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Search for singly and pair-produced leptoquarks coupling to third-generation fermions in proton-proton collisions at $\sqrt{s} = 13$ TeV

The CMS Collaboration *

CERN, Geneva, Switzerland

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ABSTRACT

A search for leptoquarks produced singly and in pairs in proton-proton collisions is presented. We consider the leptoquark (LQ) to be a scalar particle of charge $-1/3e$ coupling to a top quark plus a tau lepton ($t\tau$) or a bottom quark plus a neutrino ($b\nu$), or a vector particle of charge $+2/3e$, coupling to $t\nu$ or $b\tau$. These choices are motivated by models that can explain a series of anomalies observed in the measurement of B meson decays. In this analysis the signatures $t\tau\nu b$ and $t\tau\nu$ are probed, using data recorded by the CMS experiment at the CERN LHC at $\sqrt{s} = 13$ TeV and that correspond to an integrated luminosity of 137 fb^{-1}. These signatures have not been previously explored in a dedicated search. The data are found to be in agreement with the standard model prediction. Lower limits at 95% confidence level are set on the LQ mass in the range 0.98–1.73 TeV, depending on the LQ spin and its coupling λ to a lepton and a quark, and assuming equal couplings for the two LQ decay modes considered. These are the most stringent constraints to date on the existence of leptoquarks in this scenario.

1. Introduction

Experimental evidence has promoted the standard model (SM) to the role of a reference theory of the physics of elementary particles. Despite the theory's successes, there are several fundamental aspects of observed particle physics that lack a complete explanation. One of these is the symmetry between the quark and lepton families. Possible explanations have been offered by several models that extend the SM, such as grand unified theories [1–4], technicolor models [5–8], compositeness scenarios [9,10], and R-parity violating supersymmetry [11–20]. These theories foresee a new particle that carries both lepton number L and baryon number B, and is generically referred to as a "leptoquark" (LQ).

A leptoquark has a fractional electric charge, and can be either a scalar particle (LQ_S, with a spin of 0), or a vector particle (LQ_V, with a spin of 1), with $3B + L$ equal to either 2 or 0. At hadron colliders, leptoquarks can be produced in pairs, or singly in association with a lepton [21,22], as illustrated by the Feynman diagrams in Fig. 1. For LQ_S pair production, the cross section depends only on the LQ_S mass for the range of LQ mass and λ values investigated in this search, while for LQ_V it may depend on additional parameters [23], to comply with constraints imposed by unitarity at high energy scales. For singly produced leptoquarks, the cross section further depends on the couplings of the LQ to the quark and the lepton, and on the quark flavor.

Leptoquarks have recently gained enhanced interest, as they may provide an explanation for a series of anomalies observed in the measurement of B meson decays in charged-current $b \to c\ell\nu$ [24–33] and neutral-current $b \to s\ell\ell$ [34–41] processes. The solutions proposed to explain these anomalies favor effective couplings to third-generation SM fermions at the TeV scale, leading to processes that may be accessible at the CERN LHC. In particular, the model of Ref. [42] predicts a charge $-1/3e$ LQ_S, with $3B + L = 2$, decaying to a top quark and a τ lepton ($t\tau$), or a bottom quark and a neutrino ($b\nu_\tau$), while the model presented in Ref. [43] contains a charge $+2/3e$ LQ_V, with $3B + L = 0$, decaying to a top quark and an antineutrino ($t\bar{\nu}_\tau$) or a bottom quark and an anti-τ lepton ($b\tau^+$). Each model includes a charge-conjugate leptoquark and prefers a region of parameter space that gives equal branching fractions for the two allowed decays, rendering the $t\tau\nu b$ signature as the most frequent for pair-produced leptoquarks.

The analysis described in this Letter investigates the existence of leptoquarks produced in pairs with decays leading to the $tb\tau\nu$ signature, or singly with the decay leading to $t\tau\nu$. The models of Refs. [42,43] are considered in this analysis, relying on the implementations described in Refs. [44,45]. In these models, the parameters of interest for determining the cross section are: the LQ mass; for LQ_V, a dimensionless coupling k, set to 1 (Yang–Mills case) or 0 (minimal coupling case) [23]; and the LQ coupling (λ) to the lepton and quark, which affects the cross section for single LQ production.

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

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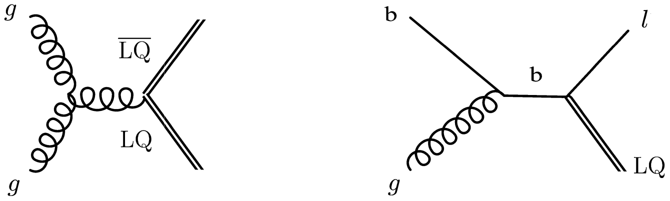

Fig. 1. Feynman diagrams for dominant leptoquark production modes at leading order: pairwise (left), and in combination with a lepton (right). In the scenarios considered the LQ$_\mathrm{S}$ may couple to tτ or bν, while the LQ$_\mathrm{V}$ may couple to tν or bτ.

We note that the analysis is designed to be agnostic to the charge of the LQ, and is thus sensitive also to models with up-type scalar LQ and down-type vector LQ, which are not directly considered below.

The most recent searches for leptoquarks have been performed at $\sqrt{s} = 13\,\mathrm{TeV}$ by the ATLAS and CMS Collaborations for couplings to (tτ, bν) and (tν, bτ) [46–53] and for couplings to other quark-lepton pairs [51,54–57].

Differently from previous searches that have separately considered single or pair LQ production, the present analysis strategy is devised to search for both production mechanisms simultaneously. The t$\tau\nu$(b) signatures are analyzed for the first time considering the inclusive hadronic decay channels of the top quark and τ lepton. We include a dedicated selection for the case of a large LQ-t mass splitting giving rise to a Lorentz-boosted top quark, whose decay products may not be resolved as individual jets.

The search is based on a data sample of proton-proton (pp) collisions at a center-of-mass energy of 13 TeV recorded by the CMS experiment at the CERN LHC in the years 2016–18, corresponding to an integrated luminosity of $137\,\mathrm{fb}^{-1}$.

2. The CMS detector

The central feature of the CMS detector is a 3.8 T superconducting solenoid magnet with an inner diameter of 6 m. Within the magnet volume are the following subdetectors: a silicon pixel and strip tracker, a lead tungstate crystal electromagnetic calorimeter (ECAL), and a brass and scintillator hadron calorimeter. Muons are detected in gas-ionization chambers embedded in the steel flux-return yoke outside the solenoid. In addition, two steel and quartz-fiber hadron forward calorimeters extend the detection coverage to regions close to the beam pipe. 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. [58]. Events of interest are selected using a two-tiered trigger system [59]. 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 time interval of about 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 around 1 kHz before data storage.

3. Simulated data samples

Monte Carlo (MC) event generators are used to simulate the SM background processes and the signal. These simulations are used to guide the design of the analysis, to estimate minor backgrounds, and to interpret the results.

Background events are generated at leading order (LO) for the W + jets and Z/γ^* + jets processes using the generator MadGraph5_amc@nlo 2.2.2 (2.4.2) [60] for simulated events matched with 2016 (2017–18) data, while the next-to-LO (NLO) generator powheg 2.0 [61–66] is used for $\mathrm{t\bar{t}}$, tW, and diboson processes, and MadGraph5_amc@nlo at NLO for $\mathrm{t\bar{t}} + \mathrm{W}$, $\mathrm{t\bar{t}} + \mathrm{Z}/\gamma^*$, $\mathrm{t\bar{t}t\bar{t}}$, tZq, and triboson production. Both MadGraph5_amc@nlo and powheg are interfaced with pythia 8.226 (8.230) [67] for parton showering and hadronization using the tune CUETP8M1 [68] or CUETP8M2T4 [69] (CP5 [70]) and the NNPDF 3.0 [71] (3.1 [72]) parton distribution functions (PDFs) for simulating all 2016 (2017–18) samples. In the following, we group these backgrounds where a genuine τ lepton is present as either “t production” or “Others”, depending on whether a top quark is produced in the SM process or not.

Signal samples are generated at LO using MadGraph5_amc@nlo interfaced with pythia for the LQ$_\mathrm{S}$ and LQ$_\mathrm{V}$ models of Refs. [42] and [43], according to the implementations of Refs. [44] and [45]. The NNPDF 3.0 [71] (3.1 [72]) parton distribution function (PDF) set is utilized with the tune CUETP8M1 [68] (CP2 [70]) for the signal events used with the 2016 (2017–18) data. The LQ mass range studied is between 0.5 and 2.3 TeV, with samples produced in steps of 0.3 TeV. We consider LQ$_\mathrm{S}$ (LQ$_\mathrm{V}$) decaying as LQ $\rightarrow$ tτ (tν) or LQ $\rightarrow$ bν (bτ). Samples of pair-produced leptoquarks are generated considering both gluon-initiated and quark-initiated mechanisms. We consider equal values of λ for leptoquarks coupled to (tτ, bν) and (tν, bτ). Samples of singly produced LQ are generated with λ values 0.1, 0.5, 1, 1.5, 2, and 2.5. In the MC simulation, the kinematic distributions of singly produced leptoquarks are independent of λ below $\lambda = 0.5$ (1) in the case of LQ$_\mathrm{S}$ (LQ$_\mathrm{V}$), and in both cases are independent of k. The dependence on λ above these values is ascribed to the contributions of virtual LQ states in the quark-gluon fusion amplitude (Fig. 1 right) that become more and more relevant compared to the resonant LQ production for increasing values of LQ mass and λ, and are manifest as off-shell events that tend to populate the low-mass tail.

Additional pp interactions within the same or nearby bunch crossings (pileup) are taken into account by superimposing simulated minimum bias interactions onto the hard scattering process, with a number distribution matching that observed in data. Simulated events are propagated through the full GEANT4 based simulation [73] of the CMS detector.

4. Particle reconstruction and identification

A particle-flow (PF) algorithm [74] is used to identify and reconstruct individual particles in the event (electrons, muons, photons, neutral and charged hadrons) through a combination of the information from the entire detector. These PF objects are used to reconstruct higher-level objects such as hadronically decaying τ leptons (τ_h), jets, and missing transverse momentum ($\vec{p}_\mathrm{T}^\mathrm{miss}$), taken as the negative vector sum of the transverse momenta ($\vec{p}_\mathrm{T}$) of all reconstructed particles in an event. The magnitudes of $\vec{p}_\mathrm{T}$ and $\vec{p}_\mathrm{T}^\mathrm{miss}$ are referred to as p_T and $p_\mathrm{T}^\mathrm{miss}$, respectively.

Jet candidates are reconstructed from PF candidates using the anti-k_T clustering algorithm [75] with a distance parameter of 0.8 (“AK8 jet”) or 0.4 (“AK4 jet”), and are selected requiring $p_\mathrm{T} > 30\,\mathrm{GeV}$ and $|\eta| < 2.4$. The jet energy scale (JES) is calibrated through correction factors dependent on the p_T, pseudorapidity (η), energy density, and the area of the jet. The jet energy resolution (JER) for the simulated jets is corrected to reproduce the resolution observed in data [76].

The AK8 jet candidates are required to have $p_\mathrm{T} > 180\,\mathrm{GeV}$, $|\eta| < 2.4$, and to be separated by $\Delta R > 0.8$ from an identified τ_h, where $\Delta R \equiv \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$ and ϕ is the azimuthal angle. They are selected if they are identified as originating from a W boson decaying to $\mathrm{q\bar{q}}'$ (denoted as “W jets”) by using a pruning algorithm [77] or from a top quark decaying fully hadronically (“t jets”). The mass of the pruned AK8 W jet is required to be within the range 65–105 GeV to select candidates consistent with W bosons and to reject quark and gluon jets. The discrimination between W jets and quark and gluon jets is further improved by requiring the ratio τ_{21} to be less than 0.35 or 0.45, depending on the year of data taking, where $\tau_{21} \equiv \tau_2/\tau_1$ and the N-subjettiness τ_n has the property that it attains a smaller value the more nearly the jet resembles a collection of n subjets [78]. In a similar way, an AK8 jet may be identified as arising from the fully hadronic decay of a top quark. These t jets are required to have $p_{\mathrm{T}} > 400\,\mathrm{GeV}$, mass of the jet reconstructed through the modified mass drop tagger algorithm [79,80] between 105 and 220 GeV, and $\tau_{32} \equiv \tau_3/\tau_2$ less than 0.81.

The τ_{h} candidates are reconstructed with the hadron-plus-strips algorithm [81], which is seeded with AK4 jets. This algorithm reconstructs τ_{h} candidates in the one-prong, one-prong plus π^0(s), and three-prong decay modes. A discriminator based on a multivariate analysis, including isolation [81] as well as lifetime information, is used to reduce the frequency of jets being misidentified as τ_{h} candidates. The typical working point used in this analysis has an efficiency of $\approx$60% for a genuine τ_{h}, with a misidentification rate for quark and gluon jets of $\approx$0.1% [81]. Electrons and muons misidentified as τ_{h} candidates are suppressed using criteria based on the consistency among the measurements in the tracker, the calorimeters, and the muon detectors. The τ_{h} candidates are required to have a minimum p_{T} of 20 GeV and $|\eta| < 2.3$.

Jets arising from a bottom quark ("b jets") are identified among AK4 jets using the combined secondary vertex algorithm [82]. We choose a "loose" working point that has an efficiency of 85% for genuine b jets and a rejection of 90% of light-flavor jets. The b jets are considered regardless of whether they are contained in top quark candidates.

Further requirements are imposed on the AK4 jets used in the construction of top and bottom quark candidates. These are required to have $p_{\mathrm{T}} > 30\,\mathrm{GeV}$ and $|\eta| < 2.4$, and to be separated by $\Delta R > 0.4$ (0.8) from an identified τ_{h} (W jet).

A hadronically decaying top quark candidate is reconstructed considering three cases: an AK8 jet identified as a t jet, a pair comprising an AK4 jet and a W jet and having combined mass closest to the top quark mass among such pairs, and the triplet of AK4 jets having a mass closest to the top quark mass. The b tagging information is not used in any of these three reconstruction processes. These cases correspond to the three possible topologies of hadronic top quark decay and are referred to as "fully merged", "partially merged", and "resolved", respectively. The reconstruction considers these cases in the order just described, removing the objects contained in a candidate from further consideration to ensure that the categories are exclusive. The efficiency for identifying W, b, and t jets in simulation is corrected to match the results found in data [82,83].

To select events from processes with fully hadronic states, a veto on electrons and muons is applied. Electron candidates are reconstructed by combining the information from the ECAL and the silicon tracker, and are identified if they satisfy quality requirements and isolation as specified in [84]; they are selected if they have $p_{\mathrm{T}} > 20\,\mathrm{GeV}$ and $|\eta| < 2.5$. Muon candidates are reconstructed by combining the information from the muon system and the silicon tracker, and are identified if they pass additional identification criteria and isolation as specified in [85]; they are selected if they have $p_{\mathrm{T}} > 20\,\mathrm{GeV}$ and $|\eta| < 2.4$.

5. Event selection

Selected events must satisfy a trigger that requires both $p_{\mathrm{T}}^{\mathrm{miss}}$ and $H_{\mathrm{T}}^{\mathrm{miss}}$ greater than 120 GeV, $H_{\mathrm{T}}^{\mathrm{miss}}$ being the magnitude of the negative summed $\vec{p}_{\mathrm{T}}$ of all the AK4 jets reconstructed with the PF algorithm.

Offline, we consider events in which both $p_{\mathrm{T}}^{\mathrm{miss}}$ and $H_{\mathrm{T}}^{\mathrm{miss}} \geq 200\,\mathrm{GeV}$, and $H_{\mathrm{T}} \geq 300\,\mathrm{GeV}$, where H_{T} is the scalar sum of the p_{T} of all AK4 jets. Events entering this region are further required to contain exactly one top quark candidate, one τ_{h} candidate, no electrons or muons, and at least one b jet. Finally, the transverse mass $m_{\mathrm{T}}(\tau_{\mathrm{h}}, p_{\mathrm{T}}^{\mathrm{miss}}) \equiv \sqrt{2 p_{\mathrm{T}}(\tau_{\mathrm{h}}) p_{\mathrm{T}}^{\mathrm{miss}} [1 - \cos \Delta\phi(\vec{p}_{\mathrm{T}}(\tau_{\mathrm{h}}), \vec{p}_{\mathrm{T}}^{\mathrm{miss}})]}$ has to exceed 300 GeV, where $\vec{p}_{\mathrm{T}}(\tau_{\mathrm{h}})$ is the transverse momentum vector of the τ_{h} candidate.

From simulation we find that the total selection efficiency, accounting for both the LQ decay branching fraction and the event selection, varies between about 2 and 9% for an LQ mass in the range 0.5–2.3 TeV for pair-produced leptoquarks. For singly produced leptoquarks, taking $\lambda = 1.5$, the signal efficiency is about 0.7% for an LQ_{S} with a mass of 1.1 TeV; the corresponding number for an LQ_{V} is 2.4 (3.1)% for $k = 0$ (1) for a mass of 1.4 TeV. The efficiency decreases for higher λ and LQ mass values. This is because of the increased impact of the virtual leptoquarks leading to the nonresonant process in which the events tend to populate the low-mass tail, as described in Section 3. The efficiency values for all the different leptoquark hypotheses and parameters investigated in this search can be found in the HEPData database [86]. The search is less sensitive to single LQ production than to pair production because of the smaller signal efficiency for higher λ and LQ mass values and the similarity of the kinematic properties to those of the expected SM background. These effects outweigh the higher relative LQ_{S} (LQ_{V} $k = 0$, LQ_{V} $k = 1$) cross section for mass values of 0.5 and 0.7 TeV (0.6 and 1.2 TeV, 1.2 and 2 TeV) at values of λ of 2 and 1.5.

The events that pass the above selection are categorized according to the number of b jets ($N_{\text{b-jet}} = 1$ or ≥ 2) and to whether the top quark candidate is selected through the fully or partially merged topology ("boosted"), or the resolved topology ("resolved"). For each of these four categories of events a distribution-based analysis is performed, searching for evidence of a signal by considering the distribution of S_{T}, which is the scalar sum of the p_{T} of the top quark candidate, the selected τ_{h}, and the $p_{\mathrm{T}}^{\mathrm{miss}}$. Fig. 2 shows the S_{T} distributions for the events passing the signal selection in the four categories of the analysis, while Table 1 gives the yields from the background estimation and the expected signal.

6. Background estimation

Several SM processes contribute as backgrounds in the signal region. We treat separately the two cases in which a genuine τ lepton is present or not in the event.

The irreducible background with a real τ lepton that decays hadronically is estimated from simulated samples, and normalized to data in a control region where we expect negligible contribution from the signal to account for residual differences between data and simulation. Processes with at least one top quark (e.g. $\mathrm{t\bar{t}}$ or $\mathrm{t\bar{t}} + \mathrm{W}$) account for most of this irreducible background, and a control region is defined by applying the requirements used for the signal region, except with $m_{\mathrm{T}}(\tau_{\mathrm{h}}, p_{\mathrm{T}}^{\mathrm{miss}}) < 80\,\mathrm{GeV}$ and $N_{\text{b-jet}} \geq 2$.

The dominant source of contamination is the reducible background, which comprises all of the processes (mainly events composed uniquely of jets produced through the strong interaction, W + jets, and $\mathrm{t\bar{t}}$) that pass the signal region selection and in which a jet is misidentified as a τ_{h} candidate. We estimate this background entirely from data by applying misidentification weights w to the yields of events selected with the same requirements as the signal region, except that the τ_{h} must pass a looser identification requirement and fail the nominal one. We refer to this sample as the application region. An estimate from simulation of the number of events entering the application region while having a genuine τ_{h} is subtracted from the application region yields. The weight w of each event depends on the probability f that a

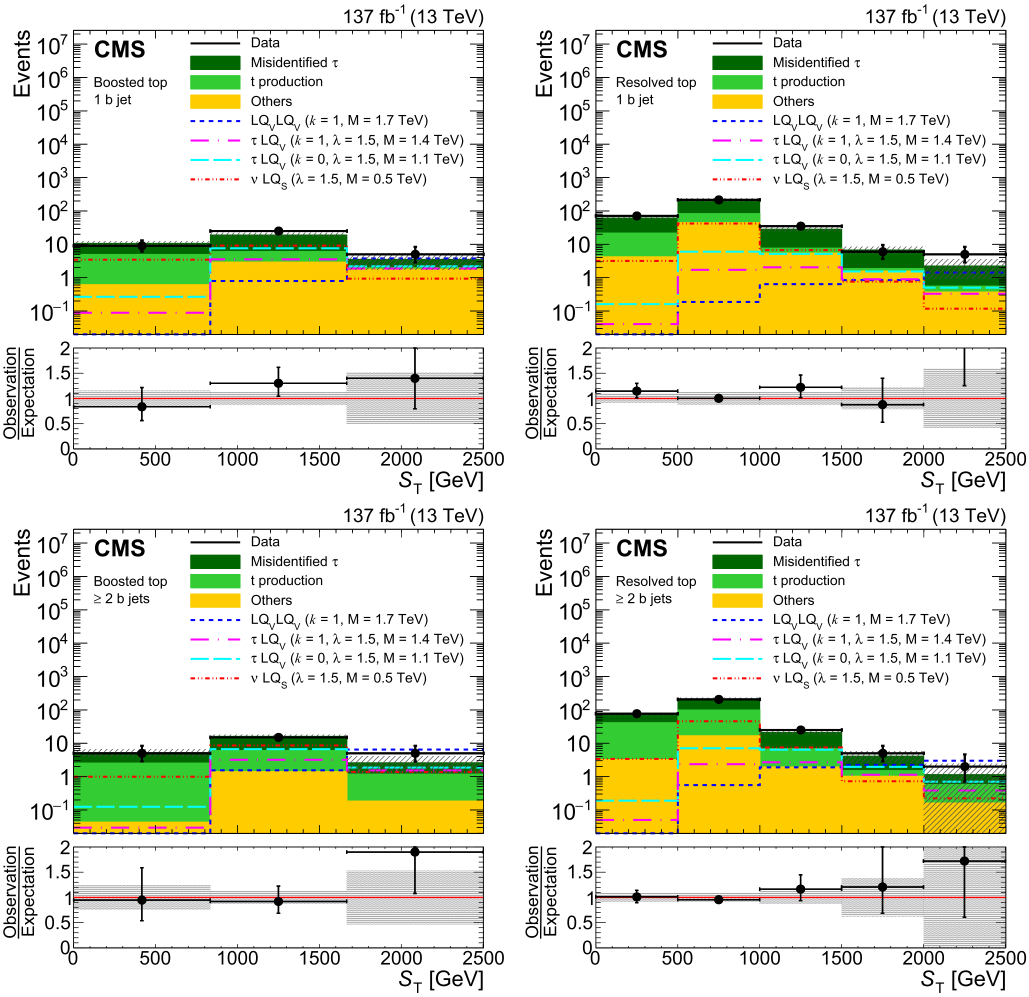

Fig. 2. Distribution of the variable S_T for events passing the signal selection for the SM background estimation (stacked filled histograms), data (black points), and different hypotheses of LQ signals (lines). Upper left: boosted top quark candidate (hadronically decaying top quark reconstructed in the fully or partially merged topology) and exactly one b jet; lower left: boosted top quark candidate and at least two b jets; upper right: resolved top quark candidate (hadronically decaying top quark reconstructed in the resolved topology) and exactly one b jet; lower-right: resolved top quark candidate and at least two b jets. The cross-hatched band in the upper panels represents the total uncertainty (statistical+systematic). The lower panel of each distribution shows the ratio, and its uncertainty, between the observation and the SM expectation.

Table 1
Yields from the SM background estimation, data, and expected signal, for the selected events, with total (statistical+systematic) uncertainties.

Category	Boosted		Resolved	
	$N_{\text{b-jet}} = 1$	$N_{\text{b-jet}} \geq 2$	$N_{\text{b-jet}} = 1$	$N_{\text{b-jet}} \geq 2$
Misidentified τ	20.5 ± 2.1	14.4 ± 1.8	199 ± 13	170 ± 12
t production	7.8 ± 2.1	8.2 ± 1.9	59 ± 5	127 ± 10
Others	5.3 ± 2.0	1.6 ± 0.8	56 ± 25	23 ± 11
Total background	33.5 ± 3.6	24.2 ± 2.7	314 ± 29	320 ± 19
Data	39	25	332	316
$\text{LQ}_\text{V}\,\overline{\text{LQ}}_\text{V}$ ($k = 1$, $m_{\text{LQ}} = 1.7\,\text{TeV}$)	4.6 ± 0.7	8.0 ± 1.2	3.1 ± 0.3	7.7 ± 0.7
τLQ_V ($k = 1$, $\lambda = 1.5$, $m_{\text{LQ}} = 1.4\,\text{TeV}$)	5.5 ± 0.4	4.8 ± 0.4	5.0 ± 0.2	6.6 ± 0.3
τLQ_V ($k = 0$, $\lambda = 1.5$, $m_{\text{LQ}} = 1.1\,\text{TeV}$)	10.1 ± 0.7	8.6 ± 0.7	13.4 ± 0.6	16.4 ± 0.8
νLQ_S ($\lambda = 1.5$, $m_{\text{LQ}} = 0.5\,\text{TeV}$)	13.5 ± 0.8	12.0 ± 0.8	52.7 ± 2.7	57.5 ± 2.9

misidentified τ_h candidate passing the relaxed criteria also passes the nominal criteria, and is given by $f/(1-f)$. The probability f is parameterized as a function of the p_T and $|\eta|$ of the jet associated with the selected τ_h candidate, within $\Delta R(\text{jet}, \tau_h) < 0.4$. It is measured in a large data sample with a high fraction of jets misidentified as τ_h. To select this sample the signal region requirements are modified by removing the thresholds on p_T^{miss} and H_T^{miss} and requiring instead the presence of a muon with p_T greater than 60 GeV. The requirement $N_{\text{b-jet}} \geq 1$ is replaced by $N_{\text{b-jet}} = 0$, to suppress $\text{t}\bar{\text{t}}$ events with genuine τ_h, and the requirement on $m_T(\tau_h, p_T^{\text{miss}})$ is replaced by $m_T(\tau_h, \mu) > 120\,\text{GeV}$, to suppress Drell–Yan events. In the resultant sample, more than 90% of the events have jets misidentified as τ_h, with W+jets contributing 60% and the rest consisting of a mixture of top, diboson, and multijet events. This estimation method has been validated in a region that passes the signal region selection, except for the modified requirement $120 < m_T(\tau_h, p_T^{\text{miss}}) < 300\,\text{GeV}$. This region is verified to have a composition of background pro-

Table 2
Lower limits on the mass in TeV of the leptoquarks $\mathrm{LQ_S}$, $\mathrm{LQ_V}$ $k = 0$, and $\mathrm{LQ_V}$ $k = 1$, based on the pair- and single-production mechanisms taken either separately or together. These lower limits are derived from the intersection of the observed 95% CL upper limits on the signal cross section and the signal cross section in Figs. 3–5. The results of the searches that depend on the λ parameter are given for values of 1.5 and 2.5. The expected limits are given in parentheses.

	$\mathrm{LQ_S}$ (TeV)		$\mathrm{LQ_V}$ $k = 0$ (TeV)		$\mathrm{LQ_V}$ $k = 1$ (TeV)	
Pair	0.95 (1.03)		1.29 (1.39)		1.65 (1.77)	
	$\lambda = 1.5$	2.5	1.5	2.5	1.5	2.5
Single	0.55 (0.56)	0.75 (0.81)	1.03 (1.12)	1.25 (1.35)	1.20 (1.29)	1.41 (1.53)
Pair+Single	0.98 (1.06)	1.02 (1.10)	1.34 (1.46)	1.41 (1.54)	1.69 (1.81)	1.73 (1.87)

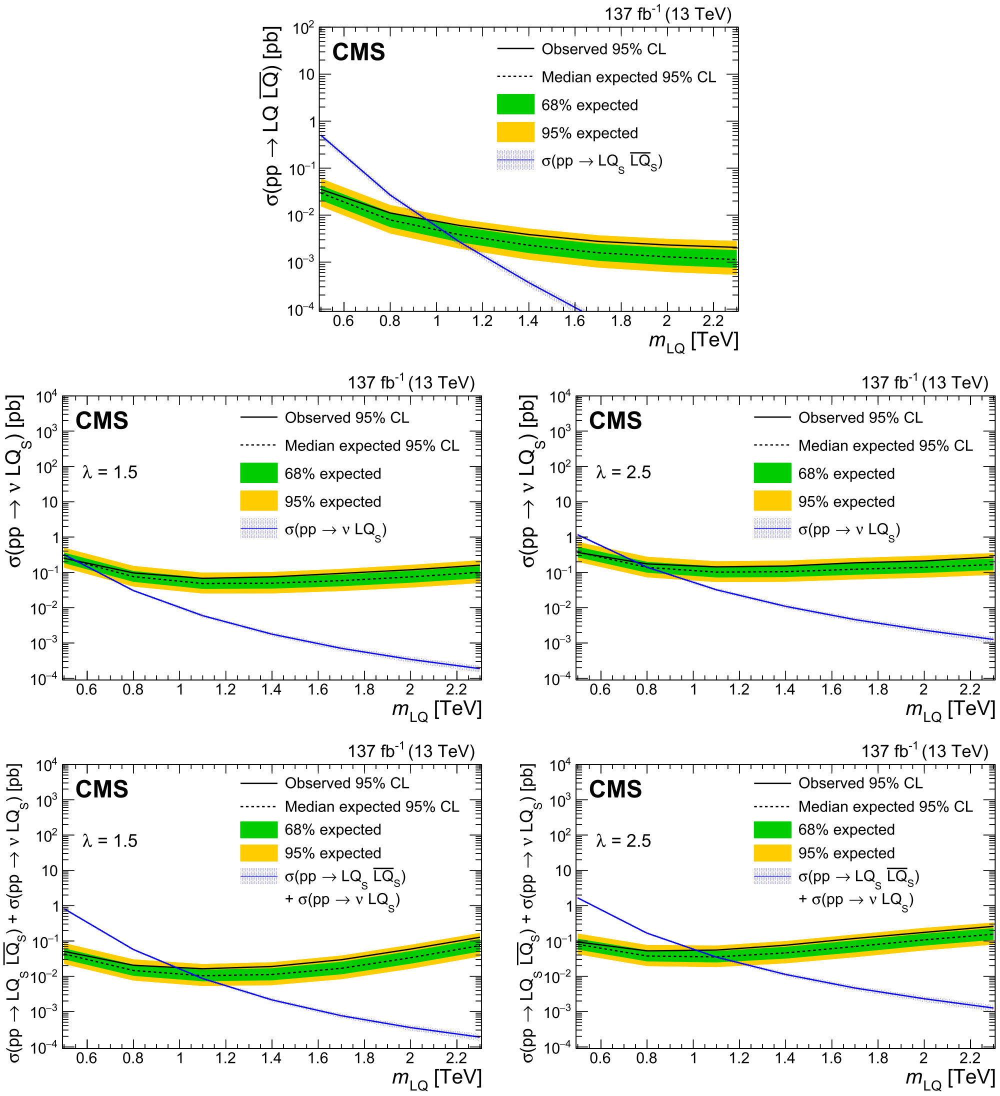

Fig. 3. The observed and expected (solid and dotted black lines) 95% CL upper limits on $\sigma(\mathrm{pp} \to \mathrm{LQ_S}\overline{\mathrm{LQ}}_\mathrm{S})$ (upper), $\sigma(\mathrm{pp} \to \nu\mathrm{LQ_S})$ with $\lambda = 1.5$ and 2.5 (middle left and right), and $\sigma(\mathrm{pp} \to \mathrm{LQ_S}\overline{\mathrm{LQ}}_\mathrm{S}) + \sigma(\mathrm{pp} \to \nu\mathrm{LQ_S})$ with $\lambda = 1.5$ and 2.5 (lower left and right), as a function of the mass of the $\mathrm{LQ_S}$. The limits apply under the assumption of equal couplings for the LQ decay to each of the two allowed lepton flavor pairings. The bands represent the one- and two-standard deviation variations of the expected limit. The solid blue curve indicates the theoretical predictions at LO, except for pair-produced $\mathrm{LQ_S}$, for which NLO values are used based on NLO quantum chromodynamics corrections [98] and the model implementation in Ref. [45].

cesses similar to that of the signal region but is dominated by events with a misidentified τ_h candidate, as determined from MC simulation. We find good agreement between the data and the estimated background in this region, as well as in a larger one with the $N_{\text{b-jet}}$ requirement released. The observed difference does not exceed 12%, and this value is therefore assigned as the systematic uncertainty in the background estimated using this method.

7. Systematic uncertainties

Systematic uncertainties from various sources are propagated to both the shape and normalization of the distributions in the discriminating variable S_T. The systematic uncertainties affect both the signal and the background, particularly the minor backgrounds (t production or "Others") that are derived relying on the MC simulation, while the main background (τ misidentification) is estimated from data.

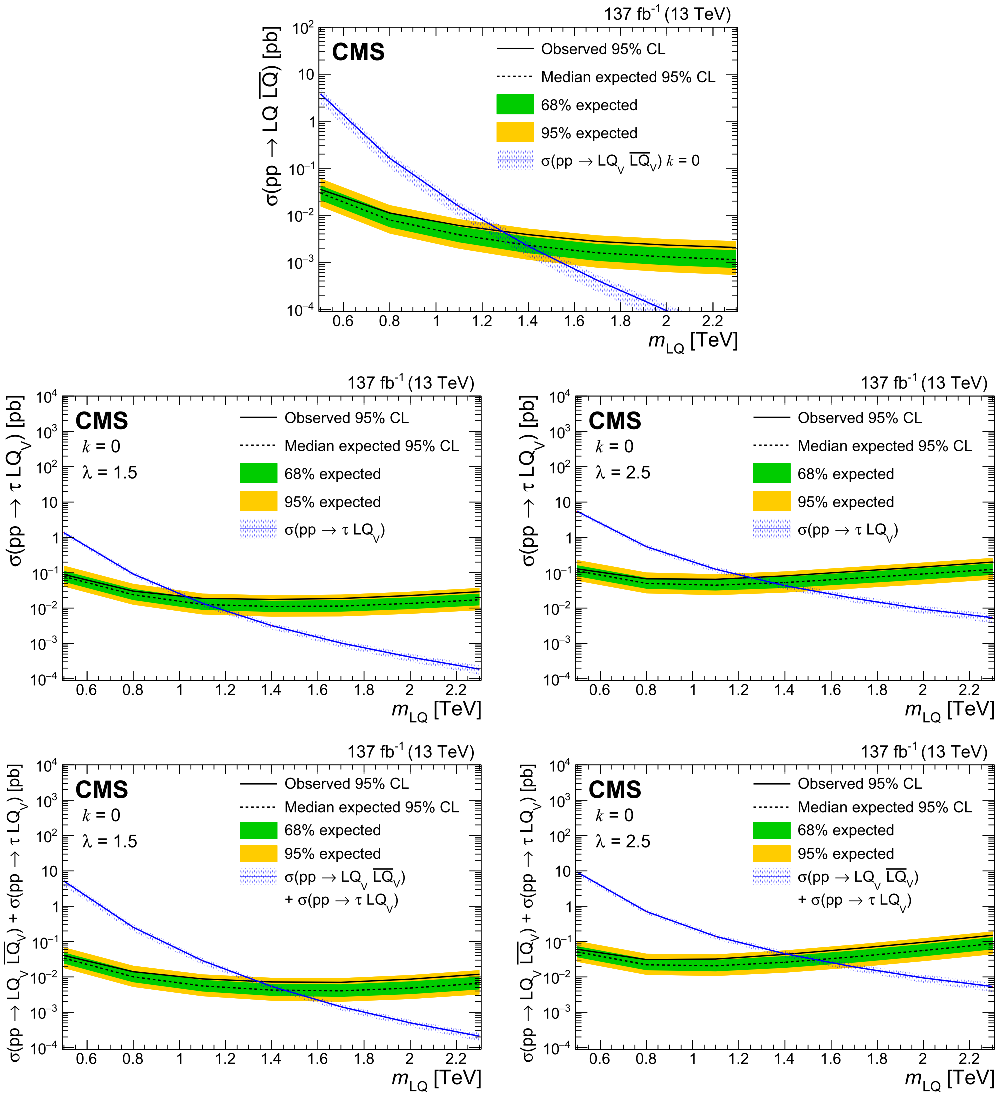

Fig. 4. The observed and expected (solid and dotted black lines) 95% CL upper limits on $\sigma(\mathrm{pp} \to \mathrm{LQ_V}\overline{\mathrm{LQ}}_\mathrm{V})$ (upper), $\sigma(\mathrm{pp} \to \tau\mathrm{LQ_V})$ with $\lambda = 1.5$ and 2.5 (middle left and right), and $\sigma(\mathrm{pp} \to \mathrm{LQ_V}\overline{\mathrm{LQ}}_\mathrm{V}) + \sigma(\mathrm{pp} \to \tau\mathrm{LQ_V})$ with $\lambda = 1.5$ and 2.5 (lower left and right), as a function of the mass of the $\mathrm{LQ_V}$, with $k = 0$. The limits apply under the assumption of equal couplings for the LQ decay to each of the two allowed lepton flavor pairings. The bands represent the one- and two-standard deviation variations of the expected limit. The solid blue curve indicates the theoretical predictions at LO.

The shape uncertainties vary according to the background process, S_T bin, and year of data taking. Thus in the following, we quote a range of values, reflecting the minimum and maximum uncertainties observed under the various conditions. The effect of the uncertainty on the simulation of pileup is estimated by varying the inelastic cross section [87] used in the simulation by 5%. This results in an uncertainty associated with the background of between 1 and 6%, and of 1% associated with the signal. The uncertainty in the acceptance associated with the PDFs is evaluated in accordance with the PDF4LHC recommendations [88], using the PDF4LHC15 Hessian PDF set with 100 eigenvectors, and is found to be less than 5% for the signal. The uncertainty related to the trigger is between 1 and 2%, for both the background and the signal. The jet four-momenta are varied within the JES and the JER uncertainties [76], resulting in an effect that ranges between 1 and 35% for the background and up to 2.5% for the signal. The above uncertainties are correlated across the years, while those discussed below are treated as uncorrelated, as they are dominated by statistical uncertainties. Corrections related to the b tagging are varied by the uncertainties that are measured with control samples in data and simulation [82], giving a systematic uncertainty in the yields in the range 3–10% for the background and 8–10% (13–23%) for single (pair) LQ production. Analogously, we take into account the uncertainty in the τ_h energy scale and identification [81], which amounts to 1–5% (less than 1%) and 5–13 (13–20)% for the background (signal). The W and t jet tagging uncertainty amounts to 2–11 (1–4)% and 3–15 (7–14)% for the background (signal). For all of the background processes, the statistical uncertainty in the samples used is included in the systematic uncertainty.

The sources of systematic uncertainty that affect only the normalization are the uncertainties in the cross sections of the backgrounds estimated from simulation (5% for top quark production and 30% for the remaining backgrounds), the uncertainty in the misidentified τ_h contribution, whose value of 12% is assigned from the consistency test discussed in Section 6, and the uncertainty in the integrated luminosity. The integrated luminosities of the 2016–18 data-taking periods are individually known with uncertainties in the 2.3–2.5% range [89–91], while the total Run 2 (2016–18) integrated luminosity has an uncertainty of 1.8%, the improvement in precision reflecting the (uncorrelated) time evolution of some systematic effects.

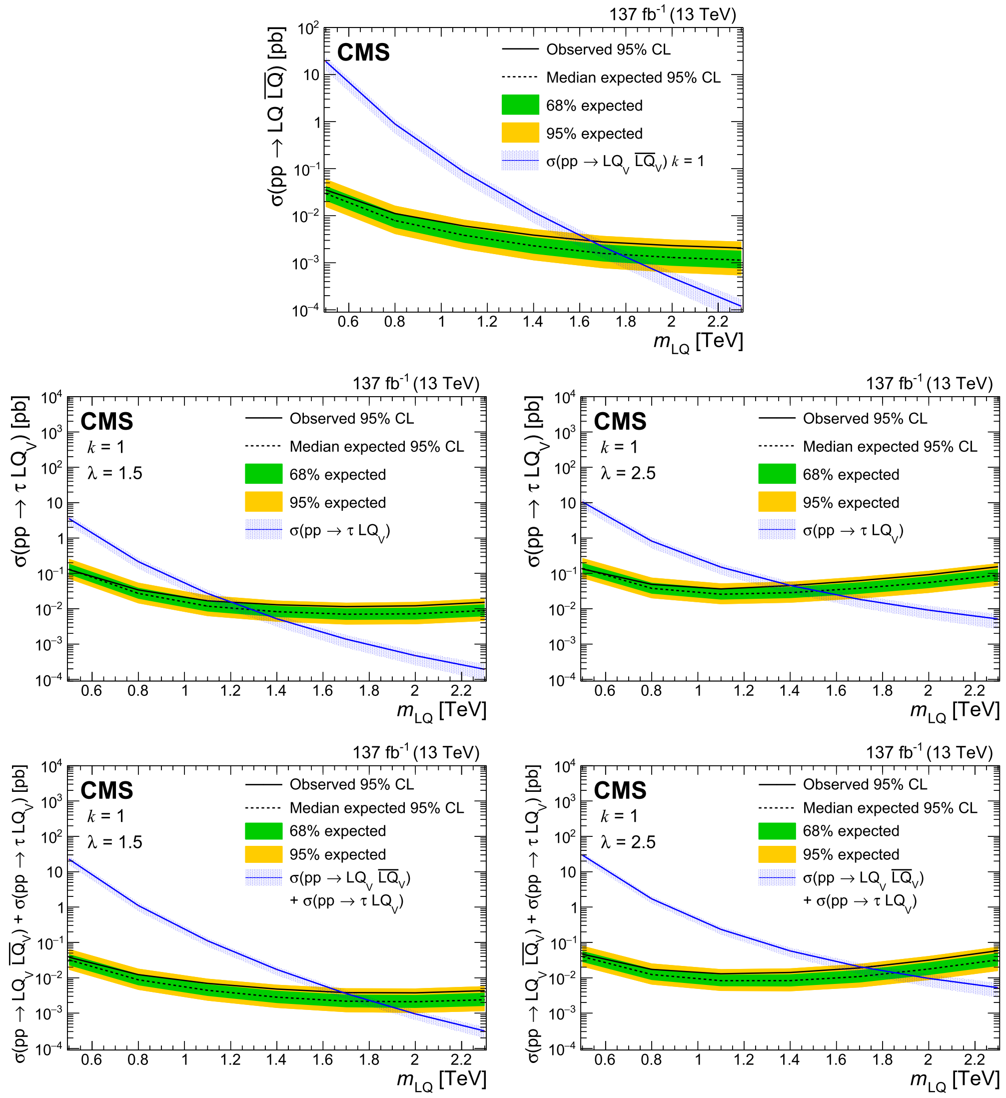

Fig. 5. The observed and expected (solid and dotted black lines) 95% CL upper limits on $\sigma(\mathrm{pp}\to\mathrm{LQ_V}\overline{\mathrm{LQ}}_\mathrm{V})$ (upper), $\sigma(\mathrm{pp}\to\tau\mathrm{LQ_V})$ with $\lambda=1.5$ and 2.5 (middle left and right), and $\sigma(\mathrm{pp}\to\mathrm{LQ_V}\overline{\mathrm{LQ}}_\mathrm{V})+\sigma(\mathrm{pp}\to\tau\mathrm{LQ_V})$ with $\lambda=1.5$ and 2.5 (lower left and right), as a function of the mass of the $\mathrm{LQ_V}$, with $k=1$. The limits apply under the assumption of equal couplings for the LQ decay to each of the two allowed lepton flavor pairings. The bands represent the one- and two-standard deviation variations of the expected limit. The solid blue curve indicates the theoretical predictions at LO.

8. Results

Fig. 2 and Table 1 show that the data are in agreement with the background expectations from the SM in all of the event categories investigated. We proceed with setting upper limits at 95% confidence level (CL) on the cross sections for the production of leptoquarks in pairs, $\sigma(\mathrm{pp}\to\mathrm{LQ}\overline{\mathrm{LQ}})$, and singly, $\sigma(\mathrm{pp}\to\ell\mathrm{LQ})$, for $\mathrm{LQ_S}$ ($\ell=\nu$), and $\mathrm{LQ_V}$ ($\ell=\tau$). We use the $\mathrm{CL_s}$ criterion [92,93] with binned templates of both background and signal as given by the distributions of Fig. 2. For each category and each bin of S_T, the observed number of events is fitted by a Poisson distribution, whose mean is the sum of the total SM expectation, determined as described in Section 6, and a potential signal contribution determined from simulation. The systematic uncertainties described in Section 7 are considered as nuisance parameters, with a lognormal distribution for the normalization parameters and a Gaussian distribution for systematic uncertainties affecting the shape.

The observed and expected upper limits on $\sigma(\mathrm{pp}\to\mathrm{LQ}\overline{\mathrm{LQ}})$, $\sigma(\mathrm{pp}\to\ell\mathrm{LQ})$, and the case where both pair and single production mechanisms are considered simultaneously, $\sigma(\mathrm{pp}\to\mathrm{LQ}\overline{\mathrm{LQ}})+\sigma(\mathrm{pp}\to\ell\mathrm{LQ})$, as a function of the mass of the leptoquarks are shown in Figs. 3–5, where the leptoquarks are $\mathrm{LQ_S}$, $\mathrm{LQ_V}$ $k=0$, and $\mathrm{LQ_V}$ $k=1$, respectively. The uncertainty in the production cross section shown in these figures is given by the sum in quadrature of contributions arising from the PDFs and the renormalization and factorization scales. To estimate the latter, we consider the effects of multiplying these scales by factors of 0.5 and 2 [94–96]. For single LQ production, the limits are shown for fixed values of $\lambda=1.5$ and 2.5. Only values of λ less than 2.5 are considered, since higher values are excluded by constraints from electroweak precision measurements [97]. The bands represent the one- and two-standard deviation variations of the expected limit. The solid blue curve indicates the theoretical prediction of $\sigma(\mathrm{pp}\to\mathrm{LQ}\overline{\mathrm{LQ}})$ and $\sigma(\mathrm{pp}\to\ell\mathrm{LQ})$, calculated at LO except for the pair production of $\mathrm{LQ_S}$, computed using NLO quantum chromodynamics corrections [98] and the model implementation in Ref. [45]. The intersection of the blue and the solid (dotted) black lines determines the observed (expected) lower limit on the LQ mass. Table 2 summarizes the observed and expected lower limits on the LQ mass inferred from Figs. 3–5 for the three cases, $\mathrm{LQ_S}$, $\mathrm{LQ_V}$ $k=0$, and $\mathrm{LQ_V}$ $k=1$. The observed limits are, respectively, 0.98–1.02, 1.34–1.41,

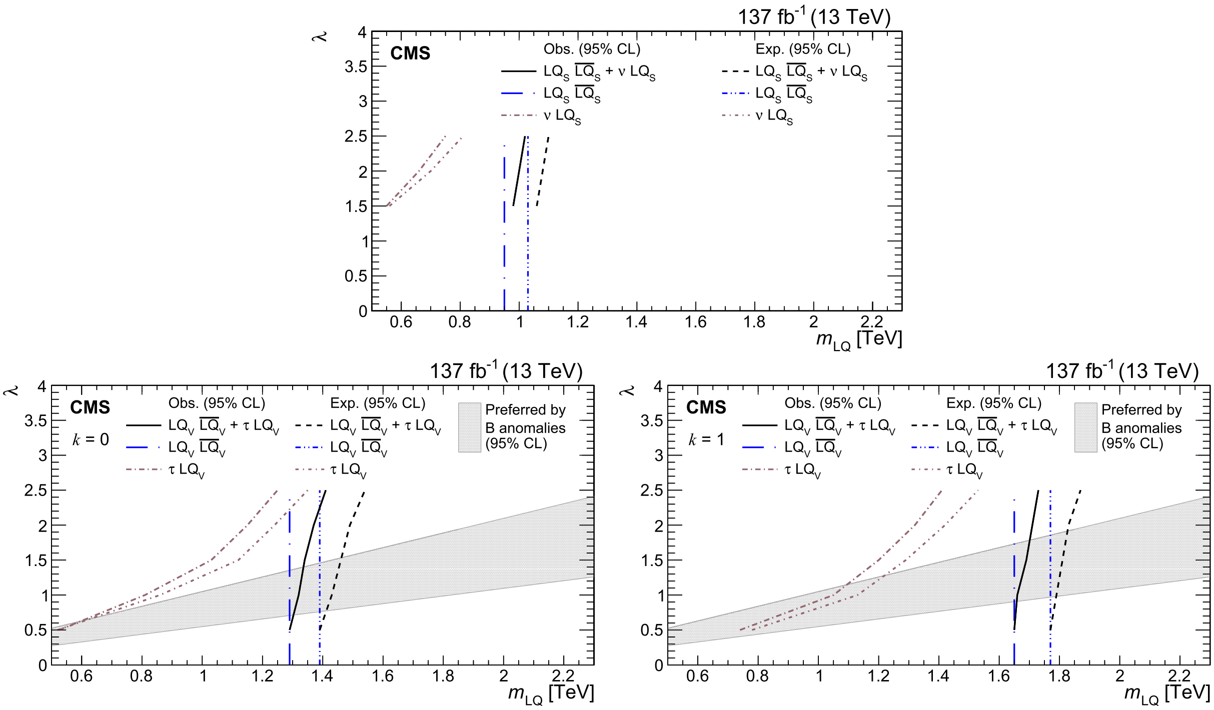

Fig. 6. The observed and expected 95% CL LQ exclusion limits in the plane of the LQ-lepton-quark coupling and the mass of the LQ for single (brown lines) and pair (blue lines) production, and considering their sum (black lines). Regions to the left of the lines are excluded. The upper plot pertains to an $\mathrm{LQ_S}$ with equal couplings to $\mathrm{t}\tau$ and $\mathrm{b}\nu$, while the lower plots are for an $\mathrm{LQ_V}$ assuming $k = 0$ (left) and 1 (right) and equal couplings to $\mathrm{t}\nu$ and $\mathrm{b}\tau$. For $\mathrm{LQ_V}$, the gray area shows the band preferred (95% CL) by the B physics anomalies: $\lambda = Cm_{\mathrm{LQ}}$, where $C = \sqrt{0.7 \pm 0.2}\,\mathrm{TeV}^{-1}$ and m_{LQ} is expressed in TeV [43].

and 1.69–1.73 TeV for values of λ between 1.5 and 2.5, based on the simultaneous search for single and pair production. The table also reports exclusion limits for the separate searches for single and pair production.

The combination of the two production mechanisms extends the exclusion on the LQ mass by 30–120 GeV depending on the type of LQ. These exclusions represent the most stringent limits to date on the existence of $\mathrm{LQ_S}$ ($\mathrm{LQ_V}$) coupled to $\mathrm{t}\tau$, $\mathrm{b}\nu$ ($\mathrm{t}\nu$, $\mathrm{b}\tau$) under the assumption of equal couplings to the lepton-quark pairs. Comparing the cases of $\lambda = 1.5$ and 2.5 in Figs. 3–5, one can see how the upper limits on the cross section increase at higher LQ masses and λ values, as a result of an increasing relative contribution of virtual LQ states in single LQ production, as discussed in Section 3, which degrades the sensitivity of the search.

Fig. 6 gives the observed and expected exclusion on the existence of leptoquarks in the $\lambda - m_{\mathrm{LQ}}$ plane, for the single and pair production mechanisms and their combination. For $\mathrm{LQ_V}$, the gray area shows the 95% CL band preferred by the B physics anomalies [43], which is given by $\lambda = Cm_{\mathrm{LQ}}$, where $C = \sqrt{0.7 \pm 0.2}\,\mathrm{TeV}^{-1}$ and m_{LQ} is expressed in TeV. A relevant portion of this parameter space is excluded.

9. Summary

A search for leptoquarks coupled to third-generation fermions, and produced in pairs and singly in association with a lepton, has been presented. The leptoquark (LQ) may couple to a top quark and a τ lepton (tτ) or a bottom quark and a neutrino (bν, scalar LQ) or else to tν and bτ (vector LQ), resulting in the tτνb and tτν signatures. The channel in which both the top quark and the τ lepton decay hadronically is investigated, including the case of a large LQ-t mass splitting giving rise to a Lorentz-boosted top quark, whose decay daughters may not be resolved as individual jets. This particular signature has not been previously examined in searches for physics beyond the standard model. The data used corresponds to an integrated luminosity of 137 fb^{-1} collected with the CMS detector at the CERN LHC in proton-proton collisions at $\sqrt{s} = 13$ TeV. The observations are found to be in agreement with the standard model predictions. Exclusion limits are given in the plane of the LQ-lepton-quark vertex coupling λ and the LQ mass for scalar and vector leptoquarks. The range of lower limits on the LQ mass, at 95% confidence level, is 0.98–1.73 TeV, depending on λ and the leptoquark spin. These results represent the most stringent limits to date on the existence of such leptoquarks for the case of equal couplings to the lepton-quark pairs. They allow a relevant portion of the parameter space preferred by the B-physics anomalies in several models [42,43] to be excluded.

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.

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The CMS Collaboration

A.M. Sirunyan[†], A. Tumasyan

Yerevan Physics Institute, Yerevan, Armenia

W. Adam, T. Bergauer, M. Dragicevic, J. Erö, A. Escalante Del Valle, R. Frühwirth[1], M. Jeitler[1], N. Krammer, L. Lechner, D. Liko, I. Mikulec, F.M. Pitters, N. Rad, J. Schieck[1], R. Schöfbeck, M. Spanring, S. Templ, W. Waltenberger, C.-E. Wulz[1], M. Zarucki

Institut für Hochenergiephysik, Wien, Austria

V. Chekhovsky, A. Litomin, V. Makarenko, J. Suarez Gonzalez

Institute for Nuclear Problems, Minsk, Belarus

M.R. Darwish[2], E.A. De Wolf, D. Di Croce, X. Janssen, T. Kello[3], A. Lelek, M. Pieters, H. Rejeb Sfar, H. Van Haevermaet, P. Van Mechelen, S. Van Putte, N. Van Remortel

Universiteit Antwerpen, Antwerpen, Belgium

F. Blekman, E.S. Bols, S.S. Chhibra, J. D'Hondt, J. De Clercq, D. Lontkovskyi, S. Lowette, I. Marchesini, S. Moortgat, A. Morton, D. Müller, Q. Python, S. Tavernier, W. Van Doninck, P. Van Mulders

Vrije Universiteit Brussel, Brussel, Belgium

D. Beghin, B. Bilin, B. Clerbaux, G. De Lentdecker, B. Dorney, L. Favart, A. Grebenyuk, A.K. Kalsi, I. Makarenko, L. Moureaux, L. Pétré, A. Popov, N. Postiau, E. Starling, L. Thomas, C. Vander Velde, P. Vanlaer, D. Vannerom, L. Wezenbeek

Université Libre de Bruxelles, Bruxelles, Belgium

T. Cornelis, D. Dobur, M. Gruchala, I. Khvastunov[4], M. Niedziela, C. Roskas, K. Skovpen, M. Tytgat, W. Verbeke, B. Vermassen, M. Vit

Ghent University, Ghent, Belgium

G. Bruno, F. Bury, C. Caputo, P. David, C. Delaere, M. Delcourt, I.S. Donertas, A. Giammanco, V. Lemaitre, K. Mondal, J. Prisciandaro, A. Taliercio, M. Teklishyn, P. Vischia, S. Wertz, S. Wuyckens

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

G.A. Alves, C. Hensel, A. Moraes

Centro Brasileiro de Pesquisas Fisicas, Rio de Janeiro, Brazil

W.L. Aldá Júnior, E. Belchior Batista Das Chagas, H. Brandao Malbouisson, W. Carvalho, J. Chinellato[5], E. Coelho, E.M. Da Costa, G.G. Da Silveira[6], D. De Jesus Damiao, S. Fonseca De Souza, J. Martins[7], D. Matos Figueiredo, M. Medina Jaime[8], C. Mora Herrera, L. Mundim, H. Nogima, P. Rebello Teles, L.J. Sanchez Rosas, A. Santoro, S.M. Silva Do Amaral, A. Sznajder, M. Thiel, F. Torres Da Silva De Araujo, A. Vilela Pereira

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

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

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

A. Aleksandrov, G. Antchev, I. Atanasov, 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, W. Fang[3], Q. Guo, H. Wang, L. Yuan

Beihang University, Beijing, China

M. Ahmad, G. Bauer, Z. Hu, Y. Wang, K. Yi[9,10]

Department of Physics, Tsinghua University, Beijing, China

E. Chapon, G.M. Chen[11], H.S. Chen[11], M. Chen, T. Javaid[11], A. Kapoor, D. Leggat, H. Liao, Z.-A. Liu[11], R. Sharma, A. Spiezia, J. Tao, J. Thomas-wilsker, J. Wang, H. Zhang, S. Zhang[11], J. Zhao

Institute of High Energy Physics, Beijing, China

A. Agapitos, Y. Ban, C. Chen, Q. Huang, A. Levin, Q. Li, M. Lu, X. Lyu, Y. Mao, S.J. Qian, D. Wang, Q. Wang, J. Xiao

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

Z. You

Sun Yat-Sen University, Guangzhou, China

X. Gao[3]

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

M. Xiao

Zhejiang University, Hangzhou, China

C. Avila, A. Cabrera, C. Florez, J. Fraga, A. Sarkar, M.A. Segura Delgado

Universidad de Los Andes, Bogota, Colombia

J. Jaramillo, J. Mejia Guisao, F. Ramirez, J.D. Ruiz Alvarez, C.A. Salazar González, N. Vanegas Arbelaez

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 [12], T. Susa

Institute Rudjer Boskovic, Zagreb, Croatia

M.W. Ather, A. Attikis, E. Erodotou, A. Ioannou, G. Kole, M. Kolosova, S. Konstantinou, J. Mousa, C. Nicolaou, F. Ptochos, P.A. Razis, H. Rykaczewski, H. Saka, D. Tsiakkouri

University of Cyprus, Nicosia, Cyprus

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

Charles University, Prague, Czech Republic

E. Ayala

Escuela Politecnica Nacional, Quito, Ecuador

E. Carrera Jarrin

Universidad San Francisco de Quito, Quito, Ecuador

S. Elgammal [14], A. Ellithi Kamel [15], S. Khalil [16]

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 [17]

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

S. Bhowmik, A. Carvalho Antunes De Oliveira, R.K. Dewanjee, K. Ehataht, M. Kadastik, M. Raidal, C. Veelken

National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

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

Department of Physics, University of Helsinki, Helsinki, Finland

E. Brücken, F. Garcia, J. Havukainen, V. Karimäki, M.S. Kim, R. Kinnunen, T. Lampén, K. Lassila-Perini, S. Lehti, T. Lindén, H. Siikonen, E. Tuominen, J. Tuominiemi

Helsinki Institute of Physics, Helsinki, Finland

P. Luukka, T. Tuuva

Lappeenranta University of Technology, Lappeenranta, Finland

C. Amendola, M. Besancon, F. Couderc, M. Dejardin, D. Denegri, J.L. Faure, F. Ferri, S. Ganjour, A. Givernaud, P. Gras, G. Hamel de Monchenault, P. Jarry, B. Lenzi, E. Locci, J. Malcles, J. Rander, A. Rosowsky, M.Ö. Sahin, A. Savoy-Navarro [18], M. Titov, G.B. Yu

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

S. Ahuja, F. Beaudette, M. Bonanomi, A. Buchot Perraguin, P. Busson, C. Charlot, O. Davignon, B. Diab, G. Falmagne, R. Granier de Cassagnac, A. Hakimi, I. Kucher, A. Lobanov, C. Martin Perez, M. Nguyen, C. Ochando, P. Paganini, J. Rembser, R. Salerno, J.B. Sauvan, Y. Sirois, A. Zabi, A. Zghiche

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

J.-L. Agram [19], J. Andrea, D. Bloch, G. Bourgatte, J.-M. Brom, E.C. Chabert, C. Collard, J.-C. Fontaine [19], D. Gelé, U. Goerlach, C. Grimault, A.-C. Le Bihan, P. Van Hove

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

E. Asilar, 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, Sa. Jain, I.B. Laktineh, H. Lattaud, A. Lesauvage, M. Lethuillier, L. Mirabito, L. Torterotot, G. Touquet, M. Vander Donckt, S. Viret

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

I. Bagaturia[20], Z. Tsamalaidze[13]

Georgian Technical University, Tbilisi, Georgia

L. Feld, K. Klein, M. Lipinski, D. Meuser, A. Pauls, M. Preuten, M.P. Rauch, J. Schulz, M. Teroerde

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

D. Eliseev, M. Erdmann, P. Fackeldey, B. Fischer, S. Ghosh, T. Hebbeker, K. Hoepfner, H. Keller, L. Mastrolorenzo, M. Merschmeyer, A. Meyer, G. Mocellin, S. Mondal, S. Mukherjee, D. Noll, A. Novak, T. Pook, A. Pozdnyakov, Y. Rath, H. Reithler, J. Roemer, A. Schmidt, S.C. Schuler, A. Sharma, S. Wiedenbeck, S. Zaleski

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

C. Dziwok, G. Flügge, W. Haj Ahmad[21], O. Hlushchenko, T. Kress, A. Nowack, C. Pistone, O. Pooth, D. Roy, H. Sert, A. Stahl[22], T. Ziemons

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

H. Aarup Petersen, M. Aldaya Martin, P. Asmuss, I. Babounikau, S. Baxter, O. Behnke, A. Bermúdez Martínez, A.A. Bin Anuar, K. Borras[23], V. Botta, D. Brunner, A. Campbell, A. Cardini, P. Connor, S. Consuegra Rodríguez, V. Danilov, A. De Wit, M.M. Defranchis, L. Didukh, D. Domínguez Damiani, G. Eckerlin, D. Eckstein, T. Eichhorn, L.I. Estevez Banos, E. Gallo[24], A. Geiser, A. Giraldi, A. Grohsjean, M. Guthoff, A. Harb, A. Jafari[25], N.Z. Jomhari, H. Jung, A. Kasem[23], M. Kasemann, H. Kaveh, C. Kleinwort, J. Knolle, D. Krücker, W. Lange, T. Lenz, J. Lidrych, K. Lipka, W. Lohmann[26], T. Madlener, R. Mankel, I.-A. Melzer-Pellmann, J. Metwally, A.B. Meyer, M. Meyer, M. Missiroli, J. Mnich, A. Mussgiller, V. Myronenko, Y. Otarid, D. Pérez Adán, S.K. Pflitsch, D. Pitzl, A. Raspereza, A. Saggio, A. Saibel, M. Savitskyi, V. Scheurer, C. Schwanenberger, A. Singh, R.E. Sosa Ricardo, N. Tonon, O. Turkot, A. Vagnerini, M. Van De Klundert, R. Walsh, D. Walter, Y. Wen, K. Wichmann, C. Wissing, S. Wuchterl, O. Zenaiev, R. Zlebcik

Deutsches Elektronen-Synchrotron, Hamburg, Germany

R. Aggleton, S. Bein, L. Benato, A. Benecke, K. De Leo, T. Dreyer, A. Ebrahimi, M. Eich, F. Feindt, A. Fröhlich, C. Garbers, E. Garutti, P. Gunnellini, J. Haller, A. Hinzmann, A. Karavdina, G. Kasieczka, R. Klanner, R. Kogler, V. Kutzner, J. Lange, T. Lange, A. Malara, C.E.N. Niemeyer, A. Nigamova, K.J. Pena Rodriguez, O. Rieger, P. Schleper, S. Schumann, J. Schwandt, D. Schwarz, J. Sonneveld, H. Stadie, G. Steinbrück, B. Vormwald, I. Zoi

University of Hamburg, Hamburg, Germany

J. Bechtel, T. Berger, E. Butz, R. Caspart, T. Chwalek, W. De Boer, A. Dierlamm, A. Droll, K. El Morabit, N. Faltermann, K. Flöh, M. Giffels, A. Gottmann, F. Hartmann[22], C. Heidecker, U. Husemann, I. Katkov[27], P. Keicher, R. Koppenhöfer, S. Maier, M. Metzler, S. Mitra, Th. Müller, M. Musich, G. Quast, K. Rabbertz, J. Rauser, D. Savoiu, D. Schäfer, M. Schnepf, M. Schröder, D. Seith, I. Shvetsov, H.J. Simonis, R. Ulrich, M. Wassmer, M. Weber, R. Wolf, S. Wozniewski

Karlsruher Institut fuer Technologie, Karlsruhe, Germany

G. Anagnostou, P. Asenov, G. Daskalakis, T. Geralis, A. Kyriakis, D. Loukas, G. Paspalaki, A. Stakia

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

M. Diamantopoulou, D. Karasavvas, G. Karathanasis, 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

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

University of Ioánnina, Ioánnina, Greece

M. Bartók[28], M. Csanad, M.M.A. Gadallah[29], S. Lökös[30], P. Major, K. Mandal, A. Mehta, G. Pasztor, O. Surányi, G.I. Veres

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

G. Bencze, C. Hajdu, D. Horvath[31], F. Sikler, V. Veszpremi, G. Vesztergombi[†]

Wigner Research Centre for Physics, Budapest, Hungary

S. Czellar, J. Karancsi[28], J. Molnar, Z. Szillasi, D. Teyssier

Institute of Nuclear Research ATOMKI, Debrecen, Hungary

P. Raics, Z.L. Trocsanyi, B. Ujvari

Institute of Physics, University of Debrecen, Debrecen, Hungary

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

Eszterhazy Karoly University, Karoly Robert Campus, Gyongyos, Hungary

S. Choudhury, J.R. Komaragiri, D. Kumar, L. Panwar, P.C. Tiwari

Indian Institute of Science (IISc), Bangalore, India

S. Bahinipati[33], D. Dash, C. Kar, P. Mal, T. Mishra, V.K. Muraleedharan Nair Bindhu, A. Nayak[34], D.K. Sahoo[33], N. Sur, S.K. Swain

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

S. Bansal, S.B. Beri, V. Bhatnagar, G. Chaudhary, S. Chauhan, N. Dhingra[35], R. Gupta, A. Kaur, S. Kaur, P. Kumari, M. Meena, K. Sandeep, S. Sharma, J.B. Singh, A.K. Virdi

Panjab University, Chandigarh, India

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

University of Delhi, Delhi, India

M. Bharti[36], R. Bhattacharya, S. Bhattacharya, D. Bhowmik, S. Dutta, S. Ghosh, B. Gomber[37], M. Maity[38], S. Nandan, P. Palit, P.K. Rout, G. Saha, B. Sahu, S. Sarkar, M. Sharan, B. Singh[36], S. Thakur[36]

Saha Institute of Nuclear Physics, HBNI, Kolkata, India

P.K. Behera, S.C. Behera, P. Kalbhor, A. Muhammad, R. Pradhan, P.R. Pujahari, A. Sharma, A.K. Sikdar

Indian Institute of Technology Madras, Madras, India

D. Dutta, V. Kumar, K. Naskar[39], P.K. Netrakanti, L.M. Pant, P. Shukla

Bhabha Atomic Research Centre, Mumbai, India

T. Aziz, M.A. Bhat, S. Dugad, R. Kumar Verma, G.B. Mohanty, U. Sarkar

Tata Institute of Fundamental Research-A, Mumbai, India

S. Banerjee, S. Bhattacharya, S. Chatterjee, R. Chudasama, M. Guchait, S. Karmakar, S. Kumar, G. Majumder, K. Mazumdar, S. Mukherjee, D. Roy

Tata Institute of Fundamental Research-B, Mumbai, India

S. Dube, B. Kansal, S. Pandey, A. Rane, A. Rastogi, S. Sharma

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

H. Bakhshiansohi[40], M. Zeinali[41]

Department of Physics, Isfahan University of Technology, Isfahan, Iran

S. Chenarani[42], S.M. Etesami, M. Khakzad, M. Mohammadi Najafabadi

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

M. Felcini, M. Grunewald

University College Dublin, Dublin, Ireland

M. Abbrescia[a,b], R. Aly[a,b,43], 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], A. Di Pilato[a,b], W. Elmetenawee[a,b], L. Fiore[a], A. Gelmi[a,b], M. Gul[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], J.A. Merlin[a], S. My[a,b], S. Nuzzo[a,b], A. Pompili[a,b], G. Pugliese[a,c], A. Ranieri[a], G. Selvaggi[a,b], L. Silvestris[a], F.M. Simone[a,b], 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], S. Braibant-Giacomelli[a,b], 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], E. Fontanesi[a,b], P. Giacomelli[a], L. Giommi[a,b], C. Grandi[a], L. Guiducci[a,b], F. Iemmi[a,b], S. Lo Meo[a,44], 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], N. Tosi[a]

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

S. Albergo[a,b,45], S. Costa[a,b], A. Di Mattia[a], R. Potenza[a,b], A. Tricomi[a,b,45], C. Tuve[a,b]

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

G. Barbagli[a], A. Cassese[a], R. Ceccarelli[a,b], V. Ciulli[a,b], C. Civinini[a], R. D'Alessandro[a,b], F. Fiori[a], 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,b], E. Robutti[a], S. Tosi[a,b]

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

A. Benaglia[a], A. Beschi[a,b], F. Brivio[a,b], F. Cetorelli[a,b], V. Ciriolo[a,b,22], 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. Malberti[a], S. Malvezzi[a], A. Massironi[a],

D. Menasce[a], F. Monti[a,b], L. Moroni[a], M. Paganoni[a,b], D. Pedrini[a], S. Ragazzi[a,b], T. Tabarelli de Fatis[a,b], D. Valsecchi[a,b,22], D. Zuolo[a,b]

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

S. Buontempo[a], N. Cavallo[a,c], A. De Iorio[a,b], F. Fabozzi[a,c], F. Fienga[a], A.O.M. Iorio[a,b], L. Lista[a,b], S. Meola[a,d,22], P. Paolucci[a,22], B. Rossi[a], C. Sciacca[a,b], E. Voevodina[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], P. De Castro Manzano[a], T. Dorigo[a], F. Gasparini[a,b], U. Gasparini[a,b], S.Y. Hoh[a,b], L. Layer[a,46], M. Margoni[a,b], A.T. Meneguzzo[a,b], M. Presilla[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. Aime[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], M. Ressegotti[a,b], 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

M. Biasini[a,b], G.M. Bilei[a], D. Ciangottini[a,b], L. Fanò[a,b], P. Lariccia[a,b], G. Mantovani[a,b], V. Mariani[a,b], M. Menichelli[a], F. Moscatelli[a], A. Piccinelli[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

K. Androsov[a], P. Azzurri[a], G. Bagliesi[a], V. Bertacchi[a,c], L. Bianchini[a], T. Boccali[a], R. Castaldi[a], M.A. Ciocci[a,b], R. Dell'Orso[a], M.R. Di Domenico[a,d], S. Donato[a], L. Giannini[a,c], A. Giassi[a], M.T. Grippo[a], F. Ligabue[a,c], E. Manca[a,c], G. Mandorli[a,c], A. Messineo[a,b], F. Palla[a], 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

F. Cavallari[a], M. Cipriani[a,b], 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,b], R. Tramontano[a,b]

[a] INFN Sezione di Roma, Rome, Italy
[b] Sapienza Università di Roma, Rome, 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], A. Cappati[a,b], N. Cartiglia[a], S. Cometti[a], M. Costa[a,b], R. Covarelli[a,b], N. Demaria[a], B. Kiani[a,b], F. Legger[a], 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], G. Ortona[a], L. Pacher[a,b], N. Pastrone[a], M. Pelliccioni[a], G.L. Pinna Angioni[a,b], M. Ruspa[a,c], R. Salvatico[a,b], 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,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], F. Vazzoler[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. Lee, S.W. Lee, C.S. Moon, Y.D. Oh, S.I. Pak, B.C. Radburn-Smith, S. Sekmen, Y.C. Yang

Kyungpook National University, Daegu, Republic of Korea

H. Kim, D.H. Moon

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

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

Hanyang University, Seoul, Republic of Korea

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

Korea University, Seoul, Republic of Korea

J. Goh, A. Gurtu

Kyung Hee University, Department of Physics, Seoul, Republic of Korea

H.S. Kim, Y. Kim

Sejong University, Seoul, Republic of Korea

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

Seoul National University, Seoul, Republic of Korea

D. Jeon, J.H. Kim, B. Ko, J.S.H. Lee, I.C. Park, Y. Roh, D. Song, I.J. Watson

University of Seoul, Seoul, Republic of Korea

H.D. Yoo

Yonsei University, Department of Physics, Seoul, Republic of Korea

Y. Choi, C. Hwang, Y. Jeong, H. Lee, Y. Lee, I. Yu

Sungkyunkwan University, Suwon, Republic of Korea

Y. Maghrbi

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

V. Veckalns[47]

Riga Technical University, Riga, Latvia

A. Juodagalvis, A. Rinkevicius, G. Tamulaitis, A. Vaitkevicius

Vilnius University, Vilnius, Lithuania

W.A.T. Wan Abdullah, M.N. Yusli, Z. Zolkapli

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

J.F. Benitez, A. Castaneda Hernandez, J.A. Murillo Quijada, L. Valencia Palomo

Universidad de Sonora (UNISON), Hermosillo, Mexico

G. Ayala, H. Castilla-Valdez, E. De La Cruz-Burelo, I. Heredia-De La Cruz[48], R. Lopez-Fernandez, C.A. Mondragon Herrera, D.A. Perez Navarro, A. Sanchez-Hernandez

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

S. Carrillo Moreno, C. Oropeza Barrera, M. Ramirez-Garcia, F. Vazquez Valencia

Universidad Iberoamericana, Mexico City, Mexico

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

Benemerita Universidad Autonoma de Puebla, Puebla, Mexico

A. Morelos Pineda

Universidad Autónoma de San Luis Potosí, San Luis Potosí, Mexico

J. Mijuskovic[4], N. Raicevic

University of Montenegro, Podgorica, Montenegro

D. Krofcheck

University of Auckland, Auckland, New Zealand

S. Bheesette, P.H. Butler

University of Canterbury, Christchurch, New Zealand

A. Ahmad, M.I. Asghar, A. Awais, M.I.M. Awan, 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, T. Frueboes, M. Górski, M. Kazana, M. Szleper, P. Traczyk, P. Zalewski

National Centre for Nuclear Research, Swierk, Poland

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

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, J. Seixas, K. Shchelina, O. Toldaiev, J. Varela

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

S. Afanasiev, V. Alexakhin, P. Bunin, M. Gavrilenko, I. Golutvin, I. Gorbunov, A. Kamenev, V. Karjavine, A. Lanev, A. Malakhov, V. Matveev[49,50], V. Palichik, V. Perelygin, M. Savina, D. Seitova, S. Shmatov, S. Shulha, V. Smirnov, O. Teryaev, N. Voytishin, B.S. Yuldashev[51], A. Zarubin

Joint Institute for Nuclear Research, Dubna, Russia

G. Gavrilov, V. Golovtcov, Y. Ivanov, V. Kim[52], E. Kuznetsova[53], V. Murzin, V. Oreshkin, I. Smirnov, D. Sosnov, V. Sulimov, L. Uvarov, S. Volkov, A. Vorobyev

Petersburg Nuclear Physics Institute, Gatchina (St. Petersburg), Russia

Yu. Andreev, A. Dermenev, S. Gninenko, N. Golubev, A. Karneyeu, M. Kirsanov, N. Krasnikov, A. Pashenkov, G. Pivovarov, D. Tlisov[†], A. Toropin

Institute for Nuclear Research, Moscow, Russia

V. Epshteyn, V. Gavrilov, N. Lychkovskaya, A. Nikitenko[54], V. Popov, G. Safronov, A. Spiridonov, A. Stepennov, M. Toms, E. Vlasov, A. Zhokin

Institute for Theoretical and Experimental Physics named by A.I. Alikhanov of NRC 'Kurchatov Institute', Moscow, Russia

T. Aushev

Moscow Institute of Physics and Technology, Moscow, Russia

R. Chistov[55], M. Danilov[56], A. Oskin, P. Parygin, S. Polikarpov[55]

National Research Nuclear University 'Moscow Engineering Physics Institute' (MEPhI), Moscow, Russia

V. Andreev, M. Azarkin, I. Dremin, M. Kirakosyan, A. Terkulov

P.N. Lebedev Physical Institute, Moscow, Russia

A. Belyaev, E. Boos, V. Bunichev, M. Dubinin[57], L. Dudko, A. Ershov, A. Gribushin, V. Klyukhin, I. Lokhtin, S. Obraztsov, M. Perfilov, V. Savrin, P. Volkov

Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow, Russia

V. Blinov[58], T. Dimova[58], L. Kardapoltsev[58], I. Ovtin[58], Y. Skovpen[58]

Novosibirsk State University (NSU), Novosibirsk, Russia

I. Azhgirey, I. Bayshev, V. Kachanov, A. Kalinin, D. Konstantinov, V. Petrov, R. Ryutin, A. Sobol, S. Troshin, N. Tyurin, A. Uzunian, A. Volkov

Institute for High Energy Physics of National Research Centre 'Kurchatov Institute', Protvino, Russia

A. Babaev, A. Iuzhakov, V. Okhotnikov, L. Sukhikh

National Research Tomsk Polytechnic University, Tomsk, Russia

V. Borchsh, V. Ivanchenko, E. Tcherniaev

Tomsk State University, Tomsk, Russia

P. Adzic[59], P. Cirkovic, M. Dordevic, P. Milenovic, J. Milosevic

University of Belgrade: Faculty of Physics and VINCA Institute of Nuclear Sciences, 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, A. García Alonso, O. Gonzalez Lopez, S. Goy Lopez, J.M. Hernandez, M.I. Josa, J. León Holgado, D. Moran, Á. Navarro Tobar, A. Pérez-Calero Yzquierdo, J. Puerta Pelayo, I. Redondo, L. Romero, S. Sánchez Navas, M.S. Soares, A. Triossi, L. Urda Gómez, C. Willmott

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

C. Albajar, J.F. de Trocóniz, R. Reyes-Almanza

Universidad Autónoma de Madrid, Madrid, Spain

B. Alvarez Gonzalez, J. Cuevas, C. Erice, J. Fernandez Menendez, S. Folgueras, I. Gonzalez Caballero, E. Palencia Cortezon, C. Ramón Álvarez, J. Ripoll Sau, V. Rodríguez Bouza, S. Sanchez Cruz, A. Trapote

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

J.A. Brochero Cifuentes, I.J. Cabrillo, A. Calderon, B. Chazin Quero, J. Duarte Campderros, M. Fernandez, P.J. Fernández Manteca, G. Gomez, C. Martinez Rivero, P. Martinez Ruiz del Arbol, F. Matorras, J. Piedra Gomez, C. Prieels, F. Ricci-Tam, T. Rodrigo, 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[60], 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, E. Auffray, G. Auzinger, J. Baechler, P. Baillon, A.H. Ball, D. Barney, J. Bendavid, N. Beni, M. Bianco, A. Bocci, E. Bossini, E. Brondolin, T. Camporesi, M. Capeans Garrido, G. Cerminara, L. Cristella, D. d'Enterria, A. Dabrowski, N. Daci, V. Daponte, A. David, A. De Roeck, M. Deile, R. Di Maria, M. Dobson, M. Dünser, N. Dupont, A. Elliott-Peisert, N. Emriskova, F. Fallavollita[61], D. Fasanella, S. Fiorendi, A. Florent, G. Franzoni, J. Fulcher, W. Funk, S. Giani, D. Gigi, K. Gill, F. Glege, L. Gouskos, M. Guilbaud, D. Gulhan, M. Haranko, J. Hegeman, Y. Iiyama, V. Innocente, T. James, P. Janot, J. Kaspar, J. Kieseler, M. Komm, N. Kratochwil, C. Lange, S. Laurila, P. Lecoq, K. Long, C. Lourenço, L. Malgeri, S. Mallios, M. Mannelli, F. Meijers, S. Mersi, E. Meschi, F. Moortgat, M. Mulders, S. Orfanelli, L. Orsini, F. Pantaleo[22], L. Pape, E. Perez, M. Peruzzi, A. Petrilli, G. Petrucciani, A. Pfeiffer, M. Pierini, T. Quast, D. Rabady, A. Racz, M. Rieger, M. Rovere, H. Sakulin, J. Salfeld-Nebgen, S. Scarfi, C. Schäfer, C. Schwick, M. Selvaggi, A. Sharma, P. Silva, W. Snoeys, P. Sphicas[62], S. Summers, V.R. Tavolaro, D. Treille, A. Tsirou, G.P. Van Onsem, A. Vartak, M. Verzetti, K.A. Wozniak, W.D. Zeuner

CERN, European Organization for Nuclear Research, Geneva, Switzerland

L. Caminada[63], W. Erdmann, R. Horisberger, Q. Ingram, H.C. Kaestli, D. Kotlinski, U. Langenegger, T. Rohe

Paul Scherrer Institut, Villigen, Switzerland

M. Backhaus, P. Berger, A. Calandri, N. Chernyavskaya, A. De Cosa, G. Dissertori, M. Dittmar, M. Donegà, C. Dorfer, T. Gadek, T.A. Gómez Espinosa, C. Grab, D. Hits, W. Lustermann, A.-M. Lyon, R.A. Manzoni, M.T. Meinhard, F. Micheli, F. Nessi-Tedaldi, J. Niedziela, F. Pauss, V. Perovic, G. Perrin, S. Pigazzini, M.G. Ratti, M. Reichmann, C. Reissel, T. Reitenspiess, B. Ristic, D. Ruini, D.A. Sanz Becerra, M. Schönenberger, V. Stampf, J. Steggemann[64], M.L. Vesterbacka Olsson, R. Wallny, D.H. Zhu

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

C. Amsler[65], C. Botta, D. Brzhechko, M.F. Canelli, R. Del Burgo, J.K. Heikkilä, M. Huwiler, A. Jofrehei, B. Kilminster, S. Leontsinis, A. Macchiolo, P. Meiring, V.M. Mikuni, U. Molinatti, I. Neutelings, G. Rauco, A. Reimers, P. Robmann, K. Schweiger, Y. Takahashi

Universität Zürich, Zurich, Switzerland

C. Adloff[66], C.M. Kuo, W. Lin, A. Roy, T. Sarkar[38], S.S. Yu

National Central University, Chung-Li, Taiwan

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

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[67], Z.S. Demiroglu, F. Dolek, C. Dozen[68], I. Dumanoglu[69], E. Eskut, G. Gokbulut, Y. Guler, E. Gurpinar Guler[70], I. Hos[71], C. Isik, E.E. Kangal[72], O. Kara, A. Kayis Topaksu, U. Kiminsu, G. Onengut, K. Ozdemir[73], A. Polatoz, A.E. Simsek, B. Tali[74], U.G. Tok, S. Turkcapar, I.S. Zorbakir, C. Zorbilmez

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

B. Isildak[75], G. Karapinar[76], K. Ocalan[77], M. Yalvac[78]

Middle East Technical University, Physics Department, Ankara, Turkey

B. Akgun, I.O. Atakisi, E. Gülmez, M. Kaya[79], O. Kaya[80], Ö. Özçelik, S. Tekten[81], E.A. Yetkin[82]

Bogazici University, Istanbul, Turkey

A. Cakir, K. Cankocak[69], Y. Komurcu, S. Sen[83]

Istanbul Technical University, Istanbul, Turkey

F. Aydogmus Sen, S. Cerci[74], B. Kaynak, S. Ozkorucuklu, D. Sunar Cerci[74]

Istanbul University, Istanbul, Turkey

B. Grynyov

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

L. Levchuk

National Scientific Center, Kharkov Institute of Physics and Technology, Kharkov, Ukraine

E. Bhal, S. Bologna, J.J. Brooke, E. Clement, D. Cussans, H. Flacher, J. Goldstein, G.P. Heath, H.F. Heath, L. Kreczko, B. Krikler, S. Paramesvaran, T. Sakuma, S. Seif El Nasr-Storey, V.J. Smith, N. Stylianou[84], J. Taylor, A. Titterton

University of Bristol, Bristol, United Kingdom

K.W. Bell, A. Belyaev[85], C. Brew, R.M. Brown, D.J.A. Cockerill, K.V. Ellis, K. Harder, S. Harper, J. Linacre, K. Manolopoulos, D.M. Newbold, E. Olaiya, D. Petyt, T. Reis, T. Schuh, C.H. Shepherd-Themistocleous, A. Thea, I.R. Tomalin, T. Williams

Rutherford Appleton Laboratory, Didcot, United Kingdom

R. Bainbridge, P. Bloch, S. Bonomally, J. Borg, S. Breeze, O. Buchmuller, A. Bundock, V. Cepaitis, G.S. Chahal[86], D. Colling, P. Dauncey, G. Davies, M. Della Negra, G. Fedi, G. Hall, G. Iles, J. Langford, L. Lyons, A.-M. Magnan, S. Malik, A. Martelli, V. Milosevic, J. Nash[87], V. Palladino, M. Pesaresi, D.M. Raymond, A. Richards, A. Rose, E. Scott, C. Seez, A. Shtipliyski, M. Stoye, A. Tapper, K. Uchida, T. Virdee[22], N. Wardle, S.N. Webb, D. Winterbottom, A.G. Zecchinelli

Imperial College, London, United Kingdom

J.E. Cole, P.R. Hobson, A. Khan, P. Kyberd, C.K. Mackay, I.D. Reid, L. Teodorescu, S. Zahid

Brunel University, Uxbridge, United Kingdom

S. Abdullin, A. Brinkerhoff, K. Call, B. Caraway, J. Dittmann, K. Hatakeyama, A.R. Kanuganti, C. Madrid, B. McMaster, N. Pastika, S. Sawant, C. Smith, J. Wilson

Baylor University, Waco, USA

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

Catholic University of America, Washington, DC, USA

A. Buccilli, O. Charaf, S.I. Cooper, S.V. Gleyzer, C. Henderson, C.U. Perez, P. Rumerio, C. West

The University of Alabama, Tuscaloosa, USA

A. Akpinar, A. Albert, D. Arcaro, C. Cosby, Z. Demiragli, D. Gastler, J. Rohlf, K. Salyer, D. Sperka, D. Spitzbart, I. Suarez, S. Yuan, D. Zou

Boston University, Boston, USA

G. Benelli, B. Burkle, X. Coubez[23], D. Cutts, Y.t. Duh, M. Hadley, U. Heintz, J.M. Hogan[88], K.H.M. Kwok, E. Laird, G. Landsberg, K.T. Lau, J. Lee, M. Narain, S. Sagir[89], R. Syarif, E. Usai, W.Y. Wong, D. Yu, W. Zhang

Brown University, Providence, USA

R. Band, C. Brainerd, R. Breedon, M. Calderon De La Barca Sanchez, M. Chertok, J. Conway, R. Conway, P.T. Cox, R. Erbacher, C. Flores, G. Funk, F. Jensen, W. Ko[†], O. Kukral, R. Lander, M. Mulhearn, D. Pellett, J. Pilot, M. Shi, D. Taylor, K. Tos, M. Tripathi, Y. Yao, F. Zhang

University of California, Davis, Davis, USA

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

University of California, Los Angeles, USA

K. Burt, Y. Chen, R. Clare, J.W. Gary, G. Hanson, G. Karapostoli, O.R. Long, N. Manganelli, M. Olmedo Negrete, M.I. Paneva, W. Si, S. Wimpenny, Y. Zhang

University of California, Riverside, Riverside, USA

J.G. Branson, P. Chang, S. Cittolin, S. Cooperstein, N. Deelen, J. Duarte, R. Gerosa, D. Gilbert, V. Krutelyov, J. Letts, M. Masciovecchio, S. May, S. Padhi, M. Pieri, V. Sharma, M. Tadel, F. Würthwein, A. Yagil

University of California, San Diego, La Jolla, USA

N. Amin, C. Campagnari, M. Citron, A. Dorsett, V. Dutta, J. Incandela, B. Marsh, H. Mei, A. Ovcharova, H. Qu, M. Quinnan, J. Richman, U. Sarica, D. Stuart, S. Wang

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

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

California Institute of Technology, Pasadena, USA

J. Alison, M.B. Andrews, T. Ferguson, T. Mudholkar, M. Paulini, M. Sun, I. Vorobiev

Carnegie Mellon University, Pittsburgh, USA

J.P. Cumalat, W.T. Ford, E. MacDonald, T. Mulholland, R. Patel, A. Perloff, K. Stenson, K.A. Ulmer, S.R. Wagner

University of Colorado Boulder, Boulder, USA

J. Alexander, Y. Cheng, J. Chu, D.J. Cranshaw, A. Datta, A. Frankenthal, K. Mcdermott, J. Monroy, J.R. Patterson, D. Quach, A. Ryd, W. Sun, S.M. Tan, Z. Tao, J. Thom, P. Wittich, M. Zientek

Cornell University, Ithaca, USA

M. Albrow, M. Alyari, G. Apollinari, A. Apresyan, A. Apyan, S. Banerjee, L.A.T. Bauerdick, A. Beretvas, D. Berry, J. Berryhill, P.C. Bhat, K. Burkett, J.N. Butler, A. Canepa, G.B. Cerati, H.W.K. Cheung, F. Chlebana, M. Cremonesi, V.D. Elvira, J. Freeman, Z. Gecse, E. Gottschalk, L. Gray, D. Green, S. Grünendahl, O. Gutsche, R.M. Harris, S. Hasegawa, R. Heller, T.C. Herwig, J. Hirschauer, B. Jayatilaka, S. Jindariani, M. Johnson, U. Joshi, P. Klabbers, T. Klijnsma, B. Klima, M.J. Kortelainen, S. Lammel, D. Lincoln, R. Lipton, M. Liu, T. Liu, J. Lykken, K. Maeshima, D. Mason, P. McBride, P. Merkel, S. Mrenna, S. Nahn, V. O'Dell, V. Papadimitriou, K. Pedro, C. Pena[57], O. Prokofyev, F. Ravera, A. Reinsvold Hall, L. Ristori, B. Schneider, E. Sexton-Kennedy, N. Smith, A. Soha, W.J. Spalding, L. Spiegel, S. Stoynev, J. Strait, L. Taylor, S. Tkaczyk, N.V. Tran, L. Uplegger, E.W. Vaandering, H.A. Weber, A. Woodard

Fermi National Accelerator Laboratory, Batavia, USA

D. Acosta, P. Avery, D. Bourilkov, L. Cadamuro, V. Cherepanov, F. Errico, R.D. Field, D. Guerrero, B.M. Joshi, M. Kim, J. Konigsberg, A. Korytov, K.H. Lo, K. Matchev, N. Menendez, G. Mitselmakher, D. Rosenzweig, K. Shi, J. Sturdy, J. Wang, S. Wang, X. Zuo

University of Florida, Gainesville, USA

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

Florida State University, Tallahassee, USA

M.M. Baarmand, S. Butalla, T. Elkafrawy[90], M. Hohlmann, D. Noonan, M. Rahmani, M. Saunders, F. Yumiceva

Florida Institute of Technology, Melbourne, USA

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

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

M. Alhusseini, K. Dilsiz[91], S. Durgut, R.P. Gandrajula, M. Haytmyradov, V. Khristenko, O.K. Köseyan, J.-P. Merlo, A. Mestvirishvili[92], A. Moeller, J. Nachtman, H. Ogul[93], Y. Onel, F. Ozok[94], A. Penzo, C. Snyder, E. Tiras, J. Wetzel

The University of Iowa, Iowa City, USA

O. Amram, B. Blumenfeld, L. Corcodilos, M. Eminizer, A.V. Gritsan, S. Kyriacou, P. Maksimovic, C. Mantilla, J. Roskes, M. Swartz, T.Á. Vámi

Johns Hopkins University, Baltimore, USA

C. Baldenegro Barrera, P. Baringer, A. Bean, A. Bylinkin, T. Isidori, S. Khalil, J. King, G. Krintiras, A. Kropivnitskaya, C. Lindsey, N. Minafra, M. Murray, C. Rogan, C. Royon, S. Sanders, E. Schmitz, J.D. Tapia Takaki, Q. Wang, J. Williams, G. Wilson

The University of Kansas, Lawrence, USA

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

Kansas State University, Manhattan, USA

F. Rebassoo, D. Wright

Lawrence Livermore National Laboratory, Livermore, USA

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

University of Maryland, College Park, USA

D. Abercrombie, B. Allen, R. Bi, S. Brandt, W. Busza, I.A. Cali, Y. Chen, M. D'Alfonso, G. Gomez Ceballos, M. Goncharov, P. Harris, D. Hsu, M. Hu, M. Klute, D. Kovalskyi, J. Krupa, Y.-J. Lee, P.D. Luckey, B. Maier, A.C. Marini, C. Mcginn, C. Mironov, S. Narayanan, X. Niu, C. Paus, D. Rankin, C. Roland, G. Roland, Z. Shi, G.S.F. Stephans, K. Sumorok, K. Tatar, D. Velicanu, J. Wang, T.W. Wang, Z. Wang, B. Wyslouch

Massachusetts Institute of Technology, Cambridge, USA

R.M. Chatterjee, A. Evans, P. Hansen, J. Hiltbrand, Sh. Jain, M. Krohn, Y. Kubota, Z. Lesko, J. Mans, M. Revering, R. Rusack, R. Saradhy, N. Schroeder, N. Strobbe, M.A. Wadud

University of Minnesota, Minneapolis, USA

J.G. Acosta, S. Oliveros

University of Mississippi, Oxford, USA

K. Bloom, S. Chauhan, D.R. Claes, C. Fangmeier, L. Finco, F. Golf, J.R. González Fernández, C. Joo, I. Kravchenko, J.E. Siado, G.R. Snow[†], W. Tabb, F. Yan

University of Nebraska-Lincoln, Lincoln, USA

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

State University of New York at Buffalo, Buffalo, USA

G. Alverson, E. Barberis, C. Freer, Y. Haddad, A. Hortiangtham, J. Li, 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, USA

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

Northwestern University, Evanston, USA

R. Bucci, N. Dev, R. Goldouzian, M. Hildreth, K. Hurtado Anampa, C. Jessop, D.J. Karmgard, K. Lannon, N. Loukas, N. Marinelli, I. Mcalister, F. Meng, K. Mohrman, Y. Musienko[49], R. Ruchti, P. Siddireddy, S. Taroni, M. Wayne, A. Wightman, M. Wolf, L. Zygala

University of Notre Dame, Notre Dame, USA

J. Alimena, B. Bylsma, B. Cardwell, L.S. Durkin, B. Francis, C. Hill, A. Lefeld, B.L. Winer, B.R. Yates

The Ohio State University, Columbus, USA

B. Bonham, P. Das, G. Dezoort, P. Elmer, B. Greenberg, N. Haubrich, S. Higginbotham, A. Kalogeropoulos, G. Kopp, S. Kwan, D. Lange, M.T. Lucchini, J. Luo, D. Marlow, K. Mei, I. Ojalvo, J. Olsen, C. Palmer, P. Piroué, D. Stickland, C. Tully

Princeton University, Princeton, USA

S. Malik, S. Norberg

University of Puerto Rico, Mayaguez, USA

V.E. Barnes, R. Chawla, S. Das, L. Gutay, M. Jones, A.W. Jung, G. Negro, N. Neumeister, C.C. Peng, S. Piperov, A. Purohit, H. Qiu, J.F. Schulte, M. Stojanovic[18], N. Trevisani, F. Wang, A. Wildridge, R. Xiao, W. Xie

Purdue University, West Lafayette, USA

J. Dolen, N. Parashar

Purdue University Northwest, Hammond, USA

A. Baty, S. Dildick, K.M. Ecklund, S. Freed, F.J.M. Geurts, M. Kilpatrick, A. Kumar, W. Li, B.P. Padley, R. Redjimi, J. Roberts[†], J. Rorie, W. Shi, A.G. Stahl Leiton

Rice University, Houston, 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

University of Rochester, Rochester, USA

B. Chiarito, J.P. Chou, A. Gandrakota, Y. Gershtein, E. Halkiadakis, A. Hart, M. Heindl, E. Hughes, S. Kaplan, O. Karacheban[26], 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, USA

H. Acharya, A.G. Delannoy, S. Spanier

University of Tennessee, Knoxville, USA

O. Bouhali[95], M. Dalchenko, A. Delgado, R. Eusebi, J. Gilmore, T. Huang, T. Kamon[96], H. Kim, S. Luo, S. Malhotra, R. Mueller, D. Overton, L. Perniè, D. Rathjens, A. Safonov

Texas A&M University, College Station, USA

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

Texas Tech University, Lubbock, USA

E. Appelt, S. Greene, A. Gurrola, R. Janjam, W. Johns, C. Maguire, A. Melo, H. Ni, K. Padeken, F. Romeo, P. Sheldon, S. Tuo, J. Velkovska

Vanderbilt University, Nashville, USA

M.W. Arenton, B. Cox, G. Cummings, J. Hakala, R. Hirosky, M. Joyce, A. Ledovskoy, A. Li, C. Neu, B. Tannenwald, Y. Wang, E. Wolfe, F. Xia

University of Virginia, Charlottesville, USA

P.E. Karchin, N. Poudyal, P. Thapa

Wayne State University, Detroit, USA

K. Black, T. Bose, J. Buchanan, C. Caillol, S. Dasu, I. De Bruyn, P. Everaerts, C. Galloni, H. He, M. Herndon, A. Hervé, U. Hussain, A. Lanaro, A. Loeliger, R. Loveless, J. Madhusudanan Sreekala, A. Mallampalli, 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

[†] Deceased.
[1] Also at Vienna University of Technology, Vienna, Austria.
[2] Also at Institute of Basic and Applied Sciences, Faculty of Engineering, Arab Academy for Science, Technology and Maritime Transport, Alexandria, Egypt.
[3] Also at Université Libre de Bruxelles, Bruxelles, Belgium.
[4] Also at IRFU, CEA, Université Paris-Saclay, Gif-sur-Yvette, France.
[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 Universidade Federal de Pelotas, Pelotas, Brazil.
[9] Also at Nanjing Normal University Department of Physics, Nanjing, China.
[10] Now at The University of Iowa, Iowa City, USA.
[11] Also at University of Chinese Academy of Sciences, Beijing, China.
[12] Also at Institute for Theoretical and Experimental Physics named by A.I. Alikhanov of NRC ‘Kurchatov Institute’, Moscow, Russia.
[13] Also at Joint Institute for Nuclear Research, Dubna, Russia.
[14] Now at British University in Egypt, Cairo, Egypt.
[15] Now at Cairo University, Cairo, Egypt.
[16] Also at Zewail City of Science and Technology, Zewail, Egypt.
[17] Now at Fayoum University, El-Fayoum, Egypt.
[18] Also at Purdue University, West Lafayette, USA.
[19] Also at Université de Haute Alsace, Mulhouse, France.
[20] Also at Ilia State University, Tbilisi, Georgia.
[21] Also at Erzincan Binali Yildirim University, Erzincan, Turkey.
[22] Also at CERN, European Organization for Nuclear Research, Geneva, Switzerland.
[23] Also at RWTH Aachen University, III. Physikalisches Institut A, Aachen, Germany.
[24] Also at University of Hamburg, Hamburg, Germany.
[25] Also at Department of Physics, Isfahan University of Technology, Isfahan, Iran.
[26] Also at Brandenburg University of Technology, Cottbus, Germany.
[27] Also at Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow, Russia.
[28] Also at Institute of Physics, University of Debrecen, Debrecen, Hungary.
[29] Also at Physics Department, Faculty of Science, Assiut University, Assiut, Egypt.
[30] Also at Eszterhazy Karoly University, Karoly Robert Campus, Gyongyos, Hungary.
[31] Also at Institute of Nuclear Research ATOMKI, Debrecen, Hungary.
[32] Also at Wigner Research Centre for Physics, Budapest, Hungary.
[33] Also at IIT Bhubaneswar, Bhubaneswar, India.
[34] Also at Institute of Physics, Bhubaneswar, India.
[35] Also at G.H.G. Khalsa College, Punjab, India.
[36] Also at Shoolini University, Solan, India.
[37] Also at University of Hyderabad, Hyderabad, India.

[38] Also at University of Visva-Bharati, Santiniketan, India.
[39] Also at Indian Institute of Technology (IIT), Mumbai, India.
[40] Also at Deutsches Elektronen-Synchrotron, Hamburg, Germany.
[41] Also at Sharif University of Technology, Tehran, Iran.
[42] Also at Department of Physics, University of Science and Technology of Mazandaran, Behshahr, Iran.
[43] Now at INFN Sezione di Bari [a], Università di Bari [b], Politecnico di Bari [c], Bari, Italy.
[44] Also at Italian National Agency for New Technologies, Energy and Sustainable Economic Development, Bologna, Italy.
[45] Also at Centro Siciliano di Fisica Nucleare e di Struttura Della Materia, Catania, Italy.
[46] Also at Università di Napoli 'Federico II', Napoli, Italy.
[47] Also at Riga Technical University, Riga, Latvia.
[48] Also at Consejo Nacional de Ciencia y Tecnología, Mexico City, Mexico.
[49] Also at Institute for Nuclear Research, Moscow, Russia.
[50] Now at National Research Nuclear University 'Moscow Engineering Physics Institute' (MEPhI), Moscow, Russia.
[51] Also at Institute of Nuclear Physics of the Uzbekistan Academy of Sciences, Tashkent, Uzbekistan.
[52] Also at St. Petersburg State Polytechnical University, St. Petersburg, Russia.
[53] Also at University of Florida, Gainesville, USA.
[54] Also at Imperial College, London, United Kingdom.
[55] Also at P.N. Lebedev Physical Institute, Moscow, Russia.
[56] Also at Moscow Institute of Physics and Technology, Moscow, Russia.
[57] Also at California Institute of Technology, Pasadena, USA.
[58] Also at Budker Institute of Nuclear Physics, Novosibirsk, Russia.
[59] Also at Faculty of Physics, University of Belgrade, Belgrade, Serbia.
[60] Also at Trincomalee Campus, Eastern University, Sri Lanka, Nilaveli, Sri Lanka.
[61] Also at INFN Sezione di Pavia [a], Università di Pavia [b], Pavia, Italy.
[62] Also at National and Kapodistrian University of Athens, Athens, Greece.
[63] Also at Universität Zürich, Zurich, Switzerland.
[64] Also at Ecole Polytechnique Fédérale Lausanne, Lausanne, Switzerland.
[65] Also at Stefan Meyer Institute for Subatomic Physics, Vienna, Austria, Vienna, Austria.
[66] Also at Laboratoire d'Annecy-le-Vieux de Physique des Particules, IN2P3-CNRS, Annecy-le-Vieux, France.
[67] Also at Şırnak University, Sirnak, Turkey.
[68] Also at Department of Physics, Tsinghua University, Beijing, China.
[69] Also at Near East University, Research Center of Experimental Health Science, Nicosia, Turkey.
[70] Also at Beykent University, Istanbul, Turkey.
[71] Also at Istanbul Aydin University, Application and Research Center for Advanced Studies (App. & Res. Cent. for Advanced Studies), Istanbul, Turkey.
[72] Also at Mersin University, Mersin, Turkey.
[73] Also at Piri Reis University, Istanbul, Turkey.
[74] Also at Adiyaman University, Adiyaman, Turkey.
[75] Also at Ozyegin University, Istanbul, Turkey.
[76] Also at Izmir Institute of Technology, Izmir, Turkey.
[77] Also at Necmettin Erbakan University, Konya, Turkey.
[78] Also at Bozok Universitetesi Rektörlügü, Yozgat, Turkey.
[79] Also at Marmara University, Istanbul, Turkey.
[80] Also at Milli Savunma University, Istanbul, Turkey.
[81] Also at Kafkas University, Kars, Turkey.
[82] Also at Istanbul Bilgi University, Istanbul, Turkey.
[83] Also at Hacettepe University, Ankara, Turkey.
[84] Also at Vrije Universiteit Brussel, Brussel, Belgium.
[85] Also at School of Physics and Astronomy, University of Southampton, Southampton, United Kingdom.
[86] Also at IPPP Durham University, Durham, United Kingdom.
[87] Also at Monash University, Faculty of Science, Clayton, Australia.
[88] Also at Bethel University, St. Paul, Minneapolis, USA, St. Paul, USA.
[89] Also at Karamanoğlu Mehmetbey University, Karaman, Turkey.
[90] Also at Ain Shams University, Cairo, Egypt.
[91] Also at Bingol University, Bingol, Turkey.
[92] Also at Georgian Technical University, Tbilisi, Georgia.
[93] Also at Sinop University, Sinop, Turkey.
[94] Also at Mimar Sinan University, Istanbul, Istanbul, Turkey.
[95] Also at Texas A&M University at Qatar, Doha, Qatar.
[96] Also at Kyungpook National University, Daegu, Republic of Korea.