Studies of Charm Quark Diffusion inside Jets Using Pb-Pb and pp Collisions at $\sqrt{s_{NN}} = 5.02$ TeV

A. M. Sirunyan et al.*
(CMS Collaboration)

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The first study of charm quark diffusion with respect to the jet axis in heavy ion collisions is presented. The measurement is performed using jets with $p_T^{jet} > 60$ GeV/c and D^0 mesons with $p_T^D > 4$ GeV/c in lead-lead (Pb-Pb) and proton-proton (pp) collisions at a nucleon-nucleon center-of-mass energy of $\sqrt{s_{NN}} = 5.02$ TeV, recorded by the CMS detector at the LHC. The radial distribution of D^0 mesons with respect to the jet axis is sensitive to the production mechanisms of the meson, as well as to the energy loss and diffusion processes undergone by its parent parton inside the strongly interacting medium produced in Pb-Pb collisions. When compared to Monte Carlo event generators, the radial distribution in pp collisions is found to be well described by PYTHIA, while the slope of the distribution predicted by POWHEG+PYTHIA is steeper than that of the data. In Pb-Pb collisions, compared to the pp results, the D^0 meson distribution for $4 < p_T^D < 20$ GeV/c hints at a larger distance on average with respect to the jet axis, reflecting a diffusion of charm quarks in the medium created in heavy ion collisions. At higher p_T^D, the Pb-Pb and pp radial distributions are found to be similar.

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The quark gluon plasma (QGP), the deconfined matter created in collisions of heavy ions accelerated to ultra-relativistic energies [1,2], can be probed by studying the remnants of hard scatterings occurring in this medium. The outgoing partons (quarks and gluons), which produce final-state jets of particles, interact strongly with the QGP and lose energy [3–5], a phenomenon known as jet quenching, as observed at the BNL Relativistic Heavy Ion Collider (RHIC) [6,7] and the CERN LHC [8–10]. Jet quenching results in modifications of the energy and structure of jets observed in heavy ion collisions, compared to proton-proton (pp) collisions. One of the most striking features of jet quenching is the enhanced production of low transverse momentum hadrons ($p_T \approx 2$–5 GeV/c) at large angles with respect to the final-state jet axis. This phenomenon manifests itself in the form of modifications of the jet fragmentation function [11–13], as well as the jet radial profile and the energy flow [14–17]. Interpretations of experimental results include medium-induced gluon radiation, modification of jet splitting functions, and medium response to the hard scattered partons [4,5,18–20].

Studying heavy flavor (HF) mesons in jets should give further insight into the origin of the observed modifications for light flavored particles [21] and can provide new information about HF jet fragmentation in both pp and lead-lead (Pb-Pb) collisions. Moreover, measurements of angular correlations between HF mesons and jets can be used to constrain parton energy loss mechanisms and to better understand the heavy quark diffusion (i.e., propagation) inside the medium [21–25]. This is complementary information to that obtained with measurements of inclusive HF meson spectra [26–30], HF meson azimuthal anisotropy [30–34], and HF-tagged jets [35,36].

In this Letter, the first measurements of the radial distributions of D^0 mesons in jets from the same parton scattering are presented, for two D^0 meson p_T intervals: a low-p_T interval $4 < p_T^D < 20$ GeV/c, and a high-p_T one, $p_T^D > 20$ GeV/c. The D^0 mesons are measured via their hadronic decay channels $D^0 \to K^-\pi^+$ and $D^0 \to K^+\pi^-$ with the CMS detector at the LHC. The observable is the normalized radial distribution of the D^0 meson with respect to the jet axis, defined as

$$\frac{1}{N_{jD}}\frac{dN_{jD}}{dr} = \frac{1}{N_{jD}}\frac{N_{jD}\,j_{\Delta r}}{\Delta r}; \qquad (1)$$

where the distance from the jet axis, $r = \sqrt{(\Delta\phi_{jD})^2 + (\Delta\eta_{jD})^2}$, is defined as the quadratic sum of the differences in pseudorapidity ($\Delta\eta_{jD}$) and azimuth ($\Delta\phi_{jD}$) of the D^0 meson with respect to the jet axis, and Δr is the width of the r interval. The quantity $j_{\Delta r}$ is the number of D^0 mesons in the Δr interval, and N_{jD} is the

*Full author list given at the end of the article.

integral of the distribution in the r region from 0 to 0.3, the distance parameter used for the jet reconstruction.

The main feature of the CMS detector [37] is a superconducting solenoid providing a magnetic field of 3.8 T. Within the solenoid volume is a silicon pixel and strip tracker, which is used to detect charged particles, a lead tungstate crystal electromagnetic calorimeter, and a brass and scintillator hadron calorimeter, each composed of a barrel and two end cap sections. Hadron forward calorimeters extend the coverage up to $|\eta| = 5.2$ and are used for collision event selection. Muons are detected in gas-ionization chambers embedded in the steel flux-return yoke outside the solenoid.

The pp (Pb-Pb) dataset used in this analysis corresponds to an integrated luminosity of 27.4 pb^{-1} (404 μb^{-1}). High-p_T jet events were selected by a high-level trigger algorithm [38] with a p_T^{jet} threshold of 60 GeV/c. For the off-line analysis, events must pass a set of selection criteria designed to reject beam-gas collisions and beam scraping events [39,40]. The Pb-Pb results are reported for the inclusive sample: no selection on centrality (i.e., the degree of overlap of the two colliding nuclei) is made.

Several Monte Carlo (MC) simulated event samples are used to evaluate the background contributions, signal efficiencies, and detector acceptance corrections. The simulated events include both prompt (produced directly from the c quark fragmentation) and nonprompt (from b hadron decays) D^0 meson events. The pp collisions are generated using PYTHIA v.8.212 [41], tune CUETP8M1 [42]. The EvtGen 1.3.0 [43] generator is used to simulate D^0 meson and b hadron decays, and final-state photon radiation in the D^0 meson decays is simulated with PHOTOS2.0 [44]. For the Pb-Pb MC samples, each PYTHIA event is embedded into a Pb-Pb collision event generated with HYDJET 1.9 [45], which is tuned to reproduce global event properties. The MC events are propagated through the CMS detector using the GEANT4 package [46].

The particle-flow (PF) algorithm [47] is used to reconstruct and identify each individual particle in a pp or Pb-Pb event. To form jets, the PF particles are clustered using an anti-k_T algorithm provided by the FastJet framework [48,49] with a distance parameter of 0.3. In order to subtract the underlying event (UE) background in Pb-Pb collisions [9,50], an iterative algorithm [51] is employed. In pp collisions, jets are reconstructed without UE subtraction. The jet energy corrections are derived from simulation, separately for pp and Pb-Pb data, and are confirmed via energy-balance methods applied to dijet, multijet, photon + jet, and leptonically decaying Z + jet events in pp data [52]. Jets with $|\eta^{\text{jet}}| < 1.6$ and corrected $p_T^{\text{jet}} > 60$ GeV/c are selected for this analysis.

The D^0 candidates are reconstructed by combining pairs of oppositely charged particle tracks with an invariant mass within 0.2 GeV/c^2 of the world-average D^0 meson mass, 1.8 GeV/c^2 [53]. They are reconstructed independently from the PF jets, which do use the same track collection. In order to suppress the combinatorial background, each track is required to have $p_T > 2$ GeV/c, to be within $|\eta| < 2$, and pass a set of quality selections [39]. For each pair of selected tracks, two D^0 candidates are created by assuming that one of the particles has the mass of the pion, while the other has the mass of the kaon, and vice versa. The D^0 candidates are required to have rapidity $|y| < 2$ and $p_T^D > 4$ GeV/c. They are further paired with every selected jet in the same event and have their invariant mass distributions recorded in two p_T^D bins, $4 < p_T^D < 20$ and $p_T^D > 20$ GeV/c, and four r bins, 0–0.05, 0.05–0.1, 0.1–0.3, and 0.3–0.5. In order to reduce further the combinatorial background, the D^0 candidates are required to pass three additional topological selections. The three-dimensional (3D) decay length (distance between the primary vertex and D^0 secondary vertex L_{3D}) normalized to its uncertainty is required to be larger than 2.34–4.00. The pointing angle θ_p (defined as the angle between the total momentum vector of the D^0 candidate and the vector connecting the primary and secondary vertices) is required to be smaller than 0.020–0.046 rad. In both cases (the 3D decay length and θ_p), the selection criteria depend on the p_T^D and r bins and are optimized separately for the pp and Pb-Pb data. The selection is optimized using a multivariate technique [54] in order to maximize the statistical significance of the D^0 meson signals. Tighter selections are found for the low-p_T^D bin, with increasing or decreasing r values, for θ_p and the 3D decay length significance, respectively. Finally, the χ^2 probability of the secondary vertex fit is required to be larger than 5%. These selections ensure a prompt D^0 meson fraction larger than 80% in both p_T^D bins of this analysis.

The D^0 meson yield in each p_T and r interval is extracted with a binned maximum likelihood fit to the invariant mass distributions in the range $1.7 < m_{\pi K} < 2.0$ GeV/c^2. The combinatorial background originating from random pairs of tracks not produced by a D^0 meson decay is modeled by a third-order polynomial. The signal shape is found to be best modeled by the sum of two Gaussian functions with the same mean but different widths. The two Gaussians are found to best capture the many contributions to the D^0 peak resolution from tracks with a highly η-dependent p_T resolution. The common mean of the Gaussian functions, the D^0 yield, and all the background parameters are free parameters in the fit. An additional Gaussian function with a larger width is used to describe the invariant mass shape of D^0 candidates with an incorrect mass assignment from the exchange of the pion and kaon designations. The widths of the Gaussian functions that describe the D^0 signal shape and the shape of the D^0 candidates with swapped mass assignments are fixed by simulation, after correcting for the difference in resolution between data and MC simulations.

The ratio between the numbers of the signal D^0 candidates and the ones with swapped mass assignments is fixed to the value extracted from simulation. No significant variation with r was observed for the shape of the combinatorial background or in the mean and in the root mean square of the distributions of signal D^0 mesons or $\bar{D}^0$ candidates with swapped mass. Two examples of D^0 candidate invariant mass distributions, for pp and Pb-Pb collisions, are available in the Supplemental Material [55].

The raw D^0 radial distributions undergo several corrections, all calculated in bins of p_T^D and r. First, the D^0 meson yields are corrected for detector acceptance and for trigger, track reconstruction, and selection inefficiencies. The correction factors are obtained from a PYTHIA (PYTHIA +HYDJET) MC sample for the pp (Pb-Pb) analysis. Second, the background contribution from combining a D^0 meson with either a jet not coming from the same hard scattering, or with a misreconstructed jet is subtracted using an event mixing technique, in which the background is estimated by combining the distributions of D^0-jet pairs formed with (i) jets from the signal event and D^0 mesons from minimum bias (MB) events [39], (ii) jets from MB events with D^0 mesons from the signal event, and (iii) jets and D^0 mesons from MB events. In this procedure, each signal event is mixed with a MB event, which has a similar primary vertex position, amount of energy deposited in the forward hadronic calorimeters, and event plane angle [56]. The resulting background radial distributions, which are in all cases less than 10%, are then subtracted from the raw D^0 radial distributions measured in the signal event. Finally, the background-subtracted radial distribution is corrected for jet resolution effects, using PYTHIA+HYDJET and PYTHIA simulations, for the Pb-Pb and pp results, respectively. The correction was calculated as the ratio between the radial distributions after and before smearing the generated p_T^{jet} by the energy and angular resolution corrections.

Several sources of systematic uncertainty are considered for the D^0 meson yield extraction and the jet reconstruction, and are studied in bins of p_T^D and r. The uncertainty in the raw yield extraction (2.6%–5.4% for pp and 1.4%–8.2% for Pb-Pb data) is evaluated by repeating the fit procedure using different background and signal fit functions and by varying the widths of the Gaussian functions that describe the D^0 signal according to the differences (up to 20%, as observed for the most forward region) between data and simulation. In the signal variation study, the sum of three Gaussian functions with the same mean but different widths is considered, while in the background variation study, a second-order polynomial function is used. This functional form gives a good description of the combinatorial background according to studies performed on same-sign pairs, which provide a pure combinatorial background with the same kinematic conditions. In these studies, the secondary vertex candidates are obtained by combining two same-sign tracks, which are assigned pion and kaon masses. The systematic uncertainty from the selection of the D^0 meson candidates (3.6% and 0.5% for the low- and high-p_T^D bin, respectively, for pp, and 3.5% and 2.7% for Pb-Pb data) is estimated by considering the differences in the D^0 kinematic variables between simulation and data when applying each of the D^0 candidate selection variables. The study is performed by varying one selection at a time and by considering the maximum relative discrepancies in the yield between data and simulation. The total uncertainty is the quadratic sum of the maximum relative discrepancy obtained by varying each of the three topological selection variables separately.

The systematic uncertainties for the jets include components for the uncertainty in the jet energy scale (JES) and jet energy resolution (JER). The systematic uncertainty pertaining to the JES is estimated by varying the p_T^{jet} by 2.8% (in both pp and Pb-Pb data), which represents the sum in quadrature of the observed data-to-simulation differences (2%) and the nonclosure (i.e., deviation from unity) in simulation, when comparing reconstructed (detector-level) versus truth (generator-level) jets smeared by the known detector and reconstruction effects. An additional uncertainty 1.8%–42% for Pb-Pb data is added to account for the different detector response to quark versus gluon jets, since in Pb-Pb events, as opposed to pp events, the quark- vs gluon-initiated jet composition is not known because of the energy loss in the medium. The largest variation is observed at high p_T^D and largest r value, a region influenced by the small sample size. The assigned uncertainty represents the maximum difference from the nominal results when applying JES corrections obtained with a pure-gluon sample or a pure-quark sample.

The systematic uncertainty due to the JER in Pb-Pb collisions is estimated by varying the p_T^{jet} energy resolution by 15% to account for an imperfect description of the fluctuations of the UE in the MC simulation. The variation considered is estimated by studying the effects of these fluctuations using two different methods: the random-cone technique [52,57] and by embedding signal PYTHIA dijet events into background HYDJET samples. The random cone method consists of reconstructing many jets in a zero bias event, clustering particles in randomly placed cones in the entire (η, ϕ) space. When the method is applied in events with negligible contribution from hard scatterings, as is the case for zero bias events, the standard deviation of the distribution of p_T^{jet} obtained with this procedure can be used to estimate the magnitude of the UE fluctuations. The relative variations in the D^0 spectra are 0.3%–3.0% in pp and 0.6%–5.6% in Pb-Pb collisions. The systematic uncertainties from the trigger efficiency correction are estimated by the difference between the result with no correction and the nominal result, which are 0.3%–2.7% in pp and 0.7%–15% in Pb-Pb data. Finally, a remaining nonclosure observed in MC simulations between generated and

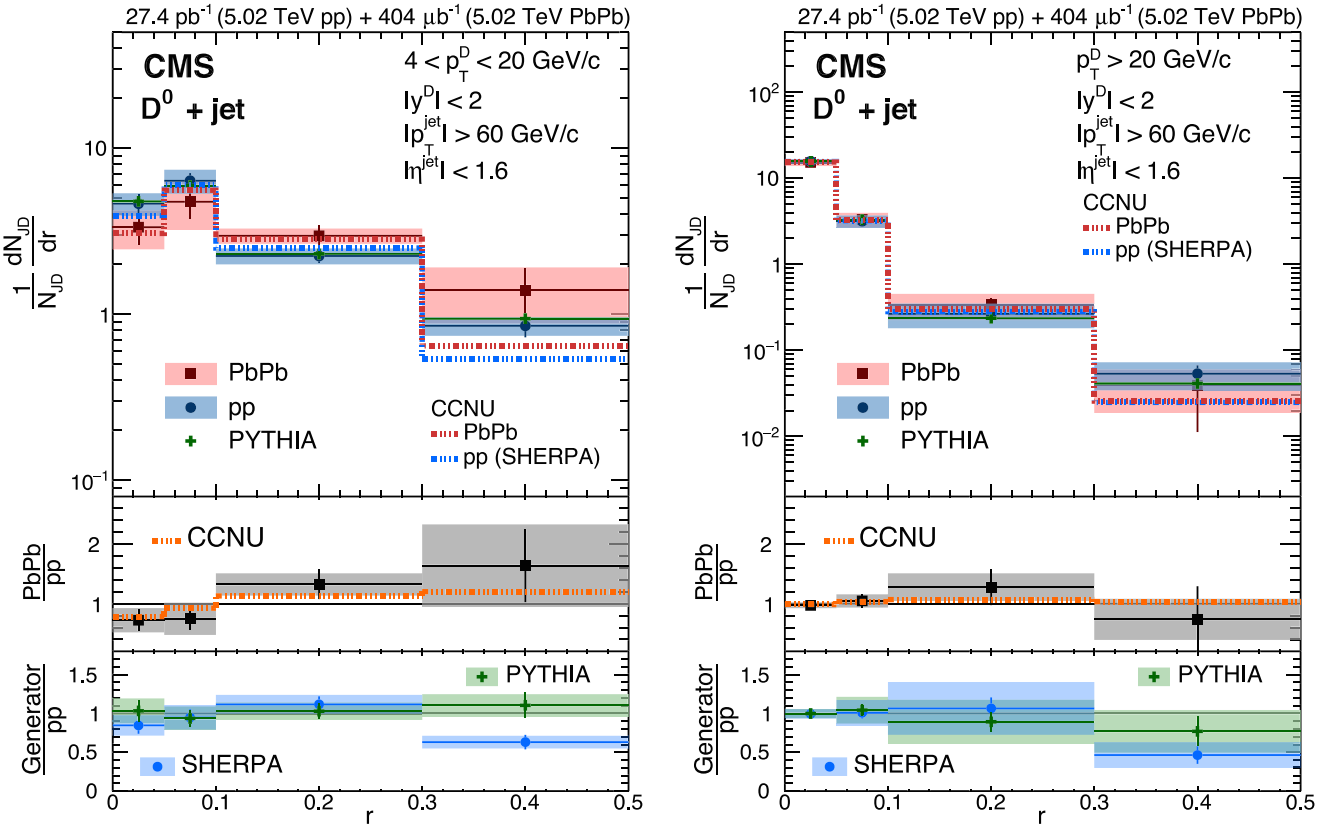

FIG. 1. Distributions of D^0 mesons in jets, as a function of the distance from the jet axis (r) for jets with $p_T^{jet} > 60$ GeV/c and $|\eta^{jet}| < 1.6$ measured in pp and Pb-Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV. The measurement is performed in the p_T^D range 4–20 GeV/c (left) and $p_T^D > 20$ GeV/c (right). Each spectrum is normalized to its integral in the region $0 < r < 0.3$. The vertical bars (boxes) correspond to statistical (systematic) uncertainties. The Pb-Pb spectra are compared to the CCNU energy loss model [21], while the pp spectra are compared with predictions from the PYTHIA and SHERPA pp MC event generators. The ratios of the D^0 meson radial distributions in Pb-Pb and pp data are shown in the middle panels. In the bottom panels, the ratios of these radial distributions of pp over the two MC event generators are presented.

reconstructed distributions of D^0 mesons in jets, is corrected bin by bin. The magnitude of the correction is quoted as the systematic uncertainty in the resolution unfolding, which varies in the range 1.3%–31% in pp and 0.7%–32% in Pb-Pb data.

The top panels of Fig. 1 show the measured D^0 meson radial distributions in pp and Pb-Pb collisions. The calculated $\langle r \rangle$ for the Pb-Pb (pp) distributions is $0.198 \pm 0.015(\text{stat}) \pm 0.005(\text{syst})$ [$0.160 \pm 0.007(\text{stat}) \pm 0.009(\text{syst})$] and $0.048 \pm 0.002(\text{stat}) \pm 0.004(\text{syst})$ [$0.046 \pm 0.001(\text{stat}) \pm 0.003(\text{syst})$], for the low- and high-p_T^D intervals, respectively. This result indicates that D^0 mesons at low p_T are farther away from the jet axis in Pb-Pb compared to pp collisions. At high p_T^D, the measured spectra in pp and Pb-Pb collisions fall rapidly, at a similar rate, as a function of r, similar to what was observed in inclusive jet-hadron correlation functions [16].

The pp results are compared to calculations from two pp MC event generators: PYTHIA [41], a leading-order matrix element event generator, and SHERPA [58], which computes the next-to-leading QCD matrix elements matched to parton shower to generate the charm-jet events [21]. For low-p_T D^0 mesons, the measured spectrum in pp collisions reaches a maximum at $0.05 < r < 0.1$, consistent with both PYTHIA and SHERPA [21]. In the $r > 0.3$ region, however, PYTHIA captures the features of the data better than SHERPA, which underpredicts the pp spectrum, in both p_T^D intervals. The Pb-Pb spectra is compared to an energy loss model, CCNU [21], which uses SHERPA for simulating the pp baseline. The CCNU calculation includes in-medium elastic (collisional) and inelastic (radiative) interactions for both the heavy and the light quarks. This model, which predicts a small depletion (increase) of the D^0 meson yield at small (large) r compared to pp collisions, is consistent with data.

To measure the medium modification of the radial profile, the ratio of Pb-Pb to pp spectra is also presented in the first subpanel of Fig. 1. In this ratio, the uncertainties from JES, JER, and D^0 candidate selections are considered uncorrelated between pp and Pb-Pb datasets and are not canceled in the ratio. The uncertainties from the modeling of the signal shape, as well as the nonclosures observed, are

partially canceled: the systematic uncertainties are reestimated directly on the ratio of the Pb-Pb to pp yields. The ratio increases slightly as a function of r at low p_T^D, corresponding to a small shift of the D^0 mesons to larger radii in Pb-Pb, while the ratio is consistent with unity within the uncertainties at high p_T^D. This shows that the modification of the radial profile of high p_T^D is small. These features of the ratios at low and high p_T^D are qualitatively different from inclusive charged particle radial distributions with respect to the jet axis measured in similar transverse momentum ranges [16]. The inclusive measurements show a ratio significantly smaller than 1, corresponding to a shift of the light quark mesons to smaller radii in Pb-Pb for all tracks with $p_T > 4$ GeV/c measured in jets with $p_T^{\text{jet}} > 120$ GeV, for $r > 0.1$ and more central Pb-Pb collisions. The CCNU model gives a good description of the ratio of Pb-Pb to pp spectra. Although this ratio is less sensitive to the choice of pp reference spectra, the pp measurements presented in this Letter could improve the description of the pp baseline.

In summary, this Letter presents the first measurement of the radial distributions of D^0 mesons with respect to the jet axis in Pb-Pb and pp collisions, performed with the CMS detector using jets with transverse momentum $p_T^{\text{jet}} > 60$ GeV/c and D^0 mesons with $p_T^D > 4$ GeV/c. When compared to the results of Monte Carlo event generators, the radial distribution in pp collisions is found to be well described by PYTHIA, while the slope of the distribution predicted by SHERPA is steeper than that of the data. The modification of the D^0 meson radial distributions in Pb-Pb collisions are studied by comparing them to those from pp collisions. The comparisons hint at a modification of the D^0 meson radial profile in Pb-Pb collisions at low p_T^D that vanishes at higher p_T^D. The results show that this modification is different from that of the light flavor hadrons. This measurement provides new experimental constraints on the mechanisms of heavy flavor production in pp collisions, as well as on the processes affecting the heavy quark propagation inside the quark-gluon plasma.

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Zou,[137] G. Benelli,[138] X. Coubez,[138] D. Cutts,[138] M. Hadley,[138] J. Hakala,[138] U. Heintz,[138] J. M. Hogan,[138,lll] K. H. M. Kwok,[138] E. Laird,[138] G. Landsberg,[138] J. Lee,[138] Z. Mao,[138] M. Narain,[138] S. Sagir,[138,mmm] R. Syarif,[138] E. Usai,[138] D. Yu,[138] R. Band,[139] C. Brainerd,[139] R. Breedon,[139] D. Burns,[139] M. Calderon De La Barca Sanchez,[139] M. Chertok,[139] J. Conway,[139] R. Conway,[139] P. T. Cox,[139] R. Erbacher,[139] C. Flores,[139] G. Funk,[139] W. Ko,[139] O. Kukral,[139] R. Lander,[139] M. Mulhearn,[139] D. Pellett,[139] J. Pilot,[139] S. Shalhout,[139] M. Shi,[139] D. Stolp,[139] D. Taylor,[139] K. Tos,[139] M. Tripathi,[139] Z. Wang,[139] F. Zhang,[139] M. Bachtis,[140] C. Bravo,[140] R. Cousins,[140] A. Dasgupta,[140] A. Florent,[140] J. Hauser,[140] M. Ignatenko,[140] N. Mccoll,[140] S. Regnard,[140] D. Saltzberg,[140] C. Schnaible,[140] V. Valuev,[140] E. Bouvier,[141] K. Burt,[141] R. Clare,[141] J. W.Gary,[141] S. M. A. Ghiasi Shirazi,[141] G. Hanson,[141] G. Karapostoli,[141] E. Kennedy,[141] F. Lacroix,[141] O. R. Long,[141] M. Olmedo Negrete,[141] M. I. Paneva,[141] W. Si,[141] L. Wang,[141] H. Wei,[141] S. Wimpenny,[141] B. R. Yates,[141] J. G.Branson,[142] P. Chang,[142] S. Cittolin,[142] M. Derdzinski,[142] R. Gerosa,[142] D. Gilbert,[142] B. Hashemi,[142] A. Holzner,[142] D. Klein,[142] G. Kole,[142] V. Krutelyov,[142] J. Letts,[142] M. Masciovecchio,[142] D. Olivito,[142] S. Padhi,[142] M. Pieri,[142] M. Sani,[142] V. Sharma,[142] S. Simon,[142] M. Tadel,[142] A. Vartak,[142] S. Wasserbaech,[142,nnn] J. Wood,[142] F. Würthwein,[142] A. Yagil,[142] G. Zevi Della Porta,[142] N. Amin,[143] R. Bhandari,[143] J. Bradmiller-Feld,[143] C. Campagnari,[143] M. Citron,[143] A. Dishaw,[143] V. Dutta,[143] M. Franco Sevilla,[143] L. Gouskos,[143] R. Heller,[143] J. Incandela,[143] A. Ovcharova,[143] H. Qu,[143] J. Richman,[143] D. Stuart,[143] I. Suarez,[143] S. Wang,[143] J. Yoo,[143] D. Anderson,[144] A. Bornheim,[144] J. M. Lawhorn,[144] H. B. Newman,[144] T. Q. Nguyen,[144] M. Spiropulu,[144] J. R. Vlimant,[144] R. Wilkinson,[144] S. Xie,[144] Z. Zhang,[144] R. Y. Zhu,[144] M. B. Andrews,[145] T. Ferguson,[145] T. Mudholkar,[145] M. Paulini,[145] M. Sun,[145] I. Vorobiev,[145] M. Weinberg,[145] J. P.Cumalat,[146] W. T. Ford,[146] F. Jensen,[146] A. Johnson,[146] M. Krohn,[146] E. MacDonald,[146] T. Mulholland,[146] R. Patel,[146] A. Perloff,[146] K. Stenson,[146] K. A. Ulmer,[146] S. R. Wagner,[146] J. Alexander,[147] J. Chaves,[147] Y. Cheng,[147] J. Chu,[147] A. Datta,[147] K. Mcdermott,[147] N. Mirman,[147] J. R. Patterson,[147]

D. Quach,[147] A. Rinkevicius,[147] A. Ryd,[147] L. Skinnari,[147] L. Soffi,[147] S. M. Tan,[147] Z. Tao,[147] J. Thom,[147] J. Tucker,[147] P. Wittich,[147] M. Zientek,[147] S. Abdullin,[148] M. Albrow,[148] M. Alyari,[148] G. Apollinari,[148] A. Apresyan,[148] A. Apyan,[148] S. Banerjee,[148] L. A. T. Bauerdick,[148] A. Beretvas,[148] J. Berryhill,[148] P. C. Bhat,[148] K. Burkett,[148] J. N. Butler,[148] A. Canepa,[148] G. B. Cerati,[148] H. W. K. Cheung,[148] F. Chlebana,[148] M. Cremonesi,[148] J. Duarte,[148] V. D. Elvira,[148] J. Freeman,[148] Z. Gecse,[148] E. Gottschalk,[148] L. Gray,[148] D. Green,[148] S. Grünendahl,[148] O. Gutsche,[148] J. Hanlon,[148] R. M. Harris,[148] S. Hasegawa,[148] J. Hirschauer,[148] Z. Hu,[148] B. Jayatilaka,[148] S. Jindariani,[148] M. Johnson,[148] U. Joshi,[148] B. Klima,[148] M. J. Kortelainen,[148] B. Kreis,[148] S. Lammel,[148] D. Lincoln,[148] R. Lipton,[148] M. Liu,[148] T. Liu,[148] J. Lykken,[148] K. Maeshima,[148] J. M. Marraffino,[148] D. Mason,[148] P. McBride,[148] P. Merkel,[148] S. Mrenna,[148] S. Nahn,[148] V. O'Dell,[148] K. Pedro,[148] C. Pena,[148] O. Prokofyev,[148] G. Rakness,[148] L. Ristori,[148] A. Savoy-Navarro,[148,ooo] B. Schneider,[148] E. Sexton-Kennedy,[148] A. Soha,[148] W. J. Spalding,[148] L. Spiegel,[148] S. Stoynev,[148] J. Strait,[148] N. Strobbe,[148] L. Taylor,[148] S. Tkaczyk,[148] N. V. Tran,[148] L. Uplegger,[148] E. W. Vaandering,[148] C. Vernieri,[148] M. Verzocchi,[148] R. Vidal,[148] M. Wang,[148] H. A. Weber,[148] A. Whitbeck,[148] D. Acosta,[149] P. Avery,[149] P. Bortignon,[149] D. Bourilkov,[149] A. Brinkerhoff,[149] L. Cadamuro,[149] A. Carnes,[149] M. Carver,[149] D. Curry,[149] R. D. Field,[149] S. V. Gleyzer,[149] B. M. Joshi,[149] J. Konigsberg,[149] A. Korytov,[149] K. H. Lo,[149] P. Ma,[149] K. Matchev,[149] H. Mei,[149] G. Mitselmakher,[149] D. Rosenzweig,[149] K. Shi,[149] D. Sperka,[149] J. Wang,[149] S. Wang,[149] X. Zuo,[149] Y. R. Joshi,[150] S. Linn,[150] A. Ackert,[151] T. Adams,[151] A. Askew,[151] S. Hagopian,[151] V. Hagopian,[151] K. F. Johnson,[151] T. Kolberg,[151] G. Martinez,[151] T. Perry,[151] H. Prosper,[151] A. Saha,[151] C. Schiber,[151] R. Yohay,[151] M. M. Baarmand,[152] V. Bhopatkar,[152] S. Colafranceschi,[152] M. Hohlmann,[152] D. Noonan,[152] M. Rahmani,[152] T. Roy,[152] F. Yumiceva,[152] M. R. Adams,[153] L. Apanasevich,[153] D. Berry,[153] R. R. Betts,[153] R. Cavanaugh,[153] X. Chen,[153] S. Dittmer,[153] O. Evdokimov,[153] C. E. Gerber,[153] D. A. Hangal,[153] D. J. Hofman,[153] K. Jung,[153] J. Kamin,[153] C. Mills,[153] I. D. Sandoval Gonzalez,[153] M. B. Tonjes,[153] H. Trauger,[153] N. Varelas,[153] H. Wang,[153] X. Wang,[153] Z. Wu,[153] J. Zhang,[153] M. Alhusseini,[154] B. Bilki,[154,ppp] W. Clarida,[154] K. Dilsiz,[154,qqq] S. Durgut,[154] R. P. Gandrajula,[154] M. Haytmyradov,[154] V. Khristenko,[154] J.-P. Merlo,[154] A. Mestvirishvili,[154] A. Moeller,[154] J. Nachtman,[154] H. Ogul,[154,rrr] Y. Onel,[154] F. Ozok,[154,sss] A. Penzo,[154] C. Snyder,[154] E. Tiras,[154] J. Wetzel,[154] B. Blumenfeld,[155] A. Cocoros,[155] N. Eminizer,[155] D. Fehling,[155] L. Feng,[155] A. V. Gritsan,[155] W. T. Hung,[155] P. Maksimovic,[155] J. Roskes,[155] U. Sarica,[155] M. Swartz,[155] M. Xiao,[155] C. You,[155] A. Al-bataineh,[156] P. Baringer,[156] A. Bean,[156] S. Boren,[156] J. Bowen,[156] A. Bylinkin,[156] J. Castle,[156] S. Khalil,[156] A. Kropivnitskaya,[156] D. Majumder,[156] W. Mcbrayer,[156] M. Murray,[156] C. Rogan,[156] S. Sanders,[156] E. Schmitz,[156] J. D. Tapia Takaki,[156] Q. Wang,[156] S. Duric,[157] A. Ivanov,[157] K. Kaadze,[157] D. Kim,[157] Y. Maravin,[157] D. R. Mendis,[157] T. Mitchell,[157] A. Modak,[157] A. Mohammadi,[157] L. K. Saini,[157] N. Skhirtladze,[157] F. Rebassoo,[158] D. Wright,[158] A. Baden,[159] O. Baron,[159] A. Belloni,[159] S. C. Eno,[159] Y. Feng,[159] C. Ferraioli,[159] N. J. Hadley,[159] S. Jabeen,[159] G. Y. Jeng,[159] R. G. Kellogg,[159] J. Kunkle,[159] A. C. Mignerey,[159] S. Nabili,[159] F. Ricci-Tam,[159] Y. H. Shin,[159] A. Skuja,[159] S. C. Tonwar,[159] K. Wong,[159] D. Abercrombie,[160] B. Allen,[160] V. Azzolini,[160] A. Baty,[160] G. Bauer,[160] R. Bi,[160] S. Brandt,[160] W. Busza,[160] I. A. Cali,[160] M. D'Alfonso,[160] Z. Demiragli,[160] G. Gomez Ceballos,[160] M. Goncharov,[160] P. Harris,[160] D. Hsu,[160] M. Hu,[160] Y. Iiyama,[160] G. M. Innocenti,[160] M. Klute,[160] D. Kovalskyi,[160] Y.-J. Lee,[160] P. D. Luckey,[160] B. Maier,[160] A. C. Marini,[160] C. Mcginn,[160] C. Mironov,[160] S. Narayanan,[160] X. Niu,[160] C. Paus,[160] C. Roland,[160] G. Roland,[160] G. S. F. Stephans,[160] K. Sumorok,[160] K. Tatar,[160] D. Velicanu,[160] J. Wang,[160] T. W. Wang,[160] B. Wyslouch,[160] S. Zhaozhong,[160] A. C. Benvenuti,[161,a] R. M. Chatterjee,[161] A. Evans,[161] P. Hansen,[161] Sh. Jain,[161] S. Kalafut,[161] Y. Kubota,[161] Z. Lesko,[161] J. Mans,[161] N. Ruckstuhl,[161] R. Rusack,[161] J. Turkewitz,[161] M. A. Wadud,[161] J. G. Acosta,[162] S. Oliveros,[162] E. Avdeeva,[163] K. Bloom,[163] D. R. Claes,[163] C. Fangmeier,[163] F. Golf,[163] R. Gonzalez Suarez,[163] R. Kamalieddin,[163] I. Kravchenko,[163] J. Monroy,[163] J. E. Siado,[163] G. R. Snow,[163] B. Stieger,[163] A. Godshalk,[164] C. Harrington,[164] I. Iashvili,[164] A. Kharchilava,[164] C. Mclean,[164] D. Nguyen,[164] A. Parker,[164] S. Rappoccio,[164] B. Roozbahani,[164] G. Alverson,[165] E. Barberis,[165] C. Freer,[165] A. Hortiangtham,[165] D. M. Morse,[165] T. Orimoto,[165] R. Teixeira De Lima,[165] T. Wamorkar,[165] B. Wang,[165] A. Wisecarver,[165] D. Wood,[165] S. Bhattacharya,[166] O. Charaf,[166] K. A. Hahn,[166] N. Mucia,[166] N. Odell,[166] M. H. Schmitt,[166] K. Sung,[166] M. Trovato,[166] M. Velasco,[166] R. Bucci,[167] N. Dev,[167] M. Hildreth,[167] K. Hurtado Anampa,[167] C. Jessop,[167] D. J. Karmgard,[167] N. Kellams,[167] K. Lannon,[167] W. Li,[167] N. Loukas,[167] N. Marinelli,[167] F. Meng,[167] C. Mueller,[167] Y. Musienko,[167,jj] M. Planer,[167] A. Reinsvold,[167] R. Ruchti,[167] P. Siddireddy,[167] G. Smith,[167] S. Taroni,[167] M. Wayne,[167] A. Wightman,[167] M. Wolf,[167] A. Woodard,[167] J. Alimena,[168] L. Antonelli,[168] B. Bylsma,[168] L. S. Durkin,[168] S. Flowers,[168] B. Francis,[168] A. Hart,[168] C. Hill,[168] W. Ji,[168] T. Y. Ling,[168] W. Luo,[168] B. L. Winer,[168] S. Cooperstein,[169] P. Elmer,[169] J. Hardenbrook,[169] S. Higginbotham,[169] A. Kalogeropoulos,[169] D. Lange,[169] M. T. Lucchini,[169] J. Luo,[169] D. Marlow,[169] K. Mei,[169] I. Ojalvo,[169]

J. Olsen,[169] C. Palmer,[169] P. Piroué,[169] J. Salfeld-Nebgen,[169] D. Stickland,[169] C. Tully,[169] S. Malik,[170] S. Norberg,[170] A. Barker,[171] V. E. Barnes,[171] S. Das,[171] L. Gutay,[171] M. Jones,[171] A. W. Jung,[171] A. Khatiwada,[171] B. Mahakud,[171] D. H. Miller,[171] N. Neumeister,[171] C. C. Peng,[171] S. Piperov,[171] H. Qiu,[171] J. F. Schulte,[171] J. Sun,[171] F. Wang,[171] R. Xiao,[171] W. Xie,[171] T. Cheng,[172] J. Dolen,[172] N. Parashar,[172] Z. Chen,[173] K. M. Ecklund,[173] S. Freed,[173] F. J. M. Geurts,[173] M. Kilpatrick,[173] W. Li,[173] B. P. Padley,[173] R. Redjimi,[173] J. Roberts,[173] J. Rorie,[173] W. Shi,[173] Z. Tu,[173] J. Zabel,[173] A. Zhang,[173] A. Bodek,[174] P. de Barbaro,[174] R. Demina,[174] Y. t. Duh,[174] J. L. Dulemba,[174] C. Fallon,[174] T. Ferbel,[174] M. Galanti,[174] A. Garcia-Bellido,[174] J. Han,[174] O. Hindrichs,[174] A. Khukhunaishvili,[174] P. Tan,[174] R. Taus,[174] A. Agapitos,[175] J. P. Chou,[175] Y. Gershtein,[175] E. Halkiadakis,[175] M. Heindl,[175] E. Hughes,[175] S. Kaplan,[175] R. Kunnawalkam Elayavalli,[175] S. Kyriacou,[175] A. Lath,[175] R. Montalvo,[175] K. Nash,[175] M. Osherson,[175] H. Saka,[175] S. Salur,[175] S. Schnetzer,[175] D. Sheffield,[175] S. Somalwar,[175] R. Stone,[175] S. Thomas,[175] P. Thomassen,[175] M. Walker,[175] A. G. Delannoy,[176] J. Heideman,[176] G. Riley,[176] S. Spanier,[176] O. Bouhali,[177,ttt] A. Celik,[177] M. Dalchenko,[177] M. De Mattia,[177] A. Delgado,[177] S. Dildick,[177] R. Eusebi,[177] J. Gilmore,[177] T. Huang,[177] T. Kamon,[177,uuu] S. Luo,[177] R. Mueller,[177] D. Overton,[177] L. Perniè,[177] D. Rathjens,[177] A. Safonov,[177] N. Akchurin,[178] J. Damgov,[178] F. De Guio,[178] P. R. Dudero,[178] S. Kunori,[178] K. Lamichhane,[178] S. W. Lee,[178] T. Mengke,[178] S. Muthumuni,[178] T. Peltola,[178] S. Undleeb,[178] I. Volobouev,[178] Z. Wang,[178] S. Greene,[179] A. Gurrola,[179] R. Janjam,[179] W. Johns,[179] C. Maguire,[179] A. Melo,[179] H. Ni,[179] K. Padeken,[179] J. D. Ruiz Alvarez,[179] P. Sheldon,[179] S. Tuo,[179] J. Velkovska,[179] M. Verweij,[179] Q. Xu,[179] M. W. Arenton,[180] P. Barria,[180] B. Cox,[180] R. Hirosky,[180] M. Joyce,[180] A. Ledovskoy,[180] H. Li,[180] C. Neu,[180] T. Sinthuprasith,[180] Y. Wang,[180] E. Wolfe,[180] F. Xia,[180] R. Harr,[181] P. E. Karchin,[181] N. Poudyal,[181] J. Sturdy,[181] P. Thapa,[181] S. Zaleski,[181] M. Brodski,[182] J. Buchanan,[182] C. Caillol,[182] D. Carlsmith,[182] S. Dasu,[182] L. Dodd,[182] B. Gomber,[182] M. Grothe,[182] M. Herndon,[182] A. Hervé,[182] U. Hussain,[182] P. Klabbers,[182] A. Lanaro,[182] K. Long,[182] R. Loveless,[182] T. Ruggles,[182] A. Savin,[182] V. Sharma,[182] N. Smith,[182] W. H. Smith,[182] and N. Woods[182]

(CMS Collaboration)

[1]Yerevan Physics Institute, Yerevan, Armenia
[2]Institut für Hochenergiephysik, Wien, Austria
[3]Institute for Nuclear Problems, Minsk, Belarus
[4]Universiteit Antwerpen, Antwerpen, Belgium
[5]Vrije Universiteit Brussel, Brussel, Belgium
[6]Université Libre de Bruxelles, Bruxelles, Belgium
[7]Ghent University, Ghent, Belgium
[8]Université Catholique de Louvain, Louvain-la-Neuve, Belgium
[9]Centro Brasileiro de Pesquisas Fisicas, Rio de Janeiro, Brazil
[10]Universidade do Estado do Rio de Janeiro, Rio de Janeiro, Brazil
[11a]Universidade Estadual Paulista, São Paulo, Brazil
[11b]Universidade Federal do ABC, São Paulo, Brazil
[12]Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Sofia, Bulgaria
[13]University of Sofia, Sofia, Bulgaria
[14]Beihang University, Beijing, China
[15]Department of Physics, Tsinghua University, Beijing, China
[16]Institute of High Energy Physics, Beijing, China
[17]State Key Laboratory of Nuclear Physics and Technology, Peking University, Beijing, China
[18]Universidad de Los Andes, Bogota, Colombia
[19]University of Split, Faculty of Electrical Engineering, Mechanical Engineering and Naval Architecture, Split, Croatia
[20]University of Split, Faculty of Science, Split, Croatia
[21]Institute Rudjer Boskovic, Zagreb, Croatia
[22]University of Cyprus, Nicosia, Cyprus
[23]Charles University, Prague, Czech Republic
[24]Escuela Politecnica Nacional, Quito, Ecuador
[25]Universidad San Francisco de Quito, Quito, Ecuador
[26]Academy of Scientific Research and Technology of the Arab Republic of Egypt, Egyptian Network of High Energy Physics, Cairo, Egypt
[27]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia
[28]Department of Physics, University of Helsinki, Helsinki, Finland

[29]Helsinki Institute of Physics, Helsinki, Finland
[30]Lappeenranta University of Technology, Lappeenranta, Finland
[31]IRFU, CEA, Université Paris-Saclay, Gif-sur-Yvette, France
[32]Laboratoire Leprince-Ringuet, CNRS/IN2P3, Ecole Polytechnique, Institut Polytechnique de Paris
[33]Université de Strasbourg, CNRS, IPHC UMR 7178, Strasbourg, France
[34]Centre de Calcul de l'Institut National de Physique Nucleaire et de Physique des Particules, CNRS/IN2P3, Villeurbanne, France
[35]Université de Lyon, Université Claude Bernard Lyon 1, CNRS-IN2P3, Institut de Physique Nucléaire de Lyon, Villeurbanne, France
[36]Georgian Technical University, Tbilisi, Georgia
[37]Tbilisi State University, Tbilisi, Georgia
[38]RWTH Aachen University, I. Physikalisches Institut, Aachen, Germany
[39]RWTH Aachen University, III. Physikalisches Institut A, Aachen, Germany
[40]RWTH Aachen University, III. Physikalisches Institut B, Aachen, Germany
[41]Deutsches Elektronen-Synchrotron, Hamburg, Germany
[42]University of Hamburg, Hamburg, Germany
[43]Karlsruher Institut fuer Technologie, Karlsruhe, Germany
[44]Institute of Nuclear and Particle Physics (INPP), NCSR Demokritos, Aghia Paraskevi, Greece
[45]National and Kapodistrian University of Athens, Athens, Greece
[46]National Technical University of Athens, Athens, Greece
[47]University of Ioánnina, Ioánnina, Greece
[48]MTA-ELTE Lendület CMS Particle and Nuclear Physics Group, Eötvös Loránd University, Budapest, Hungary
[49]Wigner Research Centre for Physics, Budapest, Hungary
[50]Institute of Nuclear Research ATOMKI, Debrecen, Hungary
[51]Institute of Physics, University of Debrecen, Debrecen, Hungary
[52]Indian Institute of Science (IISc), Bangalore, India
[53]National Institute of Science Education and Research, HBNI, Bhubaneswar, India
[54]Panjab University, Chandigarh, India
[55]University of Delhi, Delhi, India
[56]Saha Institute of Nuclear Physics, HBNI, Kolkata, India
[57]Indian Institute of Technology Madras, Madras, India
[58]Bhabha Atomic Research Centre, Mumbai, India
[59]Tata Institute of Fundamental Research-A, Mumbai, India
[60]Tata Institute of Fundamental Research-B, Mumbai, India
[61]Indian Institute of Science Education and Research (IISER), Pune, India
[62]Institute for Research in Fundamental Sciences (IPM), Tehran, Iran
[63]University College Dublin, Dublin, Ireland
[64a]INFN Sezione di Bari, Bari, Italy
[64b]Università di Bari, Bari, Italy
[64c]Politecnico di Bari, Bari, Italy
[65a]INFN Sezione di Bologna, Bologna, Italy
[65b]Università di Bologna, Bologna, Italy
[66a]INFN Sezione di Catania, Catania, Italy
[66b]Università di Catania, Catania, Italy
[67a]INFN Sezione di Firenze, Firenze, Italy
[67b]Università di Firenze, Firenze, Italy
[68]INFN Laboratori Nazionali di Frascati, Frascati, Italy
[69a]INFN Sezione di Genova, Genova, Italy
[69b]Università di Genova, Genova, Italy
[70a]INFN Sezione di Milano-Bicocca, Milano, Italy
[70b]Università di Milano-Bicocca, Milano, Italy
[71a]INFN Sezione di Napoli, Napoli, Italy
[71b]Università di Napoli 'Federico II', Napoli, Italy
[71c]Università della Basilicata, Potenza, Italy
[71d]Università G. Marconi, Roma, Italy
[72a]INFN Sezione di Padova, Padova, Italy
[72b]Università di Padova, Padova, Italy
[72c]Università di Trento, Trento, Italy
[73a]INFN Sezione di Pavia, Pavia, Italy
[73b]Università di Pavia, Pavia, Italy
[74a]INFN Sezione di Perugia, Perugia, Italy
[74b]Università di Perugia, Perugia, Italy

[75a]INFN Sezione di Pisa, Pisa, Italy
[75b]Universita` di Pisa, Pisa, Italy
[75c]Scuola Normale Superiore di Pisa, Pisa, Italy
[76a]INFN Sezione di Roma, Rome, Italy
[76b]Sapienza Universita` di Roma, Rome, Italy
[77a]INFN Sezione di Torino, Torino, Italy
[77b]Universita` di Torino, Torino, Italy
[77c]Universita` del Piemonte Orientale, Novara, Italy
[78a]INFN Sezione di Trieste, Trieste, Italy
[78b]Universita` di Trieste, Trieste, Italy
[79]Kyungpook National University, Daegu, Korea
[80]Chonnam National University, Institute for Universe and Elementary Particles, Kwangju, Korea
[81]Hanyang University, Seoul, Korea
[82]Korea University, Seoul, Korea
[83]Sejong University, Seoul, Korea
[84]Seoul National University, Seoul, Korea
[85]University of Seoul, Seoul, Korea
[86]Sungkyunkwan University, Suwon, Korea
[87]Vilnius University, Vilnius, Lithuania
[88]National Centre for Particle Physics, Universiti Malaya, Kuala Lumpur, Malaysia
[89]Universidad de Sonora (UNISON), Hermosillo, Mexico
[90]Centro de Investigacion y de Estudios Avanzados del IPN, Mexico City, Mexico
[91]Universidad Iberoamericana, Mexico City, Mexico
[92]Benemerita Universidad Autonoma de Puebla, Puebla, Mexico
[93]Universidad Autónoma de San Luis Potosí, San Luis Potosí, Mexico
[94]University of Auckland, Auckland, New Zealand
[95]University of Canterbury, Christchurch, New Zealand
[96]National Centre for Physics, Quaid-I-Azam University, Islamabad, Pakistan
[97]National Centre for Nuclear Research, Swierk, Poland
[98]Institute of Experimental Physics, Faculty of Physics, University of Warsaw, Warsaw, Poland
[99]Laboratório de Instrumentação e Física Experimental de Partículas, Lisboa, Portugal
[100]Joint Institute for Nuclear Research, Dubna, Russia
[101]Petersburg Nuclear Physics Institute, Gatchina (St.Petersburg), Russia
[102]Institute for Nuclear Research, Moscow, Russia
[103]Institute for Theoretical and Experimental Physics named by A.I. Alikhanov of NRC 'Kurchatov Institute', Moscow, Russia
[104]Moscow Institute of Physics and Technology, Moscow, Russia
[105]National Research Nuclear University 'Moscow Engineering Physics Institute' (MEPhI), Moscow, Russia
[106]P.N. Lebedev Physical Institute, Moscow, Russia
[107]Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow, Russia
[108]Novosibirsk State University (NSU), Novosibirsk, Russia
[109]Institute for High Energy Physics of National Research Centre 'Kurchatov Institute', Protvino, Russia
[110]National Research Tomsk Polytechnic University, Tomsk, Russia
[111]University of Belgrade: Faculty of Physics and VINCA Institute of Nuclear Sciences
[112]Centro de Investigaciones Energéticas Medioambientales y Tecnológicas (CIEMAT), Madrid, Spain
[113]Universidad Autónoma de Madrid, Madrid, Spain
[114]Universidad de Oviedo, Instituto Universitario de Ciencias y Tecnologías Espaciales de Asturias (ICTEA), Oviedo, Spain
[115]Instituto de Física de Cantabria (IFCA), CSIC-Universidad de Cantabria, Santander, Spain
[116]University of Ruhuna, Department of Physics, Matara, Sri Lanka
[117]CERN, European Organization for Nuclear Research, Geneva, Switzerland
[118]Paul Scherrer Institut, Villigen, Switzerland
[119]ETH Zurich—Institute for Particle Physics and Astrophysics (IPA), Zurich, Switzerland
[120]Universität Zürich, Zurich, Switzerland
[121]National Central University, Chung-Li, Taiwan
[122]National Taiwan University (NTU), Taipei, Taiwan
[123]Chulalongkorn University, Faculty of Science, Department of Physics, Bangkok, Thailand
[124]Çukurova University, Physics Department, Science and Art Faculty, Adana, Turkey
[125]Middle East Technical University, Physics Department, Ankara, Turkey
[126]Bogazici University, Istanbul, Turkey
[127]Istanbul Technical University, Istanbul, Turkey
[128]Institute for Scintillation Materials of National Academy of Science of Ukraine, Kharkov, Ukraine

[129]National Scientific Center, Kharkov Institute of Physics and Technology, Kharkov, Ukraine
[130]University of Bristol, Bristol, United Kingdom
[131]Rutherford Appleton Laboratory, Didcot, United Kingdom
[132]Imperial College, London, United Kingdom
[133]Brunel University, Uxbridge, United Kingdom
[134]Baylor University, Waco, Texas, USA
[135]Catholic University of America, Washington, DC, USA
[136]The University of Alabama, Tuscaloosa, Alabama, USA
[137]Boston University, Boston, Massachusetts, USA
[138]Brown University, Providence, Rhode Island, USA
[139]University of California, Davis, Davis, California, USA
[140]University of California, Los Angeles, California, USA
[141]University of California, Riverside, Riverside, California, USA
[142]University of California, San Diego, La Jolla, California, USA
[143]University of California, Santa Barbara—Department of Physics, Santa Barbara, California, USA
[144]California Institute of Technology, Pasadena, California, USA
[145]Carnegie Mellon University, Pittsburgh, Pennsylvania, USA
[146]University of Colorado Boulder, Boulder, Colorado, USA
[147]Cornell University, Ithaca, New York, USA
[148]Fermi National Accelerator Laboratory, Batavia, Illinois, USA
[149]University of Florida, Gainesville, Florida, USA
[150]Florida International University, Miami, Florida, USA
[151]Florida State University, Tallahassee, Florida, USA
[152]Florida Institute of Technology, Melbourne, Florida, USA
[153]University of Illinois at Chicago (UIC), Chicago, Illinois, USA
[154]The University of Iowa, Iowa City, Iowa, USA
[155]Johns Hopkins University, Baltimore, Maryland, USA
[156]The University of Kansas, Lawrence, Kansas, USA
[157]Kansas State University, Manhattan, Kansas, USA
[158]Lawrence Livermore National Laboratory, Livermore, California, USA
[159]University of Maryland, College Park, Maryland, USA
[160]Massachusetts Institute of Technology, Cambridge, Massachusetts, USA
[161]University of Minnesota, Minneapolis, Minnesota, USA
[162]University of Mississippi, Oxford, Mississippi, USA
[163]University of Nebraska-Lincoln, Lincoln, Nebraska, USA
[164]State University of New York at Buffalo, Buffalo, New York, USA
[165]Northeastern University, Boston, Massachusetts, USA
[166]Northwestern University, Evanston, Illinois, USA
[167]University of Notre Dame, Notre Dame, Indiana, USA
[168]The Ohio State University, Columbus, Ohio, USA
[169]Princeton University, Princeton, New Jersey, USA
[170]University of Puerto Rico, Mayaguez, Puerto Rico, USA
[171]Purdue University, West Lafayette, Indiana, USA
[172]Purdue University Northwest, Hammond, Indiana, USA
[173]Rice University, Houston, Texas, USA
[174]University of Rochester, Rochester, New York, USA
[175]Rutgers, The State University of New Jersey, Piscataway, New Jersey, USA
[176]University of Tennessee, Knoxville, Tennessee, USA
[177]Texas A&M University, College Station, Texas, USA
[178]Texas Tech University, Lubbock, Texas, USA
[179]Vanderbilt University, Nashville, Tennessee, USA
[180]University of Virginia, Charlottesville, Virginia, USA
[181]Wayne State University, Detroit, Michigan, USA
[182]University of Wisconsin—Madison, Madison, Wisconsin, USA

[a]Deceased.
[b]Also at Vienna University of Technology, Vienna, Austria.
[c]Also at IRFU, CEA, Université Paris-Saclay, Gif-sur-Yvette, France.
[d]Also at Universidade Estadual de Campinas, Campinas, Brazil.
[e]Also at Federal University of Rio Grande do Sul, Porto Alegre, Brazil.

[f]Also at Université Libre de Bruxelles, Bruxelles, Belgium.
[g]Also at University of Chinese Academy of Sciences, Beijing, China.
[h]Also at Institute for Theoretical and Experimental Physics named by A.I. Alikhanov of NRC 'Kurchatov Institute', Moscow, Russia.
[i]Also at Joint Institute for Nuclear Research, Dubna, Russia.
[j]Also at Cairo University, Cairo, Egypt.
[k]Also at British University in Egypt, Cairo, Egypt.
[l]Also at Fayoum University, El-Fayoum, Egypt.
[m]Also at Department of Physics, King Abdulaziz University, Jeddah, Saudi Arabia.
[n]Also at Université de Haute Alsace, Mulhouse, France.
[o]Also at Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow, Russia.
[p]Also at Tbilisi State University, Tbilisi, Georgia.
[q]Also at CERN, European Organization for Nuclear Research, Geneva, Switzerland.
[r]Also at RWTH Aachen University, III. Physikalisches Institut A, Aachen, Germany.
[s]Also at University of Hamburg, Hamburg, Germany.
[t]Also at Brandenburg University of Technology, Cottbus, Germany.
[u]Also at MTA-ELTE Lendület CMS Particle and Nuclear Physics Group, Eötvös Loránd University, Budapest, Hungary.
[v]Also at Institute of Nuclear Research ATOMKI, Debrecen, Hungary.
[w]Also at Institute of Physics, University of Debrecen, Debrecen, Hungary.
[x]Also at IIT Bhubaneswar, Bhubaneswar, India.
[y]Also at Institute of Physics, Bhubaneswar, India.
[z]Also at Shoolini University, Solan, India.
[aa]Also at University of Visva-Bharati, Santiniketan, India.
[bb]Also at Isfahan University of Technology.
[cc]Also at Plasma Physics Research Center, Science and Research Branch, Islamic Azad University, Tehran, Iran.
[dd]Also at Università degli Studi di Siena, Siena, Italy.
[ee]Also at Kyung Hee University, Department of Physics.
[ff]Also at International Islamic University of Malaysia, Kuala Lumpur, Malaysia.
[gg]Also at Malaysian Nuclear Agency, MOSTI, Kajang, Malaysia.
[hh]Also at Consejo Nacional de Ciencia y Tecnología, Mexico City, Mexico.
[ii]Also at Warsaw University of Technology, Institute of Electronic Systems, Warsaw, Poland.
[jj]Also at Institute for Nuclear Research, Moscow, Russia.
[kk]Also at National Research Nuclear University 'Moscow Engineering Physics Institute' (MEPhI), Moscow, Russia.
[ll]Also at Institute of Nuclear Physics of the Uzbekistan Academy of Sciences, Tashkent, Uzbekistan.
[mm]Also at St. Petersburg State Polytechnical University, St. Petersburg, Russia.
[nn]Also at University of Florida, Gainesville, Florida, USA.
[oo]Also at P.N. Lebedev Physical Institute, Moscow, Russia.
[pp]Also at Budker Institute of Nuclear Physics, Novosibirsk, Russia.
[qq]Also at Faculty of Physics, University of Belgrade, Belgrade, Serbia.
[rr]Also at INFN Sezione di Pavia, Università di Pavia, Pavia, Italy.
[ss]Also at University of Belgrade: Faculty of Physics and VINCA Institute of Nuclear Sciences.
[tt]Also at Scuola Normale e Sezione dell'INFN, Pisa, Italy.
[uu]Also at National and Kapodistrian University of Athens, Athens, Greece.
[vv]Also at Riga Technical University, Riga, Latvia.
[ww]Also at Universität Zürich, Zurich, Switzerland.
[xx]Also at Stefan Meyer Institute for Subatomic Physics, Vienna, Austria.
[yy]Also at Adiyaman University, Adiyaman, Turkey.
[zz]Also at Istanbul Aydin University, Application and Research Center for Advanced Studies (App. & Res. Cent. for Advanced Studies), Istanbul, Turkey.
[aaa]Also at Mersin University, Mersin, Turkey.
[bbb]Also at Piri Reis University, Istanbul, Turkey.
[ccc]Also at Ozyegin University, Istanbul, Turkey.
[ddd]Also at Izmir Institute of Technology, Izmir, Turkey.
[eee]Also at Marmara University, Istanbul, Turkey.
[fff]Also at Kafkas University, Kars, Turkey.
[ggg]Also at Istanbul Bilgi University, Istanbul, Turkey.
[hhh]Also at Hacettepe University, Ankara, Turkey.
[iii]Also at Rutherford Appleton Laboratory, Didcot, United Kingdom.
[jjj]Also at School of Physics and Astronomy, University of Southampton, Southampton, United Kingdom.
[kkk]Also at Monash University, Faculty of Science, Clayton, Australia.
[lll]Also at Bethel University, St. Paul, Minneapolis, USA.

[mmm]Also at Karamanoğlu Mehmetbey University, Karaman, Turkey.
[nnn]Also at Utah Valley University, Orem, Utah, USA.
[ooo]Also at Purdue University, West Lafayette, Indiana, USA.
[ppp]Also at Beykent University, Istanbul, Turkey.
[qqq]Also at Bingol University, Bingol, Turkey.
[rrr]Also at Sinop University, Sinop, Turkey.
[sss]Also at Mimar Sinan University, Istanbul, Istanbul, Turkey.
[ttt]Also at Texas A&M University at Qatar, Doha, Qatar.
[uuu]Also at Kyungpook National University, Daegu, Korea.