terms involving $[\eta\eta]_-$ as it is zero. This potential has an extra Goldstone boson due to the fact that $[\eta\eta]_+ = \eta_1^2 + \eta_2^2$ is equivalent to $(\eta_1 - i\eta_2)(\eta_1 + i\eta_2)$ and $[[\eta\eta]_2[\eta\eta]_2]_+ = ([\eta\eta]_+)^2$. Then, Eq. (54) is accidentally invariant under a global $U(1)$ symmetry originated from the two components of the flavor doublet scalar, η. To avoid its appearance, we softly break the accidental symmetry by introducing

$$V_{\text{soft}} = \frac{\mu_1^2}{2}\eta_1^2 + \frac{\mu_2^2}{2}\eta_2^2 - \mu_{12}^2\eta_1\eta_2. \quad (55)$$

Additionally, the fact that the heavy quark masses are simply given by $m_t \simeq y_t v_2$ and $m_b \simeq y_b v_1$ naturally points to having order one Yukawas and hierarchical VEVs in the range

$$v_2 \simeq v \quad \text{and} \quad v_1 \sim [1, 10] \text{ GeV}, \quad (56)$$

meaning that $\tan\beta \in (10, 100)$. To create such a hierarchy while maintaining all scalar masses around the electroweak scale, we need to consider $m_{22}^2 < 0$, $m_{11}^2 > 0$ and introduce the soft-breaking term

$$-m_{12}^2(\Phi_1^\dagger\Phi_2 + \text{H.c.}), \quad (57)$$

where $m_{12} \sim \mathcal{O}(10)$ GeV. By assuming $|m_{11}|, |m_{22}| \sim 100$ GeV, a straightforward calculation then leads to

$$v_2 \simeq \sqrt{\frac{-m_{22}^2}{\lambda_2}} \quad \text{and} \quad v_1 \simeq \frac{m_{12}^2 v_2}{m_{11}^2 + \lambda_{345} v_2^2}. \quad (58)$$

The smallness of v_1 is thus natural as one recovers a larger symmetry when setting it to zero.

The minimization conditions read

$$-m_{11}^2 = \lambda_1 v_1^2 + \lambda_{345} v_2^2 + (w_1^2 + w_2^2)\zeta_2 - m_{12}^2 \tan\beta,$$
$$-m_{22}^2 = \lambda_2 v_2^2 + \lambda_{345} v_1^2 + 2(w_1^2 + w_2^2)\zeta_1 - m_{12}^2 \cot\beta,$$
$$-\mu_\eta^2 = 2(w_1^2 + w_2^2)\bar{\lambda} + 2v_1^2\zeta_2 + 2v_2^2\zeta_1 + \mu_2^2 - \frac{w_1}{w_2}\mu_{12}^2,$$
$$-\mu_\eta^2 = 2(w_1^2 + w_2^2)\bar{\lambda} + 2v_1^2\zeta_2 + 2v_2^2\zeta_1 + \mu_1^2 - \frac{w_2}{w_1}\mu_{12}^2,$$

where $\bar{\lambda} = \lambda_{\eta 1} + \lambda_{\eta 2}$. The latter two conditions can only be met if

$$\mu_{12}^2 = -\frac{w_1 w_2}{w_1^2 - w_2^2}(\mu_1^2 - \mu_2^2). \quad (59)$$

The general expressions for the squared mass matrices are given in Appendix C.

In order to decouple η from the 2HDM, we assume its mass (or VEV) to be large enough and $\zeta_{1,2} \to 0$. Then, for the full potential, $V + V_{\text{soft}}$, to be bounded from below, we require the well-known relations

$$\lambda_1 \geq 0, \quad \lambda_2 \geq 0, \quad \lambda_3 \geq -\sqrt{\lambda_1\lambda_2},$$
$$\lambda_3 + \lambda_4 - |\lambda_5| \geq -\sqrt{\lambda_1\lambda_2}, \quad (60)$$

while for the new contributions

$$\lambda_{\eta 1} \geq 0 \quad \text{and} \quad \lambda_{\eta 2} \geq 0, \quad (61)$$

which all are sufficient and necessary conditions.

D. Numerical example

In the following, we give a numerical example of how the perturbations brought by the addition of η modify our initial 2HDM setup. We assign a best-fit value to our set of complex parameters $\{\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4, \epsilon_5, \epsilon_6\}$ by virtue of a χ^2 fit to the three down quark masses and four quark mixing parameters,

$$\chi^2 = \sum_{f=d,s,b} \frac{(m_f^{\text{th}} - m_f^{\text{exp}})^2}{\sigma_f^2} + \frac{(|\mathbf{V}_{12}^{\text{th}}| - |\mathbf{V}_{12}^{\text{CKM}}|)^2}{\sigma_{12}^2}$$
$$+ \frac{(|\mathbf{V}_{23}^{\text{th}}| - |\mathbf{V}_{23}^{\text{CKM}}|)^2}{\sigma_{23}^2} + \frac{(|\mathbf{V}_{13}^{\text{th}}| - |\mathbf{V}_{13}^{\text{CKM}}|)^2}{\sigma_{13}^2}$$
$$+ \frac{(J_q^{\text{th}} - J_q^{\text{exp}})^2}{\sigma_J^2}, \quad (62)$$

where the value of the masses is taken at the Z boson mass scale, M_Z, using the `RunDec` package [21],

$$m_d^{\text{exp}}(M_Z) = 0.0027^{+0.0003}_{-0.0002} \text{ GeV},$$
$$m_s^{\text{exp}}(M_Z) = 0.055^{+0.004}_{-0.002} \text{ GeV},$$
$$m_b^{\text{exp}}(M_Z) = 2.86 \pm 0.02 \text{ GeV} \quad (63)$$

and

$$|\mathbf{V}_{12}^{\text{CKM}}| = 0.22452 \pm 0.00044,$$
$$|\mathbf{V}_{23}^{\text{CKM}}| = 0.04214 \pm 0.00076,$$
$$|\mathbf{V}_{13}^{\text{CKM}}| = 0.00365 \pm 0.00012,$$
$$J_q^{\text{exp}} = (3.18 \pm 0.15) \times 10^{-5}, \quad (64)$$

as shown in the most recent global fit from the particle data group [22]. As a proof of principle, we consider a minimal scenario with the least number of parameters. We assume all of them real except for ϵ_4 which we consider it as purely imaginary and set $\epsilon_{5,6} = 0$. Also, we allow for small variations in the initial down quark Yukawa couplings appearing in Eq. (22).

The following best-fit values:

$$\epsilon_1 = 4.4634 \text{ MeV}, \qquad \epsilon_2 = 12.1428 \text{ MeV},$$
$$\epsilon_3 = 103.6520 \text{ MeV}, \qquad \epsilon_4 = -i60.9786 \text{ MeV} \quad (65)$$

reproduce the down quark masses and the observed CKM mixing at the 1σ level with a quality of fit of $\chi^2_{\text{d.o.f.}} = 0.49$.

Besides their role in mixing, the introduction of perturbations has also brought FCNC at tree level. We now show how the size of the contributions is still sufficiently small. Through the best-fit values, we calculate the unitary transformations for the left- and right-handed fields. With them, the corresponding down quark Yukawa matrices, in the mass basis, are

$$\tilde{\mathbf{\Gamma}}_1 \lesssim \begin{pmatrix} 10^{-4} & 10^{-4} & 10^{-7} \\ 10^{-4} & 10^{-3} & 10^{-5} \\ 10^{-5} & 10^{-5} & 10^{-1} \end{pmatrix} + i \begin{pmatrix} 10^{-9} & 10^{-7} & 10^{-7} \\ 10^{-7} & 10^{-8} & 10^{-6} \\ 10^{-6} & 10^{-5} & 10^{-9} \end{pmatrix},$$
$$\tilde{\mathbf{\Gamma}}_2 \lesssim \begin{pmatrix} 10^{-4} & 10^{-5} & 10^{-8} \\ 10^{-5} & 10^{-4} & 10^{-7} \\ 10^{-6} & 10^{-6} & 10^{-9} \end{pmatrix} + i \begin{pmatrix} 10^{-10} & 10^{-8} & 10^{-8} \\ 10^{-8} & 10^{-8} & 10^{-8} \\ 10^{-7} & 10^{-6} & 10^{-10} \end{pmatrix},$$
$$(66)$$

where we have assumed $v_1 \sim 10 m_b$ and $v_2 \sim m_t$ to estimate the upper bounds and which are all consistent with those presented in Refs. [10,23]. There are in fact three different scenarios from which Eq. (66) represents one of them. As all the independent perturbations defined in Eq. (45) originate from both Higgs doublets, Φ_1 and Φ_2, we can define three different benchmark scenarios as follows: all

the perturbations come from (i) Φ_1, (ii) Φ_2, or (iii) both. Our choice in Eq. (66) depicts the first case. We left for future work a detailed study of the differences between this approach and the conventional 2HDMs.

V. CONCLUSIONS

We have considered a new class of 2HDM where the conventional $\mathbb{Z}_2$ symmetry, by which FCNC can be naturally avoided, has been enlarged to $\mathcal{F} \rtimes \mathbb{Z}_2$ such that symmetry constrains the Yukawa sector but goes unnoticed by the scalar sector. In particular, we have shown that the minimal case with $\mathbb{Z}_3 \rtimes \mathbb{Z}_2$ is able to provide trivial quark and maximal atmospheric mixing at leading order. A further implication to this class of models is that couplings between the fermions to the scalars are nonuniversal, compared to the conventional types where couplings are universal. At last, we have taken the incompleteness of fermion mixing as a hint pointing toward new physics. To this end, we have included two real scalar gauge singlets which transform as a flavor doublet and are later integrated out by assuming them to be properly heavy. We have shown that quark mixing can be set in agreement with the latest global fits while the lepton mixing can become cobimaximal, i.e., maximal atmospheric mixing and maximal CP violation. We have treated the introduction of the real scalars as a new way of adding perturbations to 2HDMs in a systematic manner by demanding them to be invariant under the flavor symmetry. In general, these additions have the effect of breaking flavor conservation and tree level FCNC, mediated by the neutral scalars, are induced. However, the size of the contributions remains sufficiently small thanks to the approximate presence of a $U(2)^3$ global flavor symmetry in the light quark sector.

APPENDIX A: PRODUCT RULES OF $D_3 \simeq \mathbb{Z}_3 \rtimes \mathbb{Z}_2$

D_3 is the smallest non-Abelian discrete symmetry group. It describes the symmetrical properties of an equilateral triangle. It has three irreducible representations: two singlets, $\mathbf{1}_+$ and $\mathbf{1}_-$, and one doublet, $\mathbf{2}$. Their product rules are

$$\mathbf{1}_+ \times \mathbf{1}_+ = \mathbf{1}_+, \quad \mathbf{1}_- \times \mathbf{1}_- = \mathbf{1}_+, \quad \mathbf{1}_- \times \mathbf{1}_+ = \mathbf{1}_-,$$
$$\mathbf{1}_+ \times \mathbf{2} = \mathbf{2}, \quad \mathbf{1}_- \times \mathbf{2} = \mathbf{2}, \quad \mathbf{2} \times \mathbf{2} = \mathbf{1}_+ + \mathbf{1}_- + \mathbf{2}. \quad \text{(A1)}$$

In particular, the tensor product of two doublets, $\mathbf{a} = (a_1, a_2)^T$ and $\mathbf{b} = (b_1, b_2)^T$, is explicitly given as

$$\mathbf{a} \times \mathbf{b} = (a_1 b_1 + a_2 b_2)_{\mathbf{1}_+} + (a_1 b_2 - a_2 b_1)_{\mathbf{1}_-}$$
$$+ \begin{pmatrix} a_1 b_2 + a_2 b_1 \\ a_1 b_1 - a_2 b_2 \end{pmatrix}_{\mathbf{2}}. \quad \text{(A2)}$$

APPENDIX B: RENORMALIZATION GROUP EQUATIONS

In a model with N Higgs doublets, wherein all Higgses couple to all fermions, the fermion mass matrices are expressed as a linear combination of N Yukawa matrices times a VEV. Given an initial setup, the one-loop renormalization group equations (RGEs) tell us how stable are the initial mass matrices at higher scales and if new flavor structures may appear, giving rise to misalignments. The one-loop RGE has been calculated in Ref. [14] and reads

$$16\pi^2 \mu \frac{d}{d\mu} \mathbf{\Gamma}_k = a_{\mathbf{\Gamma}} \mathbf{\Gamma}_k$$
$$+ \sum_{l=1}^{N} [3\text{Tr}(\mathbf{\Gamma}_k \mathbf{\Gamma}_l^\dagger + \mathbf{\Delta}_k^\dagger \mathbf{\Delta}_l) + \text{Tr}(\mathbf{\Pi}_k \mathbf{\Pi}_l^\dagger)] \mathbf{\Gamma}_l$$
$$+ \sum_{l=1}^{N} (-2\mathbf{\Delta}_l \mathbf{\Delta}_k^\dagger \mathbf{\Gamma}_l + \mathbf{\Gamma}_k \mathbf{\Gamma}_l^\dagger \mathbf{\Gamma}_l)$$
$$+ \frac{1}{2} \sum_{l=1}^{N} (\mathbf{\Delta}_l \mathbf{\Delta}_l^\dagger \mathbf{\Gamma}_k + \mathbf{\Gamma}_l \mathbf{\Gamma}_l^\dagger \mathbf{\Gamma}_k), \quad \text{(B1)}$$

$$16\pi^2 \mu \frac{d}{d\mu} \mathbf{\Delta}_k = a_{\mathbf{\Delta}} \mathbf{\Delta}_k$$
$$+ \sum_{l=1}^{N} [3\text{Tr}(\mathbf{\Delta}_k \mathbf{\Delta}_l^\dagger + \mathbf{\Gamma}_k^\dagger \mathbf{\Gamma}_l) + \text{Tr}(\mathbf{\Pi}_k \mathbf{\Pi}_l^\dagger)] \mathbf{\Delta}_l$$
$$+ \sum_{l=1}^{N} (-2\mathbf{\Gamma}_l \mathbf{\Gamma}_k^\dagger \mathbf{\Delta}_l + \mathbf{\Delta}_k \mathbf{\Delta}_l^\dagger \mathbf{\Delta}_l)$$
$$+ \frac{1}{2} \sum_{l=1}^{N} (\mathbf{\Gamma}_l \mathbf{\Gamma}_l^\dagger \mathbf{\Delta}_k + \mathbf{\Delta}_l \mathbf{\Delta}_l^\dagger \mathbf{\Delta}_k), \quad \text{(B2)}$$

$$16\pi^2 \mu \frac{d}{d\mu} \mathbf{\Pi}_k = a_{\mathbf{\Pi}} \mathbf{\Pi}_k$$
$$+ \sum_{l=1}^{N} [3\text{Tr}(\mathbf{\Delta}_k \mathbf{\Delta}_l^\dagger + \mathbf{\Gamma}_k^\dagger \mathbf{\Gamma}_l) + \text{Tr}(\mathbf{\Pi}_k \mathbf{\Pi}_l^\dagger)] \mathbf{\Pi}_l$$
$$+ \sum_{l=1}^{N} \left(\mathbf{\Pi}_k \mathbf{\Pi}_l^\dagger \mathbf{\Pi}_l + \frac{1}{2} \mathbf{\Pi}_l \mathbf{\Pi}_l^\dagger \mathbf{\Pi}_k \right), \quad \text{(B3)}$$

where we have followed the notation introduced in [14]. Here μ denotes the renormalization scale and

$$a_\Gamma = -8g_s^2 - \frac{9}{4}g^2 - \frac{5}{12}g'^2,$$

$$a_\Delta = -8g_s^2 - \frac{9}{4}g^2 - \frac{17}{12}g'^2,$$

$$a_\Pi = -\frac{9}{4}g^2 - \frac{15}{4}g'^2, \tag{B4}$$

where g_s, g, and g' are the gauge couplings of the SM gauge group, $SU(3)_C \times SU(2)_L \times U(1)_Y$, respectively.

APPENDIX C: SQUARED MASS MATRICES

The squared mass matrix for the *CP*-even scalars reads

$$\mathbf{M}^2_{CP\text{-even}} = \begin{pmatrix} \mathbf{m}^2_{\phi\phi} & \mathbf{m}^2_{\phi\eta} \\ \mathbf{m}^2_{\phi\eta} & \mathbf{m}^2_{\eta\eta} \end{pmatrix}, \tag{C1}$$

where

$$\mathbf{m}^2_{\phi\phi} = \begin{pmatrix} 2v_2^2\lambda_2 + m_{12}^2\cot\beta & 2v_1v_2\lambda_{345} - m_{12}^2 \\ 2v_1v_2\lambda_{345} - m_{12}^2 & 2v_1^2\lambda_1 + m_{12}^2\tan\beta \end{pmatrix}, \tag{C2}$$

$$\mathbf{m}^2_{\phi\eta} = \begin{pmatrix} 2\sqrt{2}\zeta_1 v_2 w_1 & 2\sqrt{2}\zeta_2 v_1 w_1 \\ 2\sqrt{2}\zeta_1 v_2 w_2 & 2\sqrt{2}\zeta_2 v_1 w_2 \end{pmatrix}, \tag{C3}$$

$$\mathbf{m}^2_{\eta\eta} = \begin{pmatrix} 4\bar{\lambda}w_1w_2 - \frac{w_1w_2(\mu_1^2-\mu_2^2)}{w_2^2-w_1^2} & 4\bar{\lambda}w_2^2 + \frac{w_1^2(\mu_1^2-\mu_2^2)}{w_2^2-w_1^2} \\ 4\bar{\lambda}w_1^2 + \frac{w_2^2(\mu_1^2-\mu_2^2)}{w_2^2-w_1^2} & 4\bar{\lambda}w_1w_2 - \frac{w_1w_2(\mu_1^2-\mu_2^2)}{w_2^2-w_1^2} \end{pmatrix}, \tag{C4}$$

whereas for the *CP*-odd and charged scalars, we have

$$\mathbf{M}^2_{CP\text{-odd}} = \begin{pmatrix} 2v_2^2\lambda_5 - m_{12}^2\tan\beta & -2v_1v_2\lambda_5 + m_{12}^2 \\ -2v_1v_2\lambda_5 + m_{12}^2 & 2v_1^2\lambda_5 - m_{12}^2\cot\beta \end{pmatrix} \tag{C5}$$

and

$$\mathbf{M}^2_\pm = \begin{pmatrix} 2v_2^2(\lambda_4+\lambda_5) - m_{12}^2\tan\beta & -2v_1v_2(\lambda_4+\lambda_5) + m_{12}^2 \\ -2v_1v_2(\lambda_4+\lambda_5) + m_{12}^2 & 2v_1^2(\lambda_4+\lambda_5) - m_{12}^2\cot\beta \end{pmatrix}. \tag{C6}$$

Note that the mass matrices for the *CP*-odd and charged scalars are rank one while rank four for the *CP*-even case.

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