Search for a singly produced third-generation scalar leptoquark decaying to a \(\tau\) lepton and a bottom quark in proton-proton collisions at \(\sqrt{s} = 13\) TeV

The CMS Collaboration*

Abstract

A search is presented for a singly produced third-generation scalar leptoquark decaying to a \(\tau\) lepton and a bottom quark. Associated production of a leptoquark and a \(\tau\) lepton is considered, leading to a final state with a bottom quark and two \(\tau\) leptons. The search uses proton-proton collision data at a center-of-mass energy of 13 TeV recorded with the CMS detector, corresponding to an integrated luminosity of \(35.9\) fb\(^{-1}\). Upper limits are set at 95% confidence level on the production cross section of the third-generation scalar leptoquarks as a function of their mass. From a comparison of the results with the theoretical predictions, a third-generation scalar leptoquark decaying to a \(\tau\) lepton and a bottom quark, assuming unit Yukawa coupling (\(\lambda\)), is excluded for masses below 740 GeV. Limits are also set on \(\lambda\) of the hypothesized leptoquark as a function of its mass. Above \(\lambda = 1.4\), this result provides the best upper limit on the mass of a third-generation scalar leptoquark decaying to a \(\tau\) lepton and a bottom quark.

1 Introduction

Leptoquarks (LQs) are hypothetical color-triplet bosons, which carry both baryon and lepton quantum numbers and have fractional electric charge. They are predicted by many extensions of the standard model (SM) of particle physics, such as theories invoking grand unification [1–8], technicolor [9–11], or compositeness [12]. To satisfy experimental constraints on flavor changing neutral currents and other rare processes [13, 14], it is generally assumed that there would be three types of LQs, each type coupled to leptons and quarks of its same generation.

Third-generation scalar LQs have recently received considerable theoretical interest, as their existence can explain the anomaly in the $B \to D\tau\nu$ and $B \to D^*\tau\nu$ decay rates reported by the BaBar [15, 16], Belle [17–22], and LHCb [23] Collaborations. These decay rates collectively deviate from the SM predictions by about four standard deviations [24], and large couplings to third-generation quarks and leptons could explain this anomaly [25–28]. The LQ could also provide consistent explanations for other anomalies in B physics reported by LHCb [29–34] and Belle [35].

The production cross sections and decay widths of LQs in proton-proton (pp) collisions are determined by the LQ’s mass, $m_{LQ}$; its branching fraction $\beta$ to a charged lepton and a quark; and the Yukawa coupling $\lambda$ of the LQ-lepton-quark vertex. Leptoquarks can be produced in pairs via gluon fusion or quark-antiquark annihilation, and singly via quark-gluon fusion. Pair production of LQs does not depend on $\lambda$, while single production does, and thus the sensitivity of searches for singly-produced LQs depends on $\lambda$. At lower masses, the cross section for pair production is greater than that for single production. However, the single-LQ production cross section decreases more slowly with increasing $m_{LQ}$, eventually exceeding that for pair production. If the third-generation LQ is responsible for the observed B physics anomalies, then a large value of $\lambda$ is favored ($\lambda \sim m_{LQ}$ measured in TeV), and the cross section for single production exceeds that for pair production for $m_{LQ}$ greater than 1.0-1.5 TeV [36].

The most stringent limits on the production of a third-generation LQ decaying to a $\tau$ lepton and a bottom quark come from a search by the CMS Collaboration, in which a scalar LQ with mass below 850 GeV was excluded in a search for LQ pair production in the $\ell\tau\bb$ final state [37]. Here, $\ell$ refers to a lepton (e or $\mu$) from $\tau$ lepton decay (35% of the $\tau$ decays [38]), and $\tau_h$ denotes a hadronically decaying $\tau$ lepton (65% of the $\tau$ decays [38]). Another type of third-generation scalar LQ decaying to a $\tau$ lepton and a top quark is excluded for masses up to 900 GeV [39].

This paper presents the first search that targets singly produced third-generation scalar LQs, each decaying to a $\tau$ lepton and a bottom quark. Feynman diagrams of the signal processes at leading order (LO) are shown in Fig. 1. The final states $\ell\tau\bb$ and $\tau_h\tau_h\bb$ are considered. The search is based on a data sample of pp collisions at a center-of-mass energy of 13 TeV recorded by the CMS experiment at the CERN LHC in 2016, corresponding to an integrated luminosity of 35.9 fb$^{-1}$.

2 The CMS detector

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, there are a silicon pixel and strip tracker, a lead tungstate crystal electromagnetic calorimeter (ECAL), and a brass and scintillator hadron calorimeter, each composed of a barrel and two endcap sections. Forward
calorimeters extend the pseudorapidity 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.

Events of interest are selected using a two-tiered trigger system [40]. 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 time interval of less than 4 µs. The second level, known as the high-level trigger, 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 about 1 kHz before data storage.

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. [41].

3 Simulated samples

Samples of simulated events are used to devise selection criteria and to estimate and validate background predictions. The LQ signals are generated at LO precision using version 2.6.0 of MADGRAPH5_aMC@NLO [42] for $m_{\text{LQ}} = 200$–1000 (in steps of 100 GeV), 1200, and 1500 GeV. The particular LQ model used is $\tilde{R}_2$, as discussed in Ref. [43]. The branching fraction is assumed to be $\beta = 1$, i.e. the LQ always decays to a $\tau$ lepton and a bottom quark. The Yukawa coupling of the LQ to a $\tau$ lepton and a bottom quark is set to be $\lambda = 1$. The width $\Gamma$ is calculated to be $\Gamma = m_{\text{LQ}}\lambda^2/(16\pi)$ [44], which is narrower than the experimental resolution over the considered search range. The signal samples are normalized to the cross section calculated at LO precision, multiplied by a $K$ factor to account for higher order contributions [45]. The $K$ factors are almost constant as a function of $m_{\text{LQ}}$ and are approximately 1.4 for the bottom-quark-initiated diagrams considered in this analysis.

The main sources of background are the pair production of top quarks (t$t$), W and Z boson production in association with jets, denoted as “W+jets” and “Z+jets”, diboson (WW, WZ, ZZ), single production of top quarks, and quantum chromodynamics (QCD) production of multijet events. The W+jets and Z+jets processes are simulated using the MADGRAPH5_aMC@NLO generator (v5.2.2.2 and v5.2.3.3) at LO precision with the MLM jet matching and merging scheme [46]. The same generator is also used for diboson production simulated at next-to-leading order (NLO) with the FxFx jet matching and merging scheme [47, 48], whereas POWHEG [49–52] 2.0 and 1.0 are used for $t\bar{t}$ and single top quark production at NLO precision,
respectively [53–55]. The $t\bar{t}$ process is normalized using cross sections calculated at next-to-next-to-leading order in perturbative QCD [56].

The generators are interfaced with PYTHIA 8.212 [57] to model the parton showering and fragmentation, as well as the decay of the $\tau$ leptons. The PYTHIA parameters affecting the description of the underlying event are set to the CUETP8M1 tune [58]. The NNPDF3.0 parton distribution functions [59, 60] with the QCD order matching that of the matrix element calculations are used with all generators.

Simulated events are processed with a model of the CMS detector based on GEANT4 [61] and are reconstructed with the same algorithms used for data. The effect of pileup, additional $pp$ collisions within the same or adjacent bunch crossings, is taken into account by adding minimum bias events, generated with PYTHIA, to the hard scattering event. The additional events are weighted such that the frequency distribution matches that in data, with an average of approximately 23 interactions per bunch crossing [62].

4 Event reconstruction

The reconstruction of observed and simulated events uses a particle-flow (PF) algorithm [63], which combines the information from the CMS subdetectors to identify and reconstruct the particles emerging from $pp$ collisions: charged and neutral hadrons, photons, muons, and electrons. Combinations of these PF objects are used to reconstruct higher-level objects such as jets, $\tau$ candidates, or missing transverse momentum ($p_T^{miss}$), taken as the negative vector sum of the transverse momenta ($p_T$) of those jets.

The reconstructed vertex with the largest value of summed physics-object $p_T^2$ is taken to be the primary $pp$ collision vertex. In this case, the physics objects are the objects constructed by a jet finding algorithm [64, 65] applied to all charged tracks associated with the vertex, including tracks from lepton candidates, and the corresponding associated $p_T^{miss}$.

Electrons are identified with a multivariate (MVA) [66] discriminant combining several quantities describing the track quality, the shape of the energy deposits in the ECAL, and the compatibility of the measurements from the tracker and the ECAL [67]. The electrons must pass a cut-based discriminant to reject electrons coming from photon conversions. Muons are identified with requirements on the quality of the track reconstruction and on the number of measurements in the tracker and the muon systems [68]. Electron and muon candidates are required to have $p_T > 50$ GeV. To reject leptons that do not come from the primary vertex and particles misidentified as leptons, a relative lepton isolation $I_\ell$ ($\ell = e, \mu$) is defined as follows:

$$I_\ell = \frac{\sum_{ch} p_T + \max(0, \sum_{neut} p_T - \frac{1}{2} \sum_{ch, PU} p_T)}{p_T^\ell}.$$  

In this expression, $\sum_{ch} p_T$ is the scalar sum of the $p_T$ of the charged hadrons, electrons, and muons originating from the primary vertex and located in a cone of size $\Delta R = \sqrt{(\Delta \eta)^2 + (\Delta \phi)^2} = 0.03$ (0.04) centered on the electron (muon) direction, where $\eta$ is pseudorapidity and $\phi$ is azimuthal angle in radians. The sum $\sum_{neut} p_T$ represents the same quantity for neutral hadrons and photons. The contribution of pileup photons and neutral hadrons is estimated from the scalar sum of the $p_T$ of charged hadrons originating from pileup vertices, $\sum_{ch, PU} p_T$. This sum is multiplied by a factor of 1/2, which corresponds approximately to the ratio of neutral- to charged-hadron production in the hadronization process of inelastic $pp$ collisions, as estimated from simulation. In this analysis, $I_e < 0.10$ ($I_\mu < 0.15$) is used as an isolation requirement.
for the electron (muon). With these cut-off values, the combined efficiency of identification and isolation is around 80 (95)% for the electron (muon). Small differences, up to the 5% level, between data and simulation are corrected for by applying scale factors to simulated events.

Jets are reconstructed from PF candidates using an anti-$k_T$ clustering algorithm with a distance parameter of 0.4, implemented in the FASTJET library [65, 69]. Charged PF candidates not associated with the primary vertex of the interaction are not considered when reconstructing jets. An offset correction is applied to jet energies to take into account the contribution from additional pp collisions within the same or nearby bunch crossings. Jet energy corrections are derived from simulation to bring the average measured response of jets to that of particle-level jets [70]. Further identification requirements are applied to distinguish genuine jets from those coming from pileup [71, 72]. In this analysis, jets are required to have $p_T$ greater than 30 GeV and $|\eta|$ less than 4.7, and must be separated from the selected leptons by a $\Delta R$ of at least 0.5. Jets originating from the hadronization of bottom quarks are identified (b tagged) using the combined secondary vertex algorithm [73], which exploits observables related to the long lifetime and large mass of B hadrons. The chosen b tagging working point corresponds to an identification efficiency of approximately 60% with a misidentification rate of approximately 1%, for jets originating from light (up, down, charm, strange) quarks and gluons.

The $\tau_h$ candidates are reconstructed with the hadron-plus-strips algorithm [74, 75], which is seeded with anti-$k_T$ jets. This algorithm reconstructs $\tau_h$ candidates in the one-prong, one-prong + $\pi^0(s)$, and three-prong decay modes, based on the number of tracks and on the number of strips of ECAL crystals with energy deposits. An MVA-based discriminator, including isolation as well as lifetime information, is used to reduce the incidence of jets being misidentified as $\tau_h$ candidates. The typical working point used in this analysis has an efficiency $\approx 60\%$ for a genuine $\tau_h$, with a misidentification rate for quark and gluon jets of $\approx 0.1\%$.

Electrons and muons misidentified as $\tau_h$ candidates are suppressed using criteria based on the consistency between the measurements in the tracker, the calorimeters, and the muon detectors. The criteria are optimized separately for each final state studied.

All particles reconstructed in the event are used in the determination of $p_T^{\text{miss}}$ [76]. The calculation takes into account jet energy corrections. Corrections are applied to correct for the mismodeling of $p_T^{\text{miss}}$ in the simulated samples of the Z+jets and W+jets processes. The corrections are performed on the variable defined as the vectorial difference between the measured $p_T^{\text{miss}}$ and the total $p_T$ of neutrinos originating from the decay of the W or Z boson.

### 5 Event selection

The search for scalar LQs is performed in three channels, each containing a b-tagged jet. Channels containing in addition an electron or a muon, together with a $\tau_h$ candidate are labeled $e\tau_h$ and $\mu\tau_h$, and collectively referred to as $\ell\tau_h$. The third channel, which has two $\tau_h$ candidates in addition to the b-tagged jet, is labeled $\tau_h\tau_h$. The selection criteria have been optimized based on the expected sensitivity to a single-LQ signal.

Firstly, events are required to be compatible with $\tau\tau$ production. In the $e\tau_h$ ($\mu\tau_h$) channel, events are selected using a trigger that requires an isolated electron (muon) with $p_T > 25$ (24) GeV. Offline, the selected electron (muon) is required to have $p_T > 50$ GeV and $|\eta| < 2.1$ (2.4). The $\tau_h$ candidate is required to have $p_T > 50$ GeV and $|\eta| < 2.3$. In the $\tau_h\tau_h$ channel, events are selected online by requiring two isolated $\tau_h$ candidates with $p_T > 35$ GeV. Offline, both $\tau_h$ candidates are required to have $p_T > 50$ GeV and $|\eta| < 2.1$. The selected $\ell$ and $\tau_h$
candidate, or two $\tau_h$ candidates, must meet isolation requirements as detailed in Section 4, have opposite-sign (OS) electric charges and be separated by $\Delta R > 0.5$. They must also meet the requirement that the distance of closest approach to the primary vertex satisfies $|d_z| < 0.2$ cm along the beam direction, and $|d_{xy}| < 0.045$ cm in the transverse plane. Events with additional isolated muons or electrons ($p_T > 10$ GeV and $|\eta| < 2.4$ or $2.5$) that pass a looser identification requirement are discarded to reduce $Z$+jets and diboson backgrounds and to avoid correlations between channels.

Further event selection is applied to increase the signal purity. Since signal events contain at least one energetic bottom quark jet coming from the LQ decay, at least one b-tagged jet with $p_T > 50$ GeV and $|\eta| < 2.4$ is required. To reduce the $Z$+jets background, the invariant mass, $m_{vis}$, of the $\ell$ and $\tau_h$ candidate (two $\tau_h$ candidates), is required to be greater than 85 (95) GeV in the $\ell\tau_h$ ($\tau_h\tau_h$) channels.

The product of acceptance ($A$), efficiency ($\epsilon$), and the branching fraction ($B$) of the $\tau\tau$ to a specific final state ranges from 0.2 to 1.3% in the $e\tau_h$ channel for $m_{LQ}$ between 200 and 1500 GeV. The $\epsilon$ increases with increasing $m_{LQ}$ due to the harder $p_T$ spectra of the final state particles. Beyond 1000 GeV, however, $\epsilon$ starts to decrease, mainly because of the lower b tagging efficiency. Similarly, $A\epsilon B$ in the $\mu\tau_h$ ($\tau_h\tau_h$) channels range from 0.3 to 1.8% (0.5 to 2.5%). Figure 2 shows $A\epsilon B$ for the signal, in each final state considered in this analysis, as a function of $m_{LQ}$.

After applying the event selection, an excess of events over the SM backgrounds is searched for using the distribution of the scalar $p_T$ sum of all required final-state particles, $S_T$, which is defined as $p_T(\ell) + p_T(\tau_h) + p_T(\text{leading jet})$ for the $\ell\tau_h$ channels, and $p_T(\text{leading } \tau_h) + p_T(\text{subleading } \tau_h) + p_T(\text{leading jet})$ for the $\tau_h\tau_h$ channel, where leading and subleading refer to $p_T$. Because of the $p_T$ threshold requirements, $S_T$ is always greater than 150 GeV.

![Figure 2: The product of acceptance, efficiency, and branching fraction as a function of $m_{LQ}$ for the single production of LQs in each of the three channels considered: $\tau_h\tau_h$ (black solid line), $\mu\tau_h$ (red dashed line), and $e\tau_h$ (blue dotted line).](image-url)
6 Background estimation

The dominant background in all channels is \( t\bar{t} \) production because of the presence of genuine electrons, muons, \( \tau \) leptons, and bottom quark jets produced in the \( t\bar{t} \) decays. Additional backgrounds that satisfy the signal selection are \( W + \) jets, \( Z + \) jets, diboson, and single top quark processes, as well as QCD multijet events. In this section, background estimation methods and their validation are described separately for the \( \ell \tau_h \) and \( \tau_h \tau_h \) channels.

6.1 The \( \ell \tau_h \) channels

The normalization and shape of the \( t\bar{t} \) background are obtained from data, making use of an \( e\mu \) control region (CR), containing events with an electron, a muon, and at least one b-tagged jet. The same \( p_T \) and \( |\eta| \) requirements as in the signal region (SR) are placed on all three objects. The invariant mass of the selected electron and muon is required to be greater than 85 GeV. The purity of \( t\bar{t} \) events in this CR, estimated from simulation, is 92%, with negligible signal contamination. A good agreement between data and simulation is found for both the normalization and the shape, validating the method used to estimate the \( t\bar{t} \) background in the SR.

In order to allow for possible remaining mismodeling related to \( t\bar{t} \) backgrounds, this CR is included in the maximum likelihood fit, as described in Section 7, together with relevant nuisance parameters such as the b tagging efficiency and \( t\bar{t} \) cross section uncertainties. In this way, the normalization and the shape of the \( t\bar{t} \) backgrounds can be constrained from the data. This procedure also helps to constrain \( t\bar{t} \) backgrounds in the \( \tau_h \tau_h \) channel, although its contribution is less significant than in the \( \ell \tau_h \) channels.

For the \( W + \) jets background, the shape is taken from simulation, while the normalization is determined from data in a high (>80 GeV) transverse mass \( (m_T) \) sideband; here \( m_T \) is defined as

\[
m_T = \sqrt{2p_T^\ell |p_T^{\text{miss}}|(1 - \cos \Delta \phi)},
\]

where \( p_T^\ell \) is the lepton \( p_T \) and \( \Delta \phi \) is the azimuthal angle between the lepton direction and \( p_T^{\text{miss}} \). The normalization factor is calculated before the b tagging requirement is applied. A 30% uncertainty is assigned for the \( W + \) jets background estimate to account for the limited event counts in the high \( m_T \) sideband, as well as the extrapolation uncertainty to the SR.

The QCD multijet background, in which one of the jets is misidentified as the \( \tau_h \) candidate and another as the \( \ell \), is small and is estimated using a CR where the \( \ell \) and \( \tau_h \) candidate have same-sign (SS) electric charges. In this CR, the QCD multijet yield is obtained by subtracting from the data the contribution of the \( Z + \) jets, \( t\bar{t} \), and \( W + \) jets processes. The expected contribution of the QCD multijet background in the OS SR is then derived by rescaling the yield obtained in the SS CR by a factor of 1.06, which is measured using a pure QCD multijet sample obtained by inverting the lepton isolation requirement. To determine the uncertainty associated with this procedure, the measurement is repeated with several different \( S_T \) requirements. The maximum variation observed is 30%, and this is taken to be the uncertainty in the QCD background estimate.

Minor backgrounds such as diboson and single top quark processes are estimated from the simulation.

6.2 The \( \tau_h \tau_h \) channel

In the \( \tau_h \tau_h \) channel, the shape and normalization of all background processes with genuine hadronic \( \tau \) decays are estimated using simulated samples. The backgrounds concerned are
Z → τ_hτ_h, and contributions from the t̅t, diboson and single top quark processes.

Other backgrounds arising from jets misidentified as τ_h candidates, most of which are from QCD multijet backgrounds, are estimated from CRs in data using the fake-factor method [77, 78]. An application region (AR) is defined containing the same selection criteria as in the SR, except for an inverted τ_h isolation requirement for one of the two τ_h candidates. The AR is primarily populated by events with jets misidentified as τ_h candidates, and has a contamination from genuine hadronic τ decays at the level of a few percent or below.

The ratio of the number of events with a misidentified τ_h in the AR to the number in the SR (fake factor) is assumed to be the same as the ratio measured in samples with an SS τ_hτ_h pair. The fake factor is then applied to the number of events in the AR to estimate the number of events with a misidentified τ_h in the SR. The fake factor is calculated as a function of the p_T and decay mode of the τ_h candidate, and it ranges from 0.1 to 0.25. In order to take combinatorial effects into account, a weight factor of 0.5 is applied. Since the presence of small backgrounds in the AR that contain a genuine τ_h results in up to a 2% underestimation of the number of events with a misidentified τ_h in the SR, a correction is applied based on the fractions of these processes in simulated events. Corresponding uncertainties are incorporated in the fit model, as described in Section 7.

The fake-factor method is tested in two validation regions (VRs); one is constructed by inverting the leading jet p_T requirement (i.e. p_T < 50 GeV) and the other by using events with two τ_h candidates that do not fulfill the tight isolation criteria used to define the SR. For both VRs, all other selection criteria are kept identical to the SR, except that the b tagging requirement is removed to increase the number of events. The signal contamination is negligible in both VRs. Agreement between data and simulation is found, within statistical uncertainties, demonstrating the validity of the fake-factor method.

Finally, small contributions coming from the Z+jets background are validated using the same event selection as in the SR, except that we require m_vis < 95 GeV. Data and simulated events show agreement within statistical uncertainty. A 30% uncertainty is attributed to the Z+jets background yield due to the limited event count in this CR.

7 Systematic uncertainties and signal extraction

A binned maximum likelihood method is used for the signal extraction [79]. As discussed in Section 5, the S_T distribution for S_T greater than 150 GeV is used as the final discriminant. The fit is performed simultaneously in the eτ_h, μτ_h, and τ_hτ_h signal regions, as well as in the eμ control region, as defined in Section 6. Systematic uncertainties may affect the normalization and the shape of the S_T distribution of the signal and background processes. These uncertainties are represented by nuisance parameters in the fit, as described below. The relevant uncertainties are summarized in Table 1.

7.1 Normalization uncertainties

The uncertainty in the integrated luminosity amounts to 2.5% [62] and affects the normalization of the signal and background processes that are based on simulation. Uncertainties in the electron identification and trigger efficiency amount to 8 and 2%, respectively, while those in the muon identification and trigger efficiency amount to 2% each. The τ_h identification and trigger efficiency have been measured using the “tag-and-probe” technique [74, 75] and an uncertainty of 5% per τ_h candidate is assigned. The acceptance uncertainty due to the b tagging efficiency (misidentification rate) is taken to be 3 (5)%. A 30% uncertainty is attributed to the
W+jets, Z+jets, and QCD multijet backgrounds in the $\ell\tau_h$ channels, as discussed in Section 6. The cross section uncertainties in the $t\bar{t}$, diboson, and single top quark processes are 5.5, 6.0, and 5.5%, respectively. For events where electrons or muons are misidentified as $\tau_h$ candidates, predominantly $Z \rightarrow ee$ events in the $e\tau_h$ channel and $Z \rightarrow \mu\mu$ events in the $\mu\tau_h$ channel, rate uncertainties of 12 and 25%, respectively, are allocated, based on the tag-and-probe method.

### 7.2 Shape uncertainties

The energy scales of the $\tau_h$ candidate and the leading jet affect the shape of the $S_T$ distribution, as well as the normalization of the signal and background processes. The uncertainty is estimated by varying the $\tau_h$ and jet energies within their respective uncertainties and recomputing $S_T$ after the final selection. The uncertainty in the $\tau_h$ energy scale amounts to 3% [74], whereas the variations due to the jet energy scale are in the 1–2% range, depending on the jet $p_T$ and $\eta$ [70].

The uncertainty in the extrapolation of the $\tau_h$ identification efficiency to higher $p_T$s is treated as a shape uncertainty. It is proportional to $p_T(\tau_h)$ and has a value of $+5\%/-35\%$ at $p_T(\tau_h) = 1$ TeV. The effects of the uncertainties due to the electron and muon energy scales are found to be negligible. The probability of a jet being misidentified as a $\tau_h$ candidate has been checked using a $t\bar{t}$ control region in data. The difference between data and simulated events is fit using a linear function, and its functional form, $1.2 - 0.004\left\{\max(120, p_T)\ \text{GeV}\right\}$, is considered as a one-sided shape uncertainty for the $\tau_h$ channels.

In the $\tau_3\tau_h$ channel, additional shape uncertainties related to the fake-factor method are considered. There are eight variations coming from factors such as the finite number of events in the samples, possible neglected effects in the fake factor determination, additional uncertainties in the correction of the SS to OS extrapolation, and the uncertainties in the background composition in the AR, which is estimated with simulated events. When added in quadrature, these additional uncertainties are of order 10%.

Finally, uncertainties related to the finite number of simulated events, and to the limited number of events in data CRs, are taken into account. They are considered for all bins of the distributions that are used to extract the results. The binning of the histograms are adjusted such that the uncertainty, for a given bin, does not exceed 15%. They are uncorrelated across the different samples, and across the bins of a single distribution.

### 8 Results

Figure 3 shows the $S_T$ distributions after the combined fit to the $e\tau_h$, $\mu\tau_h$, and $\tau_h\tau_h$ signal regions, as well as to the $e\mu$ control region. The background uncertainty bands on the histograms of simulated events represent the sum in quadrature of statistical and systematic uncertainties, taking the full covariance matrix of all nuisance parameters into account. The dominant uncertainty in the background estimate comes from the limited event counts in simulated samples. However, this uncertainty is unimportant for $m_{LQ} > 500$ GeV, where the mass limit is set, and the sensitivity is ultimately constrained by the size of the data sample.

Table 2 shows the event yields for a signal-enriched region with $S_T > 500$ GeV, together with event yields expected for a representative LQ signal with $m_{LQ} = 700$ GeV.

The data are consistent with the background-only (SM) hypothesis. In the $\tau_3\tau_h$ channel, one bin at around 250 GeV shows a slight excess in data, corresponding to two standard deviations. This, however, has little impact on the results, as the sensitivity is dominated by the $S_T$ tail,
Table 1: Summary of systematic uncertainties in the signal acceptance and background estimate. The uncertainties have been grouped into those affecting the normalization of distributions and those affecting the shape, and uncertainties marked with a * are treated as correlated among channels.

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<td>Single top quark cross section *</td>
<td>5.5%</td>
<td>5.5%</td>
<td>5.5%</td>
</tr>
<tr>
<td>e → τh misidentification rate</td>
<td>12%</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>µ → τh misidentification rate</td>
<td>—</td>
<td>25%</td>
<td>—</td>
</tr>
<tr>
<td>Shape</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>τh energy scale *</td>
<td>±3%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>τh identification extrapolation *</td>
<td></td>
<td>+5%pT(τh) and −35%pT(τh)</td>
<td></td>
</tr>
<tr>
<td>Jet energy scale *</td>
<td>±1 standard deviation [70]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Jet → τh misidentification rate *</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fake-factor method</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Simulated sample size</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 2: Numbers of events observed in the eτh, µτh, τhτh, and eµ channels for ST > 500 GeV, compared to the background expectations and to the event yield expected for single-LQ processes with mLQ = 700 GeV (λ = 1 and β = 1). The “electroweak” background contains the contributions from W+jets, Z+jets, and diboson processes. The uncertainties represent the sum in quadrature of statistical and systematic contributions, and are obtained using the binned maximum likelihood fit of the ST distribution.

<table>
<thead>
<tr>
<th>Process</th>
<th>eτh</th>
<th>µτh</th>
<th>τhτh</th>
<th>eµ</th>
</tr>
</thead>
<tbody>
<tr>
<td>tt</td>
<td>114.8 ± 2.9</td>
<td>194.6 ± 4.4</td>
<td>6.7 ± 1.0</td>
<td>1895.2 ± 14.4</td>
</tr>
<tr>
<td>Single top quark</td>
<td>23.2 ± 2.2</td>
<td>36.6 ± 2.6</td>
<td>1.5 ± 0.5</td>
<td>263.4 ± 6.8</td>
</tr>
<tr>
<td>Electroweak</td>
<td>9.1 ± 2.3</td>
<td>10.9 ± 3.1</td>
<td>2.2 ± 1.0</td>
<td>16.0 ± 2.4</td>
</tr>
<tr>
<td>QCD multijet</td>
<td>4.5 ± 4.6</td>
<td>1.5 ± 5.3</td>
<td>1.9 ± 0.6</td>
<td>8.3 ± 5.6</td>
</tr>
<tr>
<td>Total expected background</td>
<td>151.6 ± 6.3</td>
<td>243.6 ± 8.0</td>
<td>12.3 ± 1.7</td>
<td>2182.9 ± 17.0</td>
</tr>
<tr>
<td>LQ signal (mLQ = 700 GeV, λ = 1, β = 1)</td>
<td>8.8 ± 0.3</td>
<td>12.9 ± 0.4</td>
<td>9.5 ± 1.2</td>
<td>4.9 ± 0.2</td>
</tr>
<tr>
<td>Observed data</td>
<td>143</td>
<td>225</td>
<td>14</td>
<td>2147</td>
</tr>
</tbody>
</table>
Figure 3: Observed $S_T$ distribution in the $e\tau_h$ (upper left), $\mu\tau_h$ (upper right), and $\tau_h\tau_h$ (lower left) signal regions, as well as in the $e\mu$ (lower right) control region, compared to the expected SM background contributions. The distribution labeled “electroweak” contains the contributions from $W$+jets, $Z$+jets, and diboson processes. The signal distributions for single-LQ production with mass 700 GeV are overlaid to illustrate the sensitivity. For the signal normalization, $\lambda = 1$ and $\beta = 1$ are assumed. The background uncertainty bands represent the sum in quadrature of statistical and systematic uncertainties obtained from the fit. The lower panels show the ratio between the observed and expected events in each bin. In all plots, the horizontal and vertical error bars on the data points represent the bin widths and the Poisson uncertainties, respectively.

rather than the main part of the distribution.

We set an upper limit on the cross section times branching fraction $\beta$ as a function of $m_{LQ}$, by using the asymptotic CL$_S$ modified frequentist criterion [79–82]. Figure 4 shows the observed and expected upper limits at 95% confidence level. The blue solid line corresponds to the theoretical cross sections [45], calculated with $\lambda = 1$ and $\beta = 1$. The intersection of the blue and the black lines determines the lower limit on $m_{LQ}$. Assuming $\lambda = 1$ and $\beta = 1$, third-generation scalar LQs with masses below 740 GeV are excluded at 95% confidence level, to be compared with an expected lower limit of 750 GeV.

The sensitivity of the analysis is dominated by the $\tau_h\tau_h$ channel, followed by the $\mu\tau_h$ channel,
Figure 4: Observed (black solid) and expected (black dotted) limits at 95% confidence level on the product of cross section $\sigma$ and branching fraction $\beta$, obtained from the combination of the $e\tau_h$, $\mu\tau_h$, and $\tau_h\tau_h$ signal regions, as well as from the $e\mu$ control region, as a function of the LQ mass. The green and yellow bands represent the one and two standard deviation uncertainties in the expected limits. The theory prediction is indicated by the blue solid line, together with systematic uncertainties due to the choice of PDF and renormalization and factorization scales [45], indicated by the blue band.

and then the $e\tau_h$ channel. The better sensitivity in the $\tau_h\tau_h$ channel comes from the larger branching fraction of $B(\tau\tau \to \tau_h\tau_h) = 42\%$, compared to $B(\tau\tau \to \mu\tau_h) = B(\tau\tau \to e\tau_h) = 21\%$. Furthermore, the $\ell\tau_h$ channels are contaminated by $t\bar{t} \to WWbb \to \ell\tau_h\nu\nu\bar{b}b$ process, in addition to the $t\bar{t} \to WWbb \to \ell\tau_h\nu\nu\bar{b}b$ background, which is not the case for the $\tau_h\tau_h$ channel. Here, $\ell\tau$ denotes a leptonically-decaying $\tau$ lepton.

Since the single-LQ signal cross section scales with $\lambda^2$, it is straightforward to recast the results presented in Fig. 4 in terms of expected and observed upper limits on $\lambda$ as a function of $m_{LQ}$, as shown in Fig. 5. Values of $\lambda$ up to 2.5 are considered, such that the width of the LQ signal stays narrow and to satisfy constraints from electroweak precision measurements [43]. Here we have made the assumption that the shape of the $S_T$ distribution does not depend on $\lambda$ over the range of $\lambda$ used in the analysis. This assumption has been verified using simulated events. The blue band shows the preferred parameter space (95% CL) for the scalar LQ preferred by the B physics anomalies: $\lambda = (0.95 \pm 0.50) m_{LQ}/(\text{TeV})$ [36]. The plot also shows the limit from the pair-produced LQ search overlaid as an orange vertical line, which does not depend on $\lambda$, as discussed in Section 1. For values of $\lambda > 1.4$, the mass limit obtained by this analysis exceeds that of the search considering pair production [37] and provides the best upper limit on $m_{LQ}$ of the third-generation scalar LQ decaying to a $\tau$ lepton and a bottom quark. For $\lambda = 2.5$ and $\beta = 1$, the observed and expected lower limits on mass are both 1050 GeV. This result, together with the pair-produced search, begins to constrain the region of parameter space implied by the B physics anomalies.
Figure 5: Expected and observed exclusion limits at 95% confidence level on the Yukawa coupling $\lambda$ at the LQ-lepton-quark vertex, as a function of the LQ mass. A unit branching fraction $\beta$ of the LQ to a $\tau$ lepton and a bottom quark is assumed. The orange vertical line indicates the limit obtained from a search for pair-produced LQs decaying to $\ell\tau_bb$ [37]. The left-hand side of the dotted (solid) line shows the expected (observed) exclusion region for the present analysis. The gray band shows ±1 standard deviations of the expected exclusion limit. The region with diagonal blue shading shows the parameter space preferred by one of the models proposed to explain anomalies observed in B physics [36].

9 Summary

A search for singly produced third-generation scalar leptoquarks, each decaying to a $\tau$ lepton and a bottom quark has been presented. The final state of an electron or a muon plus one hadronically decaying $\tau$ lepton and the final state with two hadronically decaying $\tau$ leptons are explored. In all final states at least one energetic jet identified as originating from a bottom quark is required. The search is based on a data sample of proton-proton collisions at a center-of-mass energy of 13 TeV recorded by the CMS detector, corresponding to an integrated luminosity of 35.9 fb$^{-1}$. The data are found to be in agreement with the standard model predictions. Upper limits as a function of the leptoquark mass are set on the third-generation scalar leptoquark production cross section. Results are compared with theoretical predictions to obtain lower limits on the leptoquark mass. Assuming the leptoquark always decays to a $\tau$ lepton and a bottom quark with unit Yukawa coupling $\lambda = 1$, third-generation scalar leptoquarks with mass below 740 GeV are excluded at 95% confidence level. Mass limits are also placed as a function of $\lambda$. For values of $\lambda > 1.4$, the mass limit obtained by this analysis exceeds that of the search considering pair production and provides the best upper limit. For $\lambda = 2.5$, leptoquarks are excluded in the mass range up to 1050 GeV. This is the first time that limits have been presented in the $\lambda$ versus mass plane, allowing the results to be considered in the preferred parameter space of models that invoke third-generation leptoquarks to explain anomalies observed in B hadron decays. These results thus demonstrate the important potential of single leptoquark production studies to complement pair production constraints on such
Acknowledgments

We congratulate our colleagues in the CERN accelerator departments for the excellent performance of the LHC and thank the technical and administrative staffs at CERN and at other CMS institutes for their contributions to the success of the CMS effort. In addition, we gratefully acknowledge the computing centers and personnel of the Worldwide LHC Computing Grid for delivering so effectively the computing infrastructure essential to our analyses. Finally, we acknowledge the enduring support for the construction and operation of the LHC and the CMS detector provided by the following funding agencies: BMWFW and FWF (Austria); FNRS and FWO (Belgium); CNPq, CAPES, FAPERJ, FAPERGS, and FAPESP (Brazil); MES (Bulgaria); CERN; CAS, MoST, and NSFC (China); COLCIENCIAS (Colombia); MSES and CSF (Croatia); RPF (Cyprus); SENESCYT (Ecuador); MoER, ERC IUT, and ERDF (Estonia); Academy of Finland, MEC, and HIP (Finland); CEA and CNRS/IN2P3 (France); BMBF, DFG, and HGF (Germany); GSRT (Greece); NKFIH (Hungary); DAE and DST (India); IPM (Iran); SFI (Ireland); INFN (Italy); MSIP and NRF (Republic of Korea); LAS (Lithuania); MOE and UM (Malaysia); BUAP, CINVESTAV, CONACYT, LNS, SEP, and UASLP-FAI (Mexico); MBIE (New Zealand); PAEC (Pakistan); MSHE and NSC (Poland); FCT (Portugal); JINR (Dubna); MON, RosAtom, RAS, RFBR, and NRC KI (Russia); MESTD (Serbia); SEIDI, CPAN, PCTI, and FEDER (Spain); Swiss Funding Agencies (Switzerland); MST (Taipei); ThEPCenter, IPST, STAR, and NSTDA (Thailand); TUBITAK and TAEK (Turkey); NASU and SFFR (Ukraine); STFC (United Kingdom); DOE and NSF (USA).

Individuals have received support from the Marie-Curie program and the European Research Council and Horizon 2020 Grant, contract No. 675440 (European Union); the Leventis Foundation; the A. P. Sloan Foundation; the Alexander von Humboldt Foundation; the Belgian Federal Science Policy Office; the Fonds pour la Formation à la Recherche dans l’Industrie et dans l’Agriculture (FRIA-Belgium); the Agentschap voor Innovatie door Wetenschap en Technologie (IWT-Belgium); the F.R.S.-FNRS and FWO (Belgium) under the “Excellence of Science - EOS” - be.h project n. 30820817; the Ministry of Education, Youth and Sports (MEYS) of the Czech Republic; the Lendület (“Momentum”) Program and the János Bolyai Research Scholarship of the Hungarian Academy of Sciences, the New National Excellence Program ÚNKP, the NKFIH research grants 123842, 123959, 124845, 124850 and 125105 (Hungary); the Council of Science and Industrial Research, India; the HOMING PLUS program of the Foundation for Polish Science, cofinanced from European Union, Regional Development Fund, the Mobility Plus program of the Ministry of Science and Higher Education, the National Science Center (Poland), contracts Harmonia 2014/14/M/ST2/00428, Opus 2014/13/B/ST2/02543, 2014/15/B/ST2/03998, and 2015/19/B/ST2/02861, Sonata-bis 2012/07/E/ST2/01406; the National Priorities Research Program by Qatar National Research Fund; the Programa Estatal de Fomento de la Investigación Científica y Técnica de Excelencia María de Maeztu, grant MDM-2015-0509 and the Programa Severo Ochoa del Principado de Asturias; the Thalis and Aristeia programs cofinanced by EU-ESF and the Greek NSRF; the Rachadapisek Sompot Fund for Postdoctoral Fellowship, Chulalongkorn University and the Chulalongkorn Academic into Its 2nd Century Project Advancement Project (Thailand); the Welch Foundation, contract C-1845; and the Weston Havens Foundation (USA).
References


A  The CMS Collaboration

Yerevan Physics Institute, Yerevan, Armenia
A.M. Sirunyan, A. Tumasyan

Institut für Hochenergiephysik, Wien, Austria

Institute for Nuclear Problems, Minsk, Belarus
V. Chekhovsky, V. Mossolov, J. Suarez Gonzalez

Universiteit Antwerpen, Antwerpen, Belgium

Vrije Universiteit Brussel, Brussel, Belgium

Université Libre de Bruxelles, Bruxelles, Belgium

Ghent University, Ghent, Belgium

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

Centro Brasileiro de Pesquisas Físicas, Rio de Janeiro, Brazil

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

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

Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Sofia, Bulgaria
A. Aleksandrov, R. Hadjiiska, P. Iaydjiev, A. Marinov, M. Misheva, M. Rodozov, M. Shopova, G. Sultanov
University of Sofia, Sofia, Bulgaria
A. Dimitrov, L. Litov, B. Pavlov, P. Petkov

Beihang University, Beijing, China
W. Fang, X. Gao, L. Yuan

Institute of High Energy Physics, Beijing, China

State Key Laboratory of Nuclear Physics and Technology, Peking University, Beijing, China
Y. Ban, G. Chen, A. Levin, J. Li, L. Li, Q. Li, Y. Mao, S.J. Qian, D. Wang, Z. Xu

Tsinghua University, Beijing, China
Y. Wang

Universidad de Los Andes, Bogota, Colombia
C. Avila, A. Cabrera, C.A. Carrillo Montoya, L.F. Chaparro Sierra, C. Florez, C.F. González Hernández, M.A. Segura Delgado

University of Split, Faculty of Electrical Engineering, Mechanical Engineering and Naval Architecture, Split, Croatia
B. Courbon, N. Godinovic, D. Lelas, I. Puljak, T. Sculac

University of Split, Faculty of Science, Split, Croatia
Z. Antunovic, M. Kovac

Institute Rudjer Boskovic, Zagreb, Croatia
V. Brigljevic, D. Ferencek, K. Kadija, B. Mesic, A. Starodumov, T. Susa

University of Cyprus, Nicosia, Cyprus

Charles University, Prague, Czech Republic
M. Finger, M. Finger Jr.

Escuela Politecnica Nacional, Quito, Ecuador
E. Ayala

Universidad San Francisco de Quito, Quito, Ecuador
E. Carrera Jarrin

Academy of Scientific Research and Technology of the Arab Republic of Egypt, Egyptian Network of High Energy Physics, Cairo, Egypt
Y. Assran, S. Elgammal, S. Khalil

National Institute of Chemical Physics and Biophysics, Tallinn, Estonia
S. Bhowmik, A. Carvalho Antunes De Oliveira, R.K. Dewanjee, K. Ehatiht, M. Kadastik, M. Raidal, C. Veelken

Department of Physics, University of Helsinki, Helsinki, Finland
P. Eerola, H. Kirschenmann, J. Pekkanen, M. Voutilainen
Helsinki Institute of Physics, Helsinki, Finland

Lappeenranta University of Technology, Lappeenranta, Finland
T. Tuuva

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

Laboratoire Leprince-Ringuet, Ecole polytechnique, CNRS/IN2P3, Université Paris-Saclay, Palaiseau, France

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

Centre de Calcul de l’Institut National de Physique Nucleaire et de Physique des Particules, CNRS/IN2P3, Villeurbanne, France
S. Gadrat

Université de Lyon, Université Claude Bernard Lyon 1, CNRS-IN2P3, Institut de Physique Nucléaire de Lyon, Villeurbanne, France

Georgian Technical University, Tbilisi, Georgia
A. Khvedelidze

Tbilisi State University, Tbilisi, Georgia
D. Lomidze

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

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

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

23
Deutsches Elektronen-Synchrotron, Hamburg, Germany

University of Hamburg, Hamburg, Germany

Karlsruher Institut fuer Technology

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

National and Kapodistrian University of Athens, Athens, Greece
G. Karathanasis, S. Kesisoglou, P. Kontaxakis, A. Panagiotou, N. Saoulidou, E. Tziaferi, K. Velidis

National Technical University of Athens, Athens, Greece
K. Kousouris, I. Papakrivopoulos, G. Tsipolitis

University of Ioánnina, Ioánnina, Greece

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

Wigner Research Centre for Physics, Budapest, Hungary

Institute of Nuclear Research ATOMKI, Debrecen, Hungary
N. Beni, S. Czellar, J. Karancsi, A. Makovec, J. Molnar, Z. Szillasi
Institute of Physics, University of Debrecen, Debrecen, Hungary
P. Raics, Z.L. Trocsanyi, B. Ujvari

Indian Institute of Science (IISc), Bangalore, India
S. Choudhury, J.R. Komaragiri, P.C. Tiwari

National Institute of Science Education and Research, HBNI, Bhubaneswar, India

Panjab University, Chandigarh, India

University of Delhi, Delhi, India
A. Bhardwaj, B.C. Choudhary, R.B. Garg, M. Gola, S. Keshri, Ashok Kumar, S. Malhotra, M. Naimuddin, P. Priyanka, K. Ranjan, Aashaq Shah, R. Sharma

Saha Institute of Nuclear Physics, HBNI, Kolkata, India

Indian Institute of Technology Madras, Madras, India
P.K. Behera

Bhabha Atomic Research Centre, Mumbai, India
R. Chudasama, D. Dutta, V. Jha, V. Kumar, P.K. Netrakanti, L.M. Pant, P. Shukla

Tata Institute of Fundamental Research-A, Mumbai, India
T. Aziz, M.A. Bhat, S. Dugad, G.B. Mohanty, N. Sur, B. Sutar, Ravindra Kumar Verma

Tata Institute of Fundamental Research-B, Mumbai, India

Indian Institute of Science Education and Research (IISER), Pune, India
S. Chauhan, S. Dube, V. Hegde, A. Kapoor, K. Kothekar, S. Pandey, A. Rane, S. Sharma

Institute for Research in Fundamental Sciences (IPM), Tehran, Iran
S. Chenarani26, E. Eskandari Tadavani, S.M. Etesami26, M. Khakzad, M. Mohammadi Najafabadi, M. Nasiri, F. Rezaei Hosseinabadi, B. Safarzadeh27, M. Zeinali

University College Dublin, Dublin, Ireland
M. Felcini, M. Grunewald

INFN Sezione di Bari a, Università di Bari b, Politecnico di Bari c, Bari, Italy
M. Abbresciaa,b, C. Calabriaa,b, A. Colaleoa,b, D. Creanzaa,c, L. Cristinaa,b, N. De Filippisa,c, M. De Palmaa,b, A. Di Florioa,b,f, F. Erricoa,b, L. Fiorea, A. Gelmiab,b, G. Isellia,c, M. Ineeab, S. Lezkiab,b, G. Maggia,c, M. Maggia, G. Minieloa,b, S. Myab,b, S. Nuzzoa,b, A. Pompilia,b, G. Pugliesea,c, R. Radognaa, A. Ranieri, G. Selvaggiab,b, A. Sharma, L. Silvestrais, R. Vendittia, P. Verwilligena, G. Zitoa

INFN Sezione di Bologna a, Università di Bologna b, Bologna, Italy
G. Abbiendia, C. Battilanaa,b, D. Bonacorsia,b, L. Borgonovia,b, S. Braibant-Giacomelliab, R. Campaninia,b, P. Capiluppia,b, A. Castroab, F.R. Cavalloa, S.S. Chhibraa,b, C. Cioccia,
G. Codispoti\textsuperscript{a,b}, M. Cuffiani\textsuperscript{a,b}, G.M. Dallavalle\textsuperscript{a}, F. Fabbri\textsuperscript{a}, A. Fanfani\textsuperscript{a,b}, P. Giacomelli\textsuperscript{a}, C. Grandi\textsuperscript{a}, L. Guiducci\textsuperscript{a,b}, F. Iemmi\textsuperscript{a,b}, S. Marcellini\textsuperscript{a}, G. Masetti\textsuperscript{a}, A. Montanari\textsuperscript{a}, F.L. Navarria\textsuperscript{a,b}, A. Perrotta\textsuperscript{a}, F. Primavera\textsuperscript{a,b,15}, A.M. Rossi\textsuperscript{a,b}, T. Rovelli\textsuperscript{a,b}, G.P. Siroli\textsuperscript{a,b}, N. Tosi\textsuperscript{a}

**INFN Sezione di Catania\textsuperscript{a}, Università di Catania\textsuperscript{b}, Catania, Italy**

S. Albergo\textsuperscript{a,b}, A. Di Mattia\textsuperscript{a}, R. Potenza\textsuperscript{a,b}, A. Tricomi\textsuperscript{a,b}, C. Tuve\textsuperscript{a,b}

**INFN Sezione di Firenze\textsuperscript{a}, Università di Firenze\textsuperscript{b}, Firenze, Italy**

G. Barbagli\textsuperscript{a}, K. Chatterjee\textsuperscript{a,b}, V. Ciulli\textsuperscript{a,b}, C. Civinini\textsuperscript{a}, R. D’Alessandro\textsuperscript{a,b}, E. Focardi\textsuperscript{a,b}, G. Latino, P. Lenzri\textsuperscript{a,b}, M. Meschini\textsuperscript{a}, S. Paoletti\textsuperscript{a}, L. Russo\textsuperscript{a,28}, G. Sguazzoni\textsuperscript{a}, D. Strom\textsuperscript{a}, L. Viliani\textsuperscript{a}

**INFN Laboratori Nazionali di Frascati, Frascati, Italy**

L. Benussi, S. Bianco, F. Fabbri, D. Piccolo

**INFN Sezione di Genova\textsuperscript{a}, Università di Genova\textsuperscript{b}, Genova, Italy**

F. Ferro\textsuperscript{a}, F. Ravera\textsuperscript{a,b}, E. Robutti\textsuperscript{a}, S. Tosi\textsuperscript{a,b}

**INFN Sezione di Milano-Bicocca\textsuperscript{a}, Università di Milano-Bicocca\textsuperscript{b}, Milano, Italy**

A. Benaglia\textsuperscript{a}, A. Beschi\textsuperscript{b}, L. Brianza\textsuperscript{a,b}, F. Brivio\textsuperscript{a,b}, V. Ciriolo\textsuperscript{a,b,15}, S. Di Guida\textsuperscript{a,d,15}, M.E. Dinardo\textsuperscript{a,b}, S. Fiorendi\textsuperscript{a,b}, S. Gennai\textsuperscript{a}, A. Ghezzi\textsuperscript{a,b}, P. Govoni\textsuperscript{a,b}, M. Malberti\textsuperscript{a,b}, S. Malvezzi\textsuperscript{a}, A. Massironi\textsuperscript{a,b}, D. Menasce\textsuperscript{a}, L. Moroni\textsuperscript{a}, M. Paganoni\textsuperscript{a,b}, D. Pedrini\textsuperscript{a}, S. Ragazzi\textsuperscript{a,b}, T. Tabarelli de Fatis\textsuperscript{a,b}

**INFN Sezione di Napoli\textsuperscript{a}, Università di Napoli ‘Federico II’\textsuperscript{b}, Napoli, Italy, Università della Basilicata\textsuperscript{c}, Potenza, Italy, Università G. Marconi\textsuperscript{d}, Roma, Italy**

S. Buontempo\textsuperscript{a}, N. Cavallo\textsuperscript{a,c}, A. Di Crescenzo\textsuperscript{a,b}, F. Fabozzi\textsuperscript{a,c}, F. Fienga\textsuperscript{a}, G. Galati\textsuperscript{a}, A.O.M. Iorio\textsuperscript{a,b}, W.A. Khan\textsuperscript{a}, L. Lista\textsuperscript{a}, S. Meola\textsuperscript{a,d,15}, P. Paolucci\textsuperscript{a,15}, C. Sciacca\textsuperscript{a,b}, E. Voevodina\textsuperscript{a,b}

**INFN Sezione di Padova\textsuperscript{a}, Università di Padova\textsuperscript{b}, Padova, Italy, Università di Trento\textsuperscript{c}, Trento, Italy**

P. Azzi\textsuperscript{a}, N. Bacchetta\textsuperscript{a}, D. Bisello\textsuperscript{a,b}, A. Boletti\textsuperscript{a,b}, A. Bragagnolo, R. Carlin\textsuperscript{a,b}, P. Cecchia\textsuperscript{a}, M. Dall’Osso\textsuperscript{a,b}, P. De Castro Manzano\textsuperscript{a}, T. Dorigo\textsuperscript{a}, U. Dosselli\textsuperscript{a}, F. Gasparini\textsuperscript{a,b}, U. Gasparini\textsuperscript{a,b}, A. Gozzelino\textsuperscript{a}, S. Lacaprara\textsuperscript{a}, P. Lujan, M. Margoni\textsuperscript{a,b}, A.T. Meneguzzo\textsuperscript{a,b}, J. Pazzini\textsuperscript{a,b}, P. Ronchese\textsuperscript{a,b}, R. Rossin\textsuperscript{a,b}, F. Simonetto\textsuperscript{a,b}, A. Tiko, E. Torassa\textsuperscript{a}, M. Zanetti\textsuperscript{a,b}, P. Zotto\textsuperscript{a,b}, G. Zumerle\textsuperscript{a,b}

**INFN Sezione di Pavia\textsuperscript{a}, Università di Pavia\textsuperscript{b}, Pavia, Italy**

A. Braghieri\textsuperscript{a}, A. Magnani\textsuperscript{a}, P. Montagna\textsuperscript{a,b}, S.P. Ratti\textsuperscript{a,b}, V. Re\textsuperscript{a}, M. Ressegotti\textsuperscript{a,b}, C. Riccardi\textsuperscript{a,b}, P. Salvini\textsuperscript{a}, I. Vai\textsuperscript{a,b}, P. Vitulo\textsuperscript{a,b}

**INFN Sezione di Perugia\textsuperscript{a}, Università di Perugia\textsuperscript{b}, Perugia, Italy**

L. Alunni Solestizi\textsuperscript{a,b}, M. Biasini\textsuperscript{a,b}, G.M. Bilei\textsuperscript{a}, C. Cecchi\textsuperscript{a,b}, D. Ciangottini\textsuperscript{a,b}, L. Fanò\textsuperscript{a,b}, P. Lariccia\textsuperscript{a,b}, R. Leonardi\textsuperscript{a,b}, E. Manoni\textsuperscript{a}, G. Mantovani\textsuperscript{a,b}, V. Mariani\textsuperscript{a,b}, M. Menichelli\textsuperscript{a}, A. Rossi\textsuperscript{a,b}, A. Santocchia\textsuperscript{a,b}, D. Spiga\textsuperscript{a,b}

**INFN Sezione di Pisa\textsuperscript{a}, Università di Pisa\textsuperscript{b}, Scuola Normale Superiore di Pisa\textsuperscript{c}, Pisa, Italy**

K. Androsov\textsuperscript{a}, P. Azzurri\textsuperscript{a}, G. Bagliesi\textsuperscript{a}, L. Bianchini\textsuperscript{a}, T. Boccali\textsuperscript{a}, L. Borrello, R. Castaldi\textsuperscript{a}, M.A. Ciocca\textsuperscript{a,b}, R. Dell’Orso\textsuperscript{a}, G. Fedi\textsuperscript{a}, F. Fiori\textsuperscript{a,c}, L. Giannini\textsuperscript{a,c}, A. Giassi\textsuperscript{a}, M.T. Grippo\textsuperscript{a}, F. Ligabue\textsuperscript{a,c}, E. Manca\textsuperscript{a,b,c}, G. Mandorli\textsuperscript{a,c}, A. Messineo\textsuperscript{a,b}, F. Palla\textsuperscript{a}, A. Rizzi\textsuperscript{a,b}, P. Spagnolo\textsuperscript{a}, R. Tenchini\textsuperscript{a}, G. Tonelli\textsuperscript{a,b}, A. Venturi\textsuperscript{a}, P.G. Verdini\textsuperscript{a}
INFN Sezione di Roma $^a$, Sapienza Università di Roma $^b$, Rome, Italy
L. Barone$^{a,b}$, F. Cavallari$^a$, M. Cipriani$^{a,b}$, N. Daci$^a$, D. Del Re$^{a,b}$, E. Di Marco$^{a,b}$, M. Diemoz$^a$, S. Gelli$^{a,b}$, E. Longo$^{a,b}$, B. Marzocchi$^{a,b}$, P. Meridiani$^a$, G. Organtini$^{a,b}$, F. Pandolfi$^a$, R. Paramatti$^{a,b}$, F. Preiato$^{a,b}$, S. Rahatlou$^{a,b}$, C. Rovelli$^a$, F. Santanastasio$^{a,b}$

INFN Sezione di Torino $^a$, Università di Torino $^b$, Torino, Italy, Università del Piemonte Orientale $^c$, Novara, Italy
N. Amapane$^{a,b}$, R. Arcidiacono$^{a,c}$, S. Argiro$^{a,b}$, M. Arneodo$^{a,c}$, N. Bartosik$^a$, R. Bellan$^{a,b}$, C. Biino$^a$, N. Cartiglia$^a$, F. Cenna$^{a,b}$, S. Cometti, M. Costa$^{a,b}$, R. Covarelli$^{a,b}$, N. Demaria$^a$, B. Kiani$^{a,b}$, C. Mariotti$^a$, S. Maselli$^a$, E. Migliore$^{a,b}$, V. Monaco$^{a,b}$, E. Monteil$^{a,b}$, M. Monteno$^a$, M.M. Obertino$^{a,b}$, L. Pacher$^{a,b}$, N. Pastrone$^a$, M. Pelliccioni$^a$, G.L. Pinna Angioni$^{a,b}$, A. Romero$^{a,b}$, M. Ruspa$^{a,c}$, R. Sacchi$^{a,b}$, K. Shchelina$^{a,b}$, V. Sola$^a$, A. Solano$^{a,b}$, D. Soldi, A. Staiano$^a$

INFN Sezione di Trieste $^a$, Università di Trieste $^b$, Trieste, Italy
S. Belforte$^a$, V. Candelise$^{a,b}$, M. Casarsa$^a$, F. Cossutti$^a$, G. Della Ricca$^{a,b}$, F. Vazzoler$^{a,b}$, A. Zanetti$^a$

Kyungpook National University

Chonnam National University, Institute for Universe and Elementary Particles, Kwangju, Korea
H. Kim, D.H. Moon, G. Oh

Hanyang University, Seoul, Korea
J. Goh$^{29}$, T.J. Kim

Korea University, Seoul, Korea

Sejong University, Seoul, Korea
H.S. Kim

Seoul National University, Seoul, Korea

University of Seoul, Seoul, Korea

Sungkyunkwan University, Suwon, Korea
Y. Choi, C. Hwang, J. Lee, I. Yu

Vilnius University, Vilnius, Lithuania
V. Dudenas, A. Juodagalvis, J. Vaitkus

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

Universidad de Sonora (UNISON), Hermosillo, Mexico
A. Castaneda Hernandez, J.A. Murillo Quijada
Centro de Investigacion y de Estudios Avanzados del IPN, Mexico City, Mexico
H. Castilla-Valdez, E. De La Cruz-Burelo, M.C. Duran-Osuna, I. Heredia-De La Cruz,
R. Lopez-Fernandez, J. Mejia Guisao, R.I. Rabadan-Trejo, G. Ramirez-Sanchez, R Reyes-Almanza,
A. Sanchez-Hernandez

Universidad Iberoamericana, Mexico City, Mexico
S. Carrillo Moreno, C. Oropesa Barrera, F. Vazquez Valencia

Benemerita Universidad Autonoma de Puebla, Puebla, Mexico
J. Eysermans, I. Pedraza, H.A. Salazar Ibarguen, C. Uribe Estrada

Universidad Autonoma de San Luis Potosi, San Luis Potosi, Mexico
A. Morelos Pineda

University of Auckland, Auckland, New Zealand
D. Krofcheck

University of Canterbury, Christchurch, New Zealand
S. Bheesette, P.H. Butler

National Centre for Physics, Quaid-I-Azam University, Islamabad, Pakistan
A. Ahmad, M. Ahmad, M.I. Asghar, Q. Hassan, H.R. Hoorani, A. Saddique, M.A. Shah,
M. Shoib, M. Waqas

National Centre for Nuclear Research, Swierk, Poland
H. Bialkowska, M. Bluj, B. Boimska, T. Frueboes, M. Górski, M. Kazana, K. Nawrocki,
M. Szleper, P. Traczyk, P. Zalewski

Institute of Experimental Physics, Faculty of Physics, University of Warsaw, Warsaw, Poland
K. Bunkowski, A. Byszuk, K. Doroba, A. Kalinowski, M. Konecki, J. Krolikowski, M. Misiera,
M. Olszewski, A. Pyskir, M. Walczak

Laboratório de Instrumentação e Física Experimental de Partículas, Lisboa, Portugal
P. Bargassa, C. Beirão Da Cruz E Silva, A. Di Francesco, P. Faccioli, B. Galinhas, M. Gallinaro,
J. Hollar, N. Leonardo, L. Lloret Iglesias, M.V. Nemallapudi, J. Seixas, G. Strong, O. Toldaiev,
D. Vadrucio, J. Varela

Joint Institute for Nuclear Research, Dubna, Russia
S. Afanasiev, V. Alexakhin, P. Bunin, M. Gavrilenko, A. Golunov, I. Golutvin, N. Gorbounov,
V. Karjavin, A. Lanev, A. Malakhov, V. Matveev, P. Moisenz, V. Palichik, V. Perelygin,
M. Savina, S. Shmatov, V. Smirnov, N. Voytishin, A. Zarubin

Petersburg Nuclear Physics Institute, Gatchina (St. Petersburg), Russia
V. Golovtsov, Y. Ivanov, V. Kim, E. Kuznetsova, P. Levchenko, V. Murzin, V. Oreshkin,
I. Smirnov, D. Sosnov, V. Sulimov, L. Uvarov, S. Vavilov, A. Vorobyev

Institute for Nuclear Research, Moscow, Russia
Yu. Andreev, A. Dermeniev, S. Gninenko, N. Golubev, A. Karneyeu, M. Kirsanov, N. Krasnikov,
A. Pashenkov, D. Tilov, A. Toropin

Institute for Theoretical and Experimental Physics, Moscow, Russia
V. Epshteyn, V. Gavrilov, N. Lychkovskaya, V. Popov, I. Pozdnyakov, G. Safronov,
A. Spiridonov, A. Steppennov, V. Stolin, M. Toms, E. Vlasov, A. Zhokin

Moscow Institute of Physics and Technology, Moscow, Russia
T. Aushev
National Research Nuclear University ‘Moscow Engineering Physics Institute’ (MEPhI),
Moscow, Russia
R. Chistov, M. Danilov, P. Parygin, D. Philippov, S. Polikarpov, E. Tarkovskii

P.N. Lebedev Physical Institute, Moscow, Russia
V. Andreev, M. Azarkin, I. Dremin, M. Kirakosyan, S.V. Rusakov, A. Terkulov

Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow, Russia
A. Baskakov, A. Belyaev, E. Boos, V. Bunichev, M. Dubinin, L. Dudko, A. Ershov, A. Gribushin,
V. Klyukhin, I. Lokhtin, M. Miagkov, S. Obraztsov, S. Petrushanko, V. Savrin, A. Snigirev

Novosibirsk State University (NSU), Novosibirsk, Russia
V. Blinov, T. Dimov, L. Kardapoltsev, D. Shtol, Y. Skovpen

State Research Center of Russian Federation, Institute for High Energy Physics of NRC “Kurchatov Institute”, Protvino, Russia
I. Azhgirey, I. Bayshev, V. Bitioukov, D. Elumakhov, A. Godizov, V. Kachanov, A. Kalinin,
D. Konstantinov, P. Mandrik, V. Petrov, R. Ryutin, S. Slabospitskii, A. Sobol, S. Troshin,
N. Tsyurin, A. Uzunian, A. Volkov

National Research Tomsk Polytechnic University, Tomsk, Russia
A. Babaev, S. Baidali

University of Belgrade, Faculty of Physics and Vinca Institute of Nuclear Sciences, Belgrade, Serbia
P. Adzic, P. Cirkovic, D. Devetak, M. Dordevic, J. Milosevic

Centro de Investigaciones Energéticas Medioambientales y Tecnológicas (CIEMAT), Madrid, Spain
J. Alcaraz Maestre, A. Alvarez Fernandez, I. Bachiller, M. Barrio Luna, J.A. Brochero Cifuentes,
M. Cerrada, N. Colino, B. De La Cruz, A. Delgado Peris, C. Fernandez Bedoya,
J.P. Fernandez Ramos, J. Flix, M.C. Fouz, O. Gonzalez Lopez, S. Goy Lopez, J.M. Hernandez,
M.I. Josa, D. Moran, A. Perez-Calero Yzquierdo, J. Puerta Pelayo, I. Redondo, L. Romero,
M.S. Soares, A. Triossi

Universidad Autónoma de Madrid, Madrid, Spain
C. Albajar, J.F. de Trocóniz

Universidad de Oviedo, Oviedo, Spain
J. Cuevas, C. Erice, J. Fernandez Menendez, S. Folgueras, I. Gonzalez Caballero,
J.R. Gonzalez Fernandez, E. Palencia Cortezon, V. Rodriguez Bouza, S. Sanchez Cruz, P. Vischia,
J.M. Vizan Garcia

Instituto de Física de Cantabria (IFCA), CSIC-Universidad de Cantabria, Santander, Spain
I.J. Cabrillo, A. Calderon, B. Chazin Quero, J. Duarte Campderros, M. Fernandez,
P.J. Fernandez Manteca, A. Garcia Alonso, J. Garcia-Ferrero, G. Gomez, A. Lopez Virto,
J. Marco, C. Martinez Rivero, P. Martinez Ruiz del Arbol, F. Matorras, J. Piedra Gomez,
C. Prieels, T. Rodrigo, A. Ruiz-Jimeno, L. Scodellaro, N. Trevisani, I. Vila, R. Vilar Cortabitarte

CERN, European Organization for Nuclear Research, Geneva, Switzerland
D. Abbaneo, B. Akgun, E. Auffray, P. Baillon, A.H. Ball, D. Barney, J. Bendavid, M. Bianco,
A. Bocci, C. Botta, E. Brondolin, T. Camporesi, M. Cepeda, G. Cerminara, E. Chapon, Y. Chen,
G. Cucciati, D. d’Enterria, A. Dabrowski, V. Daponte, A. David, A. De Roeck, N. Deelen,

Paul Scherrer Institut, Villigen, Switzerland

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

Universität Zürich, Zurich, Switzerland

National Central University, Chung-Li, Taiwan

National Taiwan University (NTU), Taipei, Taiwan

Chulalongkorn University, Faculty of Science, Department of Physics, Bangkok, Thailand
B. Asavapibhop, N. Srimanobhas, N. Suwonjandee

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

Middle East Technical University, Physics Department, Ankara, Turkey
B. Isildak, G. Karapinar, M. Yalvac, M. Zeyrek

Bogazici University, Istanbul, Turkey
I.O. Atakisi, E. Gülmez, M. Kaya, O. Kaya, S. Tekten, E.A. Yetkin

Istanbul Technical University, Istanbul, Turkey
M.N. Agaras, S. Atay, A. Cakir, K. Cankocak, Y. Komurcu, S. Sen

Institute for Scintillation Materials of National Academy of Science of Ukraine, Kharkov, Ukraine
B. Grynyov
National Scientific Center, Kharkov Institute of Physics and Technology, Kharkov, Ukraine
L. Levchuk

University of Bristol, Bristol, United Kingdom

Rutherford Appleton Laboratory, Didcot, United Kingdom

Imperial College, London, United Kingdom

Brunel University, Uxbridge, United Kingdom
J.E. Cole, P.R. Hobson, A. Khan, P. Kyberd, C.K. Mackay, A. Morton, I.D. Reid, L. Teodorescu, S. Zahid

Baylor University, Waco, USA
K. Call, J. Dittmann, K. Hatakeyama, H. Liu, C. Madrid, B. Mcmaster, N. Pastika, C. Smith

Catholic University of America, Washington DC, USA
R. Bartek, A. Dominguez

The University of Alabama, Tuscaloosa, USA
A. Buccilli, S.I. Cooper, C. Henderson, P. Rumerio, C. West

Boston University, Boston, USA
D. Arcaro, T. Bose, D. Gastler, D. Rankin, C. Richardson, J. Rohlf, L. Sulak, D. Zou

Brown University, Providence, USA

University of California, Davis, Davis, USA

University of California, Los Angeles, USA

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

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

California Institute of Technology, Pasadena, USA

Carnegie Mellon University, Pittsburgh, USA

University of Colorado Boulder, Boulder, USA
J.P. Cumalat, W.T. Ford, F. Jensen, A. Johnson, M. Krohn, S. Leontsinis, E. MacDonald, T. Mulholland, K. Stenson, K.A. Ulmer, S.R. Wagner

Cornell University, Ithaca, USA

Fermi National Accelerator Laboratory, Batavia, USA

University of Florida, Gainesville, USA

Florida International University, Miami, USA
Y.R. Joshi, S. Linn

Florida State University, Tallahassee, USA

Florida Institute of Technology, Melbourne, USA

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

The University of Iowa, Iowa City, USA

Johns Hopkins University, Baltimore, USA

The University of Kansas, Lawrence, USA

Kansas State University, Manhattan, USA

Lawrence Livermore National Laboratory, Livermore, USA
F. Rebassoo, D. Wright

University of Maryland, College Park, USA

Massachusetts Institute of Technology, Cambridge, USA

University of Minnesota, Minneapolis, USA

University of Mississippi, Oxford, USA
J.G. Acosta, S. Oliveros

University of Nebraska-Lincoln, Lincoln, USA

State University of New York at Buffalo, Buffalo, USA
Northeastern University, Boston, USA

Northwestern University, Evanston, USA

University of Notre Dame, Notre Dame, USA

The Ohio State University, Columbus, USA

Princeton University, Princeton, USA

University of Puerto Rico, Mayaguez, USA
S. Malik, S. Norberg

Purdue University, West Lafayette, USA

Purdue University Northwest, Hammond, USA
T. Cheng, J. Dolen, N. Parashar

Rice University, Houston, USA

University of Rochester, Rochester, USA

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

University of Tennessee, Knoxville, USA
A.G. Delannoy, J. Heideman, G. Riley, K. Rose, S. Spanier, K. Thapa

Texas A&M University, College Station, USA
Texas Tech University, Lubbock, USA

Vanderbilt University, Nashville, USA

University of Virginia, Charlottesville, USA
M.W. Arenton, P. Barria, B. Cox, R. Hirosky, M. Joyce, A. Ledovskoy, H. Li, C. Neu, T. Sinthuprasith, Y. Wang, E. Wolfe, F. Xia

Wayne State University, Detroit, USA

University of Wisconsin - Madison, Madison, WI, USA

†: Deceased
1: Also at Vienna University of Technology, Vienna, Austria
2: Also at IRFU, CEA, Université Paris-Saclay, Gif-sur-Yvette, France
3: Also at Universidade Estadual de Campinas, Campinas, Brazil
4: Also at Federal University of Rio Grande do Sul, Porto Alegre, Brazil
5: Also at Université Libre de Bruxelles, Bruxelles, Belgium
6: Also at University of Chinese Academy of Sciences, Beijing, China
7: Also at Institute for Theoretical and Experimental Physics, Moscow, Russia
8: Also at Joint Institute for Nuclear Research, Dubna, Russia
9: Also at Suez University, Suez, Egypt
10: Now at British University in Egypt, Cairo, Egypt
11: Also at Zewail City of Science and Technology, Zewail, Egypt
12: Also at Department of Physics, King Abdulaziz University, Jeddah, Saudi Arabia
13: Also at Université de Haute Alsace, Mulhouse, France
14: Also at Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow, Russia
15: Also at CERN, European Organization for Nuclear Research, Geneva, Switzerland
16: Also at RWTH Aachen University, III. Physikalisches Institut A, Aachen, Germany
17: Also at University of Hamburg, Hamburg, Germany
18: Also at Brandenburg University of Technology, Cottbus, Germany
19: Also at MTA-ELTE Lendület CMS Particle and Nuclear Physics Group, Eötvös Loránd University, Budapest, Hungary
20: Also at Institute of Nuclear Research ATOMKI, Debrecen, Hungary
21: Also at Institute of Physics, University of Debrecen, Debrecen, Hungary
22: Also at Indian Institute of Technology Bhubaneswar, Bhubaneswar, India
23: Also at Institute of Physics, Bhubaneswar, India
24: Also at Shoolini University, Solan, India
25: Also at University of Visva-Bharati, Santiniketan, India
26: Also at Isfahan University of Technology, Isfahan, Iran
27: Also at Plasma Physics Research Center, Science and Research Branch, Islamic Azad University, Tehran, Iran
28: Also at Università degli Studi di Siena, Siena, Italy
29: Also at Kyunghee University, Seoul, Korea
30: Also at International Islamic University of Malaysia, Kuala Lumpur, Malaysia
31: Also at Malaysian Nuclear Agency, MOSTI, Kajang, Malaysia
32: Also at Consejo Nacional de Ciencia y Tecnología, Mexico city, Mexico
33: Also at Warsaw University of Technology, Institute of Electronic Systems, Warsaw, Poland
34: Also at Institute for Nuclear Research, Moscow, Russia
35: Now at National Research Nuclear University ‘Moscow Engineering Physics Institute’ (MEPhI), Moscow, Russia
36: Also at St. Petersburg State Polytechnical University, St. Petersburg, Russia
37: Also at University of Florida, Gainesville, USA
38: Also at P.N. Lebedev Physical Institute, Moscow, Russia
39: Also at California Institute of Technology, Pasadena, USA
40: Also at Budker Institute of Nuclear Physics, Novosibirsk, Russia
41: Also at Faculty of Physics, University of Belgrade, Belgrade, Serbia
42: Also at INFN Sezione di Pavia $^a$, Università di Pavia $^b$, Pavia, Italy
43: Also at University of Belgrade, Faculty of Physics and Vinca Institute of Nuclear Sciences, Belgrade, Serbia
44: Also at Scuola Normale e Sezione dell’INFN, Pisa, Italy
45: Also at National and Kapodistrian University of Athens, Athens, Greece
46: Also at Riga Technical University, Riga, Latvia
47: Also at Universität Zürich, Zurich, Switzerland
48: Also at Stefan Meyer Institute for Subatomic Physics (SMI), Vienna, Austria
49: Also at Adiyaman University, Adiyaman, Turkey
50: Also at Istanbul Aydin University, Istanbul, Turkey
51: Also at Mersin University, Mersin, Turkey
52: Also at Piri Reis University, Istanbul, Turkey
53: Also at Gaziosmanpasa University, Tokat, Turkey
54: Also at Ozyegin University, Istanbul, Turkey
55: Also at Izmir Institute of Technology, Izmir, Turkey
56: Also at Marmara University, Istanbul, Turkey
57: Also at Kafkas University, Kars, Turkey
58: Also at Istanbul Bilgi University, Istanbul, Turkey
59: Also at Hacettepe University, Ankara, Turkey
60: Also at Rutherford Appleton Laboratory, Didcot, United Kingdom
61: Also at School of Physics and Astronomy, University of Southampton, Southampton, United Kingdom
62: Also at Monash University, Faculty of Science, Clayton, Australia
63: Also at Bethel University, St. Paul, USA
64: Also at Karamanoğlu Mehmetbey University, Karaman, Turkey
65: Also at Utah Valley University, Orem, USA
66: Also at Purdue University, West Lafayette, USA
67: Also at Beykent University, Istanbul, Turkey
68: Also at Bingol University, Bingol, Turkey
69: Also at Sinop University, Sinop, Turkey
70: Also at Mimar Sinan University, Istanbul, Istanbul, Turkey
71: Also at Texas A&M University at Qatar, Doha, Qatar
72: Also at Kyungpook National University, Daegu, Korea