



# Search for contact interactions using the inclusive jet $p_T$ spectrum in pp collisions at $\sqrt{s} = 7$ TeV

The CMS Collaboration\*

## Abstract

Results are reported of a search for a deviation in the jet production cross section from the prediction of perturbative quantum chromodynamics at next-to-leading order. The search is conducted using a 7 TeV proton-proton data sample corresponding to an integrated luminosity of  $5.0 \text{ fb}^{-1}$ , collected with the Compact Muon Solenoid detector at the Large Hadron Collider. A deviation could arise from interactions characterized by a mass scale  $\Lambda$  too high to be probed directly at the LHC. Such phenomena can be modeled as contact interactions. No evidence of a deviation is found. Using the  $CL_s$  criterion, lower limits are set on  $\Lambda$  of 9.9 TeV and 14.3 TeV at 95% confidence level for models with destructive and constructive interference, respectively. Limits obtained with a Bayesian method are also reported.

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## 1 Introduction

Interactions at an energy scale much lower than the mass of the mediating particle can be modeled by contact interactions (CI) [1–4] governed by a single mass scale conventionally denoted by  $\Lambda$ . A search for contact interactions is therefore a search for interactions whose detailed characteristics become manifest only at higher energies. Contact interactions can affect the jet angular distributions as well as the jet transverse momentum ( $p_T$ ) spectra, particularly for low-rapidity jets. Lower limits on  $\Lambda$  have been set by the CDF [5], D0 [6], and ATLAS [7] collaborations. The Compact Muon Solenoid (CMS) collaboration has previously measured the dijet angular distribution [8] using a data set of  $\sqrt{s} = 7$  TeV proton-proton collisions corresponding to an integrated luminosity of  $2.2 \text{ fb}^{-1}$ , and found  $\Lambda > 8.4$  TeV and  $\Lambda > 11.7$  TeV at 95% confidence level (CL), for models with destructively and constructively interfering amplitudes, respectively.

The inclusive jet  $p_T$  spectrum, i.e., the spectrum of jets in  $p + p \rightarrow \text{jet} + X$  events, where  $X$  can be any collection of particles, is generally considered to be less sensitive to the presence of contact interactions than the jet angular distribution. This perception is due to the jet  $p_T$  spectrum's greater dependence on the jet energy scale (JES) and on the parton distribution functions (PDF), which are difficult to determine accurately. However, considerable progress has been made by the CMS collaboration in understanding the JES [9]. The understanding of PDFs has also improved greatly at high parton momentum fraction [10–12], in part because of the important constraints on the gluon PDF provided by measurements at the Tevatron [13, 14]. These developments have made the jet  $p_T$  spectrum a competitive observable to search for phenomena described by contact interactions, reprising the method that was used in searches by CDF [15] and D0 [16].

In this paper, we report the results of a search for a deviation in the jet production cross section from the next-to-leading-order (NLO) quantum chromodynamics (QCD) prediction of jets produced at low-rapidity with transverse momenta  $>500$  GeV. The analysis is based on a 7 TeV proton-proton data sample corresponding to an integrated luminosity of  $5.0 \text{ fb}^{-1}$ , collected with the CMS detector at the Large Hadron Collider (LHC).

## 2 Theoretical models

The experimental results are interpreted in terms of a CI model described by the effective Lagrangian [3, 17]

$$L = \zeta \frac{2\pi}{\Lambda^2} (\bar{q}_L \gamma^\mu q_L) (\bar{q}_L \gamma_\mu q_L), \quad (1)$$

where  $q_L$  denotes a left-handed quark field and  $\zeta = +1$  or  $-1$  for destructively or constructively interfering amplitudes, respectively. The amplitude for jet production can be written as

$$a = a_{\text{SM}} + \lambda a_{\text{CI}}$$

where  $a_{\text{SM}}$  and  $a_{\text{CI}}$  are the standard model (SM) and contact interaction amplitudes, respectively. Since the amplitude is linear in  $\lambda = 1/\Lambda^2$ , the cross section  $\sigma_k$  in the  $k$ th jet  $p_T$  bin is given by

$$\sigma_k = c_k + b_k \lambda + a_k \lambda^2, \quad (2)$$

where  $c_k$ ,  $b_k$ , and  $a_k$  are jet- $p_T$ -dependent coefficients.

We use models characterized by the cross section  $\text{QCD}_{\text{NLO}} + \text{CI}(\Lambda)$ , where  $\text{QCD}_{\text{NLO}} = c_k$  is the inclusive jet cross section computed at next-to-leading order, and  $\text{CI}(\Lambda) = b_k \lambda + a_k \lambda^2$  param-

terizes the deviation of the inclusive jet cross section from the QCD prediction arising from the hypothesized contact interactions. The  $\text{QCD}_{\text{NLO}}$  cross section is calculated with version 2.1.0-1062 of the fastNLO program with scenario table fnl2332y0.tab [18] using the NLO CTEQ6.6 PDFs [19]. We do not unfold the observed inclusive jet  $p_T$  spectrum. Instead, the NLO QCD jet  $p_T$  spectrum is convolved with the CMS jet response function, where the jet energy resolution (JER)  $\sigma_{p_T}$  for low-rapidity jets is given by

$$\sigma_{p_T} = p_T \sqrt{-\frac{n^2}{p_T^2} + \frac{s^2 p_T^m}{p_T} + c^2}, \quad (3)$$

with  $n = 5.09$ ,  $s = 0.512$ ,  $m = 0.325$ ,  $c = 0.033$ , and compared directly with the observed spectrum using a likelihood function. Equation (3) is the standard form for the calorimeter resolution function, modified to account for a weak  $p_T$  dependence of the coefficient of the ( $p_T^{-1}$ ) stochastic term and to model better the resolution of low  $p_T$  jets by using a negative coefficient for the ( $p_T^{-2}$ ) noise term. For brevity, we shall refer to the smeared spectrum as the NLO QCD jet  $p_T$  spectrum.

The signal term  $\text{CI}(\Lambda)$  is modeled by subtracting the leading-order (LO) QCD jet cross section ( $\text{QCD}_{\text{LO}}$ ) from the LO jet cross section computed with a contact term. The leading-order jet  $p_T$  spectra are computed by generating events with and without a CI term using the program PYTHIA 6.422, the Z2 underlying event tune [17, 20], and the same CTEQ PDFs used to calculate  $\text{QCD}_{\text{NLO}}$ . The generated events are processed with the full CMS detector simulation program, based on GEANT4 [21]. Interactions between all quarks are included (Appendix A) and we consider models both with destructive and constructive interference between the QCD and CI amplitudes. We note that NLO corrections to the contact interaction model have recently become available [22], and we plan to use these results in future studies. These corrections are expected to change the results by less than 5%.

The jet  $p_T$  dependence of  $\text{CI}(\Lambda)$  is modeled by fitting the ratio  $f = [\text{QCD}_{\text{NLO}} + \text{CI}(\Lambda)]/\text{QCD}_{\text{NLO}}$  simultaneously to four PYTHIA CI models with  $\Lambda = 3, 5, 8$ , and 12 TeV. The fit is performed in this manner in order to construct a smooth interpolation over the four cross section ratios. Several functional forms were investigated that gave satisfactory fits, including the ansatz [23]:

$$f = 1 + p_1 \left( \frac{p_T}{100 \text{ GeV}} \right)^{p_2} \left( \frac{\Lambda}{1 \text{ TeV}^{-2}} \right) + p_3 \left( \frac{p_T}{100 \text{ GeV}} \right)^{p_4} \left( \frac{\Lambda}{1 \text{ TeV}^{-2}} \right)^2. \quad (4)$$

In a generator-level study, we verified the adequacy of the extrapolation of Eq. (4) up to 25 TeV. The results of fitting Eq. (4) to models with destructive interference are shown in Figure 1. The fit shown in Fig. 1 uses the central values of the JES, JER, and PDF parameters and the renormalization ( $\mu_r$ ) and factorization ( $\mu_f$ ) scales set to  $\mu_r = \mu_f = \text{jet } p_T$ . Models with constructive interference are obtained by reversing the sign of the parameter  $p_1$ . The fit parameters are given in Table 1. Figures 2 and 3 show model spectra in the jet  $p_T$  range  $500 \leq p_T \leq 2000 \text{ GeV}$  for values of  $\Lambda$  that are close to the limits reported in this paper. Figure 2 shows that the jet production cross section is enhanced at sufficiently high jet  $p_T$ . However, for interactions that interfere destructively, the cross section can decrease relative to the NLO QCD prediction. For example, for  $\Lambda = 10 \text{ TeV}$ , the  $\text{QCD}_{\text{NLO}} + \text{CI}$  cross section is lower than the  $\text{QCD}_{\text{NLO}}$  cross section for jet  $p_T < 1.3 \text{ TeV}$ . Figure 3 shows the contact  $p$  interaction signal,  $\text{CI}(\Lambda)$ , as a function of jet  $p_T$ .

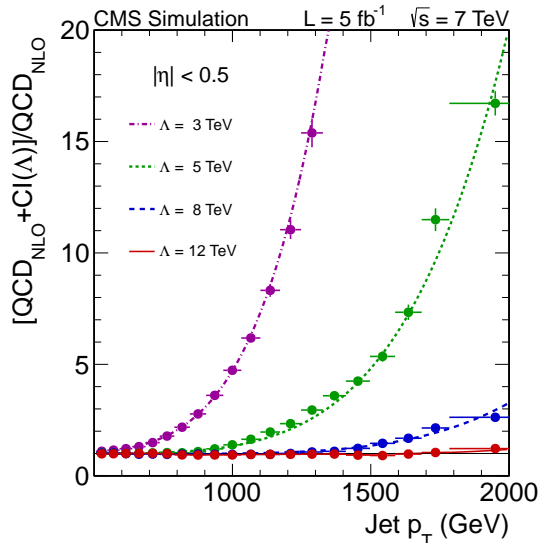


Figure 1: The cross section ratios,  $f = [\text{QCD}_{\text{NLO}} + \text{CI}(\Lambda)]/\text{QCD}_{\text{NLO}}$ , with  $\Lambda = 3, 5, 8,$  and  $12$  TeV. The points with error bars are the theoretical values of the cross section ratios. The curves are the results of a fit of Eq. (4) simultaneously to the four cross section ratios. The NLO QCD jet  $p_T$  spectrum is calculated using the nominal values of the JES, JER, PDF, renormalization and factorization scales for models with destructive interference. The values of the parameters of the fit are given in Table 1.

Table 1: The fit parameters associated with Fig. 1. The first row lists the values of the parameters  $p_1, p_2, p_3,$  and  $p_4$ , while the remaining rows list the elements of the associated covariance matrix.

	$p_1$	$p_2$	$p_3$	$p_4$
	$-1.5 \times 10^{-3}$	3.6	$1.9 \times 10^{-3}$	5.2
$p_1$	$1.4 \times 10^{-6}$	$3.6 \times 10^{-4}$	$-3.4 \times 10^{-7}$	$6.8 \times 10^{-5}$
$p_2$	$3.6 \times 10^{-4}$	$9.2 \times 10^{-2}$	$-8.4 \times 10^{-5}$	$1.7 \times 10^{-2}$
$p_3$	$-3.4 \times 10^{-7}$	$-8.4 \times 10^{-5}$	$1.0 \times 10^{-7}$	$-2.0 \times 10^{-5}$
$p_4$	$6.8 \times 10^{-5}$	$1.7 \times 10^{-2}$	$-2.0 \times 10^{-5}$	$4.1 \times 10^{-3}$

### 3 Experimental setup

The CMS coordinate system is right-handed with the origin at the center of the detector, the  $x$  axis directed toward the center of the LHC ring, the  $y$  axis directed upward, and the  $z$  axis directed along the counterclockwise proton beam. We define  $\phi$  to be the azimuthal angle,  $\theta$  to be the polar angle, and the pseudorapidity to be  $\eta \equiv -\ln[\tan(\theta/2)]$ . The central feature of the CMS apparatus is a superconducting solenoid of 6 m internal diameter, operating with a magnetic field strength of 3.8 T. Within the field volume are the silicon pixel and strip trackers and the barrel and endcap calorimeters with  $|\eta| < 3$ . Outside the field volume, in the forward region, there is an iron/quartz-fiber hadron calorimeter ( $3 < |\eta| < 5$ ). Further details about the CMS detector may be found elsewhere [24].

Jets are built from the five types of reconstructed particles: photons, neutral hadrons, charged hadrons, muons, and electrons, using the CMS particle-flow reconstruction method [25] and the anti- $k_T$  algorithm with a distance parameter of 0.7 [26–28]. The jet energy scale correction is derived as a function of the jet  $p_T$  and  $\eta$ , using a  $p_T$ -balancing technique [9], and applied to

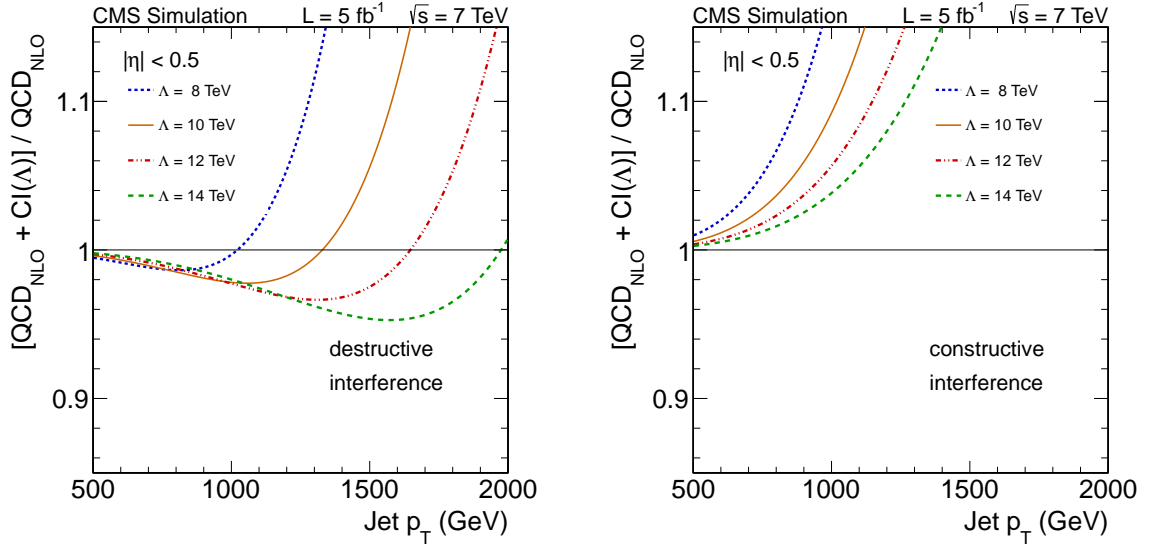


Figure 2: The cross section ratios,  $f = [\text{QCD}_{\text{NLO}} + \text{CI}(\Lambda)] / \text{QCD}_{\text{NLO}}$ , with  $\Lambda = 8, 10, 12$ , and  $14$  TeV, for models with destructive (left) and constructive (right) interference.

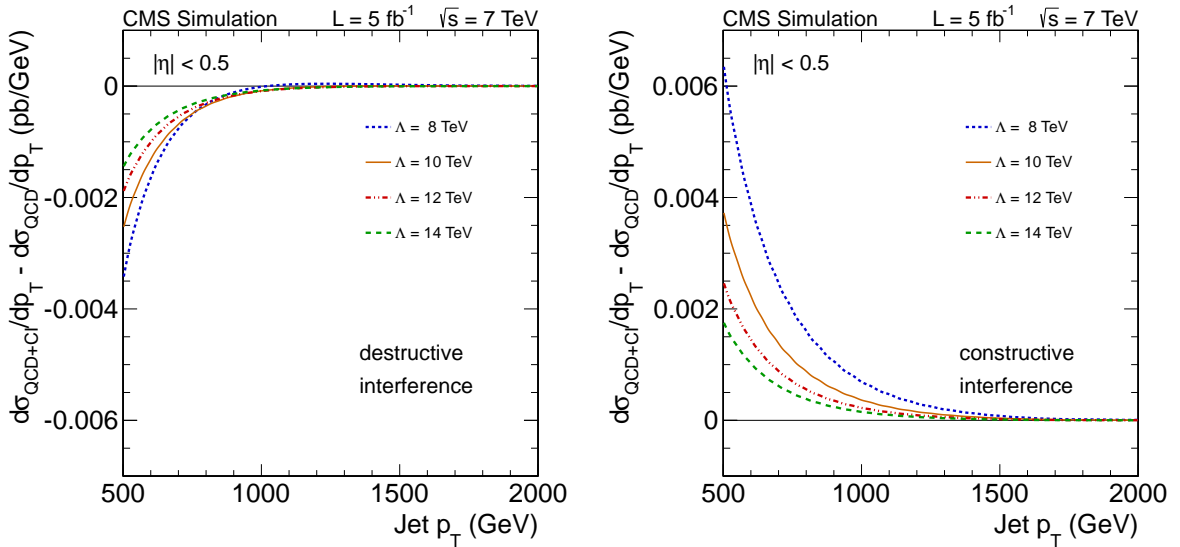


Figure 3: The CI signal spectra, defined as  $d\sigma_{\text{QCD}+\text{CI}}/dp_T - d\sigma_{\text{QCD}}/dp_T$  (pb/GeV) with  $\Lambda = 8, 10, 12$  and  $14$  TeV, for models with destructive (left) and constructive (right) interference.

all components of the jet four momentum.

The results reported are based on data collected using un-prescaled single-jet triggers with  $p_T$  thresholds that were changed in steps from 240 to 300 GeV during the data-taking period. The trigger thresholds were changed in response to the increase in instantaneous luminosity. The jet trigger efficiency is constant,  $\sim 98.8\%$ , above  $\sim 400$  GeV, well below the search region. Events with hadron calorimeter noise are removed [29] and each selected event must have a primary vertex within 24 cm of the geometric center of the detector along the  $z$  axis and within 0.2 cm in the transverse  $x$ - $y$  plane, defined by criteria described in [30]. The search is restricted to  $|\eta| < 0.5$  where the effects of contact interactions are predicted to be the largest [1–4]. The jet

$p_T$  spectrum is divided into 20  $p_T$  bins in the search region  $507 \leq p_T \leq 2116$  GeV, where the bin width is approximately equal to the jet resolution  $\sigma_{p_T}$  given in Eq. (3). No jets are observed above 2000 GeV transverse energy.

## 4 Results

In Figure 4 we compare the observed inclusive jet  $p_T$  spectrum with the NLO QCD jet  $p_T$  spectrum, which is normalized to the total observed jet count in the search region using the normalization factor  $4.007 \pm 0.009$  (stat.)  $\text{fb}^{-1}$  (Section 5). The normalization is the ratio of the observed jet count to the predicted cross section in the search region. The data and the prediction are in good agreement as indicated by two standard criteria, the Kolmogorov-Smirnov probability  $\text{Pr}(\text{KS})$  of 0.66 and the  $\chi^2$  per number of degrees of freedom (NDF) of 23.5/19. Table 2 lists the observed jet counts. Figure 5 compares the observed jet  $p_T$  spectrum in the search region with model spectra for different values of  $\Lambda$ , for models with destructive interference. Figure 6 compares the data with models with constructive interference.

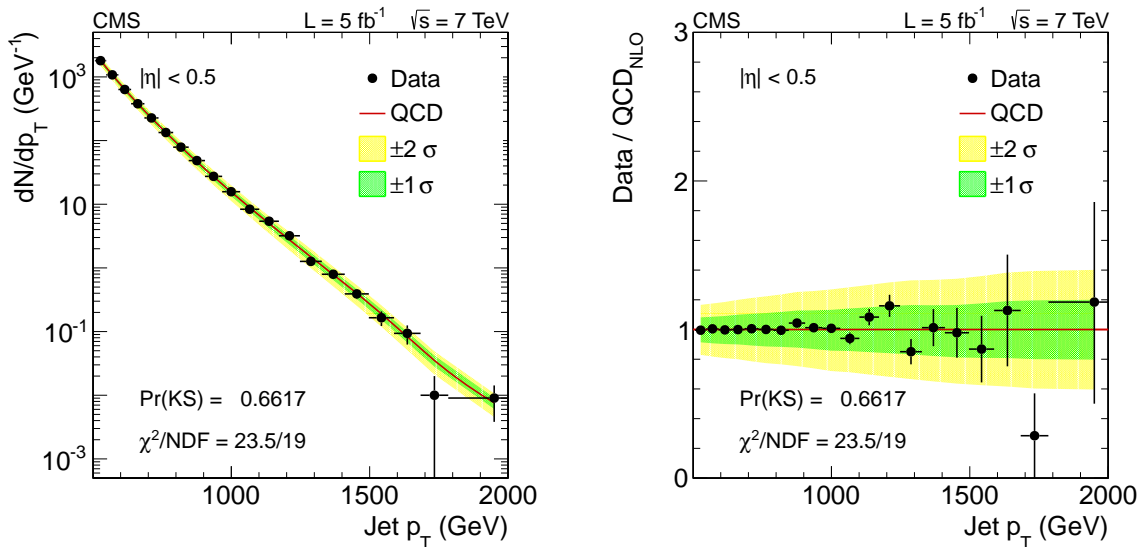


Figure 4: The observed jet  $p_T$  spectrum compared with the NLO QCD jet  $p_T$  spectrum (left). The bands represent the total uncertainty in the prediction and incorporate the uncertainties in the PDFs, jet energy scale, jet energy resolution, the renormalization and factorization scales, and the modeling of the jet  $p_T$  dependence of the parameters in Eq. (4). The ratio of the observed to the predicted spectrum (right). The error bars represent the statistical uncertainties in the expected bin count.

## 5 Statistical analysis

Since there are no significant deviations between the observed and predicted spectra, the results are interpreted in terms of lower limits on the CI scale  $\Lambda$  using the models described in Section 2. The dominant sources of systematic uncertainties are associated with the JES, the PDFs, the JER, the renormalization ( $\mu_r$ ) and factorization ( $\mu_f$ ) scales, and the modeling parameters of Eq. (4). Non-perturbative corrections are less than 1% for transverse momenta above  $\sim 400$  GeV [30], are negligible compared with other uncertainties, and are therefore not applied to our analysis.

Table 2: The observed jet count for each jet  $p_T$  bin in the range 507–2116 GeV.

Bin	$p_T$ (GeV)	Jets	Bin	$p_T$ (GeV)	Jets
1	507–548	73792	11	1032–1101	576
2	548–592	47416	12	1101–1172	384
3	592–638	29185	13	1172–1248	243
4	638–686	18187	14	1248–1327	100
5	686–737	11565	15	1327–1410	66
6	737–790	7095	16	1410–1497	34
7	790–846	4413	17	1497–1588	15
8	846–905	2862	18	1588–1684	9
9	905–967	1699	19	1684–1784	1
10	967–1032	1023	20	1784–2116	3

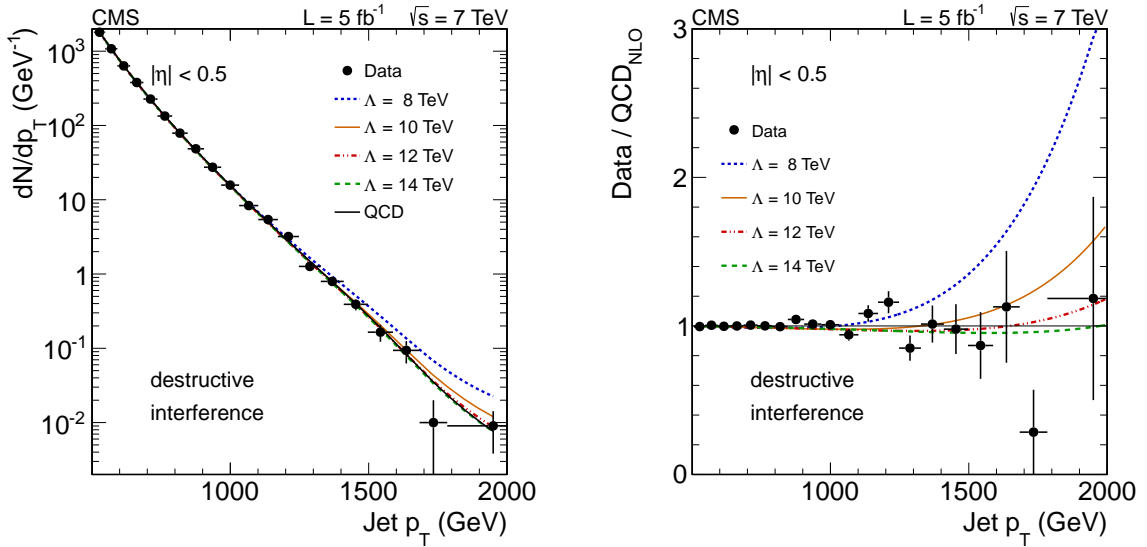


Figure 5: The data compared with model spectra for different values of  $\Lambda$  for models with destructive interference (left). The ratio of these spectra to the NLO QCD jet  $p_T$  spectrum (right).

In the search region, the inclusive jet spectrum has a range of five orders of magnitude, which causes the limits on  $\Lambda$  to be sensitive to the choice of the normalization factor and the size of the data sets. We have found that a few percent change in the normalization factor can cause limits to change by as much as 50%. Therefore, for the purpose of computing limits, we have chosen to sidestep the issue of normalization by considering only the shape of the jet  $p_T$  spectrum. This we achieve by using a multinomial distribution, which is the probability to observe  $K$  counts,  $N_j$ ,  $j = 1, \dots, K$ , given the observation of a total count  $N = \sum_{j=1}^K N_j$ . The likelihood is then defined by

$$p(D|\lambda, \omega) = \frac{N!}{N_1! \cdots N_K!} \prod_{j=1}^K \left( \frac{\sigma_j}{\sigma} \right)^{N_j}, \quad (5)$$

where  $K = 20$  is the number of bins in the search region,  $N_j$  is the jet count in the  $j$ th jet  $p_T$  bin,  $D \equiv N_1, \dots, N_K$ ,  $\sigma = \sum_{j=1}^K \sigma_j$  and  $N$  are the total cross section and total observed count, respectively, in the search region, and the symbol  $\omega$  denotes the nuisance parameters  $p_1, \dots, p_4$  in Eq. (4).



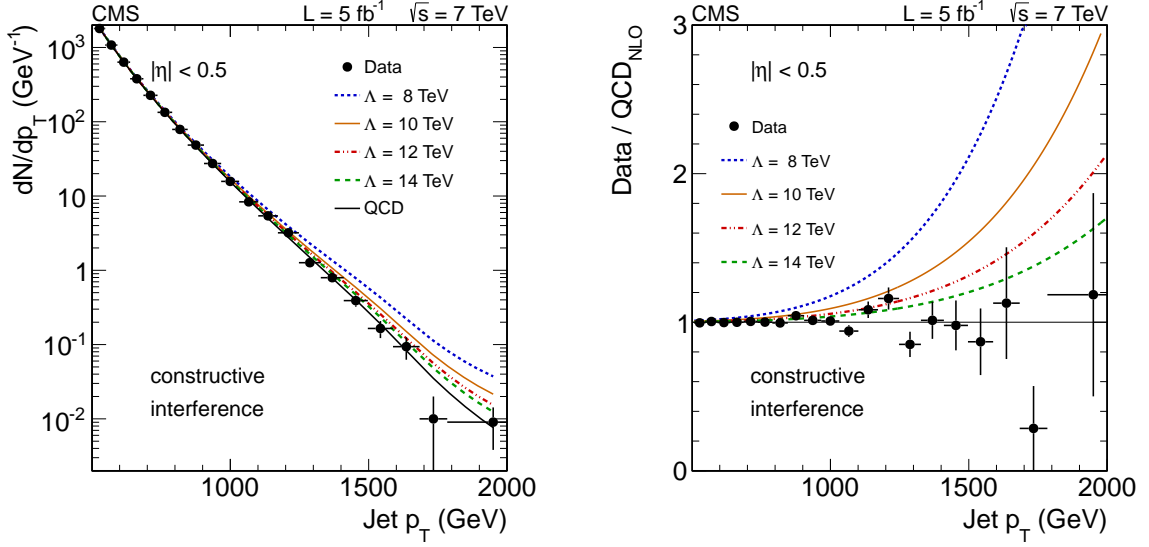


Figure 6: The data compared with model spectra for different values of  $\Lambda$  for models with constructive interference (left). The ratio of these spectra to the NLO QCD jet  $p_T$  spectrum (right).

We account for systematic uncertainties by integrating the likelihood with respect to a nuisance prior  $\pi(\omega)$ . In practice, the likelihood is averaged over the nuisance parameters,  $\omega$ , using a discrete representation of the prior  $\pi(\omega)$  constructed as described in Section 5.1. This calculation yields the marginal likelihood  $p(D|\lambda) \approx \frac{1}{M} \sum_{m=1}^M p(D|\lambda, \omega_m)$ , where  $M$  is the number of points sampled from the nuisance prior  $\pi(\omega)$  described in Appendix B.1, which is the basis of the limit calculations. The likelihood functions for models with destructive and constructive interference are shown in Figure 7.

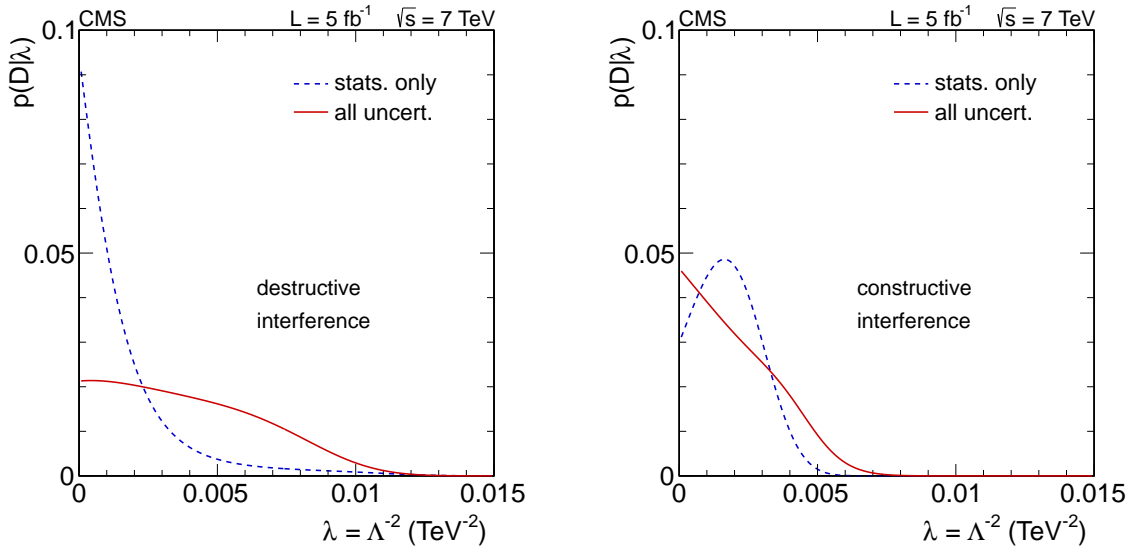


Figure 7: The likelihood functions assuming a model with either destructive (left) or constructive (right) interference. The dashed curve is the likelihood function including statistical uncertainties only and the central values of all nuisance parameters. The solid curve is the likelihood marginalized over all systematic uncertainties.

## 5.1 Uncertainties

In principle, a discrete representation of the nuisance prior  $\pi(\omega)$  can be constructed by sampling simultaneously the JES, JER, PDFs, and the three values of  $\mu_f$  and  $\mu_r$ :  $p_T/2$ ,  $p_T$ , and  $2p_T$ . However, the CTEQ collaboration [19] does not provide a sampling of PDFs. Instead, CTEQ6.6 contains 44 PDF sets in which the 22 PDF parameters are shifted by approximately  $\pm 1.64$  standard deviations. If we assume the Gaussian approximation to be valid, we can construct approximate  $20 \times 20$  covariance matrices for the jet spectra from the 44 PDF sets. Using these matrices, we generate ensembles of six correlated spectra:  $\text{QCD}_{\text{NLO}}$ ,  $\text{QCD}_{\text{LO}}$ , and  $(\text{QCD} + \text{CI}(\Lambda))_{\text{LO}}$  with  $\Lambda = 3, 5, 8$ , and 12 TeV. The generation is performed for models both with destructive and constructive interference. The details of our procedure, which also includes simultaneous sampling of the JES and JER parameters, are given in Appendix B.1.

For a given set of values for the JES, JER, PDF,  $\mu_r$ , and  $\mu_f$  parameters, Eq. (4) is fitted to the ratio  $(\text{QCD}_{\text{NLO}} + \text{CI})/\text{QCD}_{\text{NLO}}$  simultaneously to the four models with  $\Lambda = 3, 5, 8$ , and 12 TeV. We then sample a single set of the four nuisance parameters  $\omega = p_1, p_2, p_3, p_4$  from a multivariate Gaussian using the fitted values and the associated  $4 \times 4$  covariance matrix. The sampling and fitting procedure is repeated 500 times, thereby generating a discrete representation of the nuisance prior  $\pi(\omega)$  that incorporates all uncertainties. We have verified that our conclusions are robust with respect to variations in the size of the sample that represents  $\pi(\omega)$ .

## 5.2 Lower limits on $\Lambda$

We use the  $\text{CL}_s$  criterion [31, 32] to compute upper limits on  $\lambda$ . For completeness, we give the details of these calculations in Appendix B.2. Using the procedure described in the Appendix, we obtain 95% lower limits on  $\Lambda$  of 9.9 TeV and 14.3 TeV for models with destructive and constructive interference, respectively. These more stringent limits supersede those published by CMS based on a measurement of the dijet angular distribution [8]. The current search is more sensitive than the earlier dijet search as evidenced by the expected limits, which for this analysis are  $9.5 \pm 0.6$  TeV and  $13.6 \pm 1.6$  TeV, respectively, obtained using  $5 \text{ fb}^{-1}$  of data.

Limits are also computed with a Bayesian method (Appendix B.3) using the marginal likelihood  $p(D|\lambda)$  and two different priors for  $\lambda$ : a prior flat in  $\lambda$  and a reference prior [33–35]. Using a flat prior, we find lower limits on  $\Lambda$  of 10.6 TeV and 14.6 TeV at 95% confidence level for models with destructive and constructive interference, respectively. The corresponding limits using the reference prior are 10.1 TeV and 14.1 TeV at 95% confidence level, respectively.

## 6 Summary

The inclusive jet  $p_T$  spectrum of 7 TeV proton-proton collision events in the ranges  $507 \leq p_T \leq 2116 \text{ GeV}$  and  $|\eta| < 0.5$  has been studied using a data set corresponding to an integrated luminosity of  $5.0 \text{ fb}^{-1}$ . The observed jet  $p_T$  spectrum is found to be in agreement with the jet  $p_T$  spectrum predicted using perturbative QCD at NLO when the predicted spectrum is convolved with the CMS jet response function and normalized to the observed spectrum in the search region. Should additional interactions exist that can be modeled as contact interactions with either destructive or constructive interference, their scale  $\Lambda$  is above 9.9 TeV and 14.3 TeV, respectively, at 95% confidence level. We plan to extend this study to the full 8 TeV CMS data set, making use of a recently released program [36] to calculate at next-to-leading order the inclusive jet  $p_T$  spectrum with contact interactions.

It is noteworthy that the limits reported in this paper, which are the most sensitive limits pub-

lished to date, have been obtained reprising the classic method to search for contact interactions: namely, searching for deviations from QCD at high jet transverse momentum.

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## A PYTHIA 6.422 contact interaction configuration

The scale  $\Lambda$  is defined by the CI model in PYTHIA. In order to facilitate the re-interpretation of the results using a different model, we provide the details of the PYTHIA configuration in Table 3 for  $\Lambda = 8$  TeV and final state parton transverse momenta,  $\hat{p}_T$ , in the range  $170 \leq \hat{p}_T \leq 230$  GeV.

Table 3: PYTHIA 6.422 configuration for  $\Lambda = 8$  TeV contact interactions.

PYTHIA 6.422 settings specific to contact interactions	
Settings	Description
ITCM(5)=2	Switch on contact int. for all quarks
RTCM(41)=8000	Set contact scale $\Lambda$ to 8 TeV
RTCM(42)=1	Sign of contact int. is +
MSUB(381)=1	$q_i q_j \rightarrow q_i q_j$ via QCD plus a contact int.
MSUB(382)=1	$q_i \bar{q}_i \rightarrow q_k \bar{q}_k$ via QCD plus a contact int.
MSUB(13)=1	$q_i \bar{q}_i \rightarrow gg$ via normal QCD
MSUB(28)=1	$q_i g \rightarrow q_i g$ via normal QCD
MSUB(53)=1	$gg \rightarrow q_k \bar{q}_k$ via normal QCD
MSUB(68)=1	$gg \rightarrow gg$ via normal QCD
CKIN(3)=170	minimum $\hat{p}_T$ for hard int.
CKIN(4)=230	maximum $\hat{p}_T$ for hard int.

## B Statistical details

### B.1 Nuisance prior

We approximate the nuisance prior  $\pi(\omega)$  starting with two sets of ensembles. In the first, the six 20-bin model spectra  $\text{QCD}_{\text{NLO}}$ ,  $\text{QCD}_{\text{LO}}$ , and  $[\text{QCD} + \text{CI}(\Lambda)]_{\text{LO}}$  with  $\Lambda = 3, 5, 8$ , and 12 TeV are varied, reflecting random variations in the PDF parameters as well as random choices of the three  $\mu_r$  and  $\mu_f$  scales, while keeping the JES and JER parameters fixed at their central values; we call these the PDF ensembles. In the second set of ensembles, the JES and JER parameters are varied simultaneously, while keeping the PDF parameters fixed to their central values and the renormalization and factorization scales at their nominal values; we call these the JES/JER ensembles.

#### B.1.1 Generating the PDF ensembles

In the PDF ensembles, each of the six model spectra is sampled from a multivariate Gaussian distribution using the associated  $20 \times 20$  covariance matrix. For each model spectrum, the covariance matrix is approximated by

$$C_{nm} = \sum_{i=1}^{22} \sum_{j=1}^{22} \Delta X_{ni} \Delta X_{mj}, \quad (6)$$

where  $\Delta X_{ni} = (X_{ni}^+ - X_{ni}^-)/2$  and  $X_{ni}^\pm$  are the cross section values for  $n$ th jet bin associated with the + and - variations of the  $i$ th pair of CTEQ6.6 PDF sets. CTEQ [19] publishes approximate 90% intervals. We therefore approximate 68% intervals by dividing each  $\Delta X$  by 1.64. The correlation induced by the PDF uncertainties across all six model spectra is maintained by using the same set of underlying Gaussian variates during the sampling of the spectra.

#### B.1.2 Generating the JES/JER ensembles

In the JES/JER ensembles, the JES and JER parameters are sampled simultaneously for the five model spectra  $\text{QCD}_{\text{LO}}$ , and  $(\text{QCD} + \text{CI})_{\text{LO}}$  with  $\Lambda = 3, 5, 8$ , and 12 TeV, yielding ensembles of correlated shifts from the central JES, JER, and PDF values of the  $\text{QCD}_{\text{LO}}$  and  $(\text{QCD} + \text{CI})_{\text{LO}}$  spectra. For example, we compute the spectral residuals  $\delta\sigma = \text{QCD}' - \text{QCD}_{\text{central}}$ , where  $\text{QCD}'$  is the shifted jet  $p_T$  spectrum and  $\text{QCD}_{\text{central}}$  is the jet  $p_T$  spectrum computed using the central values of the JES, JER, and PDF parameters. Coherent shifts of the jet energy scale are calculated

for every jet in every simulated event. The jet  $p_T$  is shifted by  $x\delta$  for each component of the jet energy scale uncertainty, of which there are sixteen, where  $x$  is a Gaussian variate of zero mean and unit variance, and  $\delta$  is a jet-dependent uncertainty for a given component. The contributions from all uncertainty components are summed to obtain an overall shift in the jet  $p_T$ . From studies of dijet asymmetry and photon+jet  $p_T$  balancing, the uncertainty in the jet energy resolution is estimated to be 10% in the pseudorapidity range  $|\eta| < 0.5$  [30]. We sample the jet energy resolution using a procedure identical to that used to sample the jet energy scale, but using a single Gaussian variate.

### B.1.3 Generating the JES/JER/PDF ensemble

Another ensemble is created, from the PDF ensembles and the JES/JER ensembles, that approximates simultaneous sampling from the JES, JER, PDF, renormalization, and factorization parameters. We pick at random a correlated set of six spectra from the PDF ensembles, and a correlated set of five spectral residuals from the JES/JER ensembles. The JES/JER spectral residuals  $\delta\sigma$  are added to the corresponding shifted spectrum from the PDF ensembles, thereby creating a spectrum in which the JES, JER, PDF,  $\mu_r$ , and  $\mu_f$  parameters have been randomly shifted. The NLO QCD spectrum (from the PDF ensembles) is shifted using the LO QCD JES/JER spectral residuals in order to approximate the effect of the JES and JER uncertainties in this spectrum.

The result of the above procedure is an ensemble of sets of properly correlated spectra  $\text{QCD}_{\text{NLO}} + \text{CI}(\Lambda)$  with  $\Lambda = 3, 5, 8$ , and 12 TeV, in which the JES, JER, PDF,  $\mu_r$  and  $\mu_f$  parameters vary randomly. The ansatz in Eq. (4) is then fitted to the quartet of ratios  $[\text{QCD}_{\text{NLO}} + \text{CI}(\Lambda)] / \text{QCD}_{\text{NLO}}$  as described in Section 5.1 to obtain parameter values for  $p_1, p_2, p_3$ , and  $p_4$ . Five hundred sets of these parameters are generated, constituting a discrete approximation to the prior  $\pi(\omega) \equiv \pi(p_1, p_2, p_3, p_4)$ .

## B.2 CL<sub>s</sub> calculation

Since CL<sub>s</sub> is a criterion rather than a method, it is necessary to document exactly how a CL<sub>s</sub> limit is calculated. Such a calculation requires two elements: a test statistic  $Q$  that depends on the quantity of interest and its sampling distribution for two different hypotheses, here  $\lambda > 0$ , which we denote by  $H_\lambda$ , and  $\lambda = 0$ , which we denote by  $H_0$ .  $H_\lambda$  is the signal plus background hypothesis while  $H_0$  is the background-only hypothesis. For this study, we use the statistic

$$Q(\lambda) = t(D, \lambda) \equiv -2 \ln [p(D|\lambda)/p(D|0)], \quad (7)$$

where  $p(D|\lambda)$  is the marginal likelihood

$$\begin{aligned} p(D|\lambda) &= \int p(D|\lambda, \omega) \pi(\omega) d\omega, \\ &\approx \frac{1}{M} \sum_{m=1}^M p(D|\lambda, \omega_m), \end{aligned} \quad (8)$$

where  $M = 500$  is the number of points  $\omega = p_1, p_2, p_3, p_4$  sampled from the nuisance prior  $\pi(\omega)$  described in Appendix B.1. We compute the sampling distributions

$$p(Q|H_\lambda) = \int \delta[Q - t(D, \lambda)] p(D|\lambda) dD, \quad (9)$$

and

$$p(Q|H_0) = \int \delta[Q - t(D, \lambda)] p(D|0) dD, \quad (10)$$

pertaining to the hypotheses  $H_\lambda$  and  $H_0$ , respectively, and solve

$$\text{CL}_s \equiv p(\lambda)/p(0) = 0.05, \quad (11)$$

to obtain a 95 % confidence level ( $\text{CL}_s$ ) upper limit on  $\lambda$ , where the p-value  $p(\lambda)$  is defined by

$$p(\lambda) = \Pr[Q(\lambda) > Q_0(\lambda)], \quad (12)$$

and  $Q_0$  is the observed value of  $Q$ .

In practice, the  $\text{CL}_s$  limits are approximated as follows:

1. Choose a value of  $\lambda$ , say  $\lambda^*$ , and compute the observed value of  $Q$ ,  $Q_0(\lambda^*)$ .
2. Choose at random one of the  $M = 500$  sets of nuisance parameters  $p_1, p_2, p_3$ , and  $p_4$ .
3. Generate a spectrum of  $K = 20$  counts,  $D$ , according to the multinomial distribution, Eq. (5), with  $\lambda = \lambda^*$ , which corresponds to the hypothesis  $H_\lambda$ . Compute  $Q = t(D, \lambda^*)$  and keep track of how often  $Q(\lambda^*) > Q_0(\lambda^*)$ . Call this count  $n_\lambda$ .
4. Generate another set of 20 counts,  $D$ , but with  $\lambda = 0$ , corresponding to the hypothesis  $H_0$ . Compute  $Q = t(D, \lambda^*)$  and keep track of how often  $Q(\lambda^*) > Q_0(\lambda^*)$ . Call this count  $n_0$ .
5. Repeat 25,000 times steps 2 to 4, compute  $\text{CL}_s \approx n_\lambda/n_0$  and report  $\lambda = \lambda^*$  as the upper limit on  $\lambda$  at 95% CL if  $\text{CL}_s$  is sufficiently close to 0.05; otherwise, keep repeating steps 1 to 4 with different values of  $\lambda$ . The algorithm starts with two values of  $\lambda$  that are likely to bracket the solution and the solution is found using a binary search, which typically requires about 10 to 15 iterations.

### B.3 Bayesian calculation

The Bayesian limit calculations use the marginal likelihood, Eq. (8), and two different (formal) priors  $\pi(\lambda)$ : a prior flat in  $\lambda$  and a reference prior [33–35], which we calculate numerically [35]. An upper limit on  $\lambda$ ,  $\lambda^*$ , is computed by solving

$$\int_0^{\lambda^*} p(D|\lambda) \pi(\lambda) d\lambda / p(D) = 0.95, \quad (13)$$

where  $p(D)$  is a normalization constant. The integrals are performed using numerical quadrature.



## A The CMS Collaboration

### Yerevan Physics Institute, Yerevan, Armenia

S. Chatrchyan, V. Khachatryan, A.M. Sirunyan, A. Tumasyan

### Institut für Hochenergiephysik der OeAW, Wien, Austria

W. Adam, E. Aguilo, T. Bergauer, M. Dragicevic, J. Erö, C. Fabjan<sup>1</sup>, M. Friedl, R. Frühwirth<sup>1</sup>, V.M. Ghete, N. Hörmann, J. Hrubec, M. Jeitler<sup>1</sup>, W. Kiesenhofer, V. Knünz, M. Krammer<sup>1</sup>, I. Krätschmer, D. Liko, I. Mikulec, M. Pernicka<sup>†</sup>, D. Rabady<sup>2</sup>, B. Rahbaran, C. Rohringer, H. Rohringer, R. Schöfbeck, J. Strauss, A. Taurok, W. Waltenberger, C.-E. Wulz<sup>1</sup>

### National Centre for Particle and High Energy Physics, Minsk, Belarus

V. Mossolov, N. Shumeiko, J. Suarez Gonzalez

### Universiteit Antwerpen, Antwerpen, Belgium

M. Bansal, S. Bansal, T. Cornelis, E.A. De Wolf, X. Janssen, S. Luyckx, L. Mucibello, S. Ochesanu, B. Roland, R. Rougny, M. Selvaggi, H. Van Haevermaet, P. Van Mechelen, N. Van Remortel, A. Van Spilbeeck

### Vrije Universiteit Brussel, Brussel, Belgium

F. Blekman, S. Blyweert, J. D'Hondt, R. Gonzalez Suarez, A. Kalogeropoulos, M. Maes, A. Olbrechts, W. Van Doninck, P. Van Mulders, G.P. Van Onsem, I. Villella

### Université Libre de Bruxelles, Bruxelles, Belgium

B. Clerbaux, G. De Lentdecker, V. Dero, A.P.R. Gay, T. Hreus, A. Léonard, P.E. Marage, A. Mohammadi, T. Reis, L. Thomas, C. Vander Velde, P. Vanlaer, J. Wang

### Ghent University, Ghent, Belgium

V. Adler, K. Bernaert, A. Cimmino, S. Costantini, G. Garcia, M. Grunewald, B. Klein, J. Lellouch, A. Marinov, J. McCartin, A.A. Ocampo Rios, D. Ryckbosch, N. Strobbe, F. Thyssen, M. Tytgat, S. Walsh, E. Yazgan, N. Zaganidis

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

S. Basegmez, G. Bruno, R. Castello, L. Ceard, C. Delaere, T. du Pree, D. Favart, L. Forthomme, A. Giammanco<sup>3</sup>, J. Hollar, V. Lemaitre, J. Liao, O. Militaru, C. Nuttens, D. Pagano, A. Pin, K. Piotrkowski, J.M. Vizan Garcia

### Université de Mons, Mons, Belgium

N. Belyi, T. Caebergs, E. Daubie, G.H. Hammad

### Centro Brasileiro de Pesquisas Fisicas, Rio de Janeiro, Brazil

G.A. Alves, M. Correa Martins Junior, T. Martins, M.E. Pol, M.H.G. Souza

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

W.L. Aldá Júnior, W. Carvalho, A. Custódio, E.M. Da Costa, D. De Jesus Damiao, C. De Oliveira Martins, S. Fonseca De Souza, H. Malbouisson, M. Malek, D. Matos Figueiredo, L. Mundim, H. Nogima, W.L. Prado Da Silva, A. Santoro, L. Soares Jorge, A. Sznajder, A. Vilela Pereira

### Universidade Estadual Paulista <sup>a</sup>, Universidade Federal do ABC <sup>b</sup>, São Paulo, Brazil

T.S. Anjos<sup>b</sup>, C.A. Bernardes<sup>b</sup>, F.A. Dias<sup>a,4</sup>, T.R. Fernandez Perez Tomei<sup>a</sup>, E.M. Gregores<sup>b</sup>, C. Lagana<sup>a</sup>, F. Marinho<sup>a</sup>, P.G. Mercadante<sup>b</sup>, S.F. Novaes<sup>a</sup>, Sandra S. Padula<sup>a</sup>

### Institute for Nuclear Research and Nuclear Energy, Sofia, Bulgaria

V. Genchev<sup>2</sup>, P. Iaydjiev<sup>2</sup>, S. Piperov, M. Rodozov, S. Stoykova, G. Sultanov, V. Tcholakov, R. Trayanov, M. Vutova

**University of Sofia, Sofia, Bulgaria**

A. Dimitrov, R. Hadjiiska, V. Kozhuharov, L. Litov, B. Pavlov, P. Petkov

**Institute of High Energy Physics, Beijing, China**

J.G. Bian, G.M. Chen, H.S. Chen, C.H. Jiang, D. Liang, S. Liang, X. Meng, J. Tao, J. Wang, X. Wang, Z. Wang, H. Xiao, M. Xu, J. Zang, Z. Zhang

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

C. Asawatangtrakuldee, Y. Ban, Y. Guo, W. Li, S. Liu, Y. Mao, S.J. Qian, H. Teng, D. Wang, L. Zhang, W. Zou

**Universidad de Los Andes, Bogota, Colombia**

C. Avila, J.P. Gomez, B. Gomez Moreno, A.F. Osorio Oliveros, J.C. Sanabria

**Technical University of Split, Split, Croatia**

N. Godinovic, D. Lelas, R. Plestina<sup>5</sup>, D. Polic, I. Puljak<sup>2</sup>

**University of Split, Split, Croatia**

Z. Antunovic, M. Kovac

**Institute Rudjer Boskovic, Zagreb, Croatia**

V. Brigljevic, S. Duric, K. Kadija, J. Luetic, D. Mekterovic, S. Morovic

**University of Cyprus, Nicosia, Cyprus**

A. Attikis, M. Galanti, G. Mavromanolakis, J. Mousa, C. Nicolaou, F. Ptochos, P.A. Razis

**Charles University, Prague, Czech Republic**

M. Finger, M. Finger Jr.

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

Y. Assran<sup>6</sup>, S. Elgammal<sup>7</sup>, A. Ellithi Kamel<sup>8</sup>, M.A. Mahmoud<sup>9</sup>, A. Mahrous<sup>10</sup>, A. Radi<sup>11,12</sup>

**National Institute of Chemical Physics and Biophysics, Tallinn, Estonia**

M. Kadastik, M. Müntel, M. Raidal, L. Rebane, A. Tiko

**Department of Physics, University of Helsinki, Helsinki, Finland**

P. Eerola, G. Fedi, M. Voutilainen

**Helsinki Institute of Physics, Helsinki, Finland**

J. Härkönen, A. Heikkinen, V. Karimäki, R. Kinnunen, M.J. Kortelainen, T. Lampén, K. Lassila-Perini, S. Lehti, T. Lindén, P. Luukka, T. Mäenpää, T. Peltola, E. Tuominen, J. Tuominiemi, E. Tuovinen, D. Ungaro, L. Wendland

**Lappeenranta University of Technology, Lappeenranta, Finland**

K. Banzuzi, A. Karjalainen, A. Korpela, T. Tuuva

**DSM/IRFU, CEA/Saclay, Gif-sur-Yvette, France**

M. Besancon, S. Choudhury, M. Dejardin, D. Denegri, B. Fabbro, J.L. Faure, F. Ferri, S. Ganjour, A. Givernaud, P. Gras, G. Hamel de Monchenault, P. Jarry, E. Locci, J. Malcles, L. Millischer, A. Nayak, J. Rander, A. Rosowsky, M. Titov

**Laboratoire Leprince-Ringuet, Ecole Polytechnique, IN2P3-CNRS, Palaiseau, France**

S. Baffioni, F. Beaudette, L. Benhabib, L. Bianchini, M. Bluj<sup>13</sup>, P. Busson, C. Charlot, N. Daci, T. Dahms, M. Dalchenko, L. Dobrzynski, A. Florent, R. Granier de Cassagnac, M. Haguenaer, P. Miné, C. Mironov, I.N. Naranjo, M. Nguyen, C. Ochando, P. Paganini, D. Sabes, R. Salerno, Y. Sirois, C. Veelken, A. Zabi

**Institut Pluridisciplinaire Hubert Curien, Université de Strasbourg, Université de Haute Alsace Mulhouse, CNRS/IN2P3, Strasbourg, France**

J.-L. Agram<sup>14</sup>, J. Andrea, D. Bloch, D. Bodin, J.-M. Brom, M. Cardaci, E.C. Chabert, C. Collard, E. Conte<sup>14</sup>, F. Drouhin<sup>14</sup>, J.-C. Fontaine<sup>14</sup>, D. Gelé, U. Goerlach, P. Juillot, A.-C. Le Bihan, P. Van Hove

**Centre de Calcul de l'Institut National de Physique Nucleaire et de Physique des Particules, CNRS/IN2P3, Villeurbanne, France**

F. Fassi, D. Mercier

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

S. Beauceron, N. Beaupere, O. Bondu, G. Boudoul, J. Chasserat, R. Chierici<sup>2</sup>, D. Contardo, P. Depasse, H. El Mamouni, J. Fay, S. Gascon, M. Gouzevitch, B. Ille, T. Kurca, M. Lethuillier, L. Mirabito, S. Perries, L. Sgandurra, V. Sordini, Y. Tschudi, P. Verdier, S. Viret

**Institute of High Energy Physics and Informatization, Tbilisi State University, Tbilisi, Georgia**

Z. Tsamalaidze<sup>15</sup>

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

C. Autermann, S. Beranek, B. Calpas, M. Edelhoff, L. Feld, N. Heracleous, O. Hindrichs, R. Jussen, K. Klein, J. Merz, A. Ostapchuk, A. Perieanu, F. Raupach, J. Sammet, S. Schael, D. Sprenger, H. Weber, B. Wittmer, V. Zhukov<sup>16</sup>

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

M. Ata, J. Caudron, E. Dietz-Laursonn, D. Duchardt, M. Erdmann, R. Fischer, A. Güth, T. Hebbeker, C. Heidemann, K. Hoepfner, D. Klingebiel, P. Kreuzer, M. Merschmeyer, A. Meyer, M. Olschewski, P. Papacz, H. Pieta, H. Reithler, S.A. Schmitz, L. Sonnenschein, J. Steggemann, D. Teyssier, S. Thüer, M. Weber

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

M. Bontenackels, V. Cherepanov, Y. Erdogan, G. Flügge, H. Geenen, M. Geisler, W. Haj Ahmad, F. Hoehle, B. Kargoll, T. Kress, Y. Kuessel, J. Lingemann<sup>2</sup>, A. Nowack, L. Perchalla, O. Pooth, P. Sauerland, A. Stahl

**Deutsches Elektronen-Synchrotron, Hamburg, Germany**

M. Aldaya Martin, J. Behr, W. Behrenhoff, U. Behrens, M. Bergholz<sup>17</sup>, A. Bethani, K. Borras, A. Burgmeier, A. Cakir, L. Calligaris, A. Campbell, E. Castro, F. Costanza, D. Dammann, C. Diez Pardos, G. Eckerlin, D. Eckstein, G. Flucke, A. Geiser, I. Glushkov, P. Gunnellini, S. Habib, J. Hauk, G. Hellwig, H. Jung, M. Kasemann, P. Katsas, C. Kleinwort, H. Kluge, A. Knutsson, M. Krämer, D. Krücker, E. Kuznetsova, W. Lange, J. Leonard, W. Lohmann<sup>17</sup>, B. Lutz, R. Mankel, I. Marfin, M. Marienfeld, I.-A. Melzer-Pellmann, A.B. Meyer, J. Mnich, A. Mussgiller, S. Naumann-Emme, O. Novgorodova, J. Olzem, H. Perrey, A. Petrukhin, D. Pitzl, A. Raspereza, P.M. Ribeiro Cipriano, C. Riedl, E. Ron, M. Rosin, J. Salfeld-Nebgen, R. Schmidt<sup>17</sup>, T. Schoerner-Sadenius, N. Sen, A. Spiridonov, M. Stein, R. Walsh, C. Wissing

**University of Hamburg, Hamburg, Germany**

V. Blobel, H. Enderle, J. Erfle, U. Gebbert, M. Görner, M. Gosselink, J. Haller, T. Hermanns, R.S. Höing, K. Kaschube, G. Kaussen, H. Kirschenmann, R. Klanner, J. Lange, F. Nowak, T. Peiffer, N. Pietsch, D. Rathjens, C. Sander, H. Schettler, P. Schleper, E. Schlieckau, A. Schmidt, M. Schröder, T. Schum, M. Seidel, J. Sibille<sup>18</sup>, V. Sola, H. Stadie, G. Steinbrück, J. Thomsen, L. Vanelderen

**Institut für Experimentelle Kernphysik, Karlsruhe, Germany**

C. Barth, J. Berger, C. Böser, T. Chwalek, W. De Boer, A. Descroix, A. Dierlamm, M. Feindt, M. Guthoff<sup>2</sup>, C. Hackstein, F. Hartmann<sup>2</sup>, T. Hauth<sup>2</sup>, M. Heinrich, H. Held, K.H. Hoffmann, U. Husemann, I. Katkov<sup>16</sup>, J.R. Komaragiri, P. Lobelle Pardo, D. Martschei, S. Mueller, Th. Müller, M. Niegel, A. Nürnberg, O. Oberst, A. Oehler, J. Ott, G. Quast, K. Rabbertz, F. Ratnikov, N. Ratnikova, S. Röcker, F.-P. Schilling, G. Schott, H.J. Simonis, F.M. Stober, D. Troendle, R. Ulrich, J. Wagner-Kuhr, S. Wayand, T. Weiler, M. Zeise

**Institute of Nuclear Physics "Demokritos", Aghia Paraskevi, Greece**

G. Anagnostou, G. Daskalakis, T. Gerasis, S. Kesisoglou, A. Kyriakis, D. Loukas, I. Manolakos, A. Markou, C. Markou, E. Ntomari

**University of Athens, Athens, Greece**

L. Gouskos, T.J. Mertzimekis, A. Panagiotou, N. Saoulidou

**University of Ioánnina, Ioánnina, Greece**

I. Evangelou, C. Foudas, P. Kokkas, N. Manthos, I. Papadopoulos, V. Patras

**KFKI Research Institute for Particle and Nuclear Physics, Budapest, Hungary**

G. Bencze, C. Hajdu, P. Hidas, D. Horvath<sup>19</sup>, F. Sikler, V. Veszpremi, G. Vesztergombi<sup>20</sup>

**Institute of Nuclear Research ATOMKI, Debrecen, Hungary**

N. Beni, S. Czellar, J. Molnar, J. Palinkas, Z. Szillasi

**University of Debrecen, Debrecen, Hungary**

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

**Panjab University, Chandigarh, India**

S.B. Beri, V. Bhatnagar, N. Dhingra, R. Gupta, M. Kaur, M.Z. Mehta, N. Nishu, L.K. Saini, A. Sharma, J.B. Singh

**University of Delhi, Delhi, India**

Ashok Kumar, Arun Kumar, S. Ahuja, A. Bhardwaj, B.C. Choudhary, S. Malhotra, M. Naimuddin, K. Ranjan, V. Sharma, R.K. Shivpuri

**Saha Institute of Nuclear Physics, Kolkata, India**

S. Banerjee, S. Bhattacharya, S. Dutta, B. Gomber, Sa. Jain, Sh. Jain, R. Khurana, S. Sarkar, M. Sharan

**Bhabha Atomic Research Centre, Mumbai, India**

A. Abdulsalam, D. Dutta, S. Kailas, V. Kumar, A.K. Mohanty<sup>2</sup>, L.M. Pant, P. Shukla

**Tata Institute of Fundamental Research - EHEP, Mumbai, India**

T. Aziz, S. Ganguly, M. Guchait<sup>21</sup>, A. Gurtu<sup>22</sup>, M. Maity<sup>23</sup>, G. Majumder, K. Mazumdar, G.B. Mohanty, B. Parida, K. Sudhakar, N. Wickramage

**Tata Institute of Fundamental Research - HECR, Mumbai, India**

S. Banerjee, S. Dugad

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

H. Arfaei<sup>24</sup>, H. Bakhshiansohi, S.M. Etesami<sup>25</sup>, A. Fahim<sup>24</sup>, M. Hashemi<sup>26</sup>, H. Hesari, A. Jafari, M. Khakzad, M. Mohammadi Najafabadi, S. Paktinat Mehdiabadi, B. Safarzadeh<sup>27</sup>, M. Zeinali

**INFN Sezione di Bari <sup>a</sup>, Università di Bari <sup>b</sup>, Politecnico di Bari <sup>c</sup>, Bari, Italy**

M. Abbrescia<sup>a,b</sup>, L. Barbone<sup>a,b</sup>, C. Calabria<sup>a,b,2</sup>, S.S. Chhibra<sup>a,b</sup>, A. Colaleo<sup>a</sup>, D. Creanza<sup>a,c</sup>, N. De Filippis<sup>a,c,2</sup>, M. De Palma<sup>a,b</sup>, L. Fiore<sup>a</sup>, G. Iaselli<sup>a,c</sup>, G. Maggi<sup>a,c</sup>, M. Maggi<sup>a</sup>, B. Marangelli<sup>a,b</sup>,

S. My<sup>a,c</sup>, S. Nuzzo<sup>a,b</sup>, N. Pacifico<sup>a</sup>, A. Pompili<sup>a,b</sup>, G. Pugliese<sup>a,c</sup>, G. Selvaggi<sup>a,b</sup>, L. Silvestris<sup>a</sup>, G. Singh<sup>a,b</sup>, R. Venditti<sup>a,b</sup>, P. Verwilligen<sup>a</sup>, G. Zito<sup>a</sup>

**INFN Sezione di Bologna<sup>a</sup>, Università di Bologna<sup>b</sup>, Bologna, Italy**

G. Abbiendi<sup>a</sup>, A.C. Benvenuti<sup>a</sup>, D. Bonacorsi<sup>a,b</sup>, S. Braibant-Giacomelli<sup>a,b</sup>, L. Brigliadori<sup>a,b</sup>, P. Capiluppi<sup>a,b</sup>, A. Castro<sup>a,b</sup>, F.R. Cavallo<sup>a</sup>, M. Cuffiani<sup>a,b</sup>, G.M. Dallavalle<sup>a</sup>, F. Fabbri<sup>a</sup>, A. Fanfani<sup>a,b</sup>, D. Fasanella<sup>a,b</sup>, P. Giacomelli<sup>a</sup>, C. Grandi<sup>a</sup>, L. Guiducci<sup>a,b</sup>, S. Marcellini<sup>a</sup>, G. Masetti<sup>a</sup>, M. Meneghelli<sup>a,b,2</sup>, A. Montanari<sup>a</sup>, F.L. Navarria<sup>a,b</sup>, F. Odorici<sup>a</sup>, A. Perrotta<sup>a</sup>, F. Primavera<sup>a,b</sup>, A.M. Rossi<sup>a,b</sup>, T. Rovelli<sup>a,b</sup>, G.P. Siroli<sup>a,b</sup>, N. Tosi, R. Travaglini<sup>a,b</sup>

**INFN Sezione di Catania<sup>a</sup>, Università di Catania<sup>b</sup>, Catania, Italy**

S. Albergo<sup>a,b</sup>, G. Cappello<sup>a,b</sup>, M. Chiorboli<sup>a,b</sup>, S. Costa<sup>a,b</sup>, R. Potenza<sup>a,b</sup>, A. Tricomi<sup>a,b</sup>, C. Tuve<sup>a,b</sup>

**INFN Sezione di Firenze<sup>a</sup>, Università di Firenze<sup>b</sup>, Firenze, Italy**

G. Barbagli<sup>a</sup>, V. Ciulli<sup>a,b</sup>, C. Civinini<sup>a</sup>, R. D'Alessandro<sup>a,b</sup>, E. Focardi<sup>a,b</sup>, S. Frosali<sup>a,b</sup>, E. Gallo<sup>a</sup>, S. Gonzi<sup>a,b</sup>, M. Meschini<sup>a</sup>, S. Paoletti<sup>a</sup>, G. Sguazzoni<sup>a</sup>, A. Tropiano<sup>a,b</sup>

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

L. Benussi, S. Bianco, S. Colafranceschi<sup>28</sup>, F. Fabbri, D. Piccolo

**INFN Sezione di Genova<sup>a</sup>, Università di Genova<sup>b</sup>, Genova, Italy**

P. Fabbricatore<sup>a</sup>, R. Musenich<sup>a</sup>, S. Tosi<sup>a,b</sup>

**INFN Sezione di Milano-Bicocca<sup>a</sup>, Università di Milano-Bicocca<sup>b</sup>, Milano, Italy**

A. Benaglia<sup>a</sup>, F. De Guio<sup>a,b</sup>, L. Di Matteo<sup>a,b,2</sup>, S. Fiorendi<sup>a,b</sup>, S. Gennai<sup>a,2</sup>, A. Ghezzi<sup>a,b</sup>, S. Malvezzi<sup>a</sup>, R.A. Manzoni<sup>a,b</sup>, A. Martelli<sup>a,b</sup>, A. Massironi<sup>a,b</sup>, D. Menasce<sup>a</sup>, L. Moroni<sup>a</sup>, M. Paganoni<sup>a,b</sup>, D. Pedrini<sup>a</sup>, S. Ragazzi<sup>a,b</sup>, N. Redaelli<sup>a</sup>, S. Sala<sup>a</sup>, T. Tabarelli de Fatis<sup>a,b</sup>

**INFN Sezione di Napoli<sup>a</sup>, Università di Napoli 'Federico II'<sup>b</sup>, Università della Basilicata (Potenza)<sup>c</sup>, Università G. Marconi (Roma)<sup>d</sup>, Napoli, Italy**

S. Buontempo<sup>a</sup>, C.A. Carrillo Montoya<sup>a</sup>, N. Cavallo<sup>a,c</sup>, A. De Cosa<sup>a,b,2</sup>, O. Dogangun<sup>a,b</sup>, F. Fabozzi<sup>a,c</sup>, A.O.M. Iorio<sup>a,b</sup>, L. Lista<sup>a</sup>, S. Meola<sup>a,d,29</sup>, M. Merola<sup>a</sup>, P. Paolucci<sup>a,2</sup>

**INFN Sezione di Padova<sup>a</sup>, Università di Padova<sup>b</sup>, Università di Trento (Trento)<sup>c</sup>, Padova, Italy**

P. Azzi<sup>a</sup>, N. Bacchetta<sup>a,2</sup>, D. Bisello<sup>a,b</sup>, A. Branca<sup>a,b,2</sup>, R. Carlin<sup>a,b</sup>, P. Checchia<sup>a</sup>, T. Dorigo<sup>a</sup>, U. Dosselli<sup>a</sup>, F. Gasparini<sup>a,b</sup>, A. Gozzelino<sup>a</sup>, K. Kanishchev<sup>a,c</sup>, S. Lacaprara<sup>a</sup>, I. Lazzizzera<sup>a,c</sup>, M. Margoni<sup>a,b</sup>, A.T. Meneguzzo<sup>a,b</sup>, J. Pazzini<sup>a,b</sup>, N. Pozzobon<sup>a,b</sup>, P. Ronchese<sup>a,b</sup>, F. Simonetto<sup>a,b</sup>, E. Torassa<sup>a</sup>, M. Tosi<sup>a,b</sup>, S. Vanini<sup>a,b</sup>, P. Zotto<sup>a,b</sup>, A. Zucchetta<sup>a,b</sup>, G. Zumerle<sup>a,b</sup>

**INFN Sezione di Pavia<sup>a</sup>, Università di Pavia<sup>b</sup>, Pavia, Italy**

M. Gabusi<sup>a,b</sup>, S.P. Ratti<sup>a,b</sup>, C. Riccardi<sup>a,b</sup>, P. Torre<sup>a,b</sup>, P. Vitulo<sup>a,b</sup>

**INFN Sezione di Perugia<sup>a</sup>, Università di Perugia<sup>b</sup>, Perugia, Italy**

M. Biasini<sup>a,b</sup>, G.M. Bilei<sup>a</sup>, L. Fanò<sup>a,b</sup>, P. Lariccia<sup>a,b</sup>, G. Mantovani<sup>a,b</sup>, M. Menichelli<sup>a</sup>, A. Nappi<sup>a,b†</sup>, F. Romeo<sup>a,b</sup>, A. Saha<sup>a</sup>, A. Santocchia<sup>a,b</sup>, A. Spiezia<sup>a,b</sup>, S. Taroni<sup>a,b</sup>

**INFN Sezione di Pisa<sup>a</sup>, Università di Pisa<sup>b</sup>, Scuola Normale Superiore di Pisa<sup>c</sup>, Pisa, Italy**

P. Azzurri<sup>a,c</sup>, G. Bagliesi<sup>a</sup>, J. Bernardini<sup>a</sup>, T. Boccali<sup>a</sup>, G. Broccolo<sup>a,c</sup>, R. Castaldi<sup>a</sup>, R.T. D'Agnolo<sup>a,c,2</sup>, R. Dell'Orso<sup>a</sup>, F. Fiori<sup>a,b,2</sup>, L. Foà<sup>a,c</sup>, A. Giassi<sup>a</sup>, A. Kraan<sup>a</sup>, F. Ligabue<sup>a,c</sup>, T. Lomtadze<sup>a</sup>, L. Martini<sup>a,30</sup>, A. Messineo<sup>a,b</sup>, F. Palla<sup>a</sup>, A. Rizzi<sup>a,b</sup>, A.T. Serban<sup>a,31</sup>, P. Spagnolo<sup>a</sup>, P. Squillacioti<sup>a,2</sup>, R. Tenchini<sup>a</sup>, G. Tonelli<sup>a,b</sup>, A. Venturi<sup>a</sup>, P.G. Verdini<sup>a</sup>

**INFN Sezione di Roma<sup>a</sup>, Università di Roma<sup>b</sup>, Roma, Italy**

L. Barone<sup>a,b</sup>, F. Cavallari<sup>a</sup>, D. Del Re<sup>a,b</sup>, M. Diemoz<sup>a</sup>, C. Fanelli<sup>a,b</sup>, M. Grassi<sup>a,b,2</sup>, E. Longo<sup>a,b</sup>

P. Meridiani<sup>a,2</sup>, F. Micheli<sup>a,b</sup>, S. Nourbakhsh<sup>a,b</sup>, G. Organtini<sup>a,b</sup>, R. Paramatti<sup>a</sup>, S. Rahatlou<sup>a,b</sup>, M. Sigamani<sup>a</sup>, L. Soffi<sup>a,b</sup>

**INFN Sezione di Torino<sup>a</sup>, Università di Torino<sup>b</sup>, Università del Piemonte Orientale (Novara)<sup>c</sup>, Torino, Italy**

N. Amapane<sup>a,b</sup>, R. Arcidiacono<sup>a,c</sup>, S. Argiro<sup>a,b</sup>, M. Arneodo<sup>a,c</sup>, C. Biino<sup>a</sup>, N. Cartiglia<sup>a</sup>, S. Casasso<sup>a,b</sup>, M. Costa<sup>a,b</sup>, N. Demaria<sup>a</sup>, C. Mariotti<sup>a,2</sup>, S. Maselli<sup>a</sup>, E. Migliore<sup>a,b</sup>, V. Monaco<sup>a,b</sup>, M. Musich<sup>a,2</sup>, M.M. Obertino<sup>a,c</sup>, N. Pastrone<sup>a</sup>, M. Pelliccioni<sup>a</sup>, A. Potenza<sup>a,b</sup>, A. Romero<sup>a,b</sup>, M. Ruspa<sup>a,c</sup>, R. Sacchi<sup>a,b</sup>, A. Solano<sup>a,b</sup>, A. Staiano<sup>a</sup>

**INFN Sezione di Trieste<sup>a</sup>, Università di Trieste<sup>b</sup>, Trieste, Italy**

S. Belforte<sup>a</sup>, V. Candelise<sup>a,b</sup>, M. Casarsa<sup>a</sup>, F. Cossutti<sup>a</sup>, G. Della Ricca<sup>a,b</sup>, B. Gobbo<sup>a</sup>, M. Marone<sup>a,b,2</sup>, D. Montanino<sup>a,b,2</sup>, A. Penzo<sup>a</sup>, A. Schizzi<sup>a,b</sup>

**Kangwon National University, Chunchon, Korea**

T.Y. Kim, S.K. Nam

**Kyungpook National University, Daegu, Korea**

S. Chang, D.H. Kim, G.N. Kim, D.J. Kong, H. Park, D.C. Son, T. Son

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

J.Y. Kim, Zero J. Kim, S. Song

**Korea University, Seoul, Korea**

S. Choi, D. Gyun, B. Hong, M. Jo, H. Kim, T.J. Kim, K.S. Lee, D.H. Moon, S.K. Park, Y. Roh

**University of Seoul, Seoul, Korea**

M. Choi, J.H. Kim, C. Park, I.C. Park, S. Park, G. Ryu

**Sungkyunkwan University, Suwon, Korea**

Y. Choi, Y.K. Choi, J. Goh, M.S. Kim, E. Kwon, B. Lee, J. Lee, S. Lee, H. Seo, I. Yu

**Vilnius University, Vilnius, Lithuania**

M.J. Bilinskas, I. Grigelionis, M. Janulis, A. Juodagalvis

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

H. Castilla-Valdez, E. De La Cruz-Burelo, I. Heredia-de La Cruz, R. Lopez-Fernandez, J. Martínez-Ortega, A. Sanchez-Hernandez, L.M. Villasenor-Cendejas

**Universidad Iberoamericana, Mexico City, Mexico**

S. Carrillo Moreno, F. Vazquez Valencia

**Benemerita Universidad Autonoma de Puebla, Puebla, Mexico**

H.A. Salazar Ibarguen

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

E. Casimiro Linares, A. Morelos Pineda, M.A. Reyes-Santos

**University of Auckland, Auckland, New Zealand**

D. Krofcheck

**University of Canterbury, Christchurch, New Zealand**

A.J. Bell, P.H. Butler, R. Doesburg, S. Reucroft, H. Silverwood

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

M. Ahmad, M.I. Asghar, J. Butt, H.R. Hoorani, S. Khalid, W.A. Khan, T. Khurshid, S. Qazi, M.A. Shah, M. Shoaib

**National Centre for Nuclear Research, Swierk, Poland**

H. Bialkowska, B. Boimska, T. Frueboes, M. Górski, M. Kazana, K. Nawrocki, K. Romanowska-Rybinska, M. Szeleper, G. Wrochna, P. Zalewski

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

G. Brona, K. Bunkowski, M. Cwiok, W. Dominik, K. Doroba, A. Kalinowski, M. Konecki, J. Krolikowski, M. Misiura

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

N. Almeida, P. Bargassa, A. David, P. Faccioli, P.G. Ferreira Parracho, M. Gallinaro, J. Seixas, J. Varela, P. Vischia

**Joint Institute for Nuclear Research, Dubna, Russia**

P. Bunin, I. Golutvin, A. Kamenev, V. Karjavin, V. Konoplyanikov, G. Kozlov, A. Lanev, A. Malakhov, P. Moisezenz, V. Palichik, V. Perelygin, M. Savina, S. Shmatov, S. Shulha, V. Smirnov, A. Volodko, A. Zarubin

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

S. Evstyukhin, V. Golovtsov, Y. Ivanov, V. Kim, P. Levchenko, V. Murzin, V. Oreshkin, I. Smirnov, V. Sulimov, L. Uvarov, S. Vavilov, A. Vorobyev, An. Vorobyev

**Institute for Nuclear Research, Moscow, Russia**

Yu. Andreev, A. Dermenev, S. Gninenko, N. Golubev, M. Kirsanov, N. Krasnikov, V. Matveev, A. Pashenkov, D. Tlisov, A. Toropin

**Institute for Theoretical and Experimental Physics, Moscow, Russia**

V. Epshteyn, M. Erofeeva, V. Gavrilov, M. Kossov, N. Lychkovskaya, V. Popov, G. Safronov, S. Semenov, I. Shreyber, V. Stolin, E. Vlasov, A. Zhokin

**P.N. Lebedev Physical Institute, Moscow, Russia**

V. Andreev, M. Azarkin, I. Dremin, M. Kirakosyan, A. Leonidov, G. Mesyats, S.V. Rusakov, A. Vinogradov

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

A. Belyaev, E. Boos, V. Bunichev, M. Dubinin<sup>4</sup>, L. Dudko, A. Ershov, A. Gribushin, V. Klyukhin, O. Kodolova, I. Lokhtin, A. Markina, S. Obraztsov, M. Perfilov, S. Petrushanko, A. Popov, L. Sarycheva<sup>†</sup>, V. Savrin

**State Research Center of Russian Federation, Institute for High Energy Physics, Protvino, Russia**

I. Azhgirey, I. Bayshev, S. Bitioukov, V. Grishin<sup>2</sup>, V. Kachanov, D. Konstantinov, V. Krychkin, V. Petrov, R. Ryutin, A. Sobol, L. Tourtchanovitch, S. Troshin, N. Tyurin, A. Uzunian, A. Volkov

**University of Belgrade, Faculty of Physics and Vinca Institute of Nuclear Sciences, Belgrade, Serbia**

P. Adzic<sup>32</sup>, M. Djordjevic, M. Ekmedzic, D. Krpic<sup>32</sup>, J. Milosevic

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

M. Aguilar-Benitez, J. Alcaraz Maestre, P. Arce, C. Battilana, E. Calvo, M. Cerrada, M. Chamizo

Llatas, N. Colino, B. De La Cruz, A. Delgado Peris, D. Domínguez Vázquez, C. Fernandez Bedoya, J.P. Fernández Ramos, A. Ferrando, J. Flix, M.C. Fouz, P. Garcia-Abia, O. Gonzalez Lopez, S. Goy Lopez, J.M. Hernandez, M.I. Josa, G. Merino, J. Puerta Pelayo, A. Quintario Olmeda, I. Redondo, L. Romero, J. Santaolalla, M.S. Soares, C. Willmott

**Universidad Autónoma de Madrid, Madrid, Spain**

C. Albajar, G. Codispoti, J.F. de Trocóniz

**Universidad de Oviedo, Oviedo, Spain**

H. Brun, J. Cuevas, J. Fernandez Menendez, S. Folgueras, I. Gonzalez Caballero, L. Lloret Iglesias, J. Piedra Gomez

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

J.A. Brochero Cifuentes, I.J. Cabrillo, A. Calderon, S.H. Chuang, J. Duarte Campderros, M. Felcini<sup>33</sup>, M. Fernandez, G. Gomez, J. Gonzalez Sanchez, A. Graziano, C. Jorda, A. Lopez Virto, J. Marco, R. Marco, C. Martinez Rivero, F. Matorras, F.J. Munoz Sanchez, T. Rodrigo, A.Y. Rodríguez-Marrero, A. Ruiz-Jimeno, L. Scodellaro, I. Vila, R. Vilar Cortabitarte

**CERN, European Organization for Nuclear Research, Geneva, Switzerland**

D. Abbaneo, E. Auffray, G. Auzinger, M. Bachtis, P. Baillon, A.H. Ball, D. Barney, J.F. Benitez, C. Bernet<sup>5</sup>, G. Bianchi, P. Bloch, A. Bocci, A. Bonato, C. Botta, H. Breuker, T. Camporesi, G. Cerminara, T. Christiansen, J.A. Coarasa Perez, D. D'Enterria, A. Dabrowski, A. De Roeck, S. Di Guida, M. Dobson, N. Dupont-Sagorin, A. Elliott-Peisert, B. Frisch, W. Funk, G. Georgiou, M. Giffels, D. Gigi, K. Gill, D. Giordano, M. Girone, M. Giunta, F. Glege, R. Gomez-Reino Garrido, P. Govoni, S. Gowdy, R. Guida, S. Gundacker, J. Hammer, M. Hansen, P. Harris, C. Hartl, J. Harvey, B. Hegner, A. Hinzmann, V. Innocente, P. Janot, K. Kaadze, E. Karavakis, K. Kousouris, P. Lecoq, Y.-J. Lee, P. Lenzi, C. Lourenço, N. Magini, T. Mäki, M. Malberti, L. Malgeri, M. Mannelli, L. Masetti, F. Meijers, S. Mersi, E. Meschi, R. Moser, M.U. Mozer, M. Mulders, P. Musella, E. Nesvold, L. Orsini, E. Palencia Cortezon, E. Perez, L. Perrozzi, A. Petrilli, A. Pfeiffer, M. Pierini, M. Pimiä, D. Piparo, G. Polese, L. Quertenmont, A. Racz, W. Reece, J. Rodrigues Antunes, G. Rolandi<sup>34</sup>, C. Rovelli<sup>35</sup>, M. Rovere, H. Sakulin, F. Santanastasio, C. Schäfer, C. Schwick, I. Segoni, S. Sekmen, A. Sharma, P. Siegrist, P. Silva, M. Simon, P. Sphicas<sup>36</sup>, D. Spiga, A. Tsiros, G.I. Veres<sup>20</sup>, J.R. Vlimant, H.K. Wöhri, S.D. Worm<sup>37</sup>, W.D. Zeuner

**Paul Scherrer Institut, Villigen, Switzerland**

W. Bertl, K. Deiters, W. Erdmann, K. Gabathuler, R. Horisberger, Q. Ingram, H.C. Kaestli, S. König, D. Kotlinski, U. Langenegger, F. Meier, D. Renker, T. Rohe

**Institute for Particle Physics, ETH Zurich, Zurich, Switzerland**

L. Bäni, P. Bortignon, M.A. Buchmann, B. Casal, N. Chanon, A. Deisher, G. Dissertori, M. Dittmar, M. Donegà, M. Dünser, P. Eller, J. Eugster, K. Freudenreich, C. Grab, D. Hits, P. Lecomte, W. Luster, A.C. Marini, P. Martinez Ruiz del Arbol, N. Mohr, F. Moortgat, C. Nägeli<sup>38</sup>, P. Nef, F. Nessi-Tedaldi, F. Pandolfi, L. Pape, F. Pauss, M. Peruzzi, F.J. Ronga, M. Rossini, L. Sala, A.K. Sanchez, A. Starodumov<sup>39</sup>, B. Stieger, M. Takahashi, L. Tauscher<sup>†</sup>, A. Thea, K. Theofilatos, D. Treille, C. Urscheler, R. Wallny, H.A. Weber, L. Wehrli

**Universität Zürich, Zurich, Switzerland**

C. AMSLER<sup>40</sup>, V. Chiochia, S. De Visscher, C. Favaro, M. Ivova Rikova, B. Kilminster, B. Millan Mejias, P. Otiougova, P. Robmann, H. Snoek, S. Tuppiti, M. Verzetti

**National Central University, Chung-Li, Taiwan**

Y.H. Chang, K.H. Chen, C. Ferro, C.M. Kuo, S.W. Li, W. Lin, Y.J. Lu, A.P. Singh, R. Volpe, S.S. Yu



**National Taiwan University (NTU), Taipei, Taiwan**

P. Bartalini, P. Chang, Y.H. Chang, Y.W. Chang, Y. Chao, K.F. Chen, C. Dietz, U. Grundler, W.-S. Hou, Y. Hsiung, K.Y. Kao, Y.J. Lei, R.-S. Lu, D. Majumder, E. Petrakou, X. Shi, J.G. Shiu, Y.M. Tzeng, X. Wan, M. Wang

**Chulalongkorn University, Bangkok, Thailand**

B. Asavapibhop, N. Srimanobhas

**Cukurova University, Adana, Turkey**

A. Adiguzel, M.N. Bakirci<sup>41</sup>, S. Cerci<sup>42</sup>, C. Dozen, I. Dumanoglu, E. Eskut, S. Girgis, G. Gokbulut, E. Gurpinar, I. Hos, E.E. Kangal, T. Karaman, G. Karapinar<sup>43</sup>, A. Kayis Topaksu, G. Onengut, K. Ozdemir, S. Ozturk<sup>44</sup>, A. Polatoz, K. Sogut<sup>45</sup>, D. Sunar Cerci<sup>42</sup>, B. Tali<sup>42</sup>, H. Topakli<sup>41</sup>, L.N. Vergili, M. Vergili

**Middle East Technical University, Physics Department, Ankara, Turkey**

I.V. Akin, T. Aliev, B. Bilin, S. Bilmis, M. Deniz, H. Gamsizkan, A.M. Guler, K. Ocalan, A. Ozpineci, M. Serin, R. Sever, U.E. Surat, M. Yalvac, E. Yildirim, M. Zeyrek

**Bogazici University, Istanbul, Turkey**

E. Gülmez, B. Isildak<sup>46</sup>, M. Kaya<sup>47</sup>, O. Kaya<sup>47</sup>, S. Ozkorucuklu<sup>48</sup>, N. Sonmez<sup>49</sup>

**Istanbul Technical University, Istanbul, Turkey**

K. Cankocak

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

L. Levchuk

**University of Bristol, Bristol, United Kingdom**

J.J. Brooke, E. Clement, D. Cussans, H. Flacher, R. Frazier, J. Goldstein, M. Grimes, G.P. Heath, H.F. Heath, L. Kreczko, S. Metson, D.M. Newbold<sup>37</sup>, K. Nirunpong, A. Poll, S. Senkin, V.J. Smith, T. Williams

**Rutherford Appleton Laboratory, Didcot, United Kingdom**

L. Basso<sup>50</sup>, K.W. Bell, A. Belyaev<sup>50</sup>, C. Brew, R.M. Brown, D.J.A. Cockerill, J.A. Coughlan, K. Harder, S. Harper, J. Jackson, B.W. Kennedy, E. Olaiya, D. Petyt, B.C. Radburn-Smith, C.H. Shepherd-Themistocleous, I.R. Tomalin, W.J. Womersley

**Imperial College, London, United Kingdom**

R. Bainbridge, G. Ball, R. Beuselinck, O. Buchmuller, D. Colling, N. Cripps, M. Cutajar, P. Dauncey, G. Davies, M. Della Negra, W. Ferguson, J. Fulcher, D. Futyan, A. Gilbert, A. Guneratne Bryer, G. Hall, Z. Hatherell, J. Hays, G. Iles, M. Jarvis, G. Karapostoli, L. Lyons, A.-M. Magnan, J. Marrouche, B. Mathias, R. Nandi, J. Nash, A. Nikitenko<sup>39</sup>, J. Pela, M. Pesaresi, K. Petridis, M. Pioppi<sup>51</sup>, D.M. Raymond, S. Rogerson, A. Rose, M.J. Ryan, C. Seez, P. Sharp<sup>†</sup>, A. Sparrow, M. Stoye, A. Tapper, M. Vazquez Acosta, T. Virdee, S. Wakefield, N. Wardle, T. Whyntie

**Brunel University, Uxbridge, United Kingdom**

M. Chadwick, J.E. Cole, P.R. Hobson, A. Khan, P. Kyberd, D. Leggat, D. Leslie, W. Martin, I.D. Reid, P. Symonds, L. Teodorescu, M. Turner

**Baylor University, Waco, USA**

K. Hatakeyama, H. Liu, T. Scarborough

**The University of Alabama, Tuscaloosa, USA**

O. Charaf, C. Henderson, P. Rumerio

**Boston University, Boston, USA**

A. Avetisyan, T. Bose, C. Fantasia, A. Heister, P. Lawson, D. Lazic, J. Rohlf, D. Sperka, J. St. John, L. Sulak

**Brown University, Providence, USA**

J. Alimena, S. Bhattacharya, G. Christopher, D. Cutts, Z. Demiragli, A. Ferapontov, A. Garabedian, U. Heintz, S. Jabeen, G. Kukartsev, E. Laird, G. Landsberg, M. Luk, M. Narain, D. Nguyen, M. Segala, T. Sinthuprasith, T. Speer

**University of California, Davis, Davis, USA**

R. Breedon, G. Breto, M. Calderon De La Barca Sanchez, S. Chauhan, M. Chertok, J. Conway, R. Conway, P.T. Cox, J. Dolen, R. Erbacher, M. Gardner, R. Houtz, W. Ko, A. Kopecky, R. Lander, O. Mall, T. Miceli, D. Pellett, F. Ricci-Tam, B. Rutherford, M. Searle, J. Smith, M. Squires, M. Tripathi, R. Vasquez Sierra, R. Yohay

**University of California, Los Angeles, USA**

V. Andreev, D. Cline, R. Cousins, J. Duris, S. Erhan, P. Everaerts, C. Farrell, J. Hauser, M. Ignatenko, C. Jarvis, G. Rakness, P. Schlein<sup>†</sup>, P. Traczyk, V. Valuev, M. Weber

**University of California, Riverside, Riverside, USA**

J. Babb, R. Clare, M.E. Dinardo, J. Ellison, J.W. Gary, F. Giordano, G. Hanson, H. Liu, O.R. Long, A. Luthra, H. Nguyen, S. Paramesvaran, J. Sturdy, S. Sumowidagdo, R. Wilken, S. Wimpenny

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

W. Andrews, J.G. Branson, G.B. Cerati, S. Cittolin, D. Evans, A. Holzner, R. Kelley, M. Lebourgeois, J. Letts, I. Macneill, B. Mangano, S. Padhi, C. Palmer, G. Petrucciani, M. Pieri, M. Sani, V. Sharma, S. Simon, E. Sudano, M. Tadel, Y. Tu, A. Vartak, S. Wasserbaech<sup>52</sup>, F. Würthwein, A. Yagil, J. Yoo

**University of California, Santa Barbara, Santa Barbara, USA**

D. Barge, R. Bellan, C. Campagnari, M. D'Alfonso, T. Danielson, K. Flowers, P. Geffert, F. Golf, J. Incandela, C. Justus, P. Kalavase, D. Kovalskyi, V. Krutelyov, S. Lowette, R. Magaña Villalba, N. Mccoll, V. Pavlunin, J. Ribnik, J. Richman, R. Rossin, D. Stuart, W. To, C. West

**California Institute of Technology, Pasadena, USA**

A. Apresyan, A. Bornheim, Y. Chen, E. Di Marco, J. Duarte, M. Gataullin, Y. Ma, A. Mott, H.B. Newman, C. Rogan, M. Spiropulu, V. Timciuc, J. Veverka, R. Wilkinson, S. Xie, Y. Yang, R.Y. Zhu

**Carnegie Mellon University, Pittsburgh, USA**

V. Azzolini, A. Calamba, R. Carroll, T. Ferguson, Y. Iiyama, D.W. Jang, Y.F. Liu, M. Paulini, H. Vogel, I. Vorobiev

**University of Colorado at Boulder, Boulder, USA**

J.P. Cumalat, B.R. Drell, W.T. Ford, A. Gaz, E. Luiggi Lopez, J.G. Smith, K. Stenson, K.A. Ulmer, S.R. Wagner

**Cornell University, Ithaca, USA**

J. Alexander, A. Chatterjee, N. Eggert, L.K. Gibbons, B. Heltsley, W. Hopkins, A. Khukhunaishvili, B. Kreis, N. Mirman, G. Nicolas Kaufman, J.R. Patterson, A. Ryd, E. Salvati, W. Sun, W.D. Teo, J. Thom, J. Thompson, J. Tucker, J. Vaughan, Y. Weng, L. Winstrom, P. Wittich

**Fairfield University, Fairfield, USA**

D. Winn

**Fermi National Accelerator Laboratory, Batavia, USA**

S. Abdullin, M. Albrow, J. Anderson, L.A.T. Bauerdick, A. Beretvas, J. Berryhill, P.C. Bhat, K. Burkett, J.N. Butler, V. Chetluru, H.W.K. Cheung, F. Chlebana, V.D. Elvira, I. Fisk, J. Freeman, Y. Gao, D. Green, O. Gutsche, J. Hanlon, R.M. Harris, J. Hirschauer, B. Hooberman, S. Jindariani, M. Johnson, U. Joshi, B. Klima, S. Kunori, S. Kwan, C. Leonidopoulos<sup>53</sup>, J. Linacre, D. Lincoln, R. Lipton, J. Lykken, K. Maeshima, J.M. Marraffino, S. Maruyama, D. Mason, P. McBride, K. Mishra, S. Mrenna, Y. Musienko<sup>54</sup>, C. Newman-Holmes, V. O'Dell, O. Prokofyev, E. Sexton-Kennedy, S. Sharma, W.J. Spalding, L. Spiegel, L. Taylor, S. Tkaczyk, N.V. Tran, L. Uplegger, E.W. Vaandering, R. Vidal, J. Whitmore, W. Wu, F. Yang, J.C. Yun

**University of Florida, Gainesville, USA**

D. Acosta, P. Avery, D. Bourilkov, M. Chen, T. Cheng, S. Das, M. De Gruttola, G.P. Di Giovanni, D. Dobur, A. Drozdetskiy, R.D. Field, M. Fisher, Y. Fu, I.K. Furic, J. Gartner, J. Hugon, B. Kim, J. Konigsberg, A. Korytov, A. Kropivnitskaya, T. Kypreos, J.F. Low, K. Matchev, P. Milenovic<sup>55</sup>, G. Mitselmakher, L. Muniz, M. Park, R. Remington, A. Rinkevicius, P. Sellers, N. Skhirtladze, M. Snowball, J. Yelton, M. Zakaria

**Florida International University, Miami, USA**

V. Gaultney, S. Hewamanage, L.M. Lebolo, S. Linn, P. Markowitz, G. Martinez, J.L. Rodriguez

**Florida State University, Tallahassee, USA**

T. Adams, A. Askew, J. Bochenek, J. Chen, B. Diamond, S.V. Gleyzer, J. Haas, S. Hagopian, V. Hagopian, M. Jenkins, K.F. Johnson, H. Prosper, V. Veeraraghavan, M. Weinberg

**Florida Institute of Technology, Melbourne, USA**

M.M. Baarmand, B. Dorney, M. Hohlmann, H. Kalakhety, I. Vodopyanov, F. Yumiceva

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

M.R. Adams, I.M. Anghel, L. Apanasevich, Y. Bai, V.E. Bazterra, R.R. Betts, I. Bucinskaite, J. Callner, R. Cavanaugh, O. Evdokimov, L. Gauthier, C.E. Gerber, D.J. Hofman, S. Khalatyan, F. Lacroix, C. O'Brien, C. Silkworth, D. Strom, P. Turner, N. Varelas

**The University of Iowa, Iowa City, USA**

U. Akgun, E.A. Albayrak, B. Bilki<sup>56</sup>, W. Clarida, F. Duru, S. Griffiths, J.-P. Merlo, H. Mermerkaya<sup>57</sup>, A. Mestvirishvili, A. Moeller, J. Nachtman, C.R. Newsom, E. Norbeck, Y. Onel, F. Ozok<sup>58</sup>, S. Sen, P. Tan, E. Tiras, J. Wetzel, T. Yetkin, K. Yi

**Johns Hopkins University, Baltimore, USA**

B.A. Barnett, B. Blumenfeld, S. Bolognesi, D. Fehling, G. Giurgiu, A.V. Gritsan, Z.J. Guo, G. Hu, P. Maksimovic, M. Swartz, A. Whitbeck

**The University of Kansas, Lawrence, USA**

P. Baringer, A. Bean, G. Benelli, R.P. Kenny Iii, M. Murray, D. Noonan, S. Sanders, R. Stringer, G. Tinti, J.S. Wood

**Kansas State University, Manhattan, USA**

A.F. Barfuss, T. Bolton, I. Chakaberia, A. Ivanov, S. Khalil, M. Makouski, Y. Maravin, S. Shrestha, I. Svintradze

**Lawrence Livermore National Laboratory, Livermore, USA**

J. Gronberg, D. Lange, F. Rebassoo, D. Wright

**University of Maryland, College Park, USA**

A. Baden, B. Calvert, S.C. Eno, J.A. Gomez, N.J. Hadley, R.G. Kellogg, M. Kirn, T. Kolberg, Y. Lu, M. Marionneau, A.C. Mignerey, K. Pedro, A. Skuja, J. Temple, M.B. Tonjes, S.C. Tonwar

**Massachusetts Institute of Technology, Cambridge, USA**

A. Apyan, G. Bauer, J. Bendavid, W. Busza, E. Butz, I.A. Cali, M. Chan, V. Dutta, G. Gomez Ceballos, M. Goncharov, Y. Kim, M. Klute, K. Krajczar<sup>59</sup>, A. Levin, P.D. Luckey, T. Ma, S. Nahn, C. Paus, D. Ralph, C. Roland, G. Roland, M. Rudolph, G.S.F. Stephans, F. Stöckli, K. Sumorok, K. Sung, D. Velicanu, E.A. Wenger, R. Wolf, B. Wyslouch, M. Yang, Y. Yilmaz, A.S. Yoon, M. Zanetti, V. Zhukova

**University of Minnesota, Minneapolis, USA**

S.I. Cooper, B. Dahmes, A. De Benedetti, G. Franzoni, A. Gude, S.C. Kao, K. Klapoetke, Y. Kubota, J. Mans, N. Pastika, R. Rusack, M. Sasseville, A. Singovsky, N. Tambe, J. Turkewitz

**University of Mississippi, Oxford, USA**

L.M. Cremaldi, R. Kroeger, L. Perera, R. Rahmat, D.A. Sanders

**University of Nebraska-Lincoln, Lincoln, USA**

E. Avdeeva, K. Bloom, S. Bose, D.R. Claes, A. Dominguez, M. Eads, J. Keller, I. Kravchenko, J. Lazo-Flores, S. Malik, G.R. Snow

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

A. Godshalk, I. Iashvili, S. Jain, A. Kharchilava, A. Kumar, S. Rappoccio

**Northeastern University, Boston, USA**

G. Alverson, E. Barberis, D. Baumgartel, M. Chasco, J. Haley, D. Nash, T. Orimoto, D. Trocino, D. Wood, J. Zhang

**Northwestern University, Evanston, USA**

A. Anastassov, K.A. Hahn, A. Kubik, L. Lusito, N. Mucia, N. Odell, R.A. Ofierzynski, B. Pollack, A. Pozdnyakov, M. Schmitt, S. Stoynev, M. Velasco, S. Won

**University of Notre Dame, Notre Dame, USA**

L. Antonelli, D. Berry, A. Brinkerhoff, K.M. Chan, M. Hildreth, C. Jessop, D.J. Karmgard, J. Kolb, K. Lannon, W. Luo, S. Lynch, N. Marinelli, D.M. Morse, T. Pearson, M. Planer, R. Ruchti, J. Slaunwhite, N. Valls, M. Wayne, M. Wolf

**The Ohio State University, Columbus, USA**

B. Bylsma, L.S. Durkin, C. Hill, R. Hughes, K. Kotov, T.Y. Ling, D. Puigh, M. Rodenburg, C. Vuosalo, G. Williams, B.L. Winer

**Princeton University, Princeton, USA**

E. Berry, P. Elmer, V. Halyo, P. Hebda, J. Hegeman, A. Hunt, P. Jindal, S.A. Koay, D. Lopes Pegna, P. Lujan, D. Marlow, T. Medvedeva, M. Mooney, J. Olsen, P. Piroué, X. Quan, A. Raval, H. Saka, D. Stickland, C. Tully, J.S. Werner, A. Zuranski

**University of Puerto Rico, Mayaguez, USA**

E. Brownson, A. Lopez, H. Mendez, J.E. Ramirez Vargas

**Purdue University, West Lafayette, USA**

E. Alagoz, V.E. Barnes, D. Benedetti, G. Bolla, D. Bortoletto, M. De Mattia, A. Everett, Z. Hu, M. Jones, O. Koybasi, M. Kress, A.T. Laasanen, N. Leonardo, V. Maroussov, P. Merkel, D.H. Miller, N. Neumeister, I. Shipsey, D. Silvers, A. Svyatkovskiy, M. Vidal Marono, H.D. Yoo, J. Zablocki, Y. Zheng

**Purdue University Calumet, Hammond, USA**

S. Guragain, N. Parashar

**Rice University, Houston, USA**

A. Adair, B. Akgun, C. Boulahouache, K.M. Ecklund, F.J.M. Geurts, W. Li, B.P. Padley, R. Redjimi, J. Roberts, J. Zabel

**University of Rochester, Rochester, USA**

B. Betchart, A. Bodek, Y.S. Chung, R. Covarelli, P. de Barbaro, R. Demina, Y. Eshaq, T. Ferbel, A. Garcia-Bellido, P. Goldenzweig, J. Han, A. Harel, D.C. Miner, D. Vishnevskiy, M. Zielinski

**The Rockefeller University, New York, USA**

A. Bhatti, R. Ciesielski, L. Demortier, K. Goulios, G. Lungu, S. Malik, C. Mesropian

**Rutgers, the State University of New Jersey, Piscataway, USA**

S. Arora, A. Barker, J.P. Chou, C. Contreras-Campana, E. Contreras-Campana, D. Duggan, D. Ferencek, Y. Gershtein, R. Gray, E. Halkiadakis, D. Hidas, A. Lath, S. Panwalkar, M. Park, R. Patel, V. Rekovic, J. Robles, K. Rose, S. Salur, S. Schnetzer, C. Seitz, S. Somalwar, R. Stone, S. Thomas, M. Walker

**University of Tennessee, Knoxville, USA**

G. Cerizza, M. Hollingsworth, S. Spanier, Z.C. Yang, A. York

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

R. Eusebi, W. Flanagan, J. Gilmore, T. Kamon<sup>60</sup>, V. Khotilovich, R. Montalvo, I. Osipenkov, Y. Pakhotin, A. Perloff, J. Roe, A. Safonov, T. Sakuma, S. Sengupta, I. Suarez, A. Tatarinov, D. Toback

**Texas Tech University, Lubbock, USA**

N. Akchurin, J. Damgov, C. Dragoiu, P.R. Duderu, C. Jeong, K. Kovitanggoon, S.W. Lee, T. Libeiro, I. Volobouev

**Vanderbilt University, Nashville, USA**

E. Appelt, A.G. Delannoy, C. Florez, S. Greene, A. Gurrola, W. Johns, P. Kurt, C. Maguire, A. Melo, M. Sharma, P. Sheldon, B. Snook, S. Tuo, J. Velkovska

**University of Virginia, Charlottesville, USA**

M.W. Arenton, M. Balazs, S. Boutle, B. Cox, B. Francis, J. Goodell, R. Hirosky, A. Ledovskoy, C. Lin, C. Neu, J. Wood

**Wayne State University, Detroit, USA**

S. Gollapinni, R. Harr, P.E. Karchin, C. Kottachchi Kankanamge Don, P. Lamichhane, A. Sakharov

**University of Wisconsin, Madison, USA**

M. Anderson, D.A. Belknap, L. Borrello, D. Carlsmith, M. Cepeda, S. Dasu, E. Friis, L. Gray, K.S. Grogg, M. Grothe, R. Hall-Wilton, M. Herndon, A. Hervé, P. Klabbers, J. Klukas, A. Lanaro, C. Lazaridis, R. Loveless, A. Mohapatra, I. Ojalvo, F. Palmonari, G.A. Pierro, I. Ross, A. Savin, W.H. Smith, J. Swanson

†: Deceased

1: Also at Vienna University of Technology, Vienna, Austria

2: Also at CERN, European Organization for Nuclear Research, Geneva, Switzerland

3: Also at National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

4: Also at California Institute of Technology, Pasadena, USA

5: Also at Laboratoire Leprince-Ringuet, Ecole Polytechnique, IN2P3-CNRS, Palaiseau, France

6: Also at Suez Canal University, Suez, Egypt

7: Also at Zewail City of Science and Technology, Zewail, Egypt

- 8: Also at Cairo University, Cairo, Egypt
- 9: Also at Fayoum University, El-Fayoum, Egypt
- 10: Also at Helwan University, Cairo, Egypt
- 11: Also at British University in Egypt, Cairo, Egypt
- 12: Now at Ain Shams University, Cairo, Egypt
- 13: Also at National Centre for Nuclear Research, Swierk, Poland
- 14: Also at Université de Haute Alsace, Mulhouse, France
- 15: Also at Joint Institute for Nuclear Research, Dubna, Russia
- 16: Also at Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow, Russia
- 17: Also at Brandenburg University of Technology, Cottbus, Germany
- 18: Also at The University of Kansas, Lawrence, USA
- 19: Also at Institute of Nuclear Research ATOMKI, Debrecen, Hungary
- 20: Also at Eötvös Loránd University, Budapest, Hungary
- 21: Also at Tata Institute of Fundamental Research - HECR, Mumbai, India
- 22: Now at King Abdulaziz University, Jeddah, Saudi Arabia
- 23: Also at University of Visva-Bharati, Santiniketan, India
- 24: Also at Sharif University of Technology, Tehran, Iran
- 25: Also at Isfahan University of Technology, Isfahan, Iran
- 26: Also at Shiraz University, Shiraz, Iran
- 27: Also at Plasma Physics Research Center, Science and Research Branch, Islamic Azad University, Tehran, Iran
- 28: Also at Facoltà Ingegneria, Università di Roma, Roma, Italy
- 29: Also at Università degli Studi Guglielmo Marconi, Roma, Italy
- 30: Also at Università degli Studi di Siena, Siena, Italy
- 31: Also at University of Bucharest, Faculty of Physics, Bucuresti-Magurele, Romania
- 32: Also at Faculty of Physics of University of Belgrade, Belgrade, Serbia
- 33: Also at University of California, Los Angeles, USA
- 34: Also at Scuola Normale e Sezione dell'INFN, Pisa, Italy
- 35: Also at INFN Sezione di Roma, Roma, Italy
- 36: Also at University of Athens, Athens, Greece
- 37: Also at Rutherford Appleton Laboratory, Didcot, United Kingdom
- 38: Also at Paul Scherrer Institut, Villigen, Switzerland
- 39: Also at Institute for Theoretical and Experimental Physics, Moscow, Russia
- 40: Also at Albert Einstein Center for Fundamental Physics, Bern, Switzerland
- 41: Also at Gaziosmanpasa University, Tokat, Turkey
- 42: Also at Adiyaman University, Adiyaman, Turkey
- 43: Also at Izmir Institute of Technology, Izmir, Turkey
- 44: Also at The University of Iowa, Iowa City, USA
- 45: Also at Mersin University, Mersin, Turkey
- 46: Also at Ozyegin University, Istanbul, Turkey
- 47: Also at Kafkas University, Kars, Turkey
- 48: Also at Suleyman Demirel University, Isparta, Turkey
- 49: Also at Ege University, Izmir, Turkey
- 50: Also at School of Physics and Astronomy, University of Southampton, Southampton, United Kingdom
- 51: Also at INFN Sezione di Perugia; Università di Perugia, Perugia, Italy
- 52: Also at Utah Valley University, Orem, USA
- 53: Now at University of Edinburgh, Scotland, Edinburgh, United Kingdom

54: Also at Institute for Nuclear Research, Moscow, Russia

55: Also at University of Belgrade, Faculty of Physics and Vinca Institute of Nuclear Sciences, Belgrade, Serbia

56: Also at Argonne National Laboratory, Argonne, USA

57: Also at Erzincan University, Erzincan, Turkey

58: Also at Mimar Sinan University, Istanbul, Istanbul, Turkey

59: Also at KFKI Research Institute for Particle and Nuclear Physics, Budapest, Hungary

60: Also at Kyungpook National University, Daegu, Korea