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Observation of tWZ production at the CMS experiment

The CMS Collaboration*

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Abstract

The first observation of single top quark production in association with a W and a Z boson in proton-proton collisions is reported. The analysis uses data at center-of-mass energies of 13 and 13.6 TeV recorded with the CMS detector at the CERN LHC, corresponding to a total integrated luminosity of 200 fb^{-1}. Events with three or four charged leptons, which can be electrons or muons, are selected. Advanced machine-learning algorithms and improved reconstruction methods, compared to an earlier analysis, result in an unprecedented sensitivity to tWZ production. The measured cross sections for tWZ production are 248 ± 52 fb and 242 ± 77 fb for $\sqrt{s} = 13$ and 13.6 TeV, respectively. The signal is established with a statistical significance of 5.8 standard deviations, with 3.5 expected, compared to the background-only hypothesis.

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The standard model (SM) of particle physics provides a remarkably successful theoretical framework for describing the fundamental particles and their interactions through the electromagnetic, weak, and strong forces. Over the past several decades, the predictions of the SM have been extensively tested with high precision, and its theoretical consistency has withstood rigorous experimental scrutiny. Despite its successes, the SM is known to be an incomplete theory. For example, it does not account for dark matter [1], the observed matter-antimatter asymmetry in the Universe [2], neutrino masses [3], and the quantum nature of gravity [4]. Consequently, the search for phenomena not included in the SM remains a central focus of contemporary particle physics.

High sensitivity to deviations from the SM predictions, and therefore to beyond-the-SM (BSM) effects, can be achieved in direct searches [5–12], precision measurements [13], studies of loop-induced processes [14], or measurements of very rare processes. Among the rare processes predicted by the SM, the production of a single top quark t in association with a W and a Z boson in proton-proton (pp) collisions, $pp \to tWZ$, is particularly interesting [15]. This process is exceptionally rare with predicted cross sections of 136^{+9}_{-8} fb at $\sqrt{s} = 13$ TeV and 148^{+10}_{-9} fb at 13.6 TeV at next-to-leading order (NLO) accuracy in the strong coupling of quantum chromodynamics (QCD) [16, 17]. The tWZ process provides direct access to the electroweak (EW) couplings of the top quark through Feynman diagrams similar to the example shown in Fig. 1 (left). The tWZ production allows for stringent tests of the gauge structure of the SM and the underlying symmetries governing particle interactions [15, 18]. New heavy particles can induce anomalous top-quark couplings with the EW gauge bosons, as shown by the Feynman diagram in Fig. 1 (right). These would manifest as measurable deviations in the rate of tWZ production, making measurements thereof a sensitive probe of BSM physics [19, 20].

This Letter presents an analysis of pp collision data from the CERN LHC, aiming to identify events from tWZ production, characterized by the presence of multiple leptons, jets, and missing transverse momentum ($p_{\mathrm{T}}^{\mathrm{miss}}$). However, the experimental challenges are significant. The small production cross section of the tWZ process compared to backgrounds with a similar signature, namely $t\bar{t}Z$ and diboson production with additional jets, necessitates advanced analysis techniques to isolate the signal. Evidence for tWZ production has been reported by the CMS Collaboration in 2024 using $\sqrt{s} = 13$ TeV data corresponding to an integrated luminosity of 138 fb^{-1}, recorded in 2016–2018 [21]. The previous analysis reported an observed statistical significance of 3.4 standard deviations (s.d.) with 1.4 s.d. expected. The analysis presented in this Letter uses state-of-the-art machine-learning (ML) algorithms and improved reconstruction methods to study tWZ production with unprecedented sensitivity. It updates the analysis of 13 TeV data and includes, in addition, pp collision data at 13.6 TeV recorded in 2022–2023. The total integrated luminosity of the dataset is 200 fb^{-1}, of which 62 fb^{-1} were recorded at 13.6 TeV. Tabulated results are provided in the HEPData record for this analysis [22].

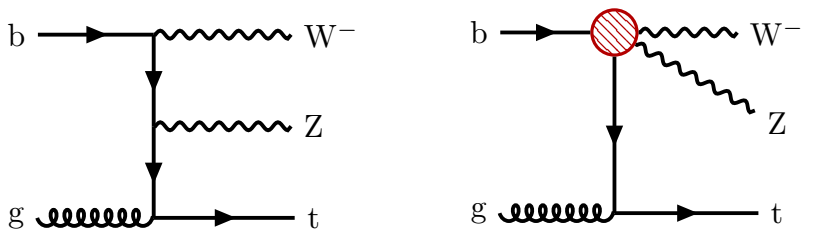


Figure 1: Example Feynman diagrams for tWZ production in the SM (left) and for anomalous tWZ production through an effective interaction (right). Charge conjugate versions of these diagrams are implied.

The CMS apparatus [23, 24] is a multipurpose, nearly hermetic detector, designed to trigger on [25–27] and identify electrons, muons, photons, and hadrons [28–30]. A global "particle-flow" (PF) algorithm [31] aims to reconstruct all individual particles in an event, combining information provided by the all-silicon inner tracker and by the crystal electromagnetic (ECAL) and brass-scintillator hadron calorimeters (HCAL), operating inside a 3.8 T superconducting solenoid, with data from the gas-ionization muon detectors embedded in the flux-return yoke outside the solenoid. The reconstructed particles are used to build τ lepton candidates, jets, and $p_{\mathrm{T}}^{\mathrm{miss}}$ [32–34].

Events of interest are selected using a two-tiered trigger system. The first level, composed of custom hardware processors, uses information from the calorimeters and muon detectors to select events at a rate of around 100 kHz within a fixed latency of about 4 μs [25]. The second level, known as the high-level trigger, consists of a farm of processors running a version of the full event reconstruction software optimized for fast processing, and reduces the event rate to a few kHz before data storage [26, 27]. Events are selected using a combination of triggers that require the presence of one, two, or three reconstructed leptons. The trigger efficiency is close to 100% for signal events passing the analysis selection [35].

The simulation of the signal is carried out using the Monte-Carlo (MC) event generator MADGRAPH5_aMC@NLO (MG) version 2.6.5 [16, 17] at NLO accuracy in perturbative QCD and in the five-flavor scheme (5FS). The factorization and renormalization scales are set to the default dynamical scales in MG, which are calculated as half the sum of all final state transverse energies [36]. The subsequent decays of the t quarks, W and Z bosons are simulated using MADSPIN [37, 38]. At leading order (LO) accuracy and in the 5FS, tWZ can be identified through the tree-level partonic process $\mathrm{gb} \to \mathrm{tWZ}$. However, at NLO, real corrections of the type $\mathrm{gg} \to \mathrm{tWZb}$ arise, that can feature a resonant top quark pair ($\mathrm{t\bar{t}}$) in the intermediate state and therefore cause overlap with the LO $\mathrm{t\bar{t}Z}$ process [18]. In other words, the emission of an extra b quark implies that the tWZb final state can also occur from the process $\mathrm{gg} \to \mathrm{t\bar{t}Z}$, with $\mathrm{t} \to \mathrm{bW}^+$ and $\bar{\mathrm{t}} \to \bar{\mathrm{b}}\mathrm{W}^-$, namely from LO $\mathrm{t\bar{t}Z}$ production. The overlap removal is performed using the MADSTR plugin [39], which implements both diagram removal (DR) and diagram subtraction (DS) techniques [40, 41]. For the signal samples, two DR options are used: DR1, which removes from the process amplitude both the squared resonant term and the interference term between resonant and nonresonant contributions, and DR2, which removes only the resonant term. The nominal samples are generated using the DR1 scheme.

The main background processes are simulated with different MC event generators. The dominant backgrounds are generated at NLO accuracy in perturbative QCD, where $\mathrm{t\bar{t}Z}$ and tZq are simulated using MG, while WZ production is simulated using POWHEG v2 [42–46]. Because of larger uncertainties in WZ production in association with a b quark compared to jets from light-flavor quarks and gluons, we split this background into WZ+b and WZ+j, respectively. Smaller backgrounds are simulated using MG, POWHEG and MCFM v7.0.1 [47–49]. These comprise di- and tri-boson processes, consolidated under VV(V) where V = W or Z, additional processes with a photon in the final state, $\mathrm{X}\gamma$, and processes in which a single top quark or a $\mathrm{t\bar{t}}$ pair is produced in association with additional particles, $\mathrm{t}(\bar{\mathrm{t}})\mathrm{X}$, grouping tW, $\mathrm{t\bar{t}H}$, $\mathrm{t\bar{t}t\bar{t}}$, $\mathrm{t\bar{t}WW}$, $\mathrm{t\bar{t}WZ}$, and $\mathrm{t\bar{t}ZZ}$. The NNPDF 3.1 next-to-NLO (NNLO) parton distribution functions (PDFs) [50] are used for the generation of all samples, together with PYTHIA 8.240 [51] for the modeling of the parton shower (PS) and hadronization. The $\mathrm{t\bar{t}Z}$ background cross section is scaled to account for approximate next-to-NNLO ($\mathrm{aN^3LO}$) QCD and NLO EW corrections [52]. The underlying event is described using the CP5 tune [53]. Matrix element calculations and PS simulations are matched using the FxFx [17] and MLM [54] algorithms for processes simulated with MG at NLO and LO, respectively. The detector response is simulated with a detailed de-

scription of the CMS apparatus based on the GEANT4 toolkit [55]. Additional pp interactions occurring in the same or adjacent bunch crossings (pileup) are modeled using PYTHIA. All simulated samples are produced taking into account the LHC and detector conditions of the different data-taking periods.

The PF algorithm [31] is used to reconstruct and identify individual particles in the event, combining information from different parts of the detector. The primary vertex (PV) is taken to be the vertex corresponding to the hardest scattering in the event, identified using the tracking information alone, as described in Section 9.4.1 of Ref. [56]. The energy of electrons is determined from a combination of the electron momentum from the reconstructed track, the energy of the corresponding ECAL cluster, and the energy sum of all bremsstrahlung photons spatially compatible with originating from the electron track. The momentum of muons is obtained from the curvature of their tracks measured in the tracking system and in the muon detectors. The energy of charged hadrons is evaluated via a combination of their momentum measured in the tracker and the matching of the ECAL and HCAL energy deposits, corrected for the response function of the calorimeters to hadronic showers. Finally, the energy of neutral hadrons is obtained from the corresponding corrected ECAL and HCAL energies.

Electrons and muons must have a transverse momentum $p_T > 10\,\text{GeV}$ for events collected at $\sqrt{s} = 13\,\text{TeV}$, and $p_T > 15\,\text{GeV}$ for events collected at $\sqrt{s} = 13.6\,\text{TeV}$. In addition, electrons must have pseudorapidity $|\eta| < 2.5$ and muons $|\eta| < 2.4$. In this Letter, nonprompt leptons denote reconstructed leptons not originating from the decay of a W or Z boson. To reduce their presence in the final selection, multivariate discriminants are employed [57], obtained from dedicated trainings on 13 TeV [58] and 13.6 TeV [59] data. The lepton identification algorithms for 13 TeV data have efficiencies of 87 and 92% for electrons and muons, respectively. An improved identification is used for 13.6 TeV data, resulting in lower efficiencies of 60 and 84% for electrons and muons, but with a threefold improvement in the rejection of nonprompt leptons.

Jets are reconstructed by clustering the PF candidates using the anti-k_T algorithm [60, 61] with a distance parameter of 0.4. Jets are required to have $p_T > 25\,\text{GeV}$, $|\eta| < 2.5$, and to be separated from selected leptons by a distance $\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2} > 0.4$. Here, $\Delta\eta$ and $\Delta\phi$ are the differences in pseudorapidity and azimuthal angle between the jet and lepton, respectively. Jets are corrected for pileup contributions and detector effects as detailed in Appendix A.1. The DEEPJET algorithm [62–64] is used in 13 TeV data to identify jets that originate from the fragmentation of b quarks (b jets). For 13.6 TeV data, an improved algorithm [65–67] is employed with better performance [68, 69]. We define b jets to be jets that pass a requirement on the algorithm score with an identification efficiency of around 80% for jets truly originating from b quarks and misidentification probabilities of about 1% for light-quark and gluon jets and about 14% for charm quark jets.

We require events in the final selection to have at least three reconstructed leptons, the p_T-leading lepton must have $p_T > 25\,\text{GeV}$ and the p_T-subleading one must have $p_T > 15\,\text{GeV}$. The events are split into different regions according to the number of leptons, jets, b jets, p_T^{miss}, and invariant mass of the lepton pairs with opposite sign and same flavor (OSSF). The OSSF lepton pairs are considered to lie inside the Z boson mass window if the invariant mass is within $m_Z \pm 15\,\text{GeV}$, where $m_Z = 91.2\,\text{GeV}$ [70]. The signal region (SR) is divided into two parts, depending on the number of leptons: events with three leptons enter the $\text{SR}_{3\ell}$, while events with four leptons are assigned to the $\text{SR}_{4\ell}$. In the $\text{SR}_{3\ell}$, one OSSF lepton pair must be present with mass within the m_Z window. The events must also contain two jets, at least one of which is b tagged. In the $\text{SR}_{4\ell}$, selected events must have exactly one OSSF lepton pair within the m_Z window. Additionally, at least one b-tagged jet must be present in the event.

In addition to the two SRs, we define four control regions (CRs) to constrain the most important backgrounds and validate their modeling. Two CRs are constructed to constrain the ZZ and WZ backgrounds. The other two help to improve the modeling of events containing nonprompt leptons, originating from Drell–Yan (DY) and $\mathrm{t\bar{t}}$ production. Events containing at least one jet and exactly four leptons with two OSSF lepton pairs inside the m_{Z} window enter the $\mathrm{CR_{ZZ}}$, which is enriched in events from ZZ production. The $\mathrm{CR_{WZ}}$ contains events with at least two jets, no b jets, three leptons, two of which are within the m_{Z} window, and $p_{\mathrm{T}}^{\mathrm{miss}} > 40\,\mathrm{GeV}$. The $\mathrm{CR_{WZ}}$ is also used to improve the description of the jet multiplicity for the WZ process, as detailed in the Appendix A.2. Events entering the $\mathrm{CR_{DY}}$ satisfy the same requirements as for the $\mathrm{CR_{WZ}}$, but with an inverted $p_{\mathrm{T}}^{\mathrm{miss}}$ selection and no requirement on the number of jets. Finally, the $\mathrm{CR_{t\bar{t}}}$ contains events with at least two jets, one of which is b tagged, three leptons but no OSSF lepton pair inside the m_{Z} window.

The contribution of the nonprompt background is estimated from a fit to data simultaneously with the signal extraction. In the fit, the misidentification rates are left as free parameters and are constrained with the help of distributions in the trailing lepton p_{T} measured in the $\mathrm{CR_{DY}}$ and $\mathrm{CR_{t\bar{t}}}$. The trailing lepton is defined as the selected lepton with the smallest p_{T}. Additional details on the estimation of the nonprompt-lepton background are provided in Appendix A.3.

A transformer ML algorithm based on the particle transformer PART architecture [65] is employed to discriminate between signal and background processes, mainly $\mathrm{t\bar{t}Z}$ and WZ production. Four different dedicated models are trained: two for $\mathrm{SR}_{3\ell}$ and two for $\mathrm{SR}_{4\ell}$, corresponding to trainings with 13 and 13.6 TeV data, respectively. In $\mathrm{SR}_{3\ell}$, the PART algorithm is set up to have four output nodes, each representing the classification as tWZ, $\mathrm{t\bar{t}Z}$, WZ, or any of the minor remaining backgrounds. The events are then divided into three categories based on the maximum value of the output nodes: tWZ, $\mathrm{t\bar{t}Z}$, and other backgrounds which combine WZ and minor backgrounds. This results in a region enriched in signal events, a second region mainly used to constrain the $\mathrm{t\bar{t}Z}$ background and related uncertainties, and a third region used to constrain other backgrounds. In $\mathrm{SR}_{4\ell}$, a binary classifier to distinguish tWZ from background is used due to the lower statistical precision of the data events with four leptons. More details on the algorithm architecture and input variables are provided in Appendix A.4.

The tWZ cross section is measured by maximizing a binned likelihood function in a fit to the data. This function combines the Poisson probabilities of the yields with the predicted signal and background estimates in each bin. It also includes all sources of systematic uncertainties, represented as nuisance parameters, which may influence the observed number of signal or background events. The fit yields the measured signal strength, defined as the ratio of the observed cross section to the expected value, along with its uncertainty. The fit is performed using the CMS statistical analysis program COMBINE [71]. Different distributions enter the fit according to the SR or CR, separately for each center-of-mass energy. Three distributions in the classifier output nodes with five bins each are measured in the $\mathrm{SR}_{3\ell}$, corresponding to the values of the tWZ, $\mathrm{t\bar{t}Z}$, and other background nodes. Two bins from the classifier output score in the $\mathrm{SR}_{4\ell}$ enter the fit. The total number of events measured in the $\mathrm{CR_{ZZ}}$ enters the fit to constrain the normalization of the ZZ background. The jet multiplicity distribution is measured in the $\mathrm{CR_{WZ}}$ to constrain the uncertainty on the modeling of additional jets produced in association with WZ. The distribution of the trailing lepton p_{T} is used for the $\mathrm{CR_{DY}}$ and $\mathrm{CR_{t\bar{t}}}$ to constrain the rates of the nonprompt-lepton identification.

The distributions in the tWZ and $\mathrm{t\bar{t}Z}$ output nodes in $\mathrm{SR}_{3\ell}$, along with the output of the classifier in $\mathrm{SR}_{4\ell}$, are shown in Fig. 2. The distributions are shown for the best fit values of the background normalizations and nuisance parameters corresponding to systematic uncertain-

ties, after a fit to the data.

Several sources of systematic uncertainties are considered, comprising experimental and theoretical components. The experimental ones are the uncertainties in the jet energy corrections and resolution [33], unclustered energy [34], the description of pileup in the simulation [72], the trigger [25, 26], b tagging [62], and lepton efficiency corrections [28, 29]. The integrated luminosity has an uncertainty of 1.6% for the 2016–2018 data-taking years [73–75], and 1.4 and 1.3% for 2022 and 2023, respectively [76, 77]. The theoretical uncertainties in the signal and main backgrounds include uncertainties from the PDFs, the matrix element renormalization and factorization scales, and the PS simulation, namely initial- and final-state radiation and the matching of the PS to the matrix-element calculations. Additional sources of uncertainty affecting the signal are taken into account by considering differences between the DR1 and DR2 subtraction schemes. Variations from DS are not considered, as these are smaller than the ones derived with DR2. The uncertainty associated with the modeling of additional jets in WZ production is also included, more details are given in the Appendix A.2. In addition, theoretical uncertainties in the cross sections of the background processes are considered. A normalization uncertainty of 7% is employed for the $\mathrm{t\bar{t}Z}$ cross section [78, 79]. Two different normalization uncertainties are considered for the WZ and ZZ processes, where we assign a 20% uncertainty on VV+b production [35] and a 10% uncertainty on VV+j [80]. An uncertainty of 11% is used for tZq production [35], and a 10% uncertainty is used for $\mathrm{VV(V)}$ [81, 82] and $\mathrm{X}\gamma$ [83, 84]. Uncertainties of 5 and 10% are applied to the $\mathrm{t\bar{t}}$ [85] and DY processes [86], respectively. A 25% uncertainty is considered for the $\mathrm{t\bar{t}W}$ process where the measurements do not agree with the SM predictions by about this amount [87], and a 20% uncertainty is assigned to $\mathrm{t(\bar{t})X}$ [58, 88, 89]. Additional uncertainties describe the rate of misidentified nonprompt leptons as detailed in Appendix A.3. Finally, uncertainties arising from the finite size of simulated samples are accounted for using the Barlow–Beeston light method [90]. We treat experimental uncertainties and the rate of misidentified nonprompt leptons as uncorrelated between the 13 and 13.6 TeV datasets, while the theoretical uncertainties and background normalizations are fully correlated.

The measured signal strength of tWZ production is $\mu_{\mathrm{tWZ}} = 1.77 \pm 0.23\,(\mathrm{stat}) \pm 0.22\,(\mathrm{syst})$ with an observed statistical significance of 5.8 s.d. compared to the background-only hypothesis, with 3.5 s.d. expected. The theoretical predictions come with an uncertainty on the signal strength of 0.06, thus the result is 2.3 s.d. larger than the SM expectation, consistent with the previous measurement [21]. The signal strength using 13 TeV data only is $1.82 \pm 0.28\,(\mathrm{stat}) \pm 0.26\,(\mathrm{syst})$, in agreement with the one from 13.6 TeV data only, $1.64 \pm 0.42\,(\mathrm{stat}) \pm 0.31\,(\mathrm{syst})$. The corresponding observed significances are 5.1 s.d. and 3.4 s.d. for 13 and 13.6 TeV data, respectively, with expected significances of 3.0 s.d. and 2.1 s.d., respectively. The measured cross sections for tWZ production are $248 \pm 38\,(\mathrm{stat}) \pm 35\,(\mathrm{syst})$ fb and $242 \pm 62\,(\mathrm{stat}) \pm 46\,(\mathrm{syst})$ fb for $\sqrt{s} = 13$ and 13.6 TeV, respectively. Signal strengths measured in the different data-taking periods and leptonic channels are presented in Appendix A.5. The dominant systematic uncertainty is the normalization of the $\mathrm{t\bar{t}Z}$ process with a contribution of 14% to the total uncertainty. Other relevant uncertainties are the normalization of the WZ+b process and the uncertainties in the jet energy corrections, with contributions of 9 and 6%, respectively. We determine the signal strengths of tWZ and $\mathrm{t\bar{t}Z}$ production in a simultaneous fit, without external constraints on the $\mathrm{t\bar{t}Z}$ cross section. The result of this fit is shown in Fig. 3. The measured signal strengths are $\mu_{\mathrm{tWZ}} = 1.88 \pm 0.30\,(\mathrm{stat}) \pm 0.15\,(\mathrm{syst})$ and $\mu_{\mathrm{t\bar{t}Z}} = 0.91 \pm 0.04\,(\mathrm{stat}) \pm 0.03\,(\mathrm{syst})$, also resulting in a significance of more than five s.d. for tWZ production. The measured $\mathrm{t\bar{t}Z}$ signal strength is compatible within two s.d. with the most recent theoretical prediction at $\mathrm{aN^3LO}$ QCD and NLO EW [52]. It is compatible with previous results on $\mathrm{t\bar{t}Z}$ production [78, 79, 91] when considering

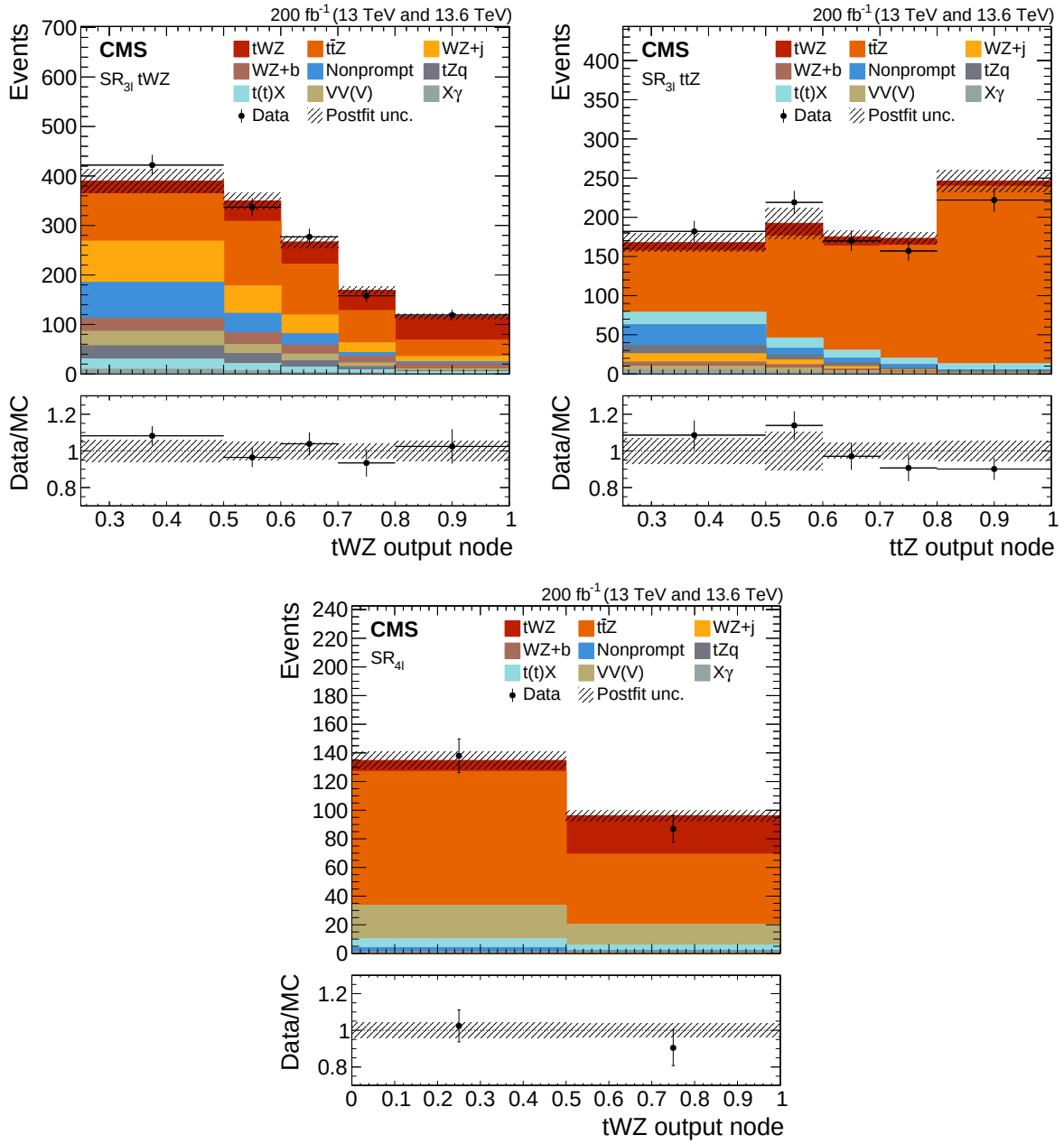


Figure 2: Distributions in the classifier output nodes for the tWZ (upper left) and $t\bar{t}Z$ (upper right) nodes in $SR_{3\ell}$, and in the classifier output node in $SR_{4\ell}$ (lower) after a fit to the data. The dashed band shows the postfit uncertainty. The results from fits to 13 and 13.6 TeV data are combined for illustration purposes. The ratio of data to the predictions from MC simulation is shown below the distributions.

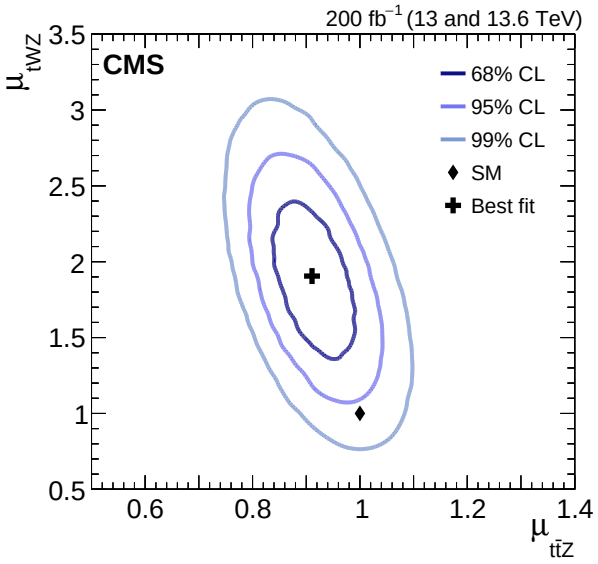


Figure 3: Likelihood scan of the signal strengths for tWZ and $t\bar{t}Z$ production. The black cross shows the best fit value, while the black diamond indicates the SM expected value. The contours in different shades of blue correspond to the 68, 95, and 99% confidence levels.

the 12% increase in the predicted cross section compared to that used in these measurements. The correlation between μ_{tWZ} and $\mu_{t\bar{t}Z}$ is reduced compared to the previous CMS analysis [21] because of the improved ML algorithm and the separation of the $SR_{3\ell}$ into three categories. The combined effect is a better constraint on μ_{tWZ} largely independent of the value of $\mu_{t\bar{t}Z}$.

In summary, a measurement of tWZ production in proton-proton (pp) collisions has been presented in events with three and four charged leptons. The analysis is performed using data recorded with the CMS detector at center-of-mass energies of 13 and 13.6 TeV, corresponding to a total integrated luminosity of 200 fb^{-1}. Advanced machine-learning algorithms are employed to significantly improve the sensitivity of the analysis compared to an earlier analysis. Analyzing the same data, an expected significance of 3.0 standard deviations (s.d.) is achieved, compared to 1.4 s.d. obtained previously. Combining the 13 and 13.6 TeV data, a significance of 5.8 s.d. is observed. The measured signal strength $\mu_{tWZ} = 1.77 \pm 0.32\,(\text{tot})$ agrees with the standard model prediction within 2.3 s.d. The measured cross sections are 248 ± 52 fb and 242 ± 77 fb for $\sqrt{s} = 13$ and 13.6 TeV, respectively. This is the first observation of tWZ production in pp collisions. This measurement represents a significant step forward in our understanding of rare processes involving the top quark and electroweak bosons. It opens up the possibility for future studies of the top quark electroweak interactions in the context of the standard model and its extensions.

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A Additional material

A.1 Pileup mitigation

Pileup can contribute additional tracks and calorimetric energy depositions to the jet momentum. For data from 2016–2018, we mitigate this effect by discarding charged particles identified to be originating from pileup vertices and apply an offset correction to correct for remaining pileup contributions [31, 72]. For 2022–2023 data, we apply the pileup-per-particle identification algorithm [72, 92], weighting all PF candidates by their probability to originate from the PV [34]. Jet energy corrections are derived from data and simulation to bring the measured response of jets to that of particle level jets on average [33]. The missing transverse momentum vector $\vec{p}_{\mathrm{T}}^{\,\mathrm{miss}}$ is the negative vector sum of the transverse momenta of all PF candidates [34, 93]. Corrections to the jet energies are propagated to $\vec{p}_{\mathrm{T}}^{\,\mathrm{miss}}$.

A.2 Jet multiplicity reweighting

The fully leptonic decay of the WZ process involves at most one jet from the matrix element calculation at NLO in QCD. Thus, additional jet emissions are primarily simulated by the PS, which may lead to mismodeling in the shape of the jet multiplicity distribution. This can be particularly relevant when selections that are not inclusive in the number of jets are applied. To improve the modeling of the jet multiplicity, a simulation-to-data reweighting is performed in the $\mathrm{CR_{WZ}}$. Simulated contributions from processes other than WZ are subtracted from data, and a correction is derived as the ratio between the observed data yield and the WZ simulation as a function of the jet multiplicity. A shape uncertainty is assigned to this correction by considering two alternative configurations: one where the correction factor is doubled and another where no correction is applied.

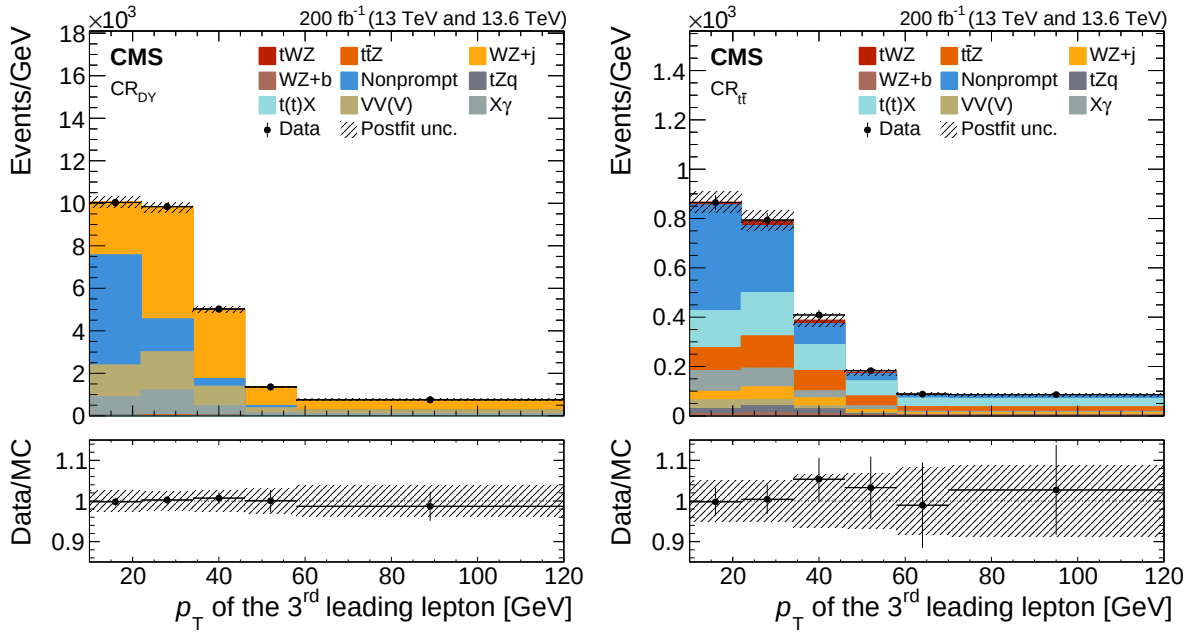


Figure A.1: Distribution in the p_{T} of the 3^{rd} leading lepton for the $\mathrm{CR_{DY}}$ (left) and $\mathrm{CR_{t\bar{t}}}$ (right) after a fit to data. The dashed band shows the postfit uncertainty. The results from fits to 13 and 13.6 TeV data are combined for illustration purposes. The ratio of data to the predictions from MC simulations is shown below the distributions.

A.3 Background from nonprompt leptons

The nonprompt-lepton contribution is estimated from a fit to data using simulated templates based on the origin of the misidentified leptons. Events containing at least one nonprompt lepton are divided into three categories: nonprompt leptons from photons, b jets, and light-quark and gluon jets. For 13.6 TeV data, nonprompt leptons from b-quark, light-quark, and gluon jets are combined into a single category because of the smaller number of events from nonprompt leptons due to the improved lepton-identification algorithm. We introduce unconstrained parameters that describe the lepton misidentification rates as functions of p_{T}. For nonprompt leptons from photons, these parameters are considered to be normal-distributed around the MC predictions, with prior uncertainties of 50%. Uncertainties accounting for shape differences in the trailing-lepton p_{T} distributions between nonprompt leptons of different flavors within the same category are considered as an additional uncertainty. We find that these have a negligible impact on the analysis. In the fit, the two distributions in the trailing-lepton p_{T} measured in the $\mathrm{CR_{DY}}$ and $\mathrm{CR_{t\bar{t}}}$ are used. These are shown in Fig. A.1 after the fit to data. The nonprompt backgrounds constitute about one-third of all selected events in these two regions. The trailing-lepton p_{T} distributions show sensitivity to the origin of the nonprompt lepton and can thus constrain the parameters describing the misidentification rates. These are measured independently for each data-taking period. The largest correction factors are measured for nonprompt leptons from light-quark and gluon jets, resulting in a nonprompt-lepton background that is 40–70% lower than the simulation-based prediction, depending on the data-taking period. The associated uncertainties are around 50%, due to the small statistical power of this category. The correction factors associated with the nonprompt leptons from b jets are closer to unity, where the largest correction shifts the prediction up by 40%, with uncertainties of about 20%.

A.4 The machine-learning algorithm

The PART algorithm takes as inputs two different set of variables: *Particles* and *Interactions*. The *Particles* input corresponds to a list of individual physics objects where each particle is described by a set of features. It is divided into two categories: *leptons* and *jets*. The components of the four-momentum of each lepton and jet in every event, as well as the $\vec{p}_{\mathrm{T}}^{\,\mathrm{miss}}$, are used as inputs. Additionally, the following set of features is considered: $\log(p_{\mathrm{T}}/\,\mathrm{GeV})$, $\log(E/\,\mathrm{GeV})$, η, ϕ, b-tagging information (only for jets), and a number that encodes the flavor of the lepton. The agreement between data and simulation has been verified for distributions in all input variables. The *interactions* encode correlations between pairs of particles considering the following variables: $\log(\Delta)$, $\log(k_{\mathrm{T}}/\,\mathrm{GeV})$, $\log(z)$, and $\log(m^2/\,\mathrm{GeV}^2)$. These are defined between two particles a and b as

$$\begin{aligned}\Delta &= \sqrt{(y_a - y_b)^2 + (\phi_a - \phi_b)^2},\\ k_{\mathrm{T}} &= \min(p_{\mathrm{T},a}, p_{\mathrm{T},b})\Delta,\\ z &= \min(p_{\mathrm{T},a}, p_{\mathrm{T},b})/(p_{\mathrm{T},a} + p_{\mathrm{T},b}),\\ m^2 &= (E_a + E_b)^2 - |\mathbf{p}_a + \mathbf{p}_b|^2,\end{aligned}$$

where y, ϕ, and $\mathbf{p}$ are the rapidity, azimuthal angle, and the three-momentum, respectively. The *interactions* allow each particle to incorporate information from all other particles using both the particle features and their pairwise relationships, enabling the network to capture both local and global event characteristics. To avoid overtraining, two versions of the PART algorithm are trained for each signal region and center-of-mass energy. An algorithm trained on one half of the simulated data is employed on the other half during the analysis. In this way, each algorithm is trained on and applied to separate halves of the simulated samples. The

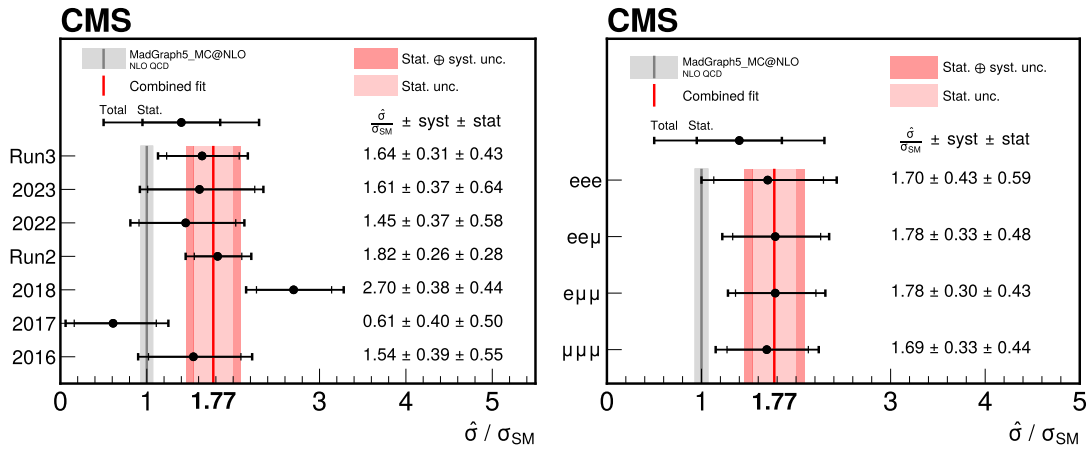


Figure A.2: Values of the signal strengths for tWZ production obtained from the different data-taking periods (left), and from events with different lepton flavors (right): three electrons (eee), two electrons and one muon (eeμ), one electron and two muons (e$\mu\mu$), and three muons ($\mu\mu\mu$). If there are more than three leptons in an event, the three p_{T}-leading leptons are used to determine the flavor. The combined results from 13 TeV data (Run 2) and from 13.6 TeV data (Run 3) are also shown. The result from the combined fit to 13 and 13.6 TeV data is shown as a red line with the corresponding uncertainty shown as a red band. The SM prediction is shown as a gray band.

agreement between data and simulation has also been verified in the $\mathrm{CR}_{\mathrm{t\bar{t}}}$ for the algorithms used in the $\mathrm{SR}_{3\ell}$, and in the $\mathrm{CR}_{\mathrm{ZZ}}$ for the algorithms employed in the $\mathrm{SR}_{4\ell}$. These CRs have the same number of physics objects as the corresponding SRs, and the data distributions in the output of the algorithms show good agreement to the simulated ones.

A.5 Individual results

The signal strength is also measured for the different data-taking periods and leptonic channels, defined by the flavor of the three leptons with the largest p_{T} in the event. Comparisons of the obtained signal strengths are shown in Fig. A.2. We find good agreement between the measured signal strengths in the different data-taking periods and among the signal strengths from different lepton flavors.

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