Search for New Resonances Decaying to Pairs of Merged Diphotons in Proton-Proton Collisions at $\sqrt{s} = 13$ TeV

A. Hayrapetyan *et al.*[*]
(CMS Collaboration)

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A search is presented for an extended Higgs sector with two new particles, X and ϕ, in the process $X \to \phi\phi \to (\gamma\gamma)(\gamma\gamma)$. Novel neural networks classify events with diphotons that are merged and determine the diphoton masses. The search uses LHC proton-proton collision data at $\sqrt{s} = 13$ TeV collected with the CMS detector, corresponding to an integrated luminosity of 138 fb^{-1}. No evidence of such resonances is seen. Upper limits are set on the production cross section for m_X between 300 and 3000 GeV and m_ϕ/m_X between 0.5% and 2.5%, representing the most sensitive search in this channel.

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Many theories of particle physics beyond the standard model (BSM) predict the existence of extended Higgs sectors [1–7]. Such extensions may include an approximate global symmetry with spontaneous symmetry breaking, which is a sufficient condition for the existence of new spin-0 particles, X and ϕ, with unknown masses m_X and m_ϕ. As long as $m_X > 2m_\phi$, $X \to \phi\phi$ is an allowed decay mode. The ϕ boson can couple to pairs of standard model (SM) particles. Thus, the ϕ decay mode can result in various final state signatures, each presenting different experimental challenges, depending on the targeted kinematic regime. The CMS Collaboration previously performed a search targeting $X \to \phi\phi$, considering $\phi \to b\bar{b}$ decays for ϕ boson masses above 25 GeV [8]. Analogously to diphoton decays of the Higgs boson, the ϕ boson can decay to pairs of photons, $\phi \to \gamma\gamma$, via loops of SM or BSM particles [9]. The $\phi \to \gamma\gamma$ channel provides sensitivity in the region of X and ϕ mass combinations that were beyond the reach of the $X \to \phi\phi \to (b\bar{b})(b\bar{b})$ search described in Ref. [8], including the region where the $(b\bar{b})(b\bar{b})$ channel is kinematically allowed but not well reconstructed. Prior searches for similar new spin-0 particles decaying to two photons were performed by the ATLAS Collaboration [10–12]. Searches for exotic decays of the Higgs boson have been performed by the CMS Collaboration; Ref. [13] searched for a four-photon final state and Ref. [14] investigated the regime in which extremely collimated photon pairs are reconstructed as a single photon by the standard CMS algorithm.

[*]Full author list given at the end of the Letter.

This Letter presents a search for the production of an X boson, decaying to a pair of ϕ bosons that themselves decay to pairs of photons, $X \to \phi\phi \to (\gamma\gamma)(\gamma\gamma)$. The analysis focuses on a broad range of m_X between 0.3 and 3 TeV, with a relative mass $\alpha = m_\phi/m_X$ ranging between 0.5% and 2.5% corresponding to events for which the angular separation (ΔR) of the photons in a pair is between 0.01 and 0.2 radians. In this range, the separation is too small for the photons to be individually identified in the CMS detector, but not so small that the signature would be consistent with a single photon in the standard CMS reconstruction [15]. These mass combinations correspond to the regime where the previous $\phi \to b\bar{b}$ search has no sensitivity. To gain sensitivity in this intermediate regime, a dedicated convolutional neural network (CNN) has been developed, which classifies energy clusters in the CMS electromagnetic calorimeter (ECAL) as originating from two overlapping photons (denoted Γ), hadronic activity, or a single photon. A second CNN is used to reconstruct the mass of the Γ candidates, similar to [16], optimized for the exploration of the α-m_X space considered in this Letter. After selecting events with two Γ candidates, the analysis searches for localized excesses over the steeply falling background distribution of their paired reconstructed mass ($m_{\Gamma\Gamma}$). The search is performed by simultaneously fitting the $m_{\Gamma\Gamma}$ spectrum in bins of the reconstructed mass ratio $\alpha^{\text{reco}} = \hat{m}_\Gamma/m_{\Gamma\Gamma}$, where $\hat{m}_\Gamma$ is the average reconstructed mass of the two Γ candidates. The α^{reco} binning is chosen based on the resolution obtained from the simulated signal samples. The signals may appear in multiple α^{reco} bins. The background in this search is derived exclusively from a parametrized fit to the data.

The search uses a dataset of proton-proton (pp) collisions at $\sqrt{s} = 13$ TeV at the CERN LHC, collected with the CMS detector in 2016–2018, corresponding to an integrated luminosity of 138 fb^{-1}. The CMS apparatus [17] is a multipurpose, nearly hermetic detector, designed to trigger on [18,19] and identify electrons, muons, photons, and hadrons [20–22]. A global reconstruction algorithm [23] combines the information provided by the all-silicon inner tracker and by the lead tungstate ECAL and brass-scintillator hadron calorimeters, operating inside a 3.8 T superconducting solenoid, with data from gas-ionization muon detectors embedded in the solenoid return yoke, to build τ leptons, jets, missing transverse momentum, and other physics objects [24–26]. Events are retained for analysis if they pass a trigger requiring two photon candidates, each with $p_{\mathrm{T}} > 60$ or 70 GeV in 2016 or 2017–2018 data, respectively. The photon identification algorithm used by the trigger only selects photons based on isolation, and not on the cluster shape, and hence has high efficiency for selecting events with two merged diphotons, provided they have sufficient p_{T}. Tabulated results for this analysis are provided in the HEPData record [27].

The ECAL barrel covers a pseudorapidity range $|\eta| < 1.4$ and consists of 61 200 individual crystals, each covering $\Delta\eta \times \Delta\phi = 0.0175 \times 0.0175$ where ϕ is the azimuthal angle. Individual photons typically deposit energy in several adjacent crystals, and are reconstructed as localized clusters of energy. For merged diphotons, such clusters may overlap. Purpose-built algorithms for identifying diphotons from the shapes of their energy distributions in the ECAL barrel are described below. To simplify the CNN implementation, this analysis uses events where both Γ candidates are reconstructed in the barrel, which account for more than 60% of the expected signal yield.

The benchmark signal model $X \to \phi\phi \to (\gamma\gamma)(\gamma\gamma)$, produced via gluon fusion in the narrow-width approximation, is generated at leading order with the MadGraph5_aMC@NLO 2.6.0 [28] generator, with up to two additional partons in the matrix element calculations. Simulated signals are generated for m_X from 0.3 to 3 TeV (at intervals ranging from 0.1 to 0.5 TeV) and for α from 0.5 to 2.5% (at 0.5% intervals). The signal production cross section is calculated numerically at next-to-next-to-leading order (NNLO) using the HqT 2.0 program [29–31], and depends on the number (N) of new Dirac quarks that receive all their mass from the X vacuum expectation value f, so that the signal cross section depends on the value $(m_X N)/f$. The background from SM production of jets and photons (γ + jets), used to optimize the analysis procedure, is also modeled at next-to-leading order with the MadGraph5_aMC@NLO generator. Hadronic objects for training of the classification CNN are taken from this sample. The parton showering and fragmentation for these samples is modeled by PYTHIA 8.240 [32]. Matching between the matrix element and parton shower jets relies on the MLM matching procedure [33]. Samples of isolated photons and diphotons with uniform energy distributions are generated with PYTHIA 8.107 [34] and are used to train the Γ identification and mass reconstruction CNNs. The CP5 [35,36] underlying event tune is used for the simulation with the NNPDF3.1 [37] NNLO parton distribution function sets. The response of the CMS detector is modeled using Geant4 [38]. The effect of extra pp interactions in the same or adjacent bunch crossings (pileup) is incorporated in the simulation, with the frequency distribution of additional vertices adjusted to match that observed in data.

Energy deposits in the ECAL barrel are clustered into Γ candidates using an algorithm inspired by the Cambridge-Aachen algorithm [39]. Beginning with the most energetic single-crystal deposit in the ECAL barrel, the nearest neighbor energy deposit is iteratively added to the cluster if the ΔR between the deposit and the energy-weighted average position of the current cluster is less than a radius $R = 0.15$, where $\Delta R = \sqrt{\Delta\eta^2 + \Delta\phi^2}$. When no new crystals can be included in a cluster, the process begins again with the highest energy unclustered deposit. The distance parameter was chosen to be large enough to capture both photons from a single ϕ boson decay in a single cluster, but not so large that the usual CMS photon identification would reconstruct two separate photons. For the range of α values considered in this analysis, the simulated efficiency of this algorithm to capture both photons in the cluster ranges from 80%–100%, while the efficiency of requiring two individually identified photons ranges from 1% to 20%.

Each Γ candidate consists of a collection of energy deposits on an array of crystals, and can be represented as a pixelated image. Convolutional neural networks developed for image recognition are well suited to extract relevant information about the Γ candidates. The clustered energy deposits are converted to a 30×30 image, centered on the lower left corner of the crystal with the most energetic deposit, where the brightness of a pixel corresponds to the energy deposited in a single crystal. Two different CNNs are used. The first separates Γ candidates arising from merged diphotons from those produced by hadronic decays and single photons. The second regresses the mass-to-energy ratio (m/E) of the Γ candidate, under the assumption that it was produced by a genuine diphoton. The architectures of both CNNs are based on the DeepTop [40] CNN, modified as described below.

For both CNNs, the inputs are the individual crystal energies of that Γ candidate, normalized such that the sum of all crystal energies is unity. These are passed through a series of four convolutional layers with kernels of sizes 7×7, 5×5, 4×4, and 3×3, with 64 output feature maps after each layer in the classification network and 16 in the mass regression network. For the classification, this is followed by one fully connected (FC) linear layer with three outputs corresponding to the output classes. A logarithmic softmax function is used to convert these to classifier scores, ranging from 0 to 1, with higher scores indicating that the cluster is more likely to belong to each category: diphoton ($\mathcal{D}_{\gamma\gamma}$), photon ($\mathcal{D}_{\gamma}$), or hadron ($\mathcal{D}_{\mathrm{had}}$),

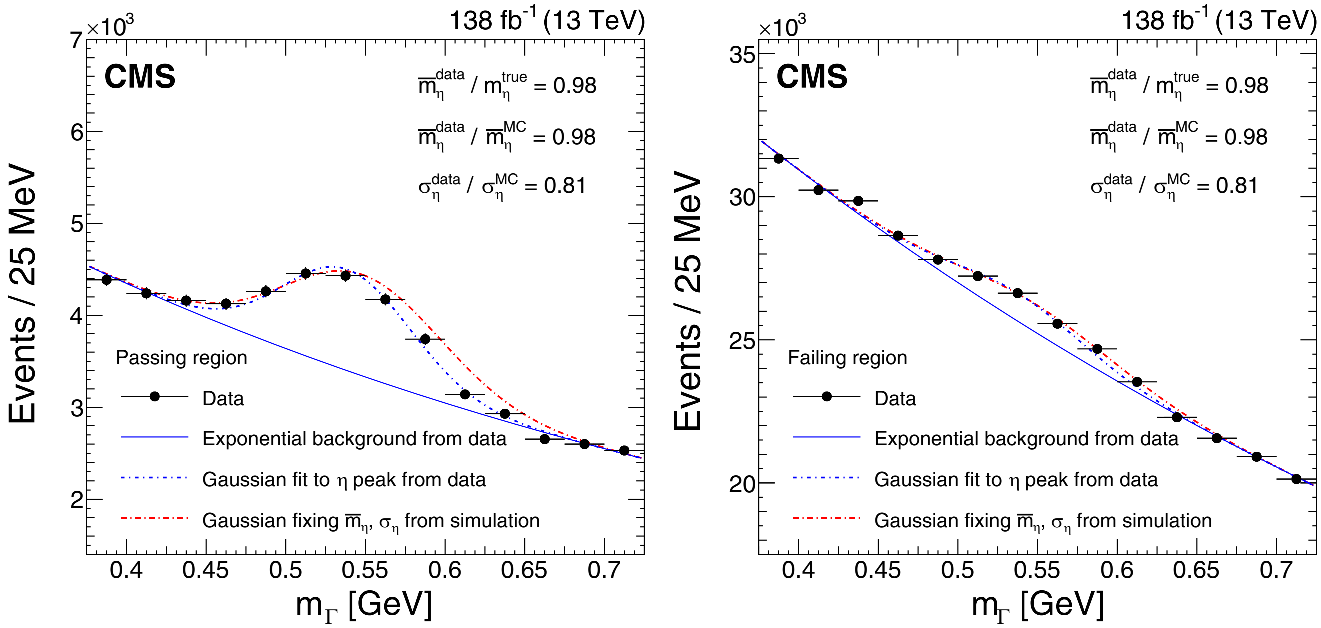

FIG. 1. Cluster mass (m_Γ) distribution in data for both the passing (left) and failing (right) regions, in the energy range for which the η meson is expected to form a single Γ candidate. The signal (background) is modeled by a Gaussian (exponential) function. Blue and red dashed lines depict Gaussian fits to the data and Monte Carlo (MC) simulation, respectively. The solid blue line shows the background component of the fit. Ratios of the Gaussian fit means ($\bar{m}$) and widths (σ) are displayed, where $m_\eta^{\rm true}$ is the true mass of the η meson.

with $\mathcal{D}_{\gamma\gamma} + \mathcal{D}_\gamma + \mathcal{D}_{\rm had} = 1$. For the mass regression, three FC layers are used with output sizes of 64, 16, and 1, respectively, and the geometric η of the Γ candidate is used as an additional input to the first FC layer. The output of the regression CNN is a single number corresponding to the predicted value of m/E.

The training of the classification CNN uses 600 000 events, divided equally between the diphoton, single photon, and hadron categories. For the regression, 500 000 simulated diphoton events are used. In both cases, diphoton events are sampled to retain a flat m/E spectrum from 0 to 0.07. The loss function used for classification is the categorical cross-entropy function; for the regression, a modified mean squared error function optimized for small positive values is used: $\sum_i -\log(e^{-(p_i-q_i)^2}) + \log(1 - e^{-(p_i-q_i)^2})$, where p_i, q_i are the true and predicted m/E values for the ith event, respectively.

To suppress the dominant background from misidentified jets, a relative isolation $r_{\rm iso}$ is defined and applied to each Γ candidate in the analysis. Jets reconstructed with the anti-$k_{\rm T}$ algorithm [41] and a distance parameter of 0.4, using the FastJet package [42], are used. If a Γ candidate overlaps with such a jet within $\Delta R < 0.15$, its $r_{\rm iso}$ is defined as the ratio of its energy to that of the jet. Otherwise, it is set to unity.

The diphoton decays of π^0 or η mesons copiously produced in hadronic showers can be used to validate the performances of the CNNs. While the technique developed in Ref. [16] utilizes π^0 decays to validate its mass regression, here the η meson is used as, in the merged signature, it has a similar Lorentz boost to the considered signals. An η meson control sample is selected to validate the efficiency of the signal classification and the scale and resolution of the m/E regression. The control sample is taken from all events passing an electron or photon trigger. The Γ candidates are required to have energies in the range 30–60 GeV and $r_{\rm iso} > 0.5$. A study made with simulated data shows that the performance of the CNNs does not depend on the energy or mass of the diphotons. This energy range is selected such that the η meson decay products form a single Γ candidate, providing a direct validation of a subset of the m/E range for which the CNNs were trained. The m_Γ distributions are compared in two subsets, depending on whether $\mathcal{D}_{\gamma\gamma} > 0.9$ or not (referred to as "passing" and "failing" regions). The m_Γ distributions of the passing and failing regions are presented in Fig. 1, showing a distinct peak at the η meson mass, providing strong evidence that the regression CNN is working as intended. Because of contamination from other particles produced in the same jet, a substantial number of η mesons decaying to collimated diphotons will appear in the failing region, resulting in the peak seen there. The data and the simulation are each fit simultaneously in the passing and failing regions; the mass of the η meson in both is reconstructed to within 2% of its true value. The classifier efficiency and the mean and width of the peak are extracted using a fit to data, where the signal (background) is modeled by a Gaussian (exponential) function. The classifier efficiency in the η meson control region, extracted from the relative yields in the passing and failing distributions, is measured to be 55 (53)% in data (simulation). The data-to-simulation efficiency ratio is consistent with unity, with a total uncertainty of 10% that is propagated to the final results. The systematic uncertainty in the m_Γ resolution is obtained from the fractional difference in the widths of the η meson peaks in data and simulation, corresponding to 23%, which is correlated across all $\alpha^{\rm reco}$ bins. Finally, the mean positions of the peaks are found to be consistent within the respective statistical uncertainties.

We further validate the performance of the regressor and classifier using a control sample of reconstructed Z bosons through the decay $Z \to e + e-$ by exploiting the case when each electron undergoes bremsstrahlung and appears consistent with a merged diphoton signature. Events are selected by requiring two clusters with $\mathcal{D}_{\gamma\gamma} > 0.75$ and $r_{\rm iso} > 0.8$. The resulting reconstructed $m_{\Gamma\Gamma}$ distribution shows a clear presence of Z bosons in both data and simulation, with nearly identical performance. The positions of the reconstructed mass peaks in data and simulation are found to be within 0.5% across a wide range of cluster $p_{\rm T}$, and this value is applied as a systematic uncertainty in the Γ candidate energy scale.

The offline analysis considers events with two Γ candidates in the ECAL barrel with $p_{\rm T} > 90$ GeV, where the trigger becomes fully efficient. Both Γ candidates must also fulfill the following requirements: $r_{\rm iso} > 0.8$ and $\mathcal{D}_{\gamma\gamma} > 0.9$. This $\mathcal{D}_{\gamma\gamma}$ requirement retains $\gtrsim$80% of simulated signal across all masses and rejects approximately 99% of the background. The mass asymmetry of the event $m_{\rm asym} = |m_{\Gamma_1} - m_{\Gamma_2}|/(m_{\Gamma_1} + m_{\Gamma_2}) < 0.25$ is required. Finally, $\Delta\eta < 1.5$ (between the candidates) is required to further suppress background from the SM production of jets and photons.

The remaining data are evaluated for localized excesses in the $m_{\Gamma\Gamma}$ distribution, in nine nonoverlapping divisions of the $\alpha^{\rm reco}$ distributions ranging from 0.3% to 3%, each determined by a combination of detector resolution and a requirement that the division contains enough events for the background estimate to converge. Any particular signal is expected to appear in only a few adjacent $\alpha^{\rm reco}$ divisions. As in previous searches [43–46], the background shape is modeled by fitting empirical functional forms to the observed data in each division, where the number of parameters in the functional forms is determined by performing Fisher F-tests [47] on progressively higher-order functions. Functions with three parameters were found to be acceptable for describing the data: the dijet function $p_0(1-x)^{p_1}/x^{p_2}$, the modified dijet function $p_0(1-x^{1/3})^{p_1}/x^{p_2}$, the diphoton function $p_0 x^{p_1+p_2 \log x}$, a power-law times an exponential function $p_0 e^{-p_1 x}/x^{p_2}$, and a four-parameter power-law function $p_0 p_1^{p_2 x + p_3/x}$, where x is $m_{\Gamma\Gamma}/\sqrt{s}$. The choice of function is encoded into the fitting procedure as a discrete parameter of the likelihood. Signal shapes are modeled by fitting a double-sided Crystal Ball function [48] to the reconstructed simulated signal $m_{\Gamma\Gamma}$ spectra, then interpolating the function parameters to generate shapes with fine spacing in m_X. To validate the robustness of the fit, a goodness-of-fit test and bias tests are performed. The bias tests use simulated events with a variety of simulated signals injected. No significant bias is observed for any X and ϕ boson mass combination. The result of the fit for one representative $\alpha^{\rm reco}$ division is shown in Fig. 2. The search uses a fit of the background function plus the simulated signal shape to the data, taking into account statistical and systematic uncertainties, and is performed for $m_{\Gamma\Gamma} > 297$ GeV and simultaneously in all bins of $\alpha^{\rm reco}$.

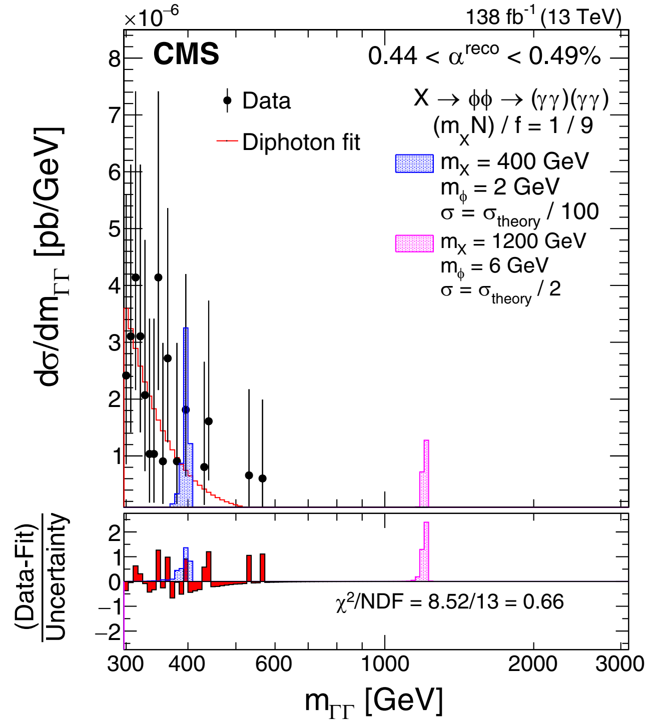

FIG. 2. Dicluster mass ($m_{\Gamma\Gamma}$) distribution for the data (points) for one of the $\alpha^{\rm reco}$ bins of the search ($0.44 < \alpha^{\rm reco} < 0.49\%$), fitted with the diphoton function (red), one of the considered five background parametrizations. Examples of two representative predicted signals are shown (blue and pink). The lower panel shows the difference between the observed data and the background prediction divided by the statistical uncertainty of the data ($\sigma_{\rm data}$), the aforementioned signals divided by $\sigma_{\rm data}$, and the goodness of fit measure χ^2/NDF (where NDF is the number of degrees of freedom).

Systematic uncertainties are modeled in the fit as nuisance parameters that affect the shapes and normalizations of signal and background processes, with log-normal priors for the uncertainties affecting only the normalization and Gaussian priors for those affecting the shapes of distributions. The main sources of systematic uncertainty in the background modeling are the choice of the background function and the background function fit parameters. The parameters of the background function are treated as freely floating nuisance parameters, and are evaluated

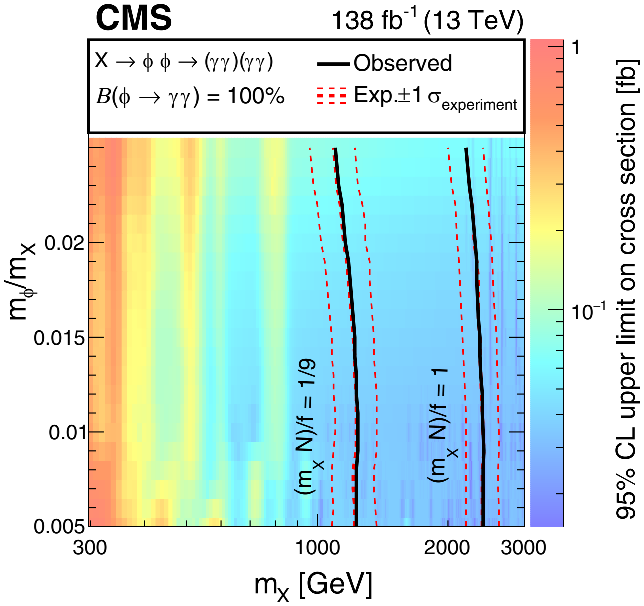

FIG. 3. Exclusion limits at 95% CL on $\sigma[X \to \phi\phi \to (\gamma\gamma)(\gamma\gamma)]$ displayed in the (m_ϕ/m_X)-m_X plane. Branching fractions ($\mathcal{B}$) of both $X \to \phi\phi$ and $\phi \to \gamma\gamma$ are assumed to be 100%. The black (red) lines represent the observed (expected) mass exclusions corresponding to different assumptions of $(m_X N)/f$. The observed upper limits on the cross section are shown on the color z axis.

via profiling. The discrete profiling method [49] is used for considering the choice of the functional form as a discrete nuisance parameter, which is profiled in an analogous way to continuous nuisance parameters. Systematic uncertainties affecting the predicted signal yield include the uncertainty in the integrated luminosity measurement (1.6%) [50–52], the diphoton classifier efficiency (10%, applied per cluster), the m_Γ resolution uncertainty (23%, affecting the yield in each α^{reco} bin), and the trigger efficiency (5%). Systematic uncertainties affecting the shape of the predicted signal distributions include the Γ energy scale uncertainty (0.5%, applied per cluster) and uncertainties in the modeling of pileup (1%–10%). The dominant systematic uncertainty in the signal modeling is due to the diphoton classifier efficiency.

No significant excesses are observed. The largest excess corresponds to $m_X \approx 720$ GeV and $\alpha = 0.7\%$ ($m_\phi \approx 5$ GeV) with a local (global) significance of 3.57 (1.07) standard deviations. The global significance accounts for the look-elsewhere effect [53] by using pseudoexperiments to compute the probability that the background hypothesis produces a signal-like fluctuation with at least the observed local significance anywhere in the sensitive range of m_X and α. The fit results are used to set 95% confidence level (CL) upper limits on the cross section $\sigma(pp \to X)$, assuming a 100% branching fraction for $X \to \phi\phi \to (\gamma\gamma)(\gamma\gamma)$. Upper limits are computed using a modified frequentist approach, based on the CL_s criterion [54–56], with the profile likelihood ratio used as the test statistic within the asymptotic approximation [57]. Observed and expected limits are computed as functions of m_X for a given assumed value of α, and compared to the theoretical estimates of $\sigma(X \to \phi\phi)$ for a set of $(m_X N)/f$ values. Figure 3 shows the observed upper limits on the cross section and the mass exclusion curves in the α-m_X plane. The observed (expected) upper limits on this process range from 0.03–1.06 (0.03-–0.79) fb, depending on m_X and m_ϕ.

In summary, a search for an extended Higgs sector with two new particles, X and ϕ, with unknown masses m_X and m_ϕ, has been presented for the decay sequence $X \to \phi\phi \to (\gamma\gamma)(\gamma\gamma)$. The search uses proton-proton collision data at $\sqrt{s} = 13$ TeV, collected with the CMS detector at the LHC in 2016–2018, corresponding to an integrated luminosity of 138 fb^{-1}. The analysis considers m_X between 0.3 and 3 TeV, and is restricted to values of m_ϕ for which the ratio m_ϕ/m_X is between 0.5% and 2.5%. As a result, the two photons from each ϕ boson overlap significantly in the electromagnetic calorimeter. Convolutional neural networks trained on clusters of calorimeter energy deposits are used to classify events containing merged diphotons and to regress the mass of the diphoton system. The dicluster mass spectra, in bins of the ratio of the average cluster mass divided by the dicluster mass, are analyzed for the presence of new resonances, and are found to be consistent with the standard model expectations. Upper limits are set at 95% confidence level on the production cross section for $X \to \phi\phi \to (\gamma\gamma)(\gamma\gamma)$, as a function of the resonance masses, where both the $X \to \phi\phi$ and $\phi \to \gamma\gamma$ branching fractions are assumed to be 100%. Observed (expected) limits range within 0.03–1.06 (0.03–0.79) fb at 95% CL for the masses considered. For the masses considered, these results represent the most sensitive search for extended Higgs sectors that have two new resonances decaying to the four-photon final state.

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Fontanesi,[142] D. Gastler,[142] F. Golf,[142] S. Jeon,[142] I. Reed,[142] J. Rohlf,[142] K. Salyer,[142] D. Sperka,[142] D. Spitzbart,[142] I. Suarez,[142] A. Tsatsos,[142] S. Yuan,[142] A. G. Zecchinelli,[142] G. Benelli,[143] X. Coubez,[143,z] D. Cutts,[143] M. Hadley,[143] U. Heintz,[143] J. M. Hogan,[143,gggg] T. Kwon,[143] G. Landsberg,[143] K. T. Lau,[143] D. Li,[143] J. Luo,[143] S. Mondal,[143] M. Narain,[143,a] N. Pervan,[143] S. Sagir,[143,hhhh] F. Simpson,[143] M. Stamenkovic,[143] N. Venkatasubramanian,[143] X. Yan,[143] W. Zhang,[143] S. Abbott,[144] J. Bonilla,[144] C. Brainerd,[144] R. Breedon,[144] H. Cai,[144] M. Calderon De La Barca Sanchez,[144] M. Chertok,[144] M. Citron,[144] J. Conway,[144] P. T. Cox,[144] R. Erbacher,[144] F. Jensen,[144] O. Kukral,[144] G. Mocellin,[144] M. Mulhearn,[144] D. Pellett,[144] W. Wei,[144] Y. Yao,[144] F. Zhang,[144] M. Bachtis,[145] R. Cousins,[145] A. Datta,[145] G. Flores Avila,[145] J. Hauser,[145] M. Ignatenko,[145] M. A. 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A. Apresyan,[153] L. A. T. Bauerdick,[153] D. Berry,[153] J. Berryhill,[153] P. C. Bhat,[153] K. Burkett,[153] J. N. Butler,[153] A. Canepa,[153] G. B. Cerati,[153] H. W. K. Cheung,[153] F. Chlebana,[153] G. Cummings,[153] J. Dickinson,[153] I. Dutta,[153] V. D. Elvira,[153] Y. Feng,[153] J. Freeman,[153] A. Gandrakota,[153] Z. Gecse,[153] L. Gray,[153] D. Green,[153] A. Grummer,[153] S. Grünendahl,[153] D. Guerrero,[153] O. Gutsche,[153] R. M. Harris,[153] R. Heller,[153] T. C. Herwig,[153] J. Hirschauer,[153] L. Horyn,[153] B. Jayatilaka,[153] S. Jindariani,[153] M. Johnson,[153] U. Joshi,[153] T. Klijnsma,[153] B. Klima,[153] K. H. M. Kwok,[153] S. Lammel,[153] D. Lincoln,[153] R. Lipton,[153] T. Liu,[153] C. Madrid,[153] K. Maeshima,[153] C. Mantilla,[153] D. Mason,[153] P. McBride,[153] P. Merkel,[153] S. Mrenna,[153] S. Nahn,[153] J. Ngadiuba,[153] D. Noonan,[153] V. Papadimitriou,[153] N. Pastika,[153] K. Pedro,[153] C. Pena,[153,iiii] F. Ravera,[153] A. Reinsvold Hall,[153,jjjj] L. Ristori,[153] E. Sexton-Kennedy,[153] N. Smith,[153] A. Soha,[153] L. Spiegel,[153] S. Stoynev,[153] J. Strait,[153] L. Taylor,[153] S. Tkaczyk,[153] N. V. Tran,[153] L. Uplegger,[153] E. W. Vaandering,[153] A. Whitbeck,[153] I. Zoi,[153] C. Aruta,[154] P. Avery,[154] D. Bourilkov,[154] L. Cadamuro,[154] P. Chang,[154] V. Cherepanov,[154] R. D. Field,[154] E. Koenig,[154] M. Kolosova,[154] J. Konigsberg,[154] A. Korytov,[154] K. Matchev,[154] N. Menendez,[154] G. Mitselmakher,[154] K. Mohrman,[154] A. Muthirakalayil Madhu,[154] N. Rawal,[154] D. Rosenzweig,[154] S. Rosenzweig,[154] J. Wang,[154] T. Adams,[155] A. Al Kadhim,[155] A. Askew,[155] S. Bower,[155] R. Habibullah,[155] V. Hagopian,[155] R. Hashmi,[155] R. S. Kim,[155] S. Kim,[155] T. Kolberg,[155] G. Martinez,[155] H. Prosper,[155] P. R. Prova,[155] M. Wulansatiti,[155] R. Yohay,[155] J. Zhang,[155] B. Alsufyani,[156] M. M. Baarmand,[156] S. Butalla,[156] S. Das,[156] T. Elkafrawy,[156,eee] M. Hohlmann,[156] R. Kumar Verma,[156] M. Rahmani,[156] E. Yanes,[156] M. R. Adams,[157] A. Baty,[157] C. Bennett,[157] R. Cavanaugh,[157] R. Escobar Franco,[157] O. Evdokimov,[157] C. E. Gerber,[157] M. Hawksworth,[157] A. Hingrajiya,[157] D. J. Hofman,[157] J. h. Lee,[157] D. S. Lemos,[157] A. H. Merrit,[157] C. Mills,[157] S. Nanda,[157] G. Oh,[157] B. Ozek,[157] D. Pilipovic,[157] R. Pradhan,[157] E. Prifti,[157] T. Roy,[157] S. Rudrabhatla,[157] M. B. Tonjes,[157] N. Varelas,[157] M. A. Wadud,[157] Z. Ye,[157] J. Yoo,[157] M. Alhusseini,[158] D. Blend,[158] K. Dilsiz,[158,kkkk] L. Emediato,[158] G. Karaman,[158] O. K. Köseyan,[158] J.-P. Merlo,[158] A. Mestvirishvili,[158,llll] J. Nachtman,[158] O. Neogi,[158] H. Ogul,[158,mmmm] Y. Onel,[158] A. Penzo,[158] C. Snyder,[158] E. Tiras,[158,nnnn] B. Blumenfeld,[159] L. Corcodilos,[159] J. Davis,[159] A. V. Gritsan,[159] L. Kang,[159] S. Kyriacou,[159] P. Maksimovic,[159] M. Roguljic,[159] J. Roskes,[159] S. Sekhar,[159] M. 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B. Bylsma,[172] M. Carrigan,[172] L. S. Durkin,[172] C. Hill,[172] M. Joyce,[172] M. Nunez Ornelas,[172] K. Wei,[172] B. L. Winer,[172] B. R. Yates,[172] F. M. Addesa,[173] H. Bouchamaoui,[173] P. Das,[173] G. Dezoort,[173] P. Elmer,[173] A. Frankenthal,[173] B. Greenberg,[173] N. Haubrich,[173] G. Kopp,[173] S. Kwan,[173] D. Lange,[173] A. Loeliger,[173] D. Marlow,[173] I. Ojalvo,[173] J. Olsen,[173] A. Shevelev,[173] D. Stickland,[173] C. Tully,[173] S. Malik,[174] A. S. Bakshi,[175] V. E. Barnes,[175] S. Chandra,[175] R. Chawla,[175] A. Gu,[175] L. Gutay,[175] M. Jones,[175] A. W. Jung,[175] D. Kondratyev,[175] A. M. Koshy,[175] M. Liu,[175] G. Negro,[175] N. Neumeister,[175] G. Paspalaki,[175] S. Piperov,[175] V. Scheurer,[175] J. F. Schulte,[175] M. Stojanovic,[175] J. Thieman,[175] A. K. Virdi,[175] F. Wang,[175] W. Xie,[175] J. Dolen,[176] N. Parashar,[176] A. Pathak,[176] D. Acosta,[177] T. Carnahan,[177] K. M. Ecklund,[177] P. J. Fernández Manteca,[177] S. Freed,[177] P. Gardner,[177] F. J. M. Geurts,[177] W. Li,[177] O. Miguel Colin,[177] B. P. Padley,[177] R. Redjimi,[177] J. Rotter,[177] E. Yigitbasi,[177] Y. Zhang,[177] A. Bodek,[178] P. de Barbaro,[178] R. Demina,[178] J. L. Dulemba,[178] A. Garcia-Bellido,[178] O. Hindrichs,[178] A. Khukhunaishvili,[178] N. Parmar,[178] P. Parygin,[178,q] E. Popova,[178,q] R. Taus,[178] K. Goulianos,[179] B. Chiarito,[180] J. P. Chou,[180] S. V. Clark,[180] D. Gadkari,[180] Y. Gershtein,[180] E. Halkiadakis,[180] M. Heindl,[180] C. Houghton,[180] D. Jaroslawski,[180] O. Karacheban,[180,cc] S. Konstantinou,[180] I. Laflotte,[180] A. Lath,[180] R. Montalvo,[180] K. Nash,[180] H. Routray,[180] P. Saha,[180] S. Salur,[180] S. Schnetzer,[180] S. Somalwar,[180] R. Stone,[180] S. A. Thayil,[180] S. Thomas,[180] J. Vora,[180] H. Wang,[180] H. Acharya,[181] D. Ally,[181] A. G. Delannoy,[181] S. Fiorendi,[181] S. Higginbotham,[181] T. Holmes,[181] A. R. Kanuganti,[181] N. Karunarathna,[181] L. Lee,[181] E. Nibigira,[181] S. Spanier,[181] D. Aebi,[182] M. Ahmad,[182] O. Bouhali,[182,pppp] R. Eusebi,[182] J. Gilmore,[182] T. Huang,[182] T. Kamon,[182,qqqq] H. Kim,[182] S. Luo,[182] R. Mueller,[182] D. Overton,[182] D. Rathjens,[182] A. Safonov,[182] N. Akchurin,[183] J. Damgov,[183] V. Hegde,[183] A. Hussain,[183] Y. Kazhykarim,[183] K. Lamichhane,[183] S. W. Lee,[183] A. Mankel,[183] T. Peltola,[183] I. Volobouev,[183] E. Appelt,[184] Y. Chen,[184] S. Greene,[184] A. Gurrola,[184] W. Johns,[184] R. Kunnawalkam Elayavalli,[184] A. Melo,[184] F. Romeo,[184] P. Sheldon,[184] S. Tuo,[184] J. Velkovska,[184] J. Viinikainen,[184] B. Cardwell,[185] B. Cox,[185] J. Hakala,[185] R. Hirosky,[185] A. Ledovskoy,[185] C. Neu,[185] C. E. Perez Lara,[185] S. Bhattacharya,[186] P. E. Karchin,[186] A. Aravind,[187] S. Banerjee,[187] K. Black,[187] T. Bose,[187] S. Dasu,[187] I. De Bruyn,[187] P. Everaerts,[187] C. Galloni,[187] H. He,[187] M. Herndon,[187] A. Herve,[187] C. K. Koraka,[187] A. Lanaro,[187] R. Loveless,[187] J. Madhusudanan Sreekala,[187] A. Mallampalli,[187] A. Mohammadi,[187] S. Mondal,[187] G. Parida,[187] L. Pétré,[187] D. Pinna,[187] A. Savin,[187] V. Shang,[187] V. Sharma,[187] W. H. Smith,[187] D. Teague,[187] H. F. Tsoi,[187] W. Vetens,[187] A. Warden,[187] S. Afanasiev,[188] V. Andreev,[188] Yu. Andreev,[188] T. Aushev,[188] M. Azarkin,[188] I. Azhgirey,[188] A. Babaev,[188] A. Belyaev,[188] V. Blinov,[188,q] E. Boos,[188] V. Borshch,[188] D. Budkouski,[188] M. Chadeeva,[188,q] V. Chekhovsky,[188] R. Chistov,[188,q] A. Dermenev,[188] T. Dimova,[188,q] D. Druzhkin,[188,rrrr] M. Dubinin,[188,iiii] L. Dudko,[188] A. Ershov,[188] G. Gavrilov,[188] V. Gavrilov,[188] S. Gninenko,[188] V. Golovtcov,[188] N. Golubev,[188] I. Golutvin,[188] I. Gorbunov,[188] A. Gribushin,[188] Y. Ivanov,[188] V. Kachanov,[188] V. Karjavine,[188] A. Karneyeu,[188] V. Kim,[188,q] M. Kirakosyan,[188] D. Kirpichnikov,[188] M. Kirsanov,[188] V. Klyukhin,[188] O. Kodolova,[188,ssss] D. Konstantinov,[188] V. Korenkov,[188] A. Kozyrev,[188,q] N. Krasnikov,[188] A. Lanev,[188] P. Levchenko,[188,tttt] N. Lychkovskaya,[188] V. Makarenko,[188] A. Malakhov,[188] V. Matveev,[188,q] V. Murzin,[188] A. Nikitenko,[188,uuuu,ssss] S. Obraztsov,[188] V. Oreshkin,[188] V. Palichik,[188] V. Perelygin,[188] S. Petrushanko,[188] S. Polikarpov,[188,q] V. Popov,[188] O. Radchenko,[188,q] R. Ryutin,[188] M. Savina,[188] V. Savrin,[188] V. Shalaev,[188] S. Shmatov,[188] S. Shulha,[188] Y. Skovpen,[188,q] S. Slabospitskii,[188] V. Smirnov,[188] A. Snigirev,[188] D. Sosnov,[188] V. Sulimov,[188] E. Tcherniaev,[188] A. Terkulov,[188] O. Teryaev,[188] I. Tlisova,[188] A. Toropin,[188] L. Uvarov,[188] A. Uzunian,[188] A. Vorobyev,[188,a] N. Voytishin,[188] B. S. Yuldashev,[188,vvvv] A. Zarubin,[188] I. Zhizhin,[188] and A. Zhokin[188]

(CMS Collaboration)

[1]*Yerevan Physics Institute, Yerevan, Armenia*
[2]*Institut für Hochenergiephysik, Vienna, Austria*
[3]*Universiteit Antwerpen, Antwerpen, Belgium*
[4]*Vrije Universiteit Brussel, Brussel, Belgium*
[5]*Université Libre de Bruxelles, Bruxelles, Belgium*

[6]Ghent University, Ghent, Belgium
[7]Université Catholique de Louvain, Louvain-la-Neuve, Belgium
[8]Centro Brasileiro de Pesquisas Fisicas, Rio de Janeiro, Brazil
[9]Universidade do Estado do Rio de Janeiro, Rio de Janeiro, Brazil
[10]Universidade Estadual Paulista, Universidade Federal do ABC, São Paulo, Brazil
[11]Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Sofia, Bulgaria
[12]University of Sofia, Sofia, Bulgaria
[13]Instituto De Alta Investigación, Universidad de Tarapacá, Casilla 7 D, Arica, Chile
[14]Beihang University, Beijing, China
[15]Department of Physics, Tsinghua University, Beijing, China
[16]Institute of High Energy Physics, Beijing, China
[17]State Key Laboratory of Nuclear Physics and Technology, Peking University, Beijing, China
[18]Sun Yat-Sen University, Guangzhou, China
[19]University of Science and Technology of China, Hefei, China
[20]Nanjing Normal University, Nanjing, China
[21]Institute of Modern Physics and Key Laboratory of Nuclear Physics and Ion-beam Application (MOE) - Fudan University, Shanghai, China
[22]Zhejiang University, Hangzhou, Zhejiang, China
[23]Universidad de Los Andes, Bogota, Colombia
[24]Universidad de Antioquia, Medellin, Colombia
[25]University of Split, Faculty of Electrical Engineering, Mechanical Engineering and Naval Architecture, Split, Croatia
[26]University of Split, Faculty of Science, Split, Croatia
[27]Institute Rudjer Boskovic, Zagreb, Croatia
[28]University of Cyprus, Nicosia, Cyprus
[29]Charles University, Prague, Czech Republic
[30]Escuela Politecnica Nacional, Quito, Ecuador
[31]Universidad San Francisco de Quito, Quito, Ecuador
[32]Academy of Scientific Research and Technology of the Arab Republic of Egypt, Egyptian Network of High Energy Physics, Cairo, Egypt
[33]Center for High Energy Physics (CHEP-FU), Fayoum University, El-Fayoum, Egypt
[34]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia
[35]Department of Physics, University of Helsinki, Helsinki, Finland
[36]Helsinki Institute of Physics, Helsinki, Finland
[37]Lappeenranta-Lahti University of Technology, Lappeenranta, Finland
[38]IRFU, CEA, Université Paris-Saclay, Gif-sur-Yvette, France
[39]Laboratoire Leprince-Ringuet, CNRS/IN2P3, Ecole Polytechnique, Institut Polytechnique de Paris, Palaiseau, France
[40]Université de Strasbourg, CNRS, IPHC UMR 7178, Strasbourg, France
[41]Institut de Physique des 2 Infinis de Lyon (IP2I), Villeurbanne, France
[42]Georgian Technical University, Tbilisi, Georgia
[43]RWTH Aachen University, I. Physikalisches Institut, Aachen, Germany
[44]RWTH Aachen University, III. Physikalisches Institut A, Aachen, Germany
[45]RWTH Aachen University, III. Physikalisches Institut B, Aachen, Germany
[46]Deutsches Elektronen-Synchrotron, Hamburg, Germany
[47]University of Hamburg, Hamburg, Germany
[48]Karlsruher Institut fuer Technologie, Karlsruhe, Germany
[49]Institute of Nuclear and Particle Physics (INPP), NCSR Demokritos, Aghia Paraskevi, Greece
[50]National and Kapodistrian University of Athens, Athens, Greece
[51]National Technical University of Athens, Athens, Greece
[52]University of Ioánnina, Ioánnina, Greece
[53]HUN-REN Wigner Research Centre for Physics, Budapest, Hungary
[54]MTA-ELTE Lendület CMS Particle and Nuclear Physics Group, Eötvös Loránd University, Budapest, Hungary
[55]Faculty of Informatics, University of Debrecen, Debrecen, Hungary
[56]Institute of Nuclear Research ATOMKI, Debrecen, Hungary
[57]Karoly Robert Campus, MATE Institute of Technology, Gyongyos, Hungary
[58]Panjab University, Chandigarh, India
[59]University of Delhi, Delhi, India
[60]Saha Institute of Nuclear Physics, HBNI, Kolkata, India
[61]Indian Institute of Technology Madras, Madras, India
[62]Tata Institute of Fundamental Research-A, Mumbai, India
[63]Tata Institute of Fundamental Research-B, Mumbai, India

[64]National Institute of Science Education and Research, An OCC of Homi Bhabha National Institute, Bhubaneswar, Odisha, India
[65]Indian Institute of Science Education and Research (IISER), Pune, India
[66]Isfahan University of Technology, Isfahan, Iran
[67]Institute for Research in Fundamental Sciences (IPM), Tehran, Iran
[68]University College Dublin, Dublin, Ireland
[69a]INFN Sezione di Bari, Bari, Italy
[69b]Università di Bari, Bari, Italy
[69c]Politecnico di Bari, Bari, Italy
[70a]INFN Sezione di Bologna, Bologna, Italy
[70b]Università di Bologna, Bologna, Italy
[71a]INFN Sezione di Catania, Catania, Italy
[71b]Università di Catania, Catania, Italy
[72a]INFN Sezione di Firenze, Firenze, Italy
[72b]Università di Firenze, Firenze, Italy
[73]INFN Laboratori Nazionali di Frascati, Frascati, Italy
[74a]INFN Sezione di Genova, Genova, Italy
[74b]Università di Genova, Genova, Italy
[75a]INFN Sezione di Milano-Bicocca, Milano, Italy
[75b]Università di Milano-Bicocca, Milano, Italy
[76a]INFN Sezione di Napoli, Napoli, Italy
[76b]Università di Napoli 'Federico II', Napoli, Italy
[76c]Università della Basilicata, Potenza, Italy
[76d]Scuola Superiore Meridionale (SSM), Napoli, Italy
[77a]INFN Sezione di Padova, Padova, Italy
[77b]Università di Padova, Padova, Italy
[77c]Università di Trento, Trento, Italy
[78a]INFN Sezione di Pavia, Pavia, Italy
[78b]Università di Pavia, Pavia, Italy
[79a]INFN Sezione di Perugia, Perugia, Italy
[79b]Università di Perugia, Perugia, Italy
[80a]INFN Sezione di Pisa, Pisa, Italy
[80b]Università di Pisa, Pisa, Italy
[80c]Scuola Normale Superiore di Pisa, Pisa, Italy
[80d]Università di Siena, Siena, Italy
[81a]INFN Sezione di Roma, Roma, Italy
[81b]Sapienza Università di Roma, Roma, Italy
[82a]INFN Sezione di Torino, Torino, Italy
[82b]Università di Torino, Torino, Italy
[82c]Università del Piemonte Orientale, Novara, Italy
[83a]INFN Sezione di Trieste, Trieste, Italy
[83b]Università di Trieste, Trieste, Italy
[84]Kyungpook National University, Daegu, Korea
[85]Department of Mathematics and Physics - GWNU, Gangneung, Korea
[86]Chonnam National University, Institute for Universe and Elementary Particles, Kwangju, Korea
[87]Hanyang University, Seoul, Korea
[88]Korea University, Seoul, Korea
[89]Kyung Hee University, Department of Physics, Seoul, Korea
[90]Sejong University, Seoul, Korea
[91]Seoul National University, Seoul, Korea
[92]University of Seoul, Seoul, Korea
[93]Yonsei University, Department of Physics, Seoul, Korea
[94]Sungkyunkwan University, Suwon, Korea
[95]College of Engineering and Technology, American University of the Middle East (AUM), Dasman, Kuwait
[96]Riga Technical University, Riga, Latvia
[97]University of Latvia (LU), Riga, Latvia
[98]Vilnius University, Vilnius, Lithuania
[99]National Centre for Particle Physics, Universiti Malaya, Kuala Lumpur, Malaysia
[100]Universidad de Sonora (UNISON), Hermosillo, Mexico
[101]Centro de Investigacion y de Estudios Avanzados del IPN, Mexico City, Mexico
[102]Universidad Iberoamericana, Mexico City, Mexico

[103]*Benemerita Universidad Autonoma de Puebla, Puebla, Mexico*
[104]*University of Montenegro, Podgorica, Montenegro*
[105]*University of Canterbury, Christchurch, New Zealand*
[106]*National Centre for Physics, Quaid-I-Azam University, Islamabad, Pakistan*
[107]*AGH University of Krakow, Faculty of Computer Science, Electronics and Telecommunications, Krakow, Poland*
[108]*National Centre for Nuclear Research, Swierk, Poland*
[109]*Institute of Experimental Physics, Faculty of Physics, University of Warsaw, Warsaw, Poland*
[110]*Warsaw University of Technology, Warsaw, Poland*
[111]*Laboratório de Instrumentação e Física Experimental de Partículas, Lisboa, Portugal*
[112]*Faculty of Physics, University of Belgrade, Belgrade, Serbia*
[113]*VINCA Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia*
[114]*Centro de Investigaciones Energéticas Medioambientales y Tecnológicas (CIEMAT), Madrid, Spain*
[115]*Universidad Autónoma de Madrid, Madrid, Spain*
[116]*Universidad de Oviedo, Instituto Universitario de Ciencias y Tecnologías Espaciales de Asturias (ICTEA), Oviedo, Spain*
[117]*Instituto de Física de Cantabria (IFCA), CSIC-Universidad de Cantabria, Santander, Spain*
[118]*University of Colombo, Colombo, Sri Lanka*
[119]*University of Ruhuna, Department of Physics, Matara, Sri Lanka*
[120]*CERN, European Organization for Nuclear Research, Geneva, Switzerland*
[121]*Paul Scherrer Institut, Villigen, Switzerland*
[122]*ETH Zurich - Institute for Particle Physics and Astrophysics (IPA), Zurich, Switzerland*
[123]*Universität Zürich, Zurich, Switzerland*
[124]*National Central University, Chung-Li, Taiwan*
[125]*National Taiwan University (NTU), Taipei, Taiwan*
[126]*High Energy Physics Research Unit, Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok, Thailand*
[127]*Çukurova University, Physics Department, Science and Art Faculty, Adana, Turkey*
[128]*Middle East Technical University, Physics Department, Ankara, Turkey*
[129]*Bogazici University, Istanbul, Turkey*
[130]*Istanbul Technical University, Istanbul, Turkey*
[131]*Istanbul University, Istanbul, Turkey*
[132]*Yildiz Technical University, Istanbul, Turkey*
[133]*Institute for Scintillation Materials of National Academy of Science of Ukraine, Kharkiv, Ukraine*
[134]*National Science Centre, Kharkiv Institute of Physics and Technology, Kharkiv, Ukraine*
[135]*University of Bristol, Bristol, United Kingdom*
[136]*Rutherford Appleton Laboratory, Didcot, United Kingdom*
[137]*Imperial College, London, United Kingdom*
[138]*Brunel University, Uxbridge, United Kingdom*
[139]*Baylor University, Waco, Texas, USA*
[140]*Catholic University of America, Washington, DC, USA*
[141]*The University of Alabama, Tuscaloosa, Alabama, USA*
[142]*Boston University, Boston, Massachusetts, USA*
[143]*Brown University, Providence, Rhode Island, USA*
[144]*University of California, Davis, Davis, California, USA*
[145]*University of California, Los Angeles, California, USA*
[146]*University of California, Riverside, Riverside, California, USA*
[147]*University of California, San Diego, La Jolla, California, USA*
[148]*University of California, Santa Barbara - Department of Physics, Santa Barbara, California, USA*
[149]*California Institute of Technology, Pasadena, California, USA*
[150]*Carnegie Mellon University, Pittsburgh, Pennsylvania, USA*
[151]*University of Colorado Boulder, Boulder, Colorado, USA*
[152]*Cornell University, Ithaca, New York, USA*
[153]*Fermi National Accelerator Laboratory, Batavia, Illinois, USA*
[154]*University of Florida, Gainesville, Florida, USA*
[155]*Florida State University, Tallahassee, Florida, USA*
[156]*Florida Institute of Technology, Melbourne, Florida, USA*
[157]*University of Illinois Chicago, Chicago, USA, Chicago, USA*
[158]*The University of Iowa, Iowa City, Iowa, USA*
[159]*Johns Hopkins University, Baltimore, Maryland, USA*
[160]*The University of Kansas, Lawrence, Kansas, USA*
[161]*Kansas State University, Manhattan, Kansas, USA*
[162]*Lawrence Livermore National Laboratory, Livermore, California, USA*

[163]*University of Maryland, College Park, Maryland, USA*
[164]*Massachusetts Institute of Technology, Cambridge, Massachusetts, USA*
[165]*University of Minnesota, Minneapolis, Minnesota, USA*
[166]*University of Mississippi, Oxford, Mississippi, USA*
[167]*University of Nebraska-Lincoln, Lincoln, Nebraska, USA*
[168]*State University of New York at Buffalo, Buffalo, New York, USA*
[169]*Northeastern University, Boston, Massachusetts, USA*
[170]*Northwestern University, Evanston, Illinois, USA*
[171]*University of Notre Dame, Notre Dame, Indiana, USA*
[172]*The Ohio State University, Columbus, Ohio, USA*
[173]*Princeton University, Princeton, New Jersey, USA*
[174]*University of Puerto Rico, Mayaguez, Puerto Rico, USA*
[175]*Purdue University, West Lafayette, Indiana, USA*
[176]*Purdue University Northwest, Hammond, Indiana, USA*
[177]*Rice University, Houston, Texas, USA*
[178]*University of Rochester, Rochester, New York, USA*
[179]*The Rockefeller University, New York, New York, USA*
[180]*Rutgers, The State University of New Jersey, Piscataway, New Jersey, USA*
[181]*University of Tennessee, Knoxville, Tennessee, USA*
[182]*Texas A&M University, College Station, Texas, USA*
[183]*Texas Tech University, Lubbock, Texas, USA*
[184]*Vanderbilt University, Nashville, Tennessee, USA*
[185]*University of Virginia, Charlottesville, Virginia, USA*
[186]*Wayne State University, Detroit, Michigan, USA*
[187]*University of Wisconsin - Madison, Madison, Wisconsin, USA*
[188]*An institute or international laboratory covered by a cooperation agreement with CERN*

[a]Deceased.
[b]Also at Yerevan State University, Yerevan, Armenia.
[c]Also at TU Wien, Vienna, Austria.
[d]Also at Institute of Basic and Applied Sciences, Faculty of Engineering, Arab Academy for Science, Technology and Maritime Transport, Alexandria, Egypt.
[e]Also at Ghent University, Ghent, Belgium.
[f]Also at Universidade Estadual de Campinas, Campinas, Brazil.
[g]Also at Federal University of Rio Grande do Sul, Porto Alegre, Brazil.
[h]Also at UFMS, Nova Andradina, Brazil.
[i]Also at Nanjing Normal University, Nanjing, China.
[j]Also at The University of Iowa, Iowa City, Iowa, USA.
[k]Also at University of Chinese Academy of Sciences, Beijing, China.
[l]Also at China Center of Advanced Science and Technology, Beijing, China.
[m]Also at University of Chinese Academy of Sciences, Beijing, China.
[n]Also at China Spallation Neutron Source, Guangdong, China.
[o]Also at Henan Normal University, Xinxiang, China.
[p]Also at Université Libre de Bruxelles, Bruxelles, Belgium.
[q]Also at Another institute or international laboratory covered by a cooperation agreement with CERN.
[r]Also at Suez University, Suez, Egypt.
[s]Also at British University in Egypt, Cairo, Egypt.
[t]Also at Purdue University, West Lafayette, Indiana, USA.
[u]Also at Université de Haute Alsace, Mulhouse, France.
[v]Also at Department of Physics, Tsinghua University, Beijing, China.
[w]Also at The University of the State of Amazonas, Manaus, Brazil.
[x]Also at Erzincan Binali Yildirim University, Erzincan, Turkey.
[y]Also at University of Hamburg, Hamburg, Germany.
[z]Also at RWTH Aachen University, III. Physikalisches Institut A, Aachen, Germany.
[aa]Also at Isfahan University of Technology, Isfahan, Iran.
[bb]Also at Bergische University Wuppertal (BUW), Wuppertal, Germany.
[cc]Also at Brandenburg University of Technology, Cottbus, Germany.
[dd]Also at Forschungszentrum Jülich, Juelich, Germany.
[ee]Also at CERN, European Organization for Nuclear Research, Geneva, Switzerland.
[ff]Also at Institute of Physics, University of Debrecen, Debrecen, Hungary.

[gg]Also at Institute of Nuclear Research ATOMKI, Debrecen, Hungary.
[hh]Also at Universitatea Babes-Bolyai—Facultatea de Fizica, Cluj-Napoca, Romania.
[ii]Also at MTA-ELTE Lendület CMS Particle and Nuclear Physics Group, Eötvös Loránd University, Budapest, Hungary.
[jj]Also at Physics Department, Faculty of Science, Assiut University, Assiut, Egypt.
[kk]Also at HUN-REN Wigner Research Centre for Physics, Budapest, Hungary.
[ll]Also at Punjab Agricultural University, Ludhiana, India.
[mm]Also at University of Visva-Bharati, Santiniketan, India.
[nn]Also at Indian Institute of Science (IISc), Bangalore, India.
[oo]Also at Birla Institute of Technology, Mesra, Mesra, India.
[pp]Also at IIT Bhubaneswar, Bhubaneswar, India.
[qq]Also at Institute of Physics, Bhubaneswar, India.
[rr]Also at University of Hyderabad, Hyderabad, India.
[ss]Also at Deutsches Elektronen-Synchrotron, Hamburg, Germany.
[tt]Also at Department of Physics, Isfahan University of Technology, Isfahan, Iran.
[uu]Also at Sharif University of Technology, Tehran, Iran.
[vv]Also at Department of Physics, University of Science and Technology of Mazandaran, Behshahr, Iran.
[ww]Also at Department of Physics, Faculty of Science, Arak University, ARAK, Iran.
[xx]Also at Helwan University, Cairo, Egypt.
[yy]Also at Italian National Agency for New Technologies, Energy and Sustainable Economic Development, Bologna, Italy.
[zz]Also at Centro Siciliano di Fisica Nucleare e di Struttura Della Materia, Catania, Italy.
[aaa]Also at Università degli Studi Guglielmo Marconi, Roma, Italy.
[bbb]Also at Scuola Superiore Meridionale, Università di Napoli "Federico II," Napoli, Italy.
[ccc]Also at Fermi National Accelerator Laboratory, Batavia, Illinois, USA.
[ddd]Also at Laboratori Nazionali di Legnaro dell'INFN, Legnaro, Italy.
[eee]Also at Ain Shams University, Cairo, Egypt.
[fff]Also at Consiglio Nazionale delle Ricerche—Istituto Officina dei Materiali, Perugia, Italy.
[ggg]Also at Department of Applied Physics, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, Bangi, Malaysia.
[hhh]Also at Consejo Nacional de Ciencia y Tecnología, Mexico City, Mexico.
[iii]Also at Trincomalee Campus, Eastern University, Sri Lanka, Nilaveli, Sri Lanka.
[jjj]Also at Saegis Campus, Nugegoda, Sri Lanka.
[kkk]Also at National and Kapodistrian University of Athens, Athens, Greece.
[lll]Also at Ecole Polytechnique Fédérale Lausanne, Lausanne, Switzerland.
[mmm]Also at Universität Zürich, Zurich, Switzerland.
[nnn]Also at Stefan Meyer Institute for Subatomic Physics, Vienna, Austria.
[ooo]Also at Laboratoire d'Annecy-le-Vieux de Physique des Particules, IN2P3-CNRS, Annecy-le-Vieux, France.
[ppp]Also at Near East University, Research Center of Experimental Health Science, Mersin, Turkey.
[qqq]Also at Konya Technical University, Konya, Turkey.
[rrr]Also at Izmir Bakircay University, Izmir, Turkey.
[sss]Also at Adiyaman University, Adiyaman, Turkey.
[ttt]Also at Bozok Universitetesi Rektörlügü, Yozgat, Turkey.
[uuu]Also at Marmara University, Istanbul, Turkey.
[vvv]Also at Milli Savunma University, Istanbul, Turkey.
[www]Also at Kafkas University, Kars, Turkey.
[xxx]Also at Istanbul Okan University, Istanbul, Turkey.
[yyy]Also at Hacettepe University, Ankara, Turkey.
[zzz]Also at Istanbul University—Cerrahpasa, Faculty of Engineering, Istanbul, Turkey.
[aaaa]Also at Yildiz Technical University, Istanbul, Turkey.
[bbbb]Also at Vrije Universiteit Brussel, Brussel, Belgium.
[cccc]Also at School of Physics and Astronomy, University of Southampton, Southampton, United Kingdom.
[dddd]Also at IPPP Durham University, Durham, United Kingdom.
[eeee]Also at Monash University, Faculty of Science, Clayton, Australia.
[ffff]Also at Università di Torino, Torino, Italy.
[gggg]Also at Bethel University, St. Paul, Minnesota, USA.
[hhhh]Also at Karamanoğlu Mehmetbey University, Karaman, Turkey.
[iiii]Also at California Institute of Technology, Pasadena, California, USA.
[jjjj]Also at United States Naval Academy, Annapolis, Maryland, USA.
[kkkk]Also at Bingol University, Bingol, Turkey.
[llll]Also at Georgian Technical University, Tbilisi, Georgia.
[mmmm]Also at Sinop University, Sinop, Turkey.
[nnnn]Also at Erciyes University, Kayseri, Turkey.

[oooo]Also at Horia Hulubei National Institute of Physics and Nuclear Engineering (IFIN-HH), Bucharest, Romania.
[pppp]Also at Texas A&M University at Qatar, Doha, Qatar.
[qqqq]Also at Kyungpook National University, Daegu, Korea.
[rrrr]Also at Universiteit Antwerpen, Antwerpen, Belgium.
[ssss]Also at Yerevan Physics Institute, Yerevan, Armenia.
[tttt]Also at Northeastern University, Boston, Massachusetts, USA.
[uuuu]Also at Imperial College, London, United Kingdom.
[vvvv]Also at Institute of Nuclear Physics of the Uzbekistan Academy of Sciences, Tashkent, Uzbekistan.