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Search for a massive scalar resonance decaying to a light scalar and a Higgs boson in the four b quarks final state with boosted topology

The CMS Collaboration *

CERN, Geneva, Switzerland

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ABSTRACT

We search for new massive scalar particles X and Y through the resonant process $X \to YH \to b\bar{b}b\bar{b}$, where H is the standard model Higgs boson. Data from CERN LHC proton-proton collisions are used, collected at a centre-of-mass energy of 13 TeV in 2016–2018 and corresponding to an integrated luminosity of 138 fb^{-1}. The search is performed in mass ranges of 0.9–4 TeV for X and 60–600 GeV for Y, where both Y and H are reconstructed as Lorentz-boosted single large-area jets. The results are interpreted in the context of the next-to-minimal supersymmetric standard model and also in an extension of the standard model with two additional singlet scalar fields. The 95% confidence level upper limits for the production cross section vary between 0.1 and 150 fb depending on the X and Y masses, and represent a significant improvement over results from previous searches.

1. Introduction

The discovery of a Higgs boson (H) of mass 125 GeV [1–3] at the CERN LHC validated the Brout–Englert–Higgs mechanism [4–9] of the standard model (SM), yet raised questions of its viability at higher energy scales [10–13]. Besides, empirical observations such as the measurements of the neutrino masses and the baryon asymmetry in the universe are inconsistent with SM expectations. Beyond the standard model (BSM) theories, including those invoking supersymmetry [14] or extra dimensions [15], seek to address many of the shortcomings of the SM. No BSM phenomena have been observed at the LHC. However, there are unexplored BSM parameter spaces, among which are areas of the scalar sector, the topic of this search.

The minimal supersymmetric extension of the SM (MSSM) [16, 17] postulates two complex scalar field doublets with SU(2) gauge symmetry. The next-to-minimal model (NMSSM) [18,19] was proposed to solve the MSSM's "unnaturalness problem" [20], where the Higgs boson mass parameter is many orders of magnitude smaller than the Planck scale. In the NMSSM, an extra complex scalar field gives a total of seven Higgs bosons: three neutral (one would be associated with H) and two charged scalar particles, as well as two neutral pseudoscalars. Searches for a heavier scalar X decaying to SM particles [21–23] have set a lower limit on its mass at $M_X = 1.5\,(1.0)$ TeV for $\tan\beta = 21\,(8)$ [21], where $\tan\beta$ is the ratio of the vacuum expectation values (VEVs) of the two Higgs doublets. The NMSSM favours low $\tan\beta$, where the current M_X bounds are the weakest.

In the NMSSM, the neutral scalar production cross sections may be suppressed because of their small couplings to SM fermions [18]. Enhanced "Higgs-to-Higgs" decays are then possible, such as $X \to YH$ [24,25], Y being the lighter scalar. Within the NMSSM, the largest branching fractions for both H and Y (for Y mass M_Y less than twice that of the top quark t) are to a b quark-antiquark pair, giving the final state $X \to YH \to b\bar{b}b\bar{b}$. For higher M_Y values the $Y \to b\bar{b}$ branching fraction is ∼10% [25,26]. The second dominant process is $X \to YH \to \tau\tau b\bar{b}$, which has been excluded [27] for $0.4 < M_X < 0.6$ TeV and $50 < M_Y < 200$ GeV, for specific values of the parameters of the model.

Another interesting model of new physics that motivates this search is the two-real-scalar-singlet extension of the SM (TRSM) [28], which introduces two additional scalar fields. This simplified model, onto which more complicated theories can be mapped, has nine degrees of freedom: the masses and VEVs of the three scalar fields, and three mixing angles. In the scenario where all three VEVs are non-zero, the three fields give rise to three massive scalars, one of which can be associated with the H boson. Depending on their masses and mixing angles, the heaviest scalar can decay to the two lighter scalars. These in turn can decay to SM particles with mass-dependent branching fractions.

* *E-mail address:* cms-publication-committee-chair@cern.ch.

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This Letter describes the search for two new scalar particles, X and Y, the former being more massive and decaying through $X \to YH$. The search uses LHC proton-proton (pp) collision data collected by the CMS experiment in 2016–2018 corresponding to a total integrated luminosity of 138 fb^{-1} [29–31]. The masses of the scalar particles satisfy $M_X > M_Y + M_H$; Y may be lighter or heavier than H and both Y and H decay to $b\bar{b}$. The search is generic, and X and Y can be associated with the particles predicted in the NMSSM or the TRSM, which are both mentioned above.

This search focuses on the kinematic region where M_X is sufficiently larger than both M_Y and M_H such that Y and H carry considerable momenta and therefore their decay products, i.e. the $b\bar{b}$ pairs, are highly collimated. We explore the mass ranges $0.9 < M_X < 4$ TeV and $60 < M_Y < 600$ GeV, complementing the $X \to YH \to \tau\tau b\bar{b}$ search [27]. In the high-momentum kinematic regime, special techniques are used to reconstruct the final states containing the collimated $b\bar{b}$ pairs, in order to increase the signal sensitivity well beyond that covered by previous searches [27].

Tabulated results for this analysis are provided in HEPData [32].

2. The CMS detector and event reconstruction

The central feature of the CMS apparatus is a superconducting solenoid of 6 m internal diameter, providing a magnetic field of 3.8 T. Within the solenoid volume are a silicon pixel and strip tracker, a lead tungstate crystal electromagnetic calorimeter (ECAL), and a brass and scintillator hadron calorimeter (HCAL), each composed of a barrel and two endcap sections. Forward calorimeters extend the pseudorapidity (η) coverage provided by the barrel and endcap detectors. Muons are measured in gas-ionization detectors embedded in the steel flux-return yoke outside the solenoid. A more detailed description of the CMS detector, together with a definition of the coordinate system used and the relevant kinematic variables, can be found in Ref. [33]. Events of interest are selected using a two-tiered trigger system. The first level, composed of custom hardware processors, uses information from the calorimeters and muon detectors to select events at a rate of around 100 kHz within a fixed latency of about 4 μs [34]. The second level, known as the high-level trigger (HLT), consists of a farm of processors running a version of the full event reconstruction software optimized for fast processing, and reduces the event rate to around 1 kHz before data storage [35].

The primary vertex is taken to be the vertex corresponding to the hardest scattering in the event, evaluated using tracking information alone, as described in Section 9.4.1 of Ref. [36].

A particle-flow algorithm (PF) [37] aims to reconstruct and identify each individual particle in an event, with an optimized combination of information from the various elements of the CMS detector. The photon energy is obtained from the ECAL measurements. The energy of electrons is determined from a combination of the electron momentum at the primary interaction vertex as determined by the tracker, the energy of the corresponding ECAL cluster, and the energy sum of all bremsstrahlung photons spatially compatible with originating from the electron track. The energy of muons is obtained from the curvature of the corresponding track. The energy of charged hadrons is determined from a combination of their momentum measured in the tracker and the matching ECAL and HCAL energy deposits, corrected for the response function of the calorimeters to hadronic showers. Finally, the energy of neutral hadrons is obtained from the corresponding corrected ECAL and HCAL energies.

Jets are clustered from PF candidates using the anti-k_T algorithm [38,39] with a distance parameter of either 0.4 (AK4 jets) or 0.8 (AK8 jets). The jet momentum is defined as the vectorial sum of all particle momenta in a jet, and is found from simulation to be, on average, within 5–10% of the true momentum over the whole transverse momentum (p_T) spectrum and detector acceptance [40]. Additional pp interactions within the same or nearby bunch crossings (pileup), averaging 23–32 in 2016–2018, can contribute additional tracks and calorimetric energy depositions to the jet momentum. The effect of pileup is mitigated using the charged-hadron subtraction (CHS) algorithm [41], whereby charged particles identified to be originating from pileup vertices are discarded and an offset correction is applied to correct for remaining contributions. Jet energy corrections are derived from simulation and data to bring the measured response of jets to that of particle level jets on average [40].

For AK8 jets, masses are computed after applying grooming [42] techniques, which remove wide-angled soft and collinear radiation from the jets, in order to mitigate the effects of contamination from initial state radiation, the underlying event, and multiple hadron scattering. The trimming algorithm [43] uses a subjet size parameter of 0.3 and a radiation fraction parameter $z = 0.1$, which determines the minimum p_T fraction that the reclustered jet constituents need to have in order not to be removed. The mass of the resultant jet is referred to as its “trimmed mass”. The “soft-drop mass” of the jet is obtained by applying the soft-drop algorithm [44,45]. Here it is obtained using a value $z = 0.1$ for the radiation fraction parameter. The angular exponent parameter is set as $\beta = 0$, so there is no dependence of the p_T fraction threshold on the distance between jet constituents.

In case of the soft-drop algorithm, the pileup per particle identification (PUPPI) [41,46] algorithm is used to mitigate the effect of pileup on AK8 jets. In PUPPI, the treatment of charged particles is similar to that in CHS. A weight between zero and one is assigned to neutral particles, larger values indicating higher probability of originating from the primary interaction vertex. The jet mass is computed from the weighted sum of the constituent four-momenta.

The missing transverse momentum vector ($\vec{p}_T^{\,miss}$) is computed as the negative vector sum of the transverse momenta of all the PF candidates in an event, and its magnitude is denoted as p_T^{miss} [47]. The $\vec{p}_T^{\,miss}$ is modified to account for corrections to the energy scale of the reconstructed jets in the event.

3. Signal and background processes

Monte Carlo simulations of the signal process $X \to YH \to b\bar{b}b\bar{b}$, with a width of 1 MeV for all the three scalars, are generated at leading order (LO) using the MadGraph5_amc@nlo2.6.5 [48] event generator. The NMSSM model [49,50] is used to produce the simulated samples. However, the kinematic parameters are model-independent, enabling the results to be interpreted using other BSM scenarios.

The two main backgrounds are $t\bar{t}$+jets events, where the top quarks decay hadronically, and events with jets arising purely from SM quantum chromodynamics (QCD) interactions (multijet events). Other sources of background like single top quark production, and Higgs boson production in association with a top quark pair or a W or Z boson are found to have negligible contributions.

The $t\bar{t}$+jets events with hadronic top quark decays are modelled using powheg2.0 [51–54], at next-to-leading order (NLO). A sample of semileptonic $t\bar{t}$ decays, with one of the top quarks decaying via $t \to Wb \to \ell\nu b$, ℓ being a lepton (electron or muon), is also simulated using the same configuration. These events are used in dedicated $t\bar{t}$ enriched control regions to derive additional data-to-simulation correction factors. The simulated $t\bar{t}$+jets event yields are scaled using a cross section of 832^{+46}_{-52} pb, calculated at next-to-next-to-leading order (NNLO) in QCD with soft gluon resummation at next-to-next-to-leading logarithmic precision [55]. The QCD multijet event samples, containing two to four jets, are simulated at LO using the MadGraph5_amc@nlo event generator and are used to develop the tools for the analysis. However, this background is estimated using data-driven techniques.

The signal and semileptonic $t\bar{t}$+jets samples are generated using the NNPDF3.1 [56] NNLO parton distribution functions (PDFs) from the LHAPDF6 PDF library [57]. The hadronic $t\bar{t}$+jets samples are generated using NNPDF3.0 [58] NLO for 2016 and NNPDF3.1 NNLO for 2017 and 2018 simulation. The multijet background samples are generated using NNPDF3.0 LO for the 2016 and NNPDF3.1 NNLO for the 2017 and 2018 simulation.

The showering and hadronization of partons are simulated with pythia8.226 [59] for 2016 and pythia8.240 for 2017 and 2018 samples. The jet-to-parton matching for all LO samples, i.e. the signal and the multijets background, use the MLM [60] scheme. The CP5 tune [61] is used for all samples, except for the 2016 $t\bar{t}$ and multijet samples, which use CUETP8M2T4 [62] and CUETP8M1 [63] tunes, respectively.

All generated events are processed through a simulation of the CMS detector based on Geant4 [64]. The effects of pileup are modelled assuming a total inelastic pp cross section of 69.2 mb [65]. All simulated event samples are weighted to match the distribution of the expected pileup profile of the data.

4. Event selection

The events are selected in two mutually-exclusive categories: an "all-jets" event sample containing only jets, and a "jets+lepton" sample, containing a lepton (electron or muon). The latter serves to derive corrections to the simulated $t\bar{t}$+jets background, in order to match the expectations in the data.

4.1. All-jets event selection

A set of triggers based on requirements on jet properties are used for online event selection in the all-jets category.

One trigger criterion required a single AK8 jet with $p_T > 450$ or 500 GeV in 2016 and in 2017–2018, respectively. A second trigger required that the scalar sum (H_T) of the p_T of all AK4 jets with $p_T > 30$ GeV and $|\eta| < 2.5$ should be greater than 800 or 900 GeV in 2016, depending on the LHC beam instantaneous luminosity. In 2017–2018, $H_T > 1050$ GeV was required.

The third trigger algorithm used required an AK8 jet with a trimmed mass >30 GeV along with $p_T > 360$ GeV (in 2016). In 2017–2018, the AK8 jet p_T threshold in this trigger was raised to 400 or 420 GeV, depending on the LHC beam instantaneous luminosity, keeping the same trimmed mass criterion. The fourth trigger required $H_T > 650$ or 700 GeV (in 2016) and $H_T > 800$ GeV (in 2017–2018), together with an AK8 jet having a trimmed mass >50 GeV.

In addition to the above, three trigger algorithms were used in 2016 only, with the following criteria: (1) two AK8 jets with $p_T > 280$ and >200 GeV with one of them having a trimmed mass >30 GeV; (2) having the same requirements as (1) and with one of the AK8 jets passing a loose b tagging criterion using the "combined secondary vertex" algorithm [66] (with efficiency $\approx 81\%$); (3) $H_T \geq 650$ GeV with a pair of AK4 jets having an invariant mass >900 GeV with their pseudorapidity separation $|\Delta\eta| < 1.5$.

The combined logical OR of all the triggers improves the overall trigger efficiency, particularly for signals with low values of M_X.

Events in the offline all-jets selection are required to have at least two AK8 jets with $p_T > 350\,(450)$ GeV and $|\eta| < 2.4\,(2.5)$ for 2016 (2017–2018). The higher p_T requirement in 2017–2018 reflects the higher trigger thresholds and ensures a trigger efficiency close to 100%. The AK8 jet pairs in multijet backgrounds tend to have a larger separation in pseudorapidity than the signal, for a given M_{JJ} range, and therefore a selection $|\Delta\eta| < 1.3$ is used to reduce such backgrounds.

The two leading-p_T jets are considered for $H \to b\bar{b}$ and $Y \to b\bar{b}$ candidates. An $H \to b\bar{b}$ candidate or an "H jet" is a jet whose soft-drop mass is $110 < M_J^H < 140$ GeV. The second jet is designated as the $Y \to b\bar{b}$ candidate or the "Y jet" if its soft-drop mass satisfies $M_J^Y > 60$ GeV. When both AK8 jets satisfy the first mass requirement, the Y jet is chosen at random. Events without either an H or a Y jet are rejected. The mass of the Y jet and the invariant mass of the H and Y jets are used to isolate the signal with approximately 15% and 9% resolution in M_J^Y and M_{JJ}, respectively.

The all-jets event category trigger efficiency is measured in the data requiring a single AK4 jet with $p_T > 260$ GeV by applying the above offline selection, and counting the number of events passing the trigger selection. It is found to be between 94 and 100%. Simulated events are weighted by this efficiency as a function of the invariant mass of the two leading-p_T AK8 jets in the event, M_{JJ}.

A graph convolutional neural network algorithm, ParticleNet [67], is employed to discriminate the decays of a boosted massive particle R, which could be an H boson or a Y resonance, to a pair of b quarks against a background of other jets, using the properties of the jet PF constituents as features. As with all heavy-flavour jet classifiers, displaced tracks and vertices are the most important features. The multiclassifier ParticleNet algorithm outputs several variables, each in the range 0–1, and each of which can be interpreted as the probability of a jet having originated from a certain decay, such as from a massive resonance $R \to b\bar{b}$ ($P(R \to b\bar{b})$) or from a light-flavoured quark or a gluon (P(QCD)). In this analysis, the ParticleNet score is defined as $P(R \to b\bar{b})/(P(R \to b\bar{b}) + P(\mathrm{QCD}))$, where $P(R \to b\bar{b})$ is a unified score for jets originating from H or Y decays.

The ParticleNet algorithm is trained [68] on AK8 jets using as the signal simulated Lorentz-boosted spin-0 particles decaying to a pair of b quarks, with a wide range of masses. The QCD multijet samples are used for the background. The wide signal mass range in the training sample ensures that the background rejection rate is decorrelated from the mass of the jet [68]. As a consequence, background enriched regions can be defined using low ParticleNet scores on jets that have the same mass spectra as that of the background in the signal region. An accurate background model can therefore be developed.

The ParticleNet scores used for selecting the $H \to b\bar{b}$ and the $Y \to b\bar{b}$ candidates ("signal jets") are either >0.98 (tight requirement) or >0.94 (loose requirement). Depending on the jet p_T, the former has an efficiency of 62–72% and a misidentification rate of 0.45%, while the latter has an efficiency of 80–85% and a misidentification rate of 1%.

The efficiency of the ParticleNet classifier is calibrated in data using a sample of jets originating from fragmentation of a gluon to $b\bar{b}$ ($g \to b\bar{b}$), which are similar to $H \to b\bar{b}$ and $Y \to b\bar{b}$ jets. Such jets are selected from the data using a boosted decision tree (BDT) classifier, such that their ensemble ParticleNet score resembles that of Y and H jets. Using simulated multijet events, the BDT is trained to separate $g \to b\bar{b}$ jets from jets of other flavours. A systematic uncertainty is assigned to account for different possible choices of such jets. The measurements give a data-to-simulation correction factor of 0.9–1.4 for the ParticleNet selection efficiencies, depending on the jet p_T and data-taking year.

The ParticleNet scores of the H and Y jets are used to classify events into either signal, sideband, or validation categories. A layout of the different regions is shown in Fig. 1.

Two signal regions are defined using the tight and the loose ParticleNet scores (Fig. 1). The "signal region 1" (SR1) and the "signal region 2" (SR2) are statistically exclusive. SR1 has a higher signal-to-background ratio and is thus more sensitive to the pres-

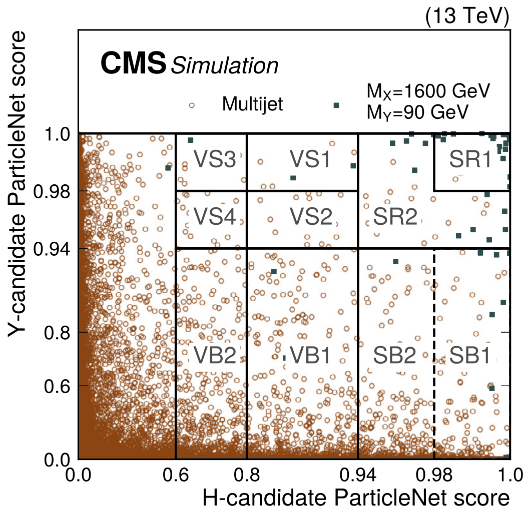

Fig. 1. Simulated ParticleNet score distributions of the H and the Y candidate jets for a signal with $M_X = 1600$ GeV and $M_Y = 90$ GeV (filled squares) and the multijets background (open circles). The grid lines show the different event categories defined using the ParticleNet scores of the two jets. A description of the regions is given in the text.

ence of signal. However, the SR2 improves the sensitivity for signal mass points with low background by increasing the signal efficiency.

Corresponding to the two signal regions, two "sideband regions" are defined for estimating the multijet background from data. They are labelled as "Sideband 1" (SB1) and "Sideband 2" (SB2) in Fig. 1. The SB2 region includes SB1 in order to provide better sideband region characteristics for estimating the multijets background in their respective signal regions.

In addition, six "validation regions" are used to validate the background estimation method. They are grouped into two sets of three regions: VS1, VS2, VB1, and VS3, VS4, VB2 as shown in Fig. 1. The labels VS and VB stand for "signal-like" and "background-like" validation regions, respectively. All these regions are enriched in QCD multijet events, and have much smaller signal-to-background ratios than the signal regions.

The signal selection efficiencies range from 1.7% to 12.6% in SR1 and 1.3% to 5.6% in SR2. Based on simulation, the background composition is about an equal proportion of $t\bar{t}$+jets and QCD multijets in the signal regions and in the corresponding validation regions, VS1–VS4. However, the sideband and validation sideband regions are composed $\approx$ 90% of multijet events.

4.2. Jets+lepton event selection

The triggers in the jets+lepton category required events to have either an isolated muon of $p_T > 24$ or 27 GeV; an isolated electron having $p_T > 27$, 32, or 35 GeV, or a photon with $p_T > 175$ or 200 GeV. The thresholds changed between data-taking years. The jets+lepton event trigger efficiencies are measured in a sample of $Z \to \ell\ell$ events and are found to be close to 100%.

Offline selection requires the events to have a lepton with $p_T > 40$ GeV and $|\eta| < 2.4$. Tight identification and isolation criteria are used for electrons [69] and muons [70]. An AK4 jet, corrected for pileup using charged hadron subtraction [41] and tagged as originating from a bottom quark (b-tagged) using the DeepJet algorithm [71], is required to be close to the lepton. The criterion is $\Delta R(\text{lepton, jet}) < 1.5$, where $\Delta R(1,2) \equiv \sqrt{(\eta_1-\eta_2)^2+(\varphi_1-\varphi_2)^2}$ is the distance between two objects in the pseudorapidity–azimuthal angle plane.

The loose DeepJet working point, with a mistag rate of 10% and approximately 90% efficiency, is used. The DeepJet score distributions of the AK4 jets are corrected using a weight extracted from measurements in the data [66]. Requirements of $p_T^{miss} > 60$ GeV and $H_T > 500$ GeV are imposed. The lepton, p_T^{miss}, and the b-tagged jet provide the signature of the leptonic decay of a top quark. A hadronically decaying top quark candidate is reconstructed from an AK8 jet with $p_T > 350\,(450)$ GeV and $|\eta| < 2.4\,(2.5)$ for 2016 (2017–2018), a soft-drop mass $>$60 GeV, and satisfying $\Delta R(\text{lepton, AK8 jet}) > 2$. Events in the jets+lepton category, which has a purity of $>$90%, are split into two regions based on whether the AK8 jet passes the tight or loose ParticleNet scores. Two separate correction factors are derived, one each for SR1 and SR2.

5. Background estimation

The analysis searches for a narrow signal in the 2-dimensional plane spanned by M_{JJ} and M_J^Y. The two-dimensional (M_{JJ}, M_J^Y) distributions of the multijet events are estimated using a pass-to-fail ratio method, described in the following paragraphs. The simulated $t\bar{t}$+jets event distributions are corrected by fitting the top quark jet mass M_J^t distributions to the data in the jets+lepton regions.

The multijet background is estimated for the three data-taking years combined. First, transfer functions, $R_{P/F}$, are defined as the ratio of event distributions in the (M_{JJ}, M_J^Y) plane in the signal regions to those in the sidebands, SR1-to-SB1 and SR2-to-SB2. These are a priori unknown, and are determined from the fit of signal and background distributions to the data.

An initial estimate $R_{P/F}^{init}$ is made using the first set of validation regions, using the data and correcting for the simulated $t\bar{t}$+jets component: VS1-to-VB1 and VS2-to-VB1. With the definition $R_{P/F} \equiv R_{P/F}^{init} R_{ratio}$, only the correction function R_{ratio} needs to be determined directly from the fit to the data. The validation regions provide a good estimate of $R_{P/F}$, because the pass-to-fail event ratios SR1-to-SB1 and SR2-to-SB2 are close to VS1-to-VB1 and VS2-to-VB1, as borne out in simulations. The values of R_{ratio} are therefore of order unity and lead to stability of the fit of signal and background models to the data.

The values of $R_{P/F}^{init}$, closely related to the loose and tight misidentification rates of the ParticleNet tagger, are determined as functions of M_J^Y only. The 1-dimensional modelling reduces the statistical uncertainties in the $R_{P/F}^{init}$. A quadratic function is found to be the best model. Furthermore, the $R_{P/F}$ dependence on M_{JJ} is weaker and is modelled through the R_{ratio}, determined directly from the fit to the data in the signal regions.

The form of the R_{ratio} is chosen to be a product of two polynomials in M_J^Y and M_{JJ}, whose parameters are determined from a simultaneous fit of the binned signal and background distributions to the data in SR1, SR2, SB1, and SB2. A variable bin width over the (M_{JJ}, M_J^Y) plane was chosen to correspond to the signal resolution while ensuring that there were no zero-event bins in the sideband regions.

A Fisher's F-test [72] is used to determine the minimum polynomial order necessary and sufficient for the model. Starting from polynomials of order one in both M_{JJ} and M_J^Y, terms are added until no significant improvement is observed. The F-test shows that linear functions in both M_{JJ} and M_J^Y are favoured at 95% confidence level (CL). The two R_{ratio} values range from 0.4 to 2.9 over the whole (M_{JJ}, M_J^Y) plane.

The simulated $t\bar{t}$+jets event distributions in (M_{JJ}, M_J^Y) for the signal regions are corrected for their shape and yield using the jets+lepton event category, which is highly enriched in this background. The AK8 jets from top quark decays fall into three categories, depending on the top quark boost. A high enough boost may result in a fully merged $t \to Wb \to q\overline{q}'b$ decay, labelled as a bqq jet. At moderate boosts, the $W \to q\overline{q}'$ may be merged to form a W jet with the b quark forming its own jet. However, such events are nearly all eliminated in the event selection. Finally, one of the quarks from the W boson decay can merge with the b quark to form a bq jet. Unmerged jets and other combinatorial backgrounds constitute a small fraction outside these three categories.

The masses of the bqq and bq jet components in the jets+lepton event category are fit to the data simultaneously with the all-jets event categories. These two mass distributions are scaled independently, with each being tied to the corresponding jet component from the $t\overline{t}$+jets in SR1 and SR2. They are independent for the three years, giving six scales in total ranging from 0.79 to 1.35.

Two sets of cross-checks are performed for the background estimation method. The first is to predict the background in the validation regions VS1 and VS2 using the validation region VB1 as a sideband. The $R^{\text{init}}_{\text{P/F}}$ are estimated from the ratios of events in the regions VS3 to VB2 and VS4 to VB2. The jets+lepton regions are treated as they would be for the true background estimation in the signal regions. Similar to the actual background estimation process, a Fisher's test is used to decide the polynomial order of the R_{ratio} function. Again, the most favoured form for R_{ratio} is found to be the product of linear functions along both M_{JJ} and in M^{Y}_{J}. A goodness-of-fit test confirmed the agreement between the data and the estimated background, with the p-value greater than 0.05.

The second check uses generated toy data sets for SR1 and SR2. A toy QCD multijets background is first obtained for these regions by applying the $R_{\text{P/F}}$ of VS1 and VS2, obtained in the first validation exercise, to SB1 and SB2, respectively. The toy multijets background is then combined with the $t\overline{t}$+jets sample and different signal strengths to get the toy data sets. The test consists of comparing the estimated and true signal strengths after the full background estimation and signal extraction procedure. The test shows no bias in the estimated signal yields for a wide range of M_{X} and M_{Y}.

6. Systematic uncertainties

Several sources of systematic uncertainty affect the (M_{JJ}, M^{Y}_{J}) shapes and the yields of the signals and backgrounds. The impact of the systematic uncertainties is reported for a signal with $M_{\text{X}} = 1.6$ TeV and $M_{\text{Y}} = 150$ GeV.

- *ParticleNet scale factor*: the uncertainty is 7–37%, depending on the AK8 jet p_{T}, and affects the signal by 15%.
- *Jet energy scale and resolution*: the uncertainties are applied to both AK4 and AK8 jets, and are fully correlated between the two sets of jets. The signal is affected by 5%.
- *Jet mass scale*: this is modelled as a ±5% shift in the AK8 jet soft-drop mass. It is uncorrelated between the bqq, the bq, and the signal jets. It affects the signal by 13%. The jet mass scale uncertainty in the $t\overline{t}$+jets background is reduced by including the jets+lepton control region.
- *Jet mass resolution*: simulated AK8 jet masses are smeared to match their distributions in the data, based on studies using Lorentz-boosted $W \to q\overline{q}'$ (W boson jets). The nominal simulated unsmeared jet mass resolution is taken as the downward uncertainty while applying a 20% larger smear [41] is used to estimate the upward uncertainty in the AK8 jet mass resolution. The resultant impact on the signal yield is an uncertainty of 4%.

The following uncertainties affect only the backgrounds.

- $t\overline{t}$ *normalization*: the uncertainties in the bqq and bq jet scale factors range from 6% to 16%.
- *Top quark p_{T} modelling in Monte Carlo simulations*: an uncertainty is assigned to the $t\overline{t}$+jets simulation process [73], resulting in a 2% uncertainty in this background.
- *Multijets background uncertainty*: the uncertainty derives mainly from the uncertainty in the $R^{\text{init}}_{\text{P/F}}(M^{\text{Y}}_{\text{J}})$, which is driven by the sample sizes in the sideband regions VS1, VS2, and VB1. It corresponds to a 7–11% change in the multijet background yields.

Other systematic uncertainties with minor impact are the following.

- *Trigger efficiency*: the difference between the jet energy scale at the HLT and in the offline reconstruction [74] is appreciable for $M_{\text{JJ}} < 1100$ GeV, resulting in the trigger efficiency dropping below 100%. An uncertainty equal to half of the difference between unity and the measured trigger efficiency is assigned. It is larger than the statistical uncertainty and is expected to cover jet energy scale uncertainties in the trigger efficiencies. Its maximum value is 3%.
- *Trigger timing correction*: during the 2016–2017 data taking, a gradual shift in the timing of the inputs of the ECAL hardware level trigger in the region of $|\eta| > 2$ caused a specific trigger inefficiency. To take this effect into account, a 2% normalization uncertainty is applied to $t\overline{t}$ events and signal for these years.
- *Integrated luminosity*: the uncertainty in the total Run 2 (2016–2018) integrated luminosity [30,31] is 1.6%.
- *Pileup*: the value of the pp total inelastic cross section that is used in the simulation of pileup events is varied upwards and downwards from its assumed value of 69.2 mb by its uncertainty of 4.6% [65].
- *PDF and scale uncertainties*: the impact of the PDF and the QCD factorization μ_{F} and renormalization μ_{R} scale uncertainties in the signal acceptance and selection is estimated to be 1%. The former is derived using the PDF4LHC procedure [75] and the NNPDF3.1 PDF sets. The latter is evaluated by separately changing μ_{R} and μ_{F} in simulation by factors of 0.5 and 2.
- *Sample size of sideband regions*: the effects of the limited sizes of the SB1 and SB2 samples are included as statistical uncertainties in the multijets background predicted in SR1 and SR2, using the Barlow–Beeston Lite prescription [76,77]. These uncertainties are small compared to the uncertainties in $R^{\text{init}}_{\text{P/F}}$.
- *Lepton ID and isolation efficiencies*: the data-to-simulation correction factors for the efficiencies have uncertainties that affect the event yields by 1–2% in the jets+lepton selection.
- *AK4 jet b-tagging data-to-simulation scale factor uncertainty*: this uncertainty amounts to about 2% and affects the semileptonic $t\overline{t}$+jets event yields.

All uncertainties affecting the signal and the $t\overline{t}$+jets samples are uncorrelated among years, except those associated with the PDF choice, the renormalization and factorization scales, the pileup correction, the integrated luminosity, and the top quark p_{T} modelling.

7. Results

The joint likelihood of the signal + background (M_{JJ}, M^{Y}_{J}) distributions in the all-jets regions (SR1 and SR2; SB1 and SB2), along with the M^{t}_{J} distributions in the jets+lepton tight and loose regions is constructed. The binned signal (M_{JJ}, M^{Y}_{J}) distributions are extracted from 260 signal hypothesis simulations. A combined three-year multijets background component is used in the likelihood distribution to reduce the statistical uncertainty. However, the likelihood has three separate $t\overline{t}$+jets and signal components, one for each data-taking year. For the three years, 2016–2018, the data

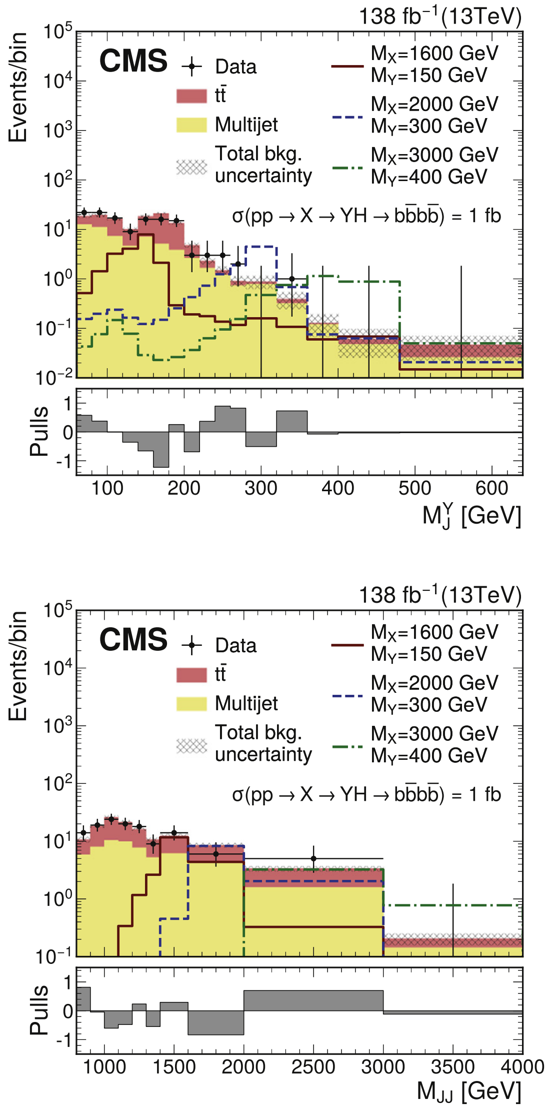

Fig. 2. The M_J^Y (upper) and M_{JJ} (lower) distributions for the number of observed events (black markers) compared with the estimated backgrounds (filled histograms) and their uncertainties (hatched areas) in SR1. The distributions expected from the signal under three M_X and M_Y hypotheses and assuming a cross section of 1 fb are also shown. The lower panels show the "Pulls" defined as (observed events−expected events)/$\sqrt{\sigma^2_{obs} - \sigma^2_{exp}}$, where σ_{obs} and σ_{exp} are the statistical and total uncertainties in the observation and the background estimation, respectively. The minus sign accounts for the correlation between data and the data-driven estimation.

distributions in the all-jets regions are added, while those for the jets+lepton regions are kept separate. The uncertainties are treated as nuisance parameters while fitting the signal+background models to the data. The distributions of the data, the post-fit background, and three representative signals in SR1 are shown in Fig. 2. The fitted distributions in the jets+lepton tight region, used for determining the corrections to the simulated $t\bar{t}$+jets events, are shown in Fig. 3 (for 2018).

The signal hypothesis with $M_X = 1.6$ TeV and $M_Y = 90$ GeV gives the highest observed local significance of 3.1σ, which becomes 0.7σ after accounting for the look-elsewhere effect [78]. However, the excess is not apparent in Fig. 2, which shows the separate 1-dimensional distributions of M_{JJ} and M_J^Y, integrated over the other variable. The estimated background is otherwise in agreement with the observed data. Upper limits on the signal cross section are calculated for various hypothesized values of M_X and M_Y.

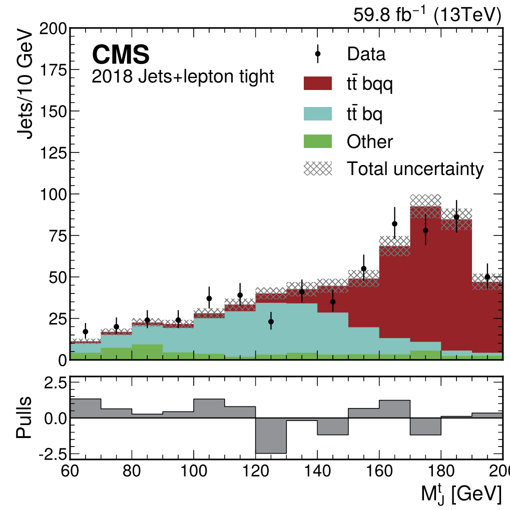

Fig. 3. The soft-drop mass distributions of the top quark candidate jets in the 2018 jets+lepton category, in the tight ParticleNet region, after the joint fit in the all-jets and jets+lepton categories. The observed data (black markers) and the post-fit estimate (filled histograms) are shown for the three jet categories. The lower panels show the "Pulls" defined as (observed events−expected events)/$\sqrt{\sigma^2_{obs} + \sigma^2_{exp}}$, where σ_{obs} and σ_{exp} are the total uncertainties in the observation and the background estimation, respectively.

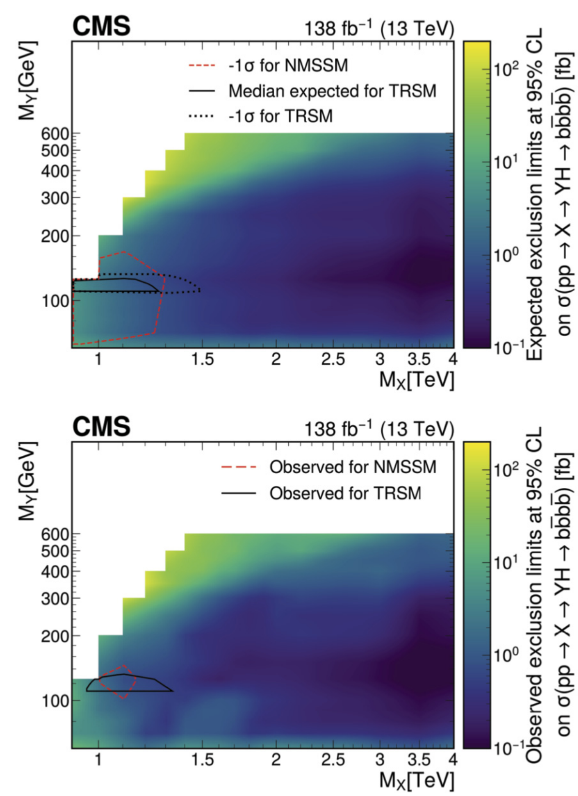

Fig. 4. The 95% confidence level expected (upper) and observed (lower) upper limits on $\sigma(pp \to X \to YH \to b\bar{b}b\bar{b})$ for different values of M_X and M_Y. The areas within the red and black contours represent the regions where the cross sections predicted by NMSSM and TRSM, respectively, are larger than the experimental limits. The areas within the dashed and dotted contours on the upper plot show the excluded masses at −1 standard deviation from the expected limits.

The upper limits are computed with a modified frequentist approach, using the CL_s criterion [79,80] with the profile likelihood ratio used as the test-statistic and with the asymptotic approximation [81]. As the signal distributions only assume that they originate from spin-0 particle decays, the limits are model-independent. The expected and observed limits at 95% CL as a function of M_X and M_Y are shown in Fig. 4, and range from 0.1 fb to 150 fb.

The cross section limits are compared with the maximally allowed cross sections in the NMSSM and TRSM. In the NMSSM, no mass range is excluded by the median expected limits. However, the observed limits exclude an area with M_X range of 1.00–1.15 TeV and M_Y range of 101–145 GeV. For TRSM, an expected exclusion area with the bounds $0.90 < M_X < 1.26$ TeV and $100 < M_Y < 126$ GeV is found while the observed exclusion range spans $0.95 < M_X < 1.33$ TeV and $110 < M_Y < 132$ GeV.

8. Summary

A search for massive scalar resonances X and Y, where X decays to Y and the standard model Higgs boson H, has been performed using proton-proton collision data collected at the LHC by the CMS detector between 2016 and 2018, and corresponding to an integrated luminosity of 138 fb^{-1}. Events are selected using jet substructure and neural network based boosted $H/Y \to b\bar{b}$ identification algorithms. Upper limits at 95% confidence level are set on the cross section of the process $pp \to X \to YH \to b\bar{b}b\bar{b}$ for assumed masses of X in the range 0.9–4 TeV and Y between 60–600 GeV. The expected and observed cross section limits for the considered process, set between 0.1 and 150 fb, are the most stringent to date over much of the explored mass range. These limits are interpreted as exclusion of possible M_X and M_Y within the frameworks of the next-to-minimal supersymmetric model and the two-real-scalar-singlet extension of the standard model.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Release and preservation of data used by the CMS Collaboration as the basis for publications is guided by the CMS policy as stated in "CMS data preservation, re-use and open access policy".

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The CMS Collaboration

A. Tumasyan [1]

Yerevan Physics Institute, Yerevan, Armenia

W. Adam, J.W. Andrejkovic, T. Bergauer, S. Chatterjee, K. Damanakis, M. Dragicevic, A. Escalante Del Valle, R. Frühwirth [2], M. Jeitler [2], N. Krammer, L. Lechner, D. Liko, I. Mikulec, P. Paulitsch, F.M. Pitters, J. Schieck [2], R. Schöfbeck, D. Schwarz, S. Templ, W. Waltenberger, C.-E. Wulz [2]

Institut für Hochenergiephysik, Vienna, Austria

M.R. Darwish [3], E.A. De Wolf, T. Janssen, T. Kello [4], A. Lelek, H. Rejeb Sfar, P. Van Mechelen, S. Van Putte, N. Van Remortel

Universiteit Antwerpen, Antwerpen, Belgium

E.S. Bols, J. D'Hondt, A. De Moor, M. Delcourt, H. El Faham, S. Lowette, S. Moortgat, A. Morton, D. Müller, A.R. Sahasransu, S. Tavernier, W. Van Doninck, D. Vannerom

Vrije Universiteit Brussel, Brussel, Belgium

D. Beghin, B. Clerbaux, G. De Lentdecker, L. Favart, K. Lee, M. Mahdavikhorrami, I. Makarenko, S. Paredes, L. Pétré, A. Popov, N. Postiau, E. Starling, L. Thomas, M. Vanden Bemden, C. Vander Velde, P. Vanlaer

Université Libre de Bruxelles, Bruxelles, Belgium

D. Dobur, J. Knolle, L. Lambrecht, G. Mestdach, M. Niedziela, C. Rendón, C. Roskas, A. Samalan, K. Skovpen, M. Tytgat, N. Van Den Bossche, B. Vermassen, L. Wezenbeek

Ghent University, Ghent, Belgium

A. Benecke, A. Bethani, G. Bruno, F. Bury, C. Caputo, P. David, C. Delaere, I.S. Donertas, A. Giammanco, K. Jaffel, Sa. Jain, V. Lemaitre, K. Mondal, J. Prisciandaro, A. Taliercio, T.T. Tran, P. Vischia, S. Wertz

Université Catholique de Louvain, Louvain-la-Neuve, Belgium

G.A. Alves, C. Hensel, A. Moraes, P. Rebello Teles

Centro Brasileiro de Pesquisas Fisicas, Rio de Janeiro, Brazil

W.L. Aldá Júnior, M. Alves Gallo Pereira, M. Barroso Ferreira Filho, H. Brandao Malbouisson, W. Carvalho, J. Chinellato [5], E.M. Da Costa, G.G. Da Silveira [6], D. De Jesus Damiao, V. Dos Santos Sousa, S. Fonseca De Souza, J. Martins [7], C. Mora Herrera, K. Mota Amarilo, L. Mundim, H. Nogima, A. Santoro, S.M. Silva Do Amaral, A. Sznajder, M. Thiel, F. Torres Da Silva De Araujo [8], A. Vilela Pereira

Universidade do Estado do Rio de Janeiro, Rio de Janeiro, Brazil

C.A. Bernardes [6], L. Calligaris, T.R. Fernandez Perez Tomei, E.M. Gregores, D.S. Lemos, P.G. Mercadante, S.F. Novaes, Sandra S. Padula

Universidade Estadual Paulista, Universidade Federal do ABC, São Paulo, Brazil

A. Aleksandrov, G. Antchev, R. Hadjiiska, P. Iaydjiev, M. Misheva, M. Rodozov, M. Shopova, G. Sultanov

Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Sofia, Bulgaria

A. Dimitrov, T. Ivanov, L. Litov, B. Pavlov, P. Petkov, A. Petrov

University of Sofia, Sofia, Bulgaria

T. Cheng, T. Javaid [9], M. Mittal, L. Yuan

Beihang University, Beijing, China

M. Ahmad, G. Bauer [10], C. Dozen, Z. Hu, Y. Wang, K. Yi [10,11]

Department of Physics, Tsinghua University, Beijing, China

E. Chapon, G.M. Chen [9], H.S. Chen [9], M. Chen, W. Fang [4], F. Iemmi, A. Kapoor, H. Liao, Z.-A. Liu [12], V. Milosevic, F. Monti, R. Sharma, J. Tao, J. Thomas-Wilsker, J. Wang, H. Zhang, J. Zhao

Institute of High Energy Physics, Beijing, China

A. Agapitos, Y. An, Y. Ban, C. Chen, A. Levin, Q. Li, X. Lyu, Y. Mao, S.J. Qian, D. Wang, J. Xiao, H. Yang

State Key Laboratory of Nuclear Physics and Technology, Peking University, Beijing, China

M. Lu, Z. You

Sun Yat-Sen University, Guangzhou, China

X. Gao [4], D. Leggat, H. Okawa, Y. Zhang

Institute of Modern Physics and Key Laboratory of Nuclear Physics and Ion-beam Application (MOE) - Fudan University, Shanghai, China

Z. Lin, M. Xiao

Zhejiang University, Hangzhou, Zhejiang, China

C. Avila, A. Cabrera, C. Florez, J. Fraga

Universidad de Los Andes, Bogota, Colombia

J. Mejia Guisao, F. Ramirez, J.D. Ruiz Alvarez

Universidad de Antioquia, Medellin, Colombia

D. Giljanovic, N. Godinovic, D. Lelas, I. Puljak

University of Split, Faculty of Electrical Engineering, Mechanical Engineering and Naval Architecture, Split, Croatia

Z. Antunovic, M. Kovac, T. Sculac

University of Split, Faculty of Science, Split, Croatia

V. Brigljevic, D. Ferencek, D. Majumder, M. Roguljic, A. Starodumov [13], T. Susa

Institute Rudjer Boskovic, Zagreb, Croatia

A. Attikis, K. Christoforou, G. Kole, M. Kolosova, S. Konstantinou, J. Mousa, C. Nicolaou, F. Ptochos, P.A. Razis, H. Rykaczewski, H. Saka

University of Cyprus, Nicosia, Cyprus

M. Finger [13], M. Finger Jr. [13], A. Kveton

Charles University, Prague, Czech Republic

E. Ayala

Escuela Politecnica Nacional, Quito, Ecuador

E. Carrera Jarrin

Universidad San Francisco de Quito, Quito, Ecuador

H. Abdalla [14], S. Khalil [15]

Academy of Scientific Research and Technology of the Arab Republic of Egypt, Egyptian Network of High Energy Physics, Cairo, Egypt

M.A. Mahmoud, Y. Mohammed

Center for High Energy Physics (CHEP-FU), Fayoum University, El-Fayoum, Egypt

S. Bhowmik, R.K. Dewanjee, K. Ehataht, M. Kadastik, S. Nandan, C. Nielsen, J. Pata, M. Raidal, L. Tani, C. Veelken

National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

P. Eerola, H. Kirschenmann, K. Osterberg, M. Voutilainen

Department of Physics, University of Helsinki, Helsinki, Finland

S. Bharthuar, E. Brücken, F. Garcia, J. Havukainen, M.S. Kim, R. Kinnunen, T. Lampén, K. Lassila-Perini, S. Lehti, T. Lindén, M. Lotti, L. Martikainen, M. Myllymäki, J. Ott, M.m. Rantanen, H. Siikonen, E. Tuominen, J. Tuominiemi

Helsinki Institute of Physics, Helsinki, Finland

P. Luukka, H. Petrow, T. Tuuva

Lappeenranta-Lahti University of Technology, Lappeenranta, Finland

C. Amendola, M. Besancon, F. Couderc, M. Dejardin, D. Denegri, J.L. Faure, F. Ferri, S. Ganjour, P. Gras, G. Hamel de Monchenault, P. Jarry, B. Lenzi, V. Lohezic, J. Malcles, J. Rander, A. Rosowsky, M.Ö. Sahin, A. Savoy-Navarro [16], P. Simkina, M. Titov

IRFU, CEA, Université Paris-Saclay, Gif-sur-Yvette, France

S. Ahuja, C. Baldenegro Barrera, F. Beaudette, M. Bonanomi, A. Buchot Perraguin, P. Busson, A. Cappati, C. Charlot, O. Davignon, B. Diab, G. Falmagne, B.A. Fontana Santos Alves, S. Ghosh, R. Granier de Cassagnac, A. Hakimi, B. Harikrishnan, J. Motta, M. Nguyen, C. Ochando, P. Paganini, L. Portales, J. Rembser, R. Salerno, U. Sarkar, J.B. Sauvan, Y. Sirois, A. Tarabini, E. Vernazza, A. Zabi, A. Zghiche

Laboratoire Leprince-Ringuet, CNRS/IN2P3, Ecole Polytechnique, Institut Polytechnique de Paris, Palaiseau, France

J.-L. Agram [17], J. Andrea, D. Apparu, D. Bloch, G. Bourgatte, J.-M. Brom, E.C. Chabert, C. Collard, D. Darej, J.-C. Fontaine [17], U. Goerlach, C. Grimault, A.-C. Le Bihan, E. Nibigira, P. Van Hove

Université de Strasbourg, CNRS, IPHC UMR 7178, Strasbourg, France

S. Beauceron, C. Bernet, G. Boudoul, C. Camen, A. Carle, N. Chanon, D. Contardo, P. Depasse, H. El Mamouni, J. Fay, S. Gascon, M. Gouzevitch, B. Ille, I.B. Laktineh, M. Lethuillier, L. Mirabito, S. Perries, K. Shchablo, V. Sordini, L. Torterotot, M. Vander Donckt, S. Viret

Institut de Physique des 2 Infinis de Lyon (IP2I), Villeurbanne, France

D. Chokheli, I. Lomidze, Z. Tsamalaidze [13]

Georgian Technical University, Tbilisi, Georgia

V. Botta, L. Feld, K. Klein, M. Lipinski, D. Meuser, A. Pauls, N. Röwert, J. Schulz, M. Teroerde

RWTH Aachen University, I. Physikalisches Institut, Aachen, Germany

A. Dodonova, N. Eich, D. Eliseev, M. Erdmann, P. Fackeldey, B. Fischer, T. Hebbeker, K. Hoepfner, F. Ivone, M.y. Lee, L. Mastrolorenzo, M. Merschmeyer, A. Meyer, S. Mondal, S. Mukherjee, D. Noll, A. Novak, A. Pozdnyakov, Y. Rath, H. Reithler, A. Schmidt, S.C. Schuler, A. Sharma, L. Vigilante, S. Wiedenbeck, S. Zaleski

RWTH Aachen University, III. Physikalisches Institut A, Aachen, Germany

C. Dziwok, G. Flügge, W. Haj Ahmad [18], O. Hlushchenko, T. Kress, A. Nowack, O. Pooth, D. Roy, A. Stahl [19], T. Ziemons, A. Zotz

RWTH Aachen University, III. Physikalisches Institut B, Aachen, Germany

H. Aarup Petersen, M. Aldaya Martin, P. Asmuss, S. Baxter, M. Bayatmakou, O. Behnke, A. Bermúdez Martínez, S. Bhattacharya, A.A. Bin Anuar, F. Blekman [20], K. Borras [21], D. Brunner, A. Campbell, A. Cardini, C. Cheng, F. Colombina, S. Consuegra Rodríguez, G. Correia Silva, M. De Silva, L. Didukh, G. Eckerlin, D. Eckstein, L.I. Estevez Banos, O. Filatov, E. Gallo [20], A. Geiser, A. Giraldi, G. Greau, A. Grohsjean, V. Guglielmi, M. Guthoff, A. Jafari [22], N.Z. Jomhari, B. Kaech, A. Kasem [21], M. Kasemann, H. Kaveh, C. Kleinwort, R. Kogler, D. Krücker, W. Lange, K. Lipka, W. Lohmann [23], R. Mankel, I.-A. Melzer-Pellmann, M. Mendizabal Morentin, J. Metwally, A.B. Meyer, M. Meyer, G. Milella, M. Mormile, A. Mussgiller, A. Nürnberg, Y. Otarid, D. Pérez Adán, D. Pitzl, A. Raspereza, B. Ribeiro Lopes, J. Rübenach, A. Saggio, A. Saibel, M. Savitskyi, M. Scham [24], V. Scheurer, S. Schnake, P. Schütze, C. Schwanenberger [20], M. Shchedrolosiev, R.E. Sosa Ricardo, D. Stafford, N. Tonon [†], M. Van De Klundert, F. Vazzoler, R. Walsh, D. Walter, Q. Wang, Y. Wen, K. Wichmann, L. Wiens, C. Wissing, S. Wuchterl, A. Zimermmane Castro Santos

Deutsches Elektronen-Synchrotron, Hamburg, Germany

R. Aggleton, S. Albrecht, S. Bein, L. Benato, P. Connor, K. De Leo, M. Eich, K. El Morabit, F. Feindt, A. Fröhlich, C. Garbers, E. Garutti, M. Hajheidari, J. Haller, A. Hinzmann, G. Kasieczka, R. Klanner, T. Kramer, V. Kutzner, J. Lange, T. Lange, A. Lobanov, A. Malara, C. Matthies, A. Mehta, L. Moureaux, A. Nigamova, K.J. Pena Rodriguez, M. Rieger, O. Rieger, P. Schleper, M. Schröder, J. Schwandt, H. Stadie, G. Steinbrück, A. Tews

University of Hamburg, Hamburg, Germany

J. Bechtel, S. Brommer, M. Burkart, E. Butz, R. Caspart, T. Chwalek, W. De Boer [†], A. Dierlamm, A. Droll, N. Faltermann, M. Giffels, J.O. Gosewisch, A. Gottmann, F. Hartmann [19], C. Heidecker, M. Horzela, U. Husemann, P. Keicher, R. Koppenhöfer, S. Maier, S. Mitra, Th. Müller, M. Neukum, G. Quast, K. Rabbertz, J. Rauser, D. Savoiu, M. Schnepf, D. Seith, I. Shvetsov, H.J. Simonis, R. Ulrich, J. van der Linden, R.F. Von Cube, M. Wassmer, M. Weber, S. Wieland, R. Wolf, S. Wozniewski, S. Wunsch

Karlsruher Institut fuer Technologie, Karlsruhe, Germany

G. Anagnostou, P. Assiouras, G. Daskalakis, A. Kyriakis, A. Stakia

Institute of Nuclear and Particle Physics (INPP), NCSR Demokritos, Aghia Paraskevi, Greece

M. Diamantopoulou, D. Karasavvas, P. Kontaxakis, C.K. Koraka, A. Manousakis-Katsikakis, A. Panagiotou, I. Papavergou, N. Saoulidou, K. Theofilatos, E. Tziaferi, K. Vellidis, E. Vourliotis

National and Kapodistrian University of Athens, Athens, Greece

G. Bakas, K. Kousouris, I. Papakrivopoulos, G. Tsipolitis, A. Zacharopoulou

National Technical University of Athens, Athens, Greece

K. Adamidis, I. Bestintzanos, I. Evangelou, C. Foudas, P. Gianneios, P. Katsoulis, P. Kokkas, N. Manthos, I. Papadopoulos, J. Strologas

University of Ioánnina, Ioánnina, Greece

M. Csanád, K. Farkas, M.M.A. Gadallah [25], S. Lökös [26], P. Major, K. Mandal, G. Pásztor, A.J. Rádl, O. Surányi, G.I. Veres

MTA-ELTE Lendület CMS Particle and Nuclear Physics Group, Eötvös Loránd University, Budapest, Hungary

M. Bartók [27], G. Bencze, C. Hajdu, D. Horvath [28,29], F. Sikler, V. Veszpremi

Wigner Research Centre for Physics, Budapest, Hungary

S. Czellar, D. Fasanella, F. Fienga, J. Karancsi [27], J. Molnar, Z. Szillasi, D. Teyssier

Institute of Nuclear Research ATOMKI, Debrecen, Hungary

P. Raics, Z.L. Trocsanyi [30], B. Ujvari [31]

Institute of Physics, University of Debrecen, Debrecen, Hungary

T. Csorgo [32], F. Nemes [32], T. Novak

Karoly Robert Campus, MATE Institute of Technology, Gyongyos, Hungary

J. Babbar, S. Bansal, S.B. Beri, V. Bhatnagar, G. Chaudhary, S. Chauhan, N. Dhingra [33], R. Gupta, A. Kaur, H. Kaur, M. Kaur, P. Kumari, M. Meena, K. Sandeep, J.B. Singh [34], A.K. Virdi

Panjab University, Chandigarh, India

A. Ahmed, A. Bhardwaj, B.C. Choudhary, M. Gola, S. Keshri, A. Kumar, M. Naimuddin, P. Priyanka, K. Ranjan, S. Saumya, A. Shah

University of Delhi, Delhi, India

R. Bhattacharya, S. Bhattacharya, D. Bhowmik, S. Dutta, S. Dutta, B. Gomber [35], M. Maity [36], P. Palit, P.K. Rout, G. Saha, B. Sahu, S. Sarkar, M. Sharan

Saha Institute of Nuclear Physics, HBNI, Kolkata, India

P.K. Behera, S.C. Behera, P. Kalbhor, J.R. Komaragiri [37], D. Kumar [37], A. Muhammad, L. Panwar [37], R. Pradhan, P.R. Pujahari, A. Sharma, A.K. Sikdar, P.C. Tiwari [37]

Indian Institute of Technology Madras, Madras, India

K. Naskar [38]

Bhabha Atomic Research Centre, Mumbai, India

T. Aziz, S. Dugad, M. Kumar, G.B. Mohanty

Tata Institute of Fundamental Research-A, Mumbai, India

S. Banerjee, R. Chudasama, M. Guchait, S. Karmakar, S. Kumar, G. Majumder, K. Mazumdar, S. Mukherjee

Tata Institute of Fundamental Research-B, Mumbai, India

S. Bahinipati [39], C. Kar, P. Mal, T. Mishra, V.K. Muraleedharan Nair Bindhu [40], A. Nayak [40], P. Saha, N. Sur, S.K. Swain, D. Vats [40]

National Institute of Science Education and Research, An OCC of Homi Bhabha National Institute, Bhubaneswar, Odisha, India

A. Alpana, S. Dube, B. Kansal, A. Laha, S. Pandey, A. Rastogi, S. Sharma

Indian Institute of Science Education and Research (IISER), Pune, India

H. Bakhshiansohi [41], E. Khazaie, M. Zeinali [42]

Isfahan University of Technology, Isfahan, Iran

S. Chenarani [43], S.M. Etesami, M. Khakzad, M. Mohammadi Najafabadi

Institute for Research in Fundamental Sciences (IPM), Tehran, Iran

M. Grunewald

University College Dublin, Dublin, Ireland

M. Abbrescia [a,b], R. Aly [a,c,44], C. Aruta [a,b], A. Colaleo [a], D. Creanza [a,c], N. De Filippis [a,c], M. De Palma [a,b], A. Di Florio [a,b], W. Elmetenawee [a,b], F. Errico [a,b], L. Fiore [a], G. Iaselli [a,c], M. Ince [a,b], S. Lezki [a,b], G. Maggi [a,c], M. Maggi [a], I. Margjeka [a,b], V. Mastrapasqua [a,b], S. My [a,b], S. Nuzzo [a,b], A. Pellecchia [a,b], A. Pompili [a,b], G. Pugliese [a,c], D. Ramos [a], A. Ranieri [a], G. Selvaggi [a,b], L. Silvestris [a], F.M. Simone [a,b], Ü. Sözbilir [a], R. Venditti [a], P. Verwilligen [a]

[a] *INFN Sezione di Bari, Bari, Italy*
[b] *Università di Bari, Bari, Italy*
[c] *Politecnico di Bari, Bari, Italy*

G. Abbiendi [a], C. Battilana [a,b], D. Bonacorsi [a,b], L. Borgonovi [a], L. Brigliadori [a], R. Campanini [a,b], P. Capiluppi [a,b], A. Castro [a,b], F.R. Cavallo [a], C. Ciocca [a], M. Cuffiani [a,b], G.M. Dallavalle [a], T. Diotalevi [a,b], F. Fabbri [a], A. Fanfani [a,b], P. Giacomelli [a], L. Giommi [a,b], C. Grandi [a], L. Guiducci [a,b], S. Lo Meo [a,45], L. Lunerti [a,b], S. Marcellini [a], G. Masetti [a], F.L. Navarria [a,b], A. Perrotta [a], F. Primavera [a,b], A.M. Rossi [a,b], T. Rovelli [a,b], G.P. Siroli [a,b]

[a] *INFN Sezione di Bologna, Bologna, Italy*
[b] *Università di Bologna, Bologna, Italy*

S. Albergo [a,b,46], S. Costa [a,b,46], A. Di Mattia [a], R. Potenza [a,b], A. Tricomi [a,b,46], C. Tuve [a,b]

[a] *INFN Sezione di Catania, Catania, Italy*
[b] *Università di Catania, Catania, Italy*

G. Barbagli [a], B. Camaiani [a,b], A. Cassese [a], R. Ceccarelli [a,b], V. Ciulli [a,b], C. Civinini [a], R. D'Alessandro [a,b], E. Focardi [a,b], G. Latino [a,b], P. Lenzi [a,b], M. Lizzo [a,b], M. Meschini [a], S. Paoletti [a], R. Seidita [a,b], G. Sguazzoni [a], L. Viliani [a]

[a] *INFN Sezione di Firenze, Firenze, Italy*
[b] *Università di Firenze, Firenze, Italy*

L. Benussi, S. Bianco, D. Piccolo

INFN Laboratori Nazionali di Frascati, Frascati, Italy

M. Bozzo [a,b], F. Ferro [a], R. Mulargia [a], E. Robutti [a], S. Tosi [a,b]

[a] *INFN Sezione di Genova, Genova, Italy*
[b] *Università di Genova, Genova, Italy*

A. Benaglia [a], G. Boldrini [a], F. Brivio [a,b], F. Cetorelli [a,b], F. De Guio [a,b], M.E. Dinardo [a,b], P. Dini [a], S. Gennai [a], A. Ghezzi [a,b], P. Govoni [a,b], L. Guzzi [a,b], M.T. Lucchini [a,b], M. Malberti [a], S. Malvezzi [a], A. Massironi [a], D. Menasce [a], L. Moroni [a], M. Paganoni [a,b], D. Pedrini [a], B.S. Pinolini [a], S. Ragazzi [a,b], N. Redaelli [a], T. Tabarelli de Fatis [a,b], D. Zuolo [a,b]

[a] INFN Sezione di Milano-Bicocca, Milano, Italy
[b] Università di Milano-Bicocca, Milano, Italy

S. Buontempo [a], F. Carnevali [a,b], N. Cavallo [a,c], A. De Iorio [a,b], F. Fabozzi [a,c], A.O.M. Iorio [a,b], L. Lista [a,b,47], S. Meola [a,d,19], P. Paolucci [a,19], B. Rossi [a], C. Sciacca [a,b]

[a] INFN Sezione di Napoli, Napoli, Italy
[b] Università di Napoli 'Federico II', Napoli, Italy
[c] Università della Basilicata, Potenza, Italy
[d] Università G. Marconi, Roma, Italy

P. Azzi [a], N. Bacchetta [a], D. Bisello [a,b], P. Bortignon [a], A. Bragagnolo [a,b], R. Carlin [a,b], P. Checchia [a], T. Dorigo [a], U. Dosselli [a], F. Gasparini [a,b], U. Gasparini [a,b], G. Grosso [a], L. Layer [a,48], E. Lusiani [a], M. Margoni [a,b], F. Marini [a], A.T. Meneguzzo [a,b], J. Pazzini [a,b], P. Ronchese [a,b], R. Rossin [a,b], F. Simonetto [a,b], G. Strong [a], M. Tosi [a,b], H. Yarar [a,b], M. Zanetti [a,b], P. Zotto [a,b], A. Zucchetta [a,b], G. Zumerle [a,b]

[a] INFN Sezione di Padova, Padova, Italy
[b] Università di Padova, Padova, Italy
[c] Università di Trento, Trento, Italy

C. Aimè [a,b], A. Braghieri [a], S. Calzaferri [a,b], D. Fiorina [a,b], P. Montagna [a,b], S.P. Ratti [a,b], V. Re [a], C. Riccardi [a,b], P. Salvini [a], I. Vai [a], P. Vitulo [a,b]

[a] INFN Sezione di Pavia, Pavia, Italy
[b] Università di Pavia, Pavia, Italy

P. Asenov [a,49], G.M. Bilei [a], D. Ciangottini [a,b], L. Fanò [a,b], M. Magherini [a,b], G. Mantovani [a,b], V. Mariani [a,b], M. Menichelli [a], F. Moscatelli [a,49], A. Piccinelli [a,b], M. Presilla [a,b], A. Rossi [a,b], A. Santocchia [a,b], D. Spiga [a], T. Tedeschi [a,b]

[a] INFN Sezione di Perugia, Perugia, Italy
[b] Università di Perugia, Perugia, Italy

P. Azzurri [a], G. Bagliesi [a], V. Bertacchi [a,c], L. Bianchini [a,b], T. Boccali [a], E. Bossini [a,b], D. Bruschini [a,c], R. Castaldi [a], M.A. Ciocci [a,b], V. D'Amante [a,d], R. Dell'Orso [a], M.R. Di Domenico [a,d], S. Donato [a], A. Giassi [a], F. Ligabue [a,c], E. Manca [a,c], G. Mandorli [a,c], D. Matos Figueiredo [a], A. Messineo [a,b], M. Musich [a,b], F. Palla [a], S. Parolia [a,b], G. Ramirez-Sanchez [a,c], A. Rizzi [a,b], G. Rolandi [a,c], S. Roy Chowdhury [a,c], A. Scribano [a], N. Shafiei [a,b], P. Spagnolo [a], R. Tenchini [a], G. Tonelli [a,b], N. Turini [a,d], A. Venturi [a], P.G. Verdini [a]

[a] INFN Sezione di Pisa, Pisa, Italy
[b] Università di Pisa, Pisa, Italy
[c] Scuola Normale Superiore di Pisa, Pisa, Italy
[d] Università di Siena, Siena, Italy

P. Barria [a], M. Campana [a,b], F. Cavallari [a], D. Del Re [a,b], E. Di Marco [a], M. Diemoz [a], E. Longo [a,b], P. Meridiani [a], G. Organtini [a,b], F. Pandolfi [a], R. Paramatti [a,b], C. Quaranta [a,b], S. Rahatlou [a,b], C. Rovelli [a], F. Santanastasio [a,b], L. Soffi [a], R. Tramontano [a,b]

[a] INFN Sezione di Roma, Roma, Italy
[b] Sapienza Università di Roma, Roma, Italy

N. Amapane [a,b], R. Arcidiacono [a,c], S. Argiro [a,b], M. Arneodo [a,c], N. Bartosik [a], R. Bellan [a,b], A. Bellora [a,b], J. Berenguer Antequera [a,b], C. Biino [a], N. Cartiglia [a], M. Costa [a,b], R. Covarelli [a,b], N. Demaria [a], M. Grippo [a,b], B. Kiani [a,b], F. Legger [a], C. Mariotti [a], S. Maselli [a], A. Mecca [a,b], E. Migliore [a,b], E. Monteil [a,b],

M. Monteno [a], M.M. Obertino [a,b], G. Ortona [a], L. Pacher [a,b], N. Pastrone [a], M. Pelliccioni [a], M. Ruspa [a,c], K. Shchelina [a], F. Siviero [a,b], V. Sola [a], A. Solano [a,b], D. Soldi [a,b], A. Staiano [a], M. Tornago [a,b], D. Trocino [a], G. Umoret [a,b], A. Vagnerini [a,b]

[a] *INFN Sezione di Torino, Torino, Italy*
[b] *Università di Torino, Torino, Italy*
[c] *Università del Piemonte Orientale, Novara, Italy*

S. Belforte [a], V. Candelise [a,b], M. Casarsa [a], F. Cossutti [a], A. Da Rold [a,b], G. Della Ricca [a,b], G. Sorrentino [a,b]

[a] *INFN Sezione di Trieste, Trieste, Italy*
[b] *Università di Trieste, Trieste, Italy*

S. Dogra, C. Huh, B. Kim, D.H. Kim, G.N. Kim, J. Kim, J. Lee, S.W. Lee, C.S. Moon, Y.D. Oh, S.I. Pak, S. Sekmen, Y.C. Yang

Kyungpook National University, Daegu, Korea

H. Kim, D.H. Moon

Chonnam National University, Institute for Universe and Elementary Particles, Kwangju, Korea

E. Asilar, B. Francois, T.J. Kim, J. Park

Hanyang University, Seoul, Korea

S. Cho, S. Choi, B. Hong, K. Lee, K.S. Lee, J. Lim, J. Park, S.K. Park, J. Yoo

Korea University, Seoul, Korea

J. Goh, A. Gurtu

Kyung Hee University, Department of Physics, Seoul, Korea

H.S. Kim, Y. Kim, G.B. Yu

Sejong University, Seoul, Korea

J. Almond, J.H. Bhyun, J. Choi, S. Jeon, J. Kim, J.S. Kim, S. Ko, H. Kwon, H. Lee, S. Lee, B.H. Oh, M. Oh, S.B. Oh, H. Seo, U.K. Yang, I. Yoon

Seoul National University, Seoul, Korea

W. Jang, D.Y. Kang, Y. Kang, S. Kim, B. Ko, J.S.H. Lee, Y. Lee, J.A. Merlin, I.C. Park, Y. Roh, M.S. Ryu, D. Song, I.J. Watson, S. Yang

University of Seoul, Seoul, Korea

S. Ha, H.D. Yoo

Yonsei University, Department of Physics, Seoul, Korea

M. Choi, H. Lee, Y. Lee, I. Yu

Sungkyunkwan University, Suwon, Korea

T. Beyrouthy, Y. Maghrbi

College of Engineering and Technology, American University of the Middle East (AUM), Dasman, Kuwait

K. Dreimanis, V. Veckalns

Riga Technical University, Riga, Latvia

M. Ambrozas, A. Carvalho Antunes De Oliveira, A. Juodagalvis, A. Rinkevicius, G. Tamulaitis

Vilnius University, Vilnius, Lithuania

N. Bin Norjoharuddeen, S.Y. Hoh [50], Z. Zolkapli

National Centre for Particle Physics, Universiti Malaya, Kuala Lumpur, Malaysia

J.F. Benitez, A. Castaneda Hernandez, H.A. Encinas Acosta, L.G. Gallegos Maríñez, M. León Coello, J.A. Murillo Quijada, A. Sehrawat, L. Valencia Palomo

Universidad de Sonora (UNISON), Hermosillo, Mexico

G. Ayala, H. Castilla-Valdez, E. De La Cruz-Burelo, I. Heredia-De La Cruz [51], R. Lopez-Fernandez, C.A. Mondragon Herrera, D.A. Perez Navarro, R. Reyes-Almanza, A. Sánchez Hernández

Centro de Investigacion y de Estudios Avanzados del IPN, Mexico City, Mexico

C. Oropeza Barrera, F. Vazquez Valencia

Universidad Iberoamericana, Mexico City, Mexico

I. Pedraza, H.A. Salazar Ibarguen, C. Uribe Estrada

Benemerita Universidad Autonoma de Puebla, Puebla, Mexico

I. Bubanja, J. Mijuskovic [52], N. Raicevic

University of Montenegro, Podgorica, Montenegro

D. Krofcheck

University of Auckland, Auckland, New Zealand

P.H. Butler

University of Canterbury, Christchurch, New Zealand

A. Ahmad, M.I. Asghar, A. Awais, M.I.M. Awan, M. Gul, H.R. Hoorani, W.A. Khan, M.A. Shah, M. Shoaib, M. Waqas

National Centre for Physics, Quaid-I-Azam University, Islamabad, Pakistan

V. Avati, L. Grzanka, M. Malawski

AGH University of Science and Technology Faculty of Computer Science, Electronics and Telecommunications, Krakow, Poland

H. Bialkowska, M. Bluj, B. Boimska, M. Górski, M. Kazana, M. Szleper, P. Zalewski

National Centre for Nuclear Research, Swierk, Poland

K. Bunkowski, K. Doroba, A. Kalinowski, M. Konecki, J. Krolikowski

Institute of Experimental Physics, Faculty of Physics, University of Warsaw, Warsaw, Poland

M. Araujo, P. Bargassa, D. Bastos, A. Boletti, P. Faccioli, M. Gallinaro, J. Hollar, N. Leonardo, T. Niknejad, M. Pisano, J. Seixas, O. Toldaiev, J. Varela

Laboratório de Instrumentação e Física Experimental de Partículas, Lisboa, Portugal

P. Adzic [53], M. Dordevic, P. Milenovic, J. Milosevic

VINCA Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

M. Aguilar-Benitez, J. Alcaraz Maestre, A. Álvarez Fernández, I. Bachiller, M. Barrio Luna, Cristina F. Bedoya, C.A. Carrillo Montoya, M. Cepeda, M. Cerrada, N. Colino, B. De La Cruz, A. Delgado Peris, J.P. Fernández Ramos, J. Flix, M.C. Fouz, O. Gonzalez Lopez, S. Goy Lopez, J.M. Hernandez, M.I. Josa, J. León Holgado, D. Moran, Á. Navarro Tobar, C. Perez Dengra, A. Pérez-Calero Yzquierdo, J. Puerta Pelayo, I. Redondo, L. Romero, S. Sánchez Navas, L. Urda Gómez, C. Willmott

Centro de Investigaciones Energéticas Medioambientales y Tecnológicas (CIEMAT), Madrid, Spain

J.F. de Trocóniz

Universidad Autónoma de Madrid, Madrid, Spain

B. Alvarez Gonzalez, J. Cuevas, J. Fernandez Menendez, S. Folgueras, I. Gonzalez Caballero, J.R. González Fernández, E. Palencia Cortezon, C. Ramón Álvarez, V. Rodríguez Bouza, A. Soto Rodríguez, A. Trapote, N. Trevisani, C. Vico Villalba

Universidad de Oviedo, Instituto Universitario de Ciencias y Tecnologías Espaciales de Asturias (ICTEA), Oviedo, Spain

J.A. Brochero Cifuentes, I.J. Cabrillo, A. Calderon, J. Duarte Campderros, M. Fernandez, C. Fernandez Madrazo, P.J. Fernández Manteca, A. García Alonso, G. Gomez, C. Martinez Rivero, P. Martinez Ruiz del Arbol, F. Matorras, P. Matorras Cuevas, J. Piedra Gomez, C. Prieels, A. Ruiz-Jimeno, L. Scodellaro, I. Vila, J.M. Vizan Garcia

Instituto de Física de Cantabria (IFCA), CSIC-Universidad de Cantabria, Santander, Spain

M.K. Jayananda, B. Kailasapathy [54], D.U.J. Sonnadara, D.D.C. Wickramarathna

University of Colombo, Colombo, Sri Lanka

W.G.D. Dharmaratna, K. Liyanage, N. Perera, N. Wickramage

University of Ruhuna, Department of Physics, Matara, Sri Lanka

T.K. Aarrestad, D. Abbaneo, J. Alimena, E. Auffray, G. Auzinger, J. Baechler, P. Baillon [†], D. Barney, J. Bendavid, M. Bianco, B. Bilin, A. Bocci, C. Caillol, T. Camporesi, M. Capeans Garrido, G. Cerminara, N. Chernyavskaya, S.S. Chhibra, S. Choudhury, M. Cipriani, L. Cristella, D. d'Enterria, A. Dabrowski, A. David, A. De Roeck, M.M. Defranchis, M. Deile, M. Dobson, M. Dünser, N. Dupont, A. Elliott-Peisert, F. Fallavollita [55], A. Florent, L. Forthomme, G. Franzoni, W. Funk, S. Ghosh, S. Giani, D. Gigi, K. Gill, F. Glege, L. Gouskos, E. Govorkova, M. Haranko, J. Hegeman, V. Innocente, T. James, P. Janot, J. Kaspar, J. Kieseler, M. Komm, N. Kratochwil, C. Lange, S. Laurila, P. Lecoq, A. Lintuluoto, C. Lourenço, B. Maier, L. Malgeri, S. Mallios, M. Mannelli, A.C. Marini, F. Meijers, S. Mersi, E. Meschi, F. Moortgat, M. Mulders, S. Orfanelli, L. Orsini, F. Pantaleo, E. Perez, M. Peruzzi, A. Petrilli, G. Petrucciani, A. Pfeiffer, M. Pierini, D. Piparo, M. Pitt, H. Qu, T. Quast, D. Rabady, A. Racz, G. Reales Gutiérrez, M. Rovere, H. Sakulin, J. Salfeld-Nebgen, S. Scarfi, M. Selvaggi, A. Sharma, P. Silva, W. Snoeys, P. Sphicas [56], A.G. Stahl Leiton, S. Summers, K. Tatar, V.R. Tavolaro, D. Treille, P. Tropea, A. Tsirou, J. Wanczyk [57], K.A. Wozniak, W.D. Zeuner

CERN, European Organization for Nuclear Research, Geneva, Switzerland

L. Caminada [58], A. Ebrahimi, W. Erdmann, R. Horisberger, Q. Ingram, H.C. Kaestli, D. Kotlinski, M. Missiroli [58], L. Noehte [58], T. Rohe

Paul Scherrer Institut, Villigen, Switzerland

K. Androsov [57], M. Backhaus, P. Berger, A. Calandri, A. De Cosa, G. Dissertori, M. Dittmar, M. Donegà, C. Dorfer, F. Eble, K. Gedia, F. Glessgen, T.A. Gómez Espinosa, C. Grab, D. Hits, W. Lustermann, A.-M. Lyon, R.A. Manzoni, L. Marchese, C. Martin Perez, A. Mascellani [57], M.T. Meinhard, F. Nessi-Tedaldi, J. Niedziela, F. Pauss, V. Perovic, S. Pigazzini, M.G. Ratti, M. Reichmann, C. Reissel, T. Reitenspiess, B. Ristic, D. Ruini, D.A. Sanz Becerra, J. Steggemann [57], D. Valsecchi [19], R. Wallny

ETH Zurich - Institute for Particle Physics and Astrophysics (IPA), Zurich, Switzerland

C. Amsler [59], P. Bärtschi, C. Botta, D. Brzhechko, M.F. Canelli, K. Cormier, A. De Wit, R. Del Burgo, J.K. Heikkilä, M. Huwiler, W. Jin, A. Jofrehei, B. Kilminster, S. Leontsinis, S.P. Liechti, A. Macchiolo, P. Meiring, V.M. Mikuni, U. Molinatti, I. Neutelings, A. Reimers, P. Robmann, S. Sanchez Cruz, K. Schweiger, M. Senger, Y. Takahashi

Universität Zürich, Zurich, Switzerland

C. Adloff [60], C.M. Kuo, W. Lin, A. Roy, T. Sarkar [36], S.S. Yu

National Central University, Chung-Li, Taiwan

L. Ceard, Y. Chao, K.F. Chen, P.H. Chen, P.s. Chen, H. Cheng, W.-S. Hou, Y.y. Li, R.-S. Lu, E. Paganis, A. Psallidas, A. Steen, H.y. Wu, E. Yazgan, P.r. Yu

National Taiwan University (NTU), Taipei, Taiwan

B. Asavapibhop, C. Asawatangtrakuldee, N. Srimanobhas

Chulalongkorn University, Faculty of Science, Department of Physics, Bangkok, Thailand

F. Boran, S. Damarseckin [61], Z.S. Demiroglu, F. Dolek, I. Dumanoglu [62], E. Eskut, Y. Guler [63], E. Gurpinar Guler [63], C. Isik, O. Kara, A. Kayis Topaksu, U. Kiminsu, G. Onengut, K. Ozdemir [64], A. Polatoz, A.E. Simsek, B. Tali [65], U.G. Tok, S. Turkcapar, I.S. Zorbakir

Çukurova University, Physics Department, Science and Art Faculty, Adana, Turkey

G. Karapinar, K. Ocalan [66], M. Yalvac [67]

Middle East Technical University, Physics Department, Ankara, Turkey

B. Akgun, I.O. Atakisi, E. Gülmez, M. Kaya [68], O. Kaya [69], Ö. Özçelik, S. Tekten [70], E.A. Yetkin [71]

Bogazici University, Istanbul, Turkey

A. Cakir, K. Cankocak [62], Y. Komurcu, S. Sen [72]

Istanbul Technical University, Istanbul, Turkey

S. Cerci [65], I. Hos [73], B. Isildak [74], B. Kaynak, S. Ozkorucuklu, H. Sert, C. Simsek, D. Sunar Cerci [65], C. Zorbilmez

Istanbul University, Istanbul, Turkey

B. Grynyov

Institute for Scintillation Materials of National Academy of Science of Ukraine, Kharkiv, Ukraine

L. Levchuk

National Science Centre, Kharkiv Institute of Physics and Technology, Kharkiv, Ukraine

D. Anthony, E. Bhal, S. Bologna, J.J. Brooke, A. Bundock, E. Clement, D. Cussans, H. Flacher, M. Glowacki, J. Goldstein, G.P. Heath, H.F. Heath, L. Kreczko, B. Krikler, S. Paramesvaran, S. Seif El Nasr-Storey, V.J. Smith, N. Stylianou [75], K. Walkingshaw Pass, R. White

University of Bristol, Bristol, United Kingdom

K.W. Bell, A. Belyaev [76], C. Brew, R.M. Brown, D.J.A. Cockerill, C. Cooke, K.V. Ellis, K. Harder, S. Harper, M.-L. Holmberg [77], J. Linacre, K. Manolopoulos, D.M. Newbold, E. Olaiya, D. Petyt, T. Reis, T. Schuh, C.H. Shepherd-Themistocleous, I.R. Tomalin, T. Williams

Rutherford Appleton Laboratory, Didcot, United Kingdom

R. Bainbridge, P. Bloch, S. Bonomally, J. Borg, S. Breeze, O. Buchmuller, V. Cepaitis, G.S. Chahal [78], D. Colling, P. Dauncey, G. Davies, M. Della Negra, S. Fayer, G. Fedi, G. Hall, M.H. Hassanshahi, G. Iles, J. Langford, L. Lyons, A.-M. Magnan, S. Malik, A. Martelli, D.G. Monk, J. Nash [79], M. Pesaresi, B.C. Radburn-Smith, D.M. Raymond, A. Richards, A. Rose, E. Scott, C. Seez, A. Shtipliyski, A. Tapper, K. Uchida, T. Virdee [19], M. Vojinovic, N. Wardle, S.N. Webb, D. Winterbottom

Imperial College, London, United Kingdom

K. Coldham, J.E. Cole, A. Khan, P. Kyberd, I.D. Reid, L. Teodorescu, S. Zahid

Brunel University, Uxbridge, United Kingdom

S. Abdullin, A. Brinkerhoff, B. Caraway, J. Dittmann, K. Hatakeyama, A.R. Kanuganti, B. McMaster, M. Saunders, S. Sawant, C. Sutantawibul, J. Wilson

Baylor University, Waco, TX, USA

R. Bartek, A. Dominguez, R. Uniyal, A.M. Vargas Hernandez

Catholic University of America, Washington, DC, USA

A. Buccilli, S.I. Cooper, D. Di Croce, S.V. Gleyzer, C. Henderson, C.U. Perez, P. Rumerio [80], C. West

The University of Alabama, Tuscaloosa, AL, USA

A. Akpinar, A. Albert, D. Arcaro, C. Cosby, Z. Demiragli, C. Erice, E. Fontanesi, D. Gastler, S. May, J. Rohlf, K. Salyer, D. Sperka, D. Spitzbart, I. Suarez, A. Tsatsos, S. Yuan

Boston University, Boston, MA, USA

G. Benelli, B. Burkle, X. Coubez [21], D. Cutts, M. Hadley, U. Heintz, J.M. Hogan [81], T. Kwon, G. Landsberg, K.T. Lau, D. Li, M. Lukasik, J. Luo, M. Narain, N. Pervan, S. Sagir [82], F. Simpson, E. Usai, W.Y. Wong, X. Yan, D. Yu, W. Zhang

Brown University, Providence, RI, USA

J. Bonilla, C. Brainerd, R. Breedon, M. Calderon De La Barca Sanchez, M. Chertok, J. Conway, P.T. Cox, R. Erbacher, G. Haza, F. Jensen, O. Kukral, R. Lander, G. Mocellin, M. Mulhearn, D. Pellett, B. Regnery, D. Taylor, Y. Yao, F. Zhang

University of California, Davis, Davis, CA, USA

M. Bachtis, R. Cousins, A. Datta, D. Hamilton, J. Hauser, M. Ignatenko, M.A. Iqbal, T. Lam, W.A. Nash, S. Regnard, D. Saltzberg, B. Stone, V. Valuev

University of California, Los Angeles, CA, USA

Y. Chen, R. Clare, J.W. Gary, M. Gordon, G. Hanson, G. Karapostoli, O.R. Long, N. Manganelli, W. Si, S. Wimpenny, Y. Zhang

University of California, Riverside, Riverside, CA, USA

J.G. Branson, P. Chang, S. Cittolin, S. Cooperstein, D. Diaz, J. Duarte, R. Gerosa, L. Giannini, J. Guiang, R. Kansal, V. Krutelyov, R. Lee, J. Letts, M. Masciovecchio, F. Mokhtar, M. Pieri, B.V. Sathia Narayanan, V. Sharma, M. Tadel, F. Würthwein, Y. Xiang, A. Yagil

University of California, San Diego, La Jolla, CA, USA

N. Amin, C. Campagnari, M. Citron, G. Collura, A. Dorsett, V. Dutta, J. Incandela, M. Kilpatrick, J. Kim, B. Marsh, H. Mei, M. Oshiro, M. Quinnan, J. Richman, U. Sarica, F. Setti, J. Sheplock, P. Siddireddy, D. Stuart, S. Wang

University of California, Santa Barbara - Department of Physics, Santa Barbara, CA, USA

A. Bornheim, O. Cerri, I. Dutta, J.M. Lawhorn, N. Lu, J. Mao, H.B. Newman, T.Q. Nguyen, M. Spiropulu, J.R. Vlimant, C. Wang, S. Xie, Z. Zhang, R.Y. Zhu

California Institute of Technology, Pasadena, CA, USA

J. Alison, S. An, M.B. Andrews, P. Bryant, T. Ferguson, A. Harilal, C. Liu, T. Mudholkar, M. Paulini, A. Sanchez, W. Terrill

Carnegie Mellon University, Pittsburgh, PA, USA

J.P. Cumalat, W.T. Ford, A. Hassani, G. Karathanasis, E. MacDonald, R. Patel, A. Perloff, C. Savard, N. Schonbeck, K. Stenson, K.A. Ulmer, S.R. Wagner, N. Zipper

University of Colorado Boulder, Boulder, CO, USA

J. Alexander, S. Bright-Thonney, X. Chen, Y. Cheng, D.J. Cranshaw, J. Fan, X. Fan, D. Gadkari, S. Hogan, J. Monroy, J.R. Patterson, D. Quach, J. Reichert, M. Reid, A. Ryd, J. Thom, P. Wittich, R. Zou

Cornell University, Ithaca, NY, USA

M. Albrow, M. Alyari, G. Apollinari, A. Apresyan, A. Apyan, L.A.T. Bauerdick, D. Berry, J. Berryhill, P.C. Bhat, K. Burkett, J.N. Butler, A. Canepa, G.B. Cerati, H.W.K. Cheung, F. Chlebana, K.F. Di Petrillo, J. Dickinson, V.D. Elvira, Y. Feng, J. Freeman, A. Gandrakota, Z. Gecse, L. Gray, D. Green, S. Grünendahl, O. Gutsche, R.M. Harris, R. Heller, T.C. Herwig, J. Hirschauer, B. Jayatilaka, S. Jindariani, M. Johnson, U. Joshi, T. Klijnsma, B. Klima, K.H.M. Kwok, S. Lammel, D. Lincoln, R. Lipton, T. Liu, C. Madrid, K. Maeshima, C. Mantilla, D. Mason, P. McBride, P. Merkel, S. Mrenna, S. Nahn, J. Ngadiuba, V. Papadimitriou, N. Pastika, K. Pedro, C. Pena [83], F. Ravera, A. Reinsvold Hall [84], L. Ristori, E. Sexton-Kennedy, N. Smith, A. Soha, L. Spiegel, J. Strait, L. Taylor, S. Tkaczyk, N.V. Tran, L. Uplegger, E.W. Vaandering, H.A. Weber, I. Zoi

Fermi National Accelerator Laboratory, Batavia, IL, USA

P. Avery, D. Bourilkov, L. Cadamuro, V. Cherepanov, R.D. Field, D. Guerrero, M. Kim, E. Koenig, J. Konigsberg, A. Korytov, K.H. Lo, K. Matchev, N. Menendez, G. Mitselmakher, A. Muthirakalayil Madhu, N. Rawal, D. Rosenzweig, S. Rosenzweig, K. Shi, J. Wang, Z. Wu, E. Yigitbasi, X. Zuo

University of Florida, Gainesville, FL, USA

T. Adams, A. Askew, R. Habibullah, V. Hagopian, K.F. Johnson, R. Khurana, T. Kolberg, G. Martinez, H. Prosper, C. Schiber, O. Viazlo, R. Yohay, J. Zhang

Florida State University, Tallahassee, FL, USA

M.M. Baarmand, S. Butalla, T. Elkafrawy [85], M. Hohlmann, R. Kumar Verma, D. Noonan, M. Rahmani, F. Yumiceva

Florida Institute of Technology, Melbourne, FL, USA

M.R. Adams, H. Becerril Gonzalez, R. Cavanaugh, S. Dittmer, O. Evdokimov, C.E. Gerber, D.J. Hofman, A.H. Merrit, C. Mills, G. Oh, T. Roy, S. Rudrabhatla, M.B. Tonjes, N. Varelas, J. Viinikainen, X. Wang, Z. Ye

University of Illinois at Chicago (UIC), Chicago, IL, USA

M. Alhusseini, K. Dilsiz [86], L. Emediato, R.P. Gandrajula, O.K. Köseyan, J.-P. Merlo, A. Mestvirishvili [87], J. Nachtman, H. Ogul [88], Y. Onel, A. Penzo, C. Snyder, E. Tiras [89]

The University of Iowa, Iowa City, IA, USA

O. Amram, B. Blumenfeld, L. Corcodilos, J. Davis, S. Kyriacou, P. Maksimovic, J. Roskes, M. Swartz, T.Á. Vámi

Johns Hopkins University, Baltimore, MD, USA

A. Abreu, J. Anguiano, P. Baringer, A. Bean, Z. Flowers, T. Isidori, S. Khalil, J. King, G. Krintiras, A. Kropivnitskaya, M. Lazarovits, C. Le Mahieu, C. Lindsey, J. Marquez, N. Minafra, M. Murray, M. Nickel, C. Rogan, C. Royon, R. Salvatico, S. Sanders, E. Schmitz, C. Smith, Q. Wang, Z. Warner, J. Williams, G. Wilson

The University of Kansas, Lawrence, KS, USA

S. Duric, A. Ivanov, K. Kaadze, D. Kim, Y. Maravin, T. Mitchell, A. Modak, K. Nam

Kansas State University, Manhattan, KS, USA

F. Rebassoo, D. Wright

Lawrence Livermore National Laboratory, Livermore, CA, USA

E. Adams, A. Baden, O. Baron, A. Belloni, S.C. Eno, N.J. Hadley, S. Jabeen, R.G. Kellogg, T. Koeth, Y. Lai, S. Lascio, A.C. Mignerey, S. Nabili, C. Palmer, M. Seidel, A. Skuja, L. Wang, K. Wong

University of Maryland, College Park, MD, USA

D. Abercrombie, G. Andreassi, R. Bi, W. Busza, I.A. Cali, Y. Chen, M. D'Alfonso, J. Eysermans, C. Freer, G. Gomez-Ceballos, M. Goncharov, P. Harris, M. Hu, M. Klute, D. Kovalskyi, J. Krupa, Y.-J. Lee, K. Long, C. Mironov, C. Paus, D. Rankin, C. Roland, G. Roland, Z. Shi, G.S.F. Stephans, J. Wang, Z. Wang, B. Wyslouch

Massachusetts Institute of Technology, Cambridge, MA, USA

R.M. Chatterjee, A. Evans, J. Hiltbrand, Sh. Jain, B.M. Joshi, M. Krohn, Y. Kubota, J. Mans, M. Revering, R. Rusack, R. Saradhy, N. Schroeder, N. Strobbe, M.A. Wadud

University of Minnesota, Minneapolis, MN, USA

K. Bloom, M. Bryson, S. Chauhan, D.R. Claes, C. Fangmeier, L. Finco, F. Golf, C. Joo, I. Kravchenko, I. Reed, J.E. Siado, G.R. Snow[†], W. Tabb, A. Wightman, F. Yan, A.G. Zecchinelli

University of Nebraska-Lincoln, Lincoln, NE, USA

G. Agarwal, H. Bandyopadhyay, L. Hay, I. Iashvili, A. Kharchilava, C. McLean, D. Nguyen, J. Pekkanen, S. Rappoccio, A. Williams

State University of New York at Buffalo, Buffalo, NY, USA

G. Alverson, E. Barberis, Y. Haddad, Y. Han, A. Hortiangtham, A. Krishna, J. Li, J. Lidrych, G. Madigan, B. Marzocchi, D.M. Morse, V. Nguyen, T. Orimoto, A. Parker, L. Skinnari, A. Tishelman-Charny, T. Wamorkar, B. Wang, A. Wisecarver, D. Wood

Northeastern University, Boston, MA, USA

S. Bhattacharya, J. Bueghly, Z. Chen, A. Gilbert, T. Gunter, K.A. Hahn, Y. Liu, N. Odell, M.H. Schmitt, M. Velasco

Northwestern University, Evanston, IL, USA

R. Band, R. Bucci, M. Cremonesi, A. Das, R. Goldouzian, M. Hildreth, K. Hurtado Anampa, C. Jessop, K. Lannon, J. Lawrence, N. Loukas, L. Lutton, J. Mariano, N. Marinelli, I. Mcalister, T. McCauley, C. Mcgrady, K. Mohrman, C. Moore, Y. Musienko[13], R. Ruchti, A. Townsend, M. Wayne, M. Zarucki, L. Zygala

University of Notre Dame, Notre Dame, IN, USA

B. Bylsma, L.S. Durkin, B. Francis, C. Hill, A. Lesauvage, M. Nunez Ornelas, K. Wei, B.L. Winer, B.R. Yates

The Ohio State University, Columbus, OH, USA

F.M. Addesa, B. Bonham, P. Das, G. Dezoort, P. Elmer, A. Frankenthal, B. Greenberg, N. Haubrich, S. Higginbotham, A. Kalogeropoulos, G. Kopp, S. Kwan, D. Lange, D. Marlow, K. Mei, I. Ojalvo, J. Olsen, D. Stickland, C. Tully

Princeton University, Princeton, NJ, USA

S. Malik, S. Norberg

University of Puerto Rico, Mayaguez, PR, USA

A.S. Bakshi, V.E. Barnes, R. Chawla, S. Das, L. Gutay, M. Jones, A.W. Jung, D. Kondratyev, A.M. Koshy, M. Liu, G. Negro, N. Neumeister, G. Paspalaki, S. Piperov, A. Purohit, J.F. Schulte, M. Stojanovic, J. Thieman, F. Wang, R. Xiao, W. Xie

Purdue University, West Lafayette, IN, USA

J. Dolen, N. Parashar

Purdue University Northwest, Hammond, IN, USA

D. Acosta, A. Baty, T. Carnahan, M. Decaro, S. Dildick, K.M. Ecklund, S. Freed, P. Gardner, F.J.M. Geurts, A. Kumar, W. Li, B.P. Padley, R. Redjimi, J. Rotter, W. Shi, S. Yang, L. Zhang [90], Y. Zhang

Rice University, Houston, TX, USA

A. Bodek, P. de Barbaro, R. Demina, J.L. Dulemba, C. Fallon, T. Ferbel, M. Galanti, A. Garcia-Bellido, O. Hindrichs, A. Khukhunaishvili, E. Ranken, R. Taus, G.P. Van Onsem

University of Rochester, Rochester, NY, USA

K. Goulianos

The Rockefeller University, New York, NY, USA

B. Chiarito, J.P. Chou, Y. Gershtein, E. Halkiadakis, A. Hart, M. Heindl, O. Karacheban [23], I. Laflotte, A. Lath, R. Montalvo, K. Nash, M. Osherson, S. Salur, S. Schnetzer, S. Somalwar, R. Stone, S.A. Thayil, S. Thomas, H. Wang

Rutgers, The State University of New Jersey, Piscataway, NJ, USA

H. Acharya, A.G. Delannoy, S. Fiorendi, T. Holmes, S. Spanier

University of Tennessee, Knoxville, TN, USA

O. Bouhali [91], M. Dalchenko, A. Delgado, R. Eusebi, J. Gilmore, T. Huang, T. Kamon [92], H. Kim, S. Luo, S. Malhotra, R. Mueller, D. Overton, D. Rathjens, A. Safonov

Texas A&M University, College Station, TX, USA

N. Akchurin, J. Damgov, V. Hegde, K. Lamichhane, S.W. Lee, T. Mengke, S. Muthumuni, T. Peltola, I. Volobouev, Z. Wang, A. Whitbeck

Texas Tech University, Lubbock, TX, USA

E. Appelt, S. Greene, A. Gurrola, W. Johns, A. Melo, F. Romeo, P. Sheldon, S. Tuo, J. Velkovska

Vanderbilt University, Nashville, TN, USA

M.W. Arenton, B. Cardwell, B. Cox, G. Cummings, J. Hakala, R. Hirosky, M. Joyce, A. Ledovskoy, A. Li, C. Neu, C.E. Perez Lara, B. Tannenwald, S. White

University of Virginia, Charlottesville, VA, USA

N. Poudyal

Wayne State University, Detroit, MI, USA

S. Banerjee, K. Black, T. Bose, S. Dasu, I. De Bruyn, P. Everaerts, C. Galloni, H. He, M. Herndon, A. Herve, U. Hussain, A. Lanaro, A. Loeliger, R. Loveless, J. Madhusudanan Sreekala, A. Mallampalli, A. Mohammadi, D. Pinna, A. Savin, V. Shang, V. Sharma, W.H. Smith, D. Teague, S. Trembath-Reichert, W. Vetens

University of Wisconsin - Madison, Madison, WI, USA

S. Afanasiev, V. Andreev, Yu. Andreev, T. Aushev, M. Azarkin, A. Babaev, A. Belyaev, V. Blinov [93], E. Boos, V. Borshch, D. Budkouski, V. Bunichev, O. Bychkova, V. Chekhovsky, R. Chistov [93], M. Danilov [93], A. Dermenev, T. Dimova [93], I. Dremin, M. Dubinin [83], L. Dudko, V. Epshteyn [94], G. Gavrilov, V. Gavrilov, S. Gninenko, V. Golovtcov, N. Golubev, I. Golutvin, I. Gorbunov, A. Gribushin, V. Ivanchenko, Y. Ivanov, V. Kachanov, L. Kardapoltsev [93], V. Karjavine, A. Karneyeu, V. Kim [93], M. Kirakosyan, D. Kirpichnikov, M. Kirsanov, V. Klyukhin, O. Kodolova [95], D. Konstantinov, V. Korenkov, A. Kozyrev [93], N. Krasnikov, E. Kuznetsova [96], A. Lanev, A. Litomin, N. Lychkovskaya, V. Makarenko, A. Malakhov, V. Matveev [93], V. Murzin, A. Nikitenko [97], S. Obraztsov, V. Okhotnikov, V. Oreshkin, A. Oskin, I. Ovtin [93], V. Palichik, P. Parygin [98], A. Pashenkov, V. Perelygin, M. Perfilov, S. Petrushanko, G. Pivovarov, S. Polikarpov [93], V. Popov, O. Radchenko [93], M. Savina, V. Savrin, V. Shalaev, S. Shmatov, S. Shulha, Y. Skovpen [93], S. Slabospitskii, I. Smirnov, V. Smirnov, D. Sosnov, A. Stepennov, V. Sulimov, E. Tcherniaev, A. Terkulov, O. Teryaev, M. Toms [99], A. Toropin, L. Uvarov, A. Uzunian, E. Vlasov [100], S. Volkov, A. Vorobyev, N. Voytishin, B.S. Yuldashev [101], A. Zarubin, I. Zhizhin, A. Zhokin

Authors affiliated with an institute or an international laboratory covered by a cooperation agreement with CERN

[†] Deceased.
[1] Also at Yerevan State University, Yerevan, Armenia.
[2] Also at TU Wien, Vienna, Austria.
[3] Also at Institute of Basic and Applied Sciences, Faculty of Engineering, Arab Academy for Science, Technology and Maritime Transport, Alexandria, Egypt.
[4] Also at Université Libre de Bruxelles, Bruxelles, Belgium.
[5] Also at Universidade Estadual de Campinas, Campinas, Brazil.
[6] Also at Federal University of Rio Grande do Sul, Porto Alegre, Brazil.
[7] Also at UFMS, Nova Andradina, Brazil.
[8] Also at The University of the State of Amazonas, Manaus, Brazil.
[9] Also at University of Chinese Academy of Sciences, Beijing, China.
[10] Also at Nanjing Normal University Department of Physics, Nanjing, China.
[11] Now at The University of Iowa, Iowa City, Iowa, USA.
[12] Also at University of Chinese Academy of Sciences, Beijing, China.
[13] Also at an institute or an international laboratory covered by a cooperation agreement with CERN.
[14] Also at Cairo University, Cairo, Egypt.
[15] Also at Zewail City of Science and Technology, Zewail, Egypt.
[16] Also at Purdue University, West Lafayette, Indiana, USA.
[17] Also at Université de Haute Alsace, Mulhouse, France.
[18] Also at Erzincan Binali Yildirim University, Erzincan, Turkey.
[19] Also at CERN, European Organization for Nuclear Research, Geneva, Switzerland.
[20] Also at University of Hamburg, Hamburg, Germany.
[21] Also at RWTH Aachen University, III. Physikalisches Institut A, Aachen, Germany.
[22] Also at Isfahan University of Technology, Isfahan, Iran.
[23] Also at Brandenburg University of Technology, Cottbus, Germany.
[24] Also at Forschungszentrum Jülich, Juelich, Germany.
[25] Also at Physics Department, Faculty of Science, Assiut University, Assiut, Egypt.
[26] Also at Karoly Robert Campus, MATE Institute of Technology, Gyongyos, Hungary.
[27] Also at Institute of Physics, University of Debrecen, Debrecen, Hungary.
[28] Also at Institute of Nuclear Research ATOMKI, Debrecen, Hungary.
[29] Now at Universitatea Babes-Bolyai - Facultatea de Fizica, Cluj-Napoca, Romania.
[30] Also at MTA-ELTE Lendület CMS Particle and Nuclear Physics Group, Eötvös Loránd University, Budapest, Hungary.
[31] Also at Faculty of Informatics, University of Debrecen, Debrecen, Hungary.
[32] Also at Wigner Research Centre for Physics, Budapest, Hungary.
[33] Also at Punjab Agricultural University, Ludhiana, India.
[34] Also at UPES - University of Petroleum and Energy Studies, Dehradun, India.
[35] Also at University of Hyderabad, Hyderabad, India.
[36] Also at University of Visva-Bharati, Santiniketan, India.
[37] Also at Indian Institute of Science (IISc), Bangalore, India.
[38] Also at Indian Institute of Technology (IIT), Mumbai, India.
[39] Also at IIT Bhubaneswar, Bhubaneswar, India.
[40] Also at Institute of Physics, Bhubaneswar, India.
[41] Also at Deutsches Elektronen-Synchrotron, Hamburg, Germany.
[42] Also at Sharif University of Technology, Tehran, Iran.

[43] Also at Department of Physics, University of Science and Technology of Mazandaran, Behshahr, Iran.
[44] Also at Helwan University, Cairo, Egypt.
[45] Also at Italian National Agency for New Technologies, Energy and Sustainable Economic Development, Bologna, Italy.
[46] Also at Centro Siciliano di Fisica Nucleare e di Struttura Della Materia, Catania, Italy.
[47] Also at Scuola Superiore Meridionale, Università di Napoli 'Federico II', Napoli, Italy.
[48] Also at Università di Napoli 'Federico II', Napoli, Italy.
[49] Also at Consiglio Nazionale delle Ricerche - Istituto Officina dei Materiali, Perugia, Italy.
[50] Also at Department of Applied Physics, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, Bangi, Malaysia.
[51] Also at Consejo Nacional de Ciencia y Tecnología, Mexico City, Mexico.
[52] Also at IRFU, CEA, Université Paris-Saclay, Gif-sur-Yvette, France.
[53] Also at Faculty of Physics, University of Belgrade, Belgrade, Serbia.
[54] Also at Trincomalee Campus, Eastern University, Sri Lanka, Nilaveli, Sri Lanka.
[55] Also at INFN Sezione di Pavia, Università di Pavia, Pavia, Italy.
[56] Also at National and Kapodistrian University of Athens, Athens, Greece.
[57] Also at Ecole Polytechnique Fédérale Lausanne, Lausanne, Switzerland.
[58] Also at Universität Zürich, Zurich, Switzerland.
[59] Also at Stefan Meyer Institute for Subatomic Physics, Vienna, Austria.
[60] Also at Laboratoire d'Annecy-le-Vieux de Physique des Particules, IN2P3-CNRS, Annecy-le-Vieux, France.
[61] Also at Şırnak University, Sirnak, Turkey.
[62] Also at Near East University, Research Center of Experimental Health Science, Mersin, Turkey.
[63] Also at Konya Technical University, Konya, Turkey.
[64] Also at Izmir Bakircay University, Izmir, Turkey.
[65] Also at Adiyaman University, Adiyaman, Turkey.
[66] Also at Necmettin Erbakan University, Konya, Turkey.
[67] Also at Bozok Universitetesi Rektörlügü, Yozgat, Turkey.
[68] Also at Marmara University, Istanbul, Turkey.
[69] Also at Milli Savunma University, Istanbul, Turkey.
[70] Also at Kafkas University, Kars, Turkey.
[71] Also at Istanbul Bilgi University, Istanbul, Turkey.
[72] Also at Hacettepe University, Ankara, Turkey.
[73] Also at Istanbul University - Cerrahpasa, Faculty of Engineering, Istanbul, Turkey.
[74] Also at Ozyegin University, Istanbul, Turkey.
[75] Also at Vrije Universiteit Brussel, Brussel, Belgium.
[76] Also at School of Physics and Astronomy, University of Southampton, Southampton, United Kingdom.
[77] Also at University of Bristol, Bristol, United Kingdom.
[78] Also at IPPP Durham University, Durham, United Kingdom.
[79] Also at Monash University, Faculty of Science, Clayton, Australia.
[80] Also at Università di Torino, Torino, Italy.
[81] Also at Bethel University, St. Paul, Minnesota, USA.
[82] Also at Karamanoğlu Mehmetbey University, Karaman, Turkey.
[83] Also at California Institute of Technology, Pasadena, California, USA.
[84] Also at United States Naval Academy, Annapolis, Maryland, USA.
[85] Also at Ain Shams University, Cairo, Egypt.
[86] Also at Bingol University, Bingol, Turkey.
[87] Also at Georgian Technical University, Tbilisi, Georgia.
[88] Also at Sinop University, Sinop, Turkey.
[89] Also at Erciyes University, Kayseri, Turkey.
[90] Also at Institute of Modern Physics and Key Laboratory of Nuclear Physics and Ion-beam Application (MOE) - Fudan University, Shanghai, China.
[91] Also at Texas A&M University at Qatar, Doha, Qatar.
[92] Also at Kyungpook National University, Daegu, Korea.
[93] Also at another institute or international laboratory covered by a cooperation agreement with CERN.
[94] Now at Istanbul University, Istanbul, Turkey.
[95] Also at Yerevan Physics Institute, Yerevan, Armenia.
[96] Now at University of Florida, Gainesville, Florida, USA.
[97] Also at Imperial College, London, United Kingdom.
[98] Now at University of Rochester, Rochester, New York, USA.
[99] Now at Baylor University, Waco, Texas, USA.
[100] Now at INFN Sezione di Torino, Università di Torino, Torino, Italy; Università del Piemonte Orientale, Novara, Italy.
[101] Also at Institute of Nuclear Physics of the Uzbekistan Academy of Sciences, Tashkent, Uzbekistan.