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Search for charged Higgs bosons decaying into top and bottom quarks in lepton+jets final states in proton-proton collisions at $\sqrt{s} = 13$ TeV

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Abstract

A search is presented for charged Higgs bosons ($H^\pm$) in proton-proton (pp) collision events via the $pp \rightarrow (b)H^\pm$ processes, with $H^\pm$ decaying into top (t) and bottom (b) quarks. The search targets final states with one lepton, missing transverse momentum, and two or more b jets. The analysis is based on data collected at a center-of-mass energy of 13 TeV with the CMS detector at the LHC, corresponding to an integrated luminosity of 138 fb^{-1} . We search for charged Higgs bosons in the 200 GeV to 1 TeV mass range. The results are interpreted within the generalized two-Higgs-doublet model (g2HDM). This model predicts additional Yukawa couplings of the Higgs bosons to the top quark ρ_{tt} , the top and charm quark ρ_{tc} , and the top and up quark ρ_{tu} . This search focuses on the real components of ρ_{tt} and ρ_{tc} , which are probed up to values of unity. An excess is observed with respect to the standard model expectation with a local significance of 2.4 standard deviations for a signal with an $H^\pm$ boson mass ($m_{H^\pm}$) of 600 GeV. Limits are derived on the product of the cross section $\sigma(pp \rightarrow (b)H^\pm)$ and branching fraction $\mathcal{B}(H^\pm \rightarrow tb, t \rightarrow b\ell\nu)$, where $\ell = e, \mu$. The values of $\rho_{tc} \gtrsim 0.15\text{--}0.5$ are excluded at 95% confidence level, depending on the $m_{H^\pm}$ and ρ_{tt} assumptions. The results represent the first search for charged Higgs bosons within the g2HDM framework and complement the existing results on additional neutral Higgs bosons.

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1 Introduction

In 2012, the LHC experiments discovered a scalar boson with a mass of 125 GeV [1–3]. The properties of this boson have been scrutinized in great detail and found consistent with those predicted for the Higgs boson in the standard model (SM) [4, 5]. The CERN LHC Run 2 (2015–2018) data enabled more precise measurements of the Higgs boson properties and put further constraints on possible contributions from new physics beyond the SM. The ATLAS and CMS experiments have measured the Yukawa couplings of the 125 GeV Higgs boson to the top quark (t) [6–8], bottom quark (b) [9, 10], tau lepton (τ) [11, 12], and the muon (μ) [13, 14], as well as constrained the couplings to charm quarks (c) [15, 16]. Although the measured couplings in all cases are found to be consistent with the SM expectations within uncertainties, having established the existence of one scalar doublet, it is natural to question if a second doublet exists.

A second doublet is predicted in the two-Higgs-doublet model (2HDM) framework, implying the existence of two charged Higgs bosons ($H^\pm$), a new scalar boson (H), and a pseudoscalar boson (A), in addition to the SM-like Higgs boson (h). There are several main classes of 2HDM extensions [17]:

- *2HDM-I*: All quarks and charged leptons couple to the same Higgs doublet.
- *2HDM-II*: The u-type quarks couple to one doublet, while d-type quarks and charged leptons couple to the other.
- *2HDM-X*: All quarks couple to one doublet, and charged leptons couple to the other.
- *2HDM-Y*: This is the flipped version of the 2HDM-X.
- *2HDM-III* or *generalized 2HDM (g2HDM)*: Extra Yukawa couplings are present, and unlike the other types listed above, no $\mathbb{Z}_2$ symmetry is imposed.

Earlier LHC searches for $H^\pm$ were performed in the context of the 2HDM-II, including Run 2 results presented in Refs. [18–29].

In the g2HDM, the absence of a $\mathbb{Z}_2$ symmetry allows for flavor-changing neutral current (FCNC) interactions involving the A and H bosons, while such interactions remain suppressed for the h boson. In the g2HDM, the couplings of the spin-0 particles h, H, A, and $H^\pm$ to fermions are regulated by the Yukawa couplings, the mixing angle (γ) between the h and H scalar particles, and the elements of the Cabibbo–Kobayashi–Maskawa (CKM) matrix [30]. The largest contributions to the $cbH^\pm$ and $tbH^\pm$ couplings come from $\rho_{tc}V_{tb}$ and $\rho_{tt}V_{tb}$, respectively. Unlike in the 2HDM-II, where the corresponding couplings are CKM-suppressed, here, the $\rho_{tc}V_{tb}$ and $\rho_{tt}V_{tb}$ terms appear without suppression. As a result, the $H^\pm$ production cross section in the g2HDM can be significantly larger than in the 2HDM-II. A more detailed discussion can be found in Ref. [31].

With the additional Yukawa couplings, many parameters and extra processes become possible, but there are tight constraints from electroweak precision measurements, flavor physics, and direct searches at the LHC. However, extra Higgs bosons at mass scales <1 TeV at the LHC could still be hidden by the fermion mass-mixing hierarchy [32] or the alignment mechanisms [33], where the mixing angle γ between the two CP -even scalars is close to $\pi/2$, i.e., $\cos \gamma \approx 0$. Therefore, the lack of a hint of FCNC interactions of the SM Higgs boson at the LHC may be a result of the amplitude suppression by the alignment mechanism. The extra Yukawa couplings of the additional Higgs bosons to the top quark ρ_{tt} , to the top and charm quark ρ_{tc} , and to the top and up quark ρ_{tu} can assume large values [33], and combined with the Higgs quartic couplings of order 1, they can also explain electroweak baryogenesis [31, 34–36]. These

arguments strongly motivate direct experimental searches for extra Yukawa couplings.

Previous searches for extra Yukawa couplings based on the g2HDM were focused on A and H bosons and no significant excess above the background prediction was observed in either case, leading to strong bounds on ρ_{tu} [37, 38]. In this paper, we focus on $H^\pm$ and further explore the extra Yukawa couplings ρ_{tc} and ρ_{tt} , while setting ρ_{tu} to zero. We consider $H^\pm$ production in proton-proton (pp) collisions in the $pp \rightarrow (q)H^\pm \rightarrow (q)tb$ channels, with q being a b or c quark. This process is dominated by the $pp \rightarrow H^\pm$ and $pp \rightarrow bH^\pm$ contributions. The $pp \rightarrow cH^\pm$ is suppressed by the parton distribution function (PDF) of the bottom quark in the proton. This process is taken into account for completeness and is categorized together with $pp \rightarrow H^\pm$. Representative Feynman diagrams for the signal processes are displayed in Fig. 1. Considering the decay $H^\pm \rightarrow tb$ and top quark decays with one isolated electron or muon in the final state, the signature is expected to contain two or three b quarks at tree level, as well as a lepton and missing transverse momentum (p_T^{miss}). In the 2HDM-II, $H^\pm$ production via these processes is suppressed, resulting in negligible cross sections and limited experimental sensitivity. Consequently, such channels have not been the focus of previous experimental searches. In contrast, in the g2HDM, they become dominant because of the presence of an additional Yukawa coupling ρ_{tc} . These processes result in low jet multiplicity events, which are enhanced in the g2HDM but not in the 2HDM-II. The $qg \rightarrow tH^\pm$ processes, permitted in both the 2HDM-II and g2HDM, are omitted from this study because their cross sections are at least an order of magnitude smaller (for $\rho_{tt} \sim \rho_{tc} \sim 1$) than those of the processes considered in this search.

The paper is organized as follows: Section 2 describes the CMS detector. In Section 3, descriptions of the data and the simulation samples used in the analysis are given. The event selection and reconstruction procedure of the physics objects are given in Sections 4 and 5, respectively. Background estimation from control samples in the data is discussed in Section 6, and the signal extraction procedure in Section 7. Section 8 discusses the sources of systematic uncertainty. The results of the analysis are presented in Section 9. Finally, a summary of the paper is given in Section 10. Tabulated results are accessible from the HEPData record for this analysis [39].

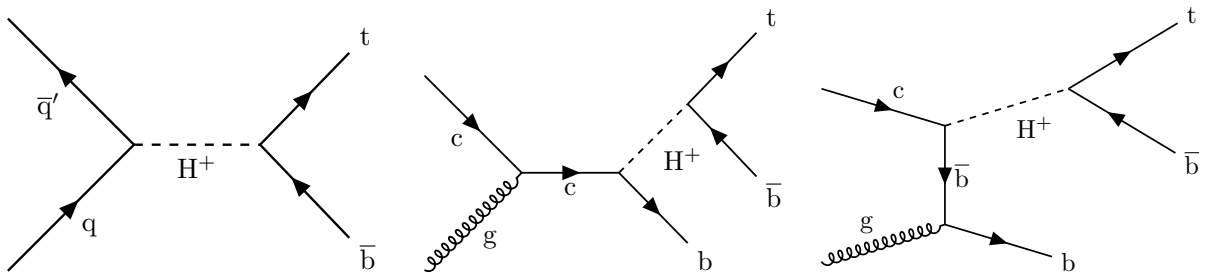


Figure 1: Representative tree-level Feynman diagrams for the signal processes: $pp \rightarrow H^+$, $H^+ \rightarrow t\bar{b}$ (left), and $pp \rightarrow bH^+$, $H^+ \rightarrow t\bar{b}$ (middle and right).

2 The CMS detector

The CMS apparatus [40, 41] is a multipurpose, nearly hermetic detector, designed to trigger on [42–44] and identify electrons, muons, photons, and (charged and neutral) hadrons [45–47]. Its central feature is a superconducting solenoid of 6 m internal diameter, providing a magnetic field of 3.8 T. Within the solenoid volume are a silicon pixel and strip tracker, a lead tungstate crystal electromagnetic calorimeter (ECAL), and a brass and scintillator hadron calorimeter, each composed of a barrel and two endcap sections. Forward calorimeters extend the pseudo-

rapidity (η) coverage provided by the barrel and endcap detectors. Muons are reconstructed using gas-ionization detectors embedded in the steel flux-return yoke outside the solenoid. More detailed descriptions of the CMS detector, together with a definition of the coordinate system used and the relevant kinematic variables, can be found in Refs. [40, 41].

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 $4\ \mu\text{s}$ [42]. The second level, known as the high-level trigger, consists of a farm of processors running a version of the full event reconstruction software optimized for fast processing, and reduces the event rate to around 1 kHz before data storage [43, 44].

3 Data and simulated event samples

The data were collected with the CMS detector at the LHC during the years 2016 to 2018, and correspond to an integrated luminosity of $138\ \text{fb}^{-1}$. Data are selected online with a combination of single-muon, single-electron, and single-photon triggers to maximize signal efficiency. In particular, single-photon triggers were used to recover the efficiency for high-energy electrons.

The signal and background processes are simulated using several Monte Carlo (MC) generators. The $(q)H^\pm$ signal samples are simulated at leading order (LO) in perturbative quantum chromodynamics (QCD), with up to two additional noncollinear high-transverse momentum (p_T) partons in the matrix element calculations using MADGRAPH5_aMC@NLO v2.6.5 [48], and the hard scattering simulation is interfaced with parton shower jets using the MLM [49] matching prescription. Several signal samples are simulated assuming nonzero values of ρ_{tt} and ρ_{tc} selected from 0.1, 0.4, 0.6, and 1, and assuming an $H^\pm$ boson mass ($m_{H^\pm}$) between 200 and 1000 GeV. Nine $H^\pm$ boson mass points are considered from 200 to 1000 GeV in 100 GeV steps, chosen based on the mass resolution, and one more point at 350 GeV is added to improve the sensitivity around the $t\bar{t}$ threshold. In this analysis, $H^\pm$ decays to H or A are not considered.

Background events generated by MADGRAPH5_aMC@NLO at next-to-LO (NLO) in perturbative QCD (pQCD) are $t\bar{t}W$, tZ , VVV , s -channel single top quark production, and Z +jets processes, and the ones generated at LO precision are $t\bar{t}Z$, W +jets, $t\bar{t}VV$, $t\bar{t}Vh$, $t\bar{t}hh$, $t\bar{t}tj$, $t\bar{t}tW$, $t\bar{t}t\bar{t}$, and multijet production. Multijet events refer to the events composed uniquely of jets produced through the QCD interaction. Here, V represents a W or Z boson. Among these processes, FxFx matching [50] is used for $t\bar{t}W$ and Z +jets, while MLM matching [49] is used for W +jets. The POWHEG v2.0 generator [51–53] is used to simulate events at NLO in pQCD for $t\bar{t}$ [54], $W^\pm W^\mp$ [55], single top quark production in association with a W boson (tW) [56], single top quark t -channel production [57], and $t\bar{t}h$ production [58]. The PYTHIA v8.240 [59] generator is used to simulate WZ and WW events at LO. If a higher-order cross section calculation exists, the yields of backgrounds are normalized to the corresponding value, as discussed below.

The predicted $t\bar{t}$ production cross section is $834^{+38}_{-43}\ \text{pb}$ as calculated with the TOP++ v2.0 program at next-to-NLO (NNLO) in pQCD, including soft-gluon resummation to next-to-next-to-leading logarithmic (NNLL) order (as discussed in Ref. [60] and references therein), and assuming a top quark mass $m_t = 172.5\ \text{GeV}$. The predicted cross sections of single top quark and single top antiquark production in the t channel are $\sigma(tq) = 134.2^{+1.9}_{-1.3}\ \text{pb}$ and $\sigma(\bar{t}q) = 80.0^{+2.3}_{-1.8}\ \text{pb}$, respectively. The cross sections were calculated with the MCFM program [61] at NNLO in pQCD assuming $m_t = 172.5\ \text{GeV}$. For both $t\bar{t}$ and single top quark cross sections quoted above, the uncertainties include the ones due to the choice of the renormalization and factorization scales, μ_r and μ_f , the uncertainties in the PDFs and α_s . The inclusive tW production cross section is

calculated at NLO in pQCD with the addition of third-order corrections of soft-gluon emissions by resumming NNLL terms [62]. For single top quark s -channel production, the cross section at NLO in pQCD is calculated using the HATHOR v2.1 program [63, 64].

The cross sections for W +jets events are normalized to NNLO calculations using the FEWZ v3.1 program [65]. The inclusive cross section for $t\bar{t}Z$, calculated at NLO+NNLL, is taken from Ref. [66]. Cross sections at NLO are used for $t\bar{t}W$ [67], $t\bar{t}h$ [68], $t\bar{t}hh$ [69], $t\bar{t}Vh$ [68], $t\bar{t}VV$ [70], tZ [71], and $t\bar{t}t\bar{t}$ [72] processes.

Simulated samples are interfaced with PYTHIA v8.240 for parton showering, fragmentation, and hadronization. The underlying event is also modeled with PYTHIA v8, using the CP5 tune [73]. The PDFs are taken from the NNPDF3.1 NNLO set [74]. Finally, for simulated event samples, the detector response is modeled with the GEANT4 package [75].

The simulated events include effects of additional pp interactions within the same or nearby bunch crossings (pileup) by overlaying simulated minimum bias collisions on the hard scattering interaction, with the multiplicity matched to that observed in data [76]. To match the measured top quark p_T [77] distribution, the simulated $t\bar{t}$ events are reweighted according to the NNLO-to-NLO k -factor, by multiplying the p_T of the top quarks at the generator level (p_T^t) by the function $\exp(0.0615 - 0.0005p_T^t / \text{GeV})$.

4 Event reconstruction

A global “particle-flow” (PF) algorithm [78] aims to reconstruct all individual particles in an event (PF candidates), combining information provided by the inner tracker and the calorimeters, with data from the muon detectors.

The primary vertex (PV) is taken to be the vertex corresponding to the hardest scattering in the event, evaluated using tracking information alone, as described in Section 9.4.1 of Ref. [79].

Muons are reconstructed within $|\eta| < 2.4$ via a combination of the measurements with the tracker and the muon spectrometers in a global fit [46]. Electrons are reconstructed combining the tracker and ECAL measurements [45] within $|\eta| < 2.5$. Electrons that fall in the region between the ECAL barrel and endcaps ($1.442 < |\eta| < 1.556$) are discarded.

Jets are built from PF candidates using the anti- k_T algorithm [80, 81] with a distance parameter of 0.4. Pileup interactions can contribute additional tracks and calorimetric energy depositions, increasing the apparent jet momentum. To mitigate this effect, tracks identified to be originating from pileup are discarded, and an offset correction is applied to correct for remaining contributions [76]. Jet energy corrections are derived from simulation studies so that the average measured energy of jets becomes identical to that of particle-level jets. In situ measurements of the momentum balance in dijet, photon+jet, Z +jets, and multijet events are used to determine any residual differences between the jet energy scale in data and in simulation, and appropriate corrections are made [82]. The energy of each jet is smeared by an amount depending on its p_T and η to adjust the jet energy resolution in simulation to match the one in data. Additional selection criteria are applied to each jet to remove jets potentially dominated by instrumental effects or reconstruction failures [76].

The vector $\vec{p}_T^{\text{miss}}$ is computed as the negative vector sum of the p_T of all the PF candidates in an event, and its magnitude is denoted as p_T^{miss} [83]. The $\vec{p}_T^{\text{miss}}$ is modified to account for corrections to the energy scale of the reconstructed jets in the event.

Hadronic τ lepton decays (τ_h) are reconstructed from jets, using the hadrons-plus-strips al-

gorithm [84], which combines one or three tracks with energy deposits in the calorimeters, to identify the tau decay modes. The DEEPTAU algorithm [85] is used to distinguish genuine τ_h decays from jets originating from electrons, muons, or the hadronization of quarks or gluons. The chosen working point provides a τ_h identification efficiency of approximately 90% and a misidentification rate of about 5% for τ_h candidates with p_T up to 200 GeV [85, 86]. The events that contain τ_h candidates with $p_T > 20$ GeV and $|\eta| < 2.3$ are vetoed.

5 Event selection

Events are selected to reduce contributions from nonprompt leptons. In this analysis, “prompt leptons” refer to electrons and muons originating directly from the prompt decay of vector bosons, while “nonprompt leptons” refer to those originating from semileptonic decays of heavy quarks, hadrons misidentified as leptons, electrons from photon conversions, or jets misidentified as leptons. Charged leptons are required to originate from the PV to reject contributions from pileup by restricting the impact parameter (IP), defined as the distance to the point of closest approach of the track to the PV. The IP defined in the plane transverse to the beams is required to be $|d_{xy}| < 0.05$ cm, while in the longitudinal direction it must satisfy $|d_z| < 0.1$ cm. In addition, charged leptons are required to have an IP significance (SIP_{3D}) less than 8, where SIP_{3D} is defined as the ratio between the IP of the associated track and its uncertainty calculated in three dimensions. The number of electrons originating from asymmetric photon conversions is reduced by requiring the track associated with each electron has no missing hits in the innermost layers of the silicon tracker. An isolation variable, defined relative to the lepton p_T , is used to reduce the effect of hadronic activity in the event not connected with the lepton of interest. The isolation variable, I_{mini} , is defined by $I_{\text{mini}} = S_I(R)/p_T^\ell$, with $R(p_T^\ell) = 10 \text{ GeV} / \min(\max(p_T^\ell, 50 \text{ GeV}), 200 \text{ GeV})$, where $S_I(R)$ is the scalar p_T sum of charged and neutral hadrons, and photon PF candidates inside a cone with a variable radius $R(p_T^\ell)$ around the lepton in the η - ϕ plane [87], and p_T^ℓ is the p_T of the lepton. The isolation variable I_{mini} is calculated for each lepton, where the cone size decreases with increasing p_T^ℓ , reducing the probability of the overlap with a jet for Lorentz-boosted topologies. For this analysis, muons and electrons are required to have $I_{\text{mini}} < 0.4$.

A boosted decision tree (BDT) is employed for the separation of “prompt leptons” and “nonprompt leptons” [88, 89]. The BDT is trained separately for electrons and muons based on the identification methods developed for various CMS measurements [90–94] targeting the leptons from the top quark decay chain and vector boson decays, or from particles beyond the SM [95]. Based on thresholds on the BDT discriminant value, “loose” and “tight” leptons (muons and electrons) are defined, with efficiencies of approximately 96 and 89%, respectively. Selected leptons are those that pass the kinematic selection criteria of $p_T > 30$ (35) GeV and $|\eta| < 2.4$ (2.5) for muons (electrons). Events are corrected for the differences between data and simulation for trigger efficiencies, lepton identification, and lepton isolation. The corrections are determined using the “tag-and-probe” method applied to Z boson candidate events [96] and are parameterized as functions of the lepton p_T and η .

The jets are required to have $p_T > 30$ GeV and to be within $|\eta| < 2.4$ for 2016 data and $|\eta| < 2.5$ for 2017–2018 data. In addition, jets are required to be separated from the identified leptons by $\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2} > 0.4$. The charged-hadron subtraction algorithm is used to mitigate the effect of pileup [82]. Jets with $p_T < 50$ GeV that originate from pileup events are suppressed by a “pileup jet identification” algorithm [76]. For jets with $p_T > 50$ GeV no pileup identification is applied. The working point that corresponds to a 99% efficiency for prompt jets and

1% misidentification rate for pileup jets within $|\eta| < 2.5$ is used. The jets originating from b quarks (b jets) are tagged using the DEEPJET [97, 98] deep neural network algorithm utilizing global variables, as well as charged and neutral particle, and secondary vertex features in a jet to perform flavor tagging. The thresholds used for the DEEPJET discriminant for b jets in this analysis correspond to a mistagging probability of 1% for jets initiated by light quarks or gluons. This choice of thresholds provides an efficiency of approximately 81% for jets initiated by b quarks. Scale factors (SF) have been applied to the simulation to correct for the differences with respect to the data, depending on the jet flavor, p_T , and $|\eta|$ [99].

The signal signature is one lepton, p_T^{miss} , and b-tagged jets. The main event selection requirements are no hadronic τ lepton decay, $p_T^{\text{miss}} > 35$ GeV, and exactly one “tight” lepton. An additional selection on the scalar p_T sum of the jets, $H_T > 200$ GeV, is applied to enhance the signal purity. Events with additional “loose” leptons with $p_T > 10$ GeV are rejected. We define signal regions (SRs) depending on the number of b-tagged jets and jets, namely 2b2j, 2b3j, 2b4j, 3b3j, and 3b4j. The numbers preceding b and j indicate the number of b-tagged jets and jets, respectively. Regions labeled with 4j include at least four jets, while those labeled with 3b include at least three b-tagged jets. Different SRs are sensitive to different signature and mass assumptions. The 2b and 3b SRs are defined mainly to separate s -channel production from the one in association with a quark, which is predominantly a b quark. The signal selection efficiencies range from ≈ 3 to 30%, depending on the SR and the assumed $m_{H^\pm}$, with the highest efficiencies corresponding to the 2b2j SR, and the lowest efficiencies corresponding to the 3b SRs.

For each event, the top quark and $H^\pm$ boson masses are reconstructed. As the signal signature contains a W boson originating from a top quark decay, the first step is to form the W boson from its decay products. The W boson four-momentum is obtained by summing the neutrino and lepton four-momenta. To achieve this, neutrino kinematic distributions are inferred using techniques described in Refs. [100, 101]. It is assumed that the x and y components of the $\vec{p}_T^{\text{miss}}$ are entirely due to the escaping neutrino, and the W boson mass (m_W) is taken to be equal to its world average value of 80.4 GeV [102] to extract the unknown z component of the neutrino (p_z^ν). In $\approx 75\%$ of the cases p_z^ν has two real solutions, and we select the one that has the smaller magnitude. In $\approx 25\%$ of the cases, the reconstructed transverse mass of the W boson is larger than m_W , leading to complex solutions for p_z^ν . In those cases, only the real part of the solution is kept. Once the neutrino and the W boson are reconstructed, in a second step, we evaluate the four-momentum of the top quark candidate. When coupled with the reconstructed W boson, the b jet that results in a reconstructed m_t closest to the nominal value [102] is chosen to be the b jet candidate from the top quark decay. The efficiency of the top quark kinematic reconstruction, based on generator-level information about the b quark origin and defined as the fraction of events for which the b jet is correctly assigned to the top quark that match a reconstructed b jet, varies between 61 and 94%, depending on $m_{H^\pm}$. The b jet candidate combined with the top quark candidate that gives the highest $m_{H^\pm}$ is selected to be the b jet from the $H^\pm$ boson decay. The reconstruction efficiency of $H^\pm$ rises from 27% at $m_{H^\pm} = 200$ GeV to 93% at $m_{H^\pm} = 1$ TeV. The reconstructed distributions of the two discriminating variables, $m_{H^\pm}$ and H_T , in the 2b2j, 2b3j, 2b4j, 3b3j, and 3b4j regions are displayed in Figs. 2–3. A good agreement is observed between data and the sum of the background predictions within the uncertainties. Backgrounds are detailed in Section 6.

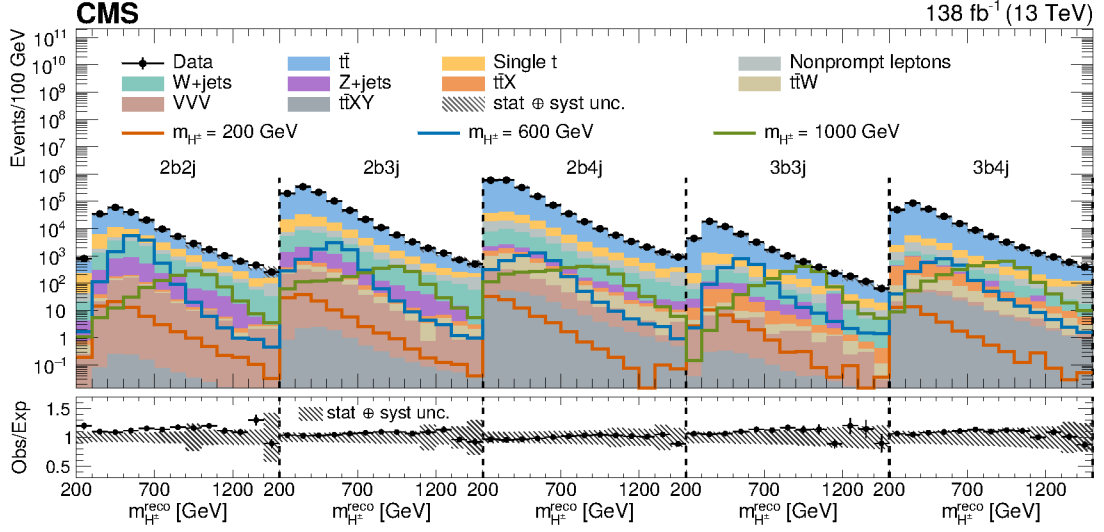


Figure 2: The reconstructed $H^\pm$ boson mass distributions in each SR in the combined data set. Predictions for the signal with $m_{H^\pm} = 200, 600$, and 1000 GeV, normalized to a cross section of 1 pb, are also shown. Beneath each plot, the ratio of data to predictions is shown. The error bars only consider statistical uncertainties in data, while the hashed bands include both statistical and systematic uncertainties.

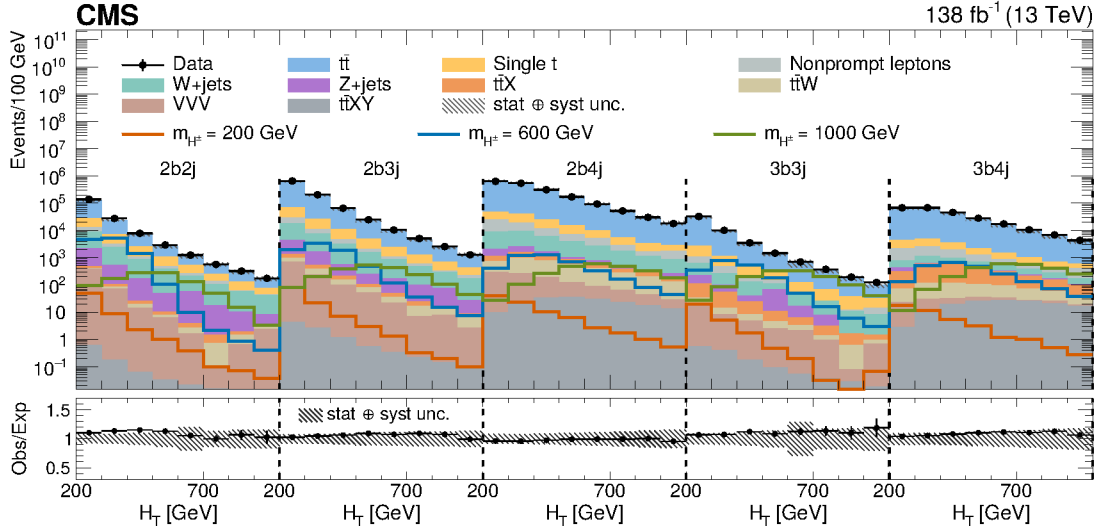


Figure 3: The reconstructed H_T distributions in each SR in the combined data set. Predictions for the signal with $m_{H^\pm} = 200, 600$, and 1000 GeV, normalized to a cross section of 1 pb, are also shown. Beneath each plot, the ratio of data to predictions is shown. The error bars only consider statistical uncertainties in data, while the hashed bands include both statistical and systematic uncertainties.

6 Background estimation from control samples in data

Several processes can mimic the signature of the signal events. After selection, these backgrounds are dominated by $t\bar{t}$ and single top quark, and W +jets production, and by jets misreconstructed as leptons (“nonprompt”). Minor contributions come from Z +jets, $t\bar{t}W$, $t\bar{t}X$ ($t\bar{t}Z$ and $t\bar{t}h$) events and even smaller contributions from $t\bar{t}XY$ ($t\bar{t}hh$, $t\bar{t}tj$, $t\bar{t}t\bar{t}$, $t\bar{t}tW$, $t\bar{t}Wh$, $t\bar{t}WW$, $t\bar{t}WZ$, $t\bar{t}Zh$, and $t\bar{t}ZZ$ events), and VVV production are considered as well. All backgrounds

except the nonprompt lepton contribution are estimated using simulated event samples. The nonprompt lepton background is derived from data control regions using the “tight-to-loose” ratio method (discussed, e.g., in Refs. [103–107]). The nonprompt leptons originate from heavy-flavor hadron decays, misidentified hadrons, decay products of light-meson decays, or photon conversions in jets. The derivation is done in two main steps: First, we estimate the misidentification rate and calculate weights; then, these weights are used to extrapolate the background from an application region to the SR. This method requires “tight” and “loose” lepton candidates that correspond to signal and nonprompt leptons, respectively, and then the “tight-to-loose” ratio is measured in a data control region. The muon and electron misidentification rates are measured using the following selection: exactly one muon or electron that passes the “tight” object selection or the nonprompt-lepton selection, no additional muons or electrons that pass the “loose” selection, $p_T^{\text{miss}} < 35 \text{ GeV}$, and exactly one b-tagged jet (medium WP) with $p_T > 30 \text{ GeV}$ and $|\eta| < 2.4$.

A multijet-enriched sample is selected from data, from which the probability for a “loose” nonprompt lepton to also pass the “tight” lepton selection criteria, f_p , is estimated in bins of p_T and $|\eta|$. The nonprompt-lepton background contribution is then estimated by applying f_p to events in a data control sample in which at least one lepton fails the “tight” lepton selection criteria. The most dominant contribution of the nonprompt lepton background originates from QCD multijet events. A 50% uncertainty in the nonprompt lepton background rate is assigned. We validated the “tight-to-loose” method by doing a closure test using simulated multijet samples requiring one b-tagged jet and no requirement on p_T^{miss} .

Table 1: Input variables of the pDNN_{2b} and pDNN_{3b}. Indices $i < j$ run up to including 2 for pDNN_{2b} and 3 for pDNN_{3b}.

$p_T(\ell)$	Transverse momentum of the lepton
p_T^{miss}	Missing transverse momentum
$\Delta R(\mathbf{b}_i, \ell)$	Angular separation between b jet and lepton
$\Delta R(\mathbf{b}_i, \mathbf{b}_j)$	Angular separation between b jets
$p_T(\mathbf{b}_i)$	Transverse momentum of b jets
H_T	Scalar p_T sum of the jets
$m(\ell, \mathbf{b}_i, \mathbf{b}_j)$	Invariant mass of b jets and lepton
$m(\ell, \mathbf{b}_i)$	Invariant mass of b jet and lepton
$\Delta\phi(p_T^{\text{miss}}, \ell)$	Azimuthal angle difference between missing transverse momentum and lepton
$m_{H^\pm}^{\text{reco}}$	Invariant mass of the reconstructed $H^\pm$

7 Signal extraction

Parametric deep neural network (pDNN) [108] distributions are used to separate signal and background events. The pDNN input features used in the analysis in the 2b (pDNN_{2b}) and 3b (pDNN_{3b}) SRs are listed in Table 1. The input features are selected based on the correlation between features and the results of the Boruta algorithm [109]. This algorithm shuffles the original features to create copies of them, called shadow features, and trains a random forest classifier on the extended data set. The features that have lower variable importance than the highest rated shadow feature are regarded as unimportant and are removed. Consistent features in the 2b and 3b regions are selected for simplicity, with no loss in performance. In the pDNN, the neural network is parametrized by $m_{H^\pm}$, which is taken as an additional input variable

of the network. This feature is assigned to be the generated $m_{H^\pm}$ for the signal and assigned randomly from the $m_{H^\pm}$ values for the background. The pDNN interpolates between different $m_{H^\pm}$ hypotheses. Additionally, it provides effective interpolation for the mass input to pDNN for modeling the background. However, for the signal, since the input kinematic distributions change in a nontrivial way, interpolation can not fully capture the differences. Therefore, we provide results on specific mass hypotheses. Separate trainings are performed for 2016 and 2017–2018 data to take into account the changing detector conditions. The pDNNs are trained separately for the 2b2j, 2b3j+2b4j, 3b3j, and 3b4j SRs and the two data-taking periods. The signal is extracted from the pDNN score distributions combining all data-taking periods in each SR.

Reweightings are performed among signal samples, so that each mass hypothesis enters with the same weight. The weight assigned to each background sample during the training is proportional to its expected event yield. The pDNN design contains three hidden layers. Hyperparameter tuning is performed using part of the training data set to minimize the loss function, which is chosen to be the binary cross entropy. The k -fold ($k = 5$) strategy is used to avoid overtraining. We first split the data set into an application sample and a training+validation sample. Then, the training+validation sample is used for k -fold training, so the application sample remains independent of the training and validation. Using the Adam algorithm [110] employing the Nesterov momentum [111] to minimize the binary cross entropy loss function, the model is trained for 250 epochs. The final model is the ensemble of the models produced from k -fold training weighted with inverse of its loss in the k -fold test. Receiver operating characteristic curves in each fold and the comparison between validation and training distributions are used to check the performance and potential overtraining of the pDNN.

The bins of the pDNN score distribution are optimized in several steps. First, the pDNN distribution is constructed with 10 bins of equal size. Second, the bins are combined so that the yield in each bin is at least 10 events. In the next step, the pDNN distribution is rebinned using the Bayesian block algorithm [112, 113] based on the signal distribution, to ensure the stability of the signal extraction procedure. Further optimization is performed in order to avoid large differences of bin widths between two consecutive bins. This last step of the optimization procedure is not applied to the lowest and highest bins.

8 Systematic uncertainties

Systematic uncertainties, arising from various sources, such as detector effects, theoretical uncertainties, and mismodeling, are evaluated and categorized in two main groups: experimental and modeling uncertainties. The systematic uncertainties are modeled as nuisance parameters in the maximum likelihood estimation procedure used for determining the best fit signal strength $\hat{\mu}$, defined as the ratio of the measured cross section to the signal expectation in the g2HDM model. The nuisance parameters can modify the shape and normalization of the background and signal distributions in the fit using the CMS statistical analysis tool COMBINE [114]. The chosen probability density function (pdf) used for the interpolation between nominal and modified templates is dependent on whether the associated nuisance parameter can also affect the shape of the nominal template or not. Log-normal pdfs are used for nuisance parameters that only affect the distribution normalizations, whereas Gaussian pdfs are used for those that can affect the shape as well. Experimental uncertainties, where appropriate, and all modeling uncertainties are taken as correlated across the data-taking periods, SRs, and channels. The effect of the limited number of simulated events is estimated using the Barlow–Beeston “light” method [115].

The experimental uncertainties are described below. The integrated luminosity measurements of CMS for the 2016, 2017, and 2018 data-taking periods are described in Refs. [116–118]. The uncertainty in the integrated luminosity has an effect on the background and signal yields. The combined uncertainty for 2016–2018 is 1.6%. To estimate the effect of mismodeling of the pileup, the total inelastic cross section of 69.2 mb [76] is varied by $\pm 4.6\%$. The variations are treated as fully correlated between the different data-taking years. In 2016 and 2017, a time jitter of the trigger signal in the muon [119] and ECAL [42] detectors, led to a loss of events of the order of $\lesssim 0.5\%$. These effects are corrected for by applying dedicated SFs to the simulation. The associated uncertainties are evaluated by varying the SFs within their uncertainties.

The trigger SF uncertainties are assumed to be uncorrelated between the data-taking periods. The uncertainties in the electron reconstruction efficiency SFs are considered to be correlated across the data-taking years. For the uncertainties in the SFs related to lepton identification, isolation, energy scale, and resolution, the statistical and systematic components are merged, and therefore, for both muons and electrons, nuisance parameters are considered correlated across years.

For the b tagging and misidentification efficiencies, two nuisance parameters are considered for light-quark/gluon and heavy-flavor jets [99]. Each of them have components correlated/un-correlated across the data-taking periods. The variations of jet four-momenta using the full set of uncertainty sources and corresponding correlations from Ref. [82] are used. The uncertainties in the jet energy resolution in different data-taking periods are considered uncorrelated, and in different channels fully correlated. The uncertainties in jet energy scale and resolution, as well as the variation of the unclustered energy, are propagated into p_T^{miss} . The uncertainty in p_T^{miss} is taken as uncorrelated across the three data-taking years.

Finally, two separate nuisance parameters are used for the nonprompt lepton background estimate from data: a normalization uncertainty of 50% and a shape uncertainty estimated from the difference between the 1b and 2b nonprompt lepton background distributions. The normalization uncertainty is uncorrelated across the SRs and channels.

In the following, we describe the sources of modeling uncertainty. The uncertainties in the signal, $t\bar{t}$, and W +jets backgrounds are included as separate nuisance parameters that affect the shape of the distributions, and additional parameters are included that affect their normalization. For the other backgrounds, which are estimated using simulated event samples, the corresponding uncertainties in the cross section calculations are used, and nuisance parameters are included that only affect the yields. For the top quark p_T reweighting, which only affects the $t\bar{t}$ background, uncertainties related to the correction from NLO to NNLO predictions are estimated using the difference between the NNLO and NLO predictions. These uncertainties are treated as uncorrelated across the SRs.

Variations of μ_r and μ_f by factors of 0.5 and 2 are considered and assumed uncorrelated with each other. This uncertainty is taken correlated across years and channels. The uncertainties due to the PDF set used in the simulation are estimated using the Hessian variations of the NNPDF3.1 NNLO set. The effects are propagated through event weights [120]. The effect of the variation of α_s on the PDF set is also taken into account. The PDF uncertainties are considered fully correlated across the data-taking years. The parton shower scale choice is varied by a factor of 0.5 and 2 for initial-state and final-state radiation separately, using event weights for the signal, $t\bar{t}$, and W +jets samples. This uncertainty is considered correlated for the same process across the years and channels.

9 Results

The signal is extracted by simultaneously fitting the pDNN distributions across two channels (e and μ), and five SRs (2b2j, 2b3j, 2b4j, 3b3j, and 3b4j) combining all data-taking periods. For the background processes, the yields and shapes are taken directly from the simulation except for the nonprompt lepton background. Figures 4 and 5 display the postfit pDNN discriminant distributions used for the signal extraction in the 2b2j and 3b3j SRs for the e and μ channels, for $m_{H^\pm} = 600$ and 1000 GeV, respectively. Summary of the decomposition of the systematic uncertainties with respect to the total uncertainty on the signal strength for $m_{H^\pm} = 200, 600$, and 1000 GeV are shown in Tables 2–4.

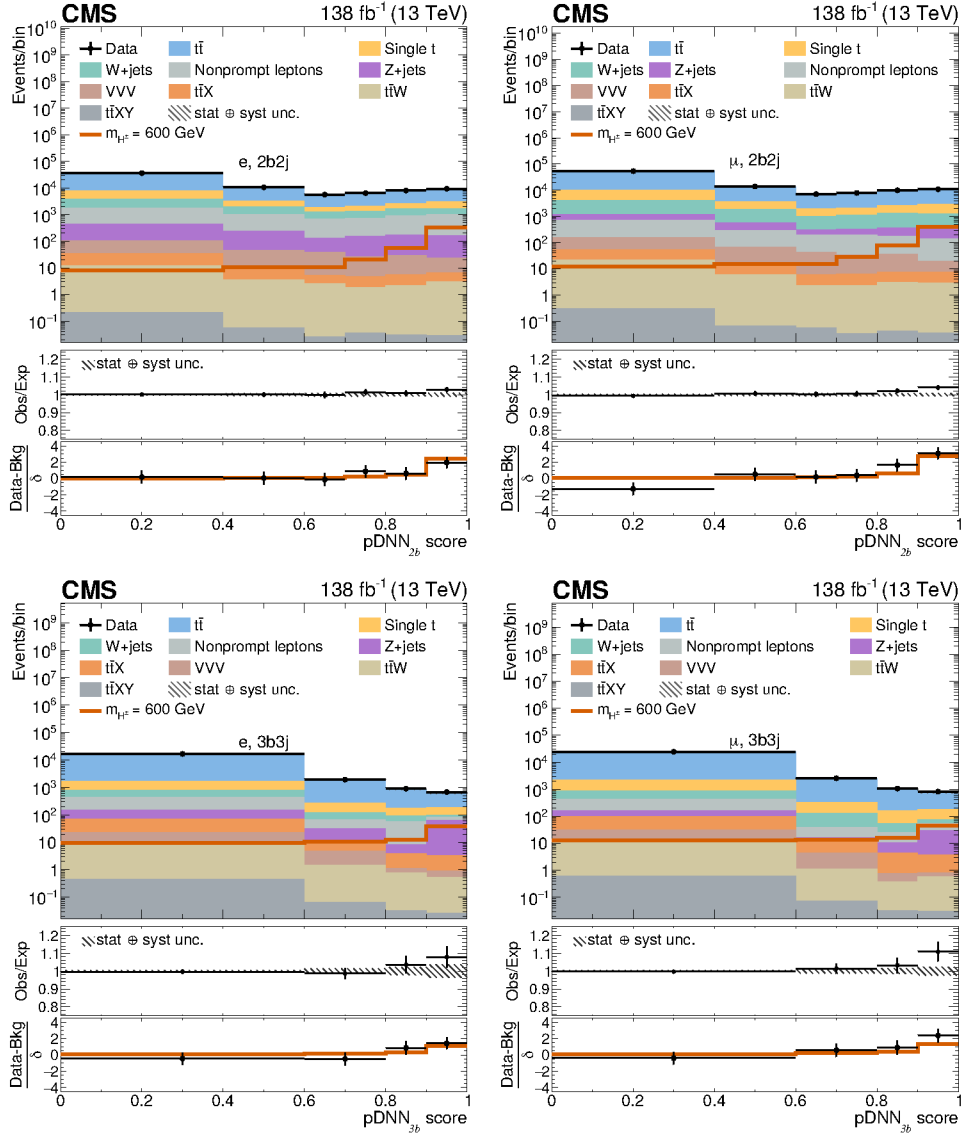


Figure 4: The postfit pDNN distributions in the SR 2b2j (upper) and 3b3j (lower) for electron (left) and muon (right) channels assuming $m_{H^\pm} = 600$ GeV. Postfit signal for $m_{H^\pm} = 600$ GeV is also shown. Lower panels display the difference between data and the sum of the SM background predictions, normalized by the combined statistical and systematic uncertainty, δ . The error bars only consider statistical uncertainties in data, while the hashed bands include both statistical and systematic uncertainties.

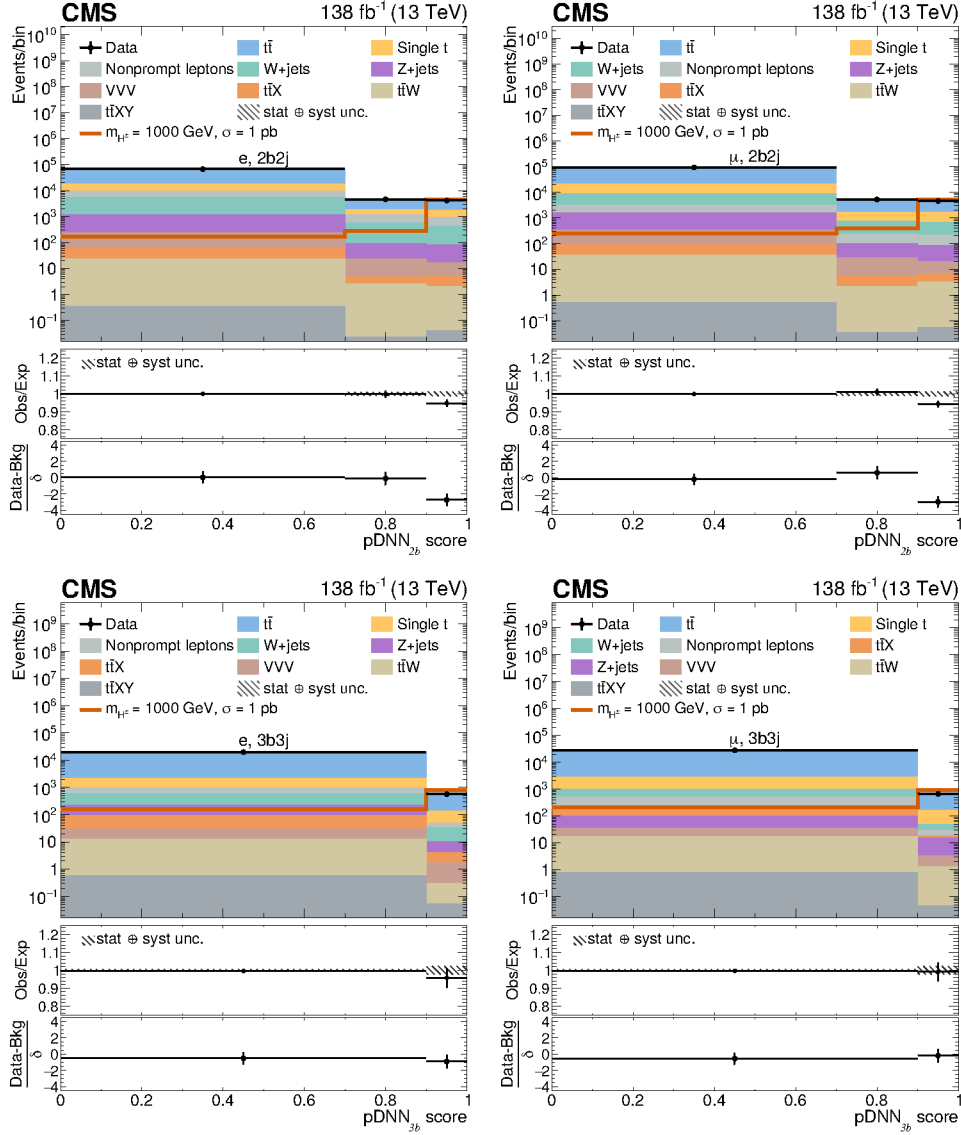


Figure 5: The postfit pDNN distributions in the SR 2b2j (upper) and 3b3j (lower) for electron (left) and muon (right) channels assuming $m_{H^\pm} = 1$ TeV. The signal for $m_{H^\pm} = 1$ TeV is also shown before the fit, assuming a cross section of 1 pb. Lower panels display the difference between data and the sum of the SM background predictions, normalized by the combined statistical and systematic uncertainty, δ . The error bars only consider statistical uncertainties in data, while the hashed bands include both statistical and systematic uncertainties.

The results of the search are interpreted in terms of upper limits on the product of the cross section $\sigma(\text{pp} \rightarrow (b)H^\pm)$ and branching fraction $\mathcal{B}(H^\pm \rightarrow tb, t \rightarrow b\ell\nu)$ in the g2HDM, where $\ell = e, \mu$. The upper limits on cross sections are calculated at 95% confidence level (CL) using a modified frequentist method [121–123] within an asymptotic approximation [124]. The expected 95% CL on the production cross section and the regions containing 68 and 95% of the distribution of the limits expected under the background-only hypothesis are calculated with pseudo-experiments using background-only samples. Modifying the extra Yukawa couplings in the range 0.1–1.0 does not impact the limits significantly, and they remain within the 68% CL band. The $H^\pm$ boson width increases with the mass and the strength of the extra Yukawa couplings. The analysis is not sensitive to the width up to 10%, and the largest $H^\pm$ boson width

in the signal phase space probed in this analysis is $\sim 12\%$, which is obtained for $m_{H^\pm} = 1$ TeV and $\rho_{tt} = \rho_{tc} = 1$. Figure 6 displays the observed and expected 95% CL upper limits on the cross section times branching fraction, along with the corresponding observed and expected local significances, p-value [124], as a function of $m_{H^\pm}$. The smallest p-value is observed for a signal with $m_{H^\pm} = 600$ GeV, corresponding to a local significance of 2.4 standard deviations (SD). Figure 7 displays the excluded phase space regions as functions of $m_{H^\pm}$ and ρ_{tc} for various assumed ρ_{tt} values based on the g2HDM with all the extra Yukawa couplings except ρ_{tt} and ρ_{tc} set to zero. The largest exclusion region is observed around $m_{H^\pm} = 400$ GeV, excluding values of $\rho_{tc} > 0.16$ (0.21) for $\rho_{tt} = 1.0$ (0.3) at 95% CL. For $\rho_{tt} = 1$, values of $\rho_{tc} > 0.57$ are excluded at 95% CL for the entire mass range tested, for $m_{H^\pm}$ from 200 to 1000 GeV.

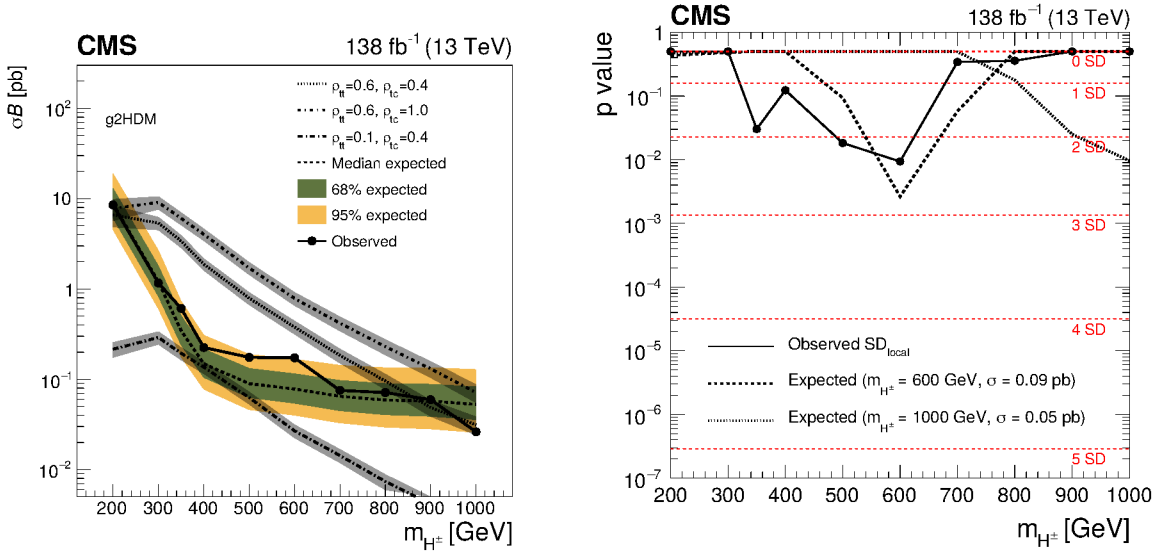


Figure 6: Left: observed and expected 95% CL limits on the cross section times branching fraction ($\sigma\mathcal{B}$) for different $H^\pm$ boson mass hypotheses with $\rho_{tc} = 0.4$ and $\rho_{tt} = 0.6$. The inner (green) band and the outer (yellow) band represent the regions containing 68 and 95%, respectively, of the distribution of limits expected under the background-only hypothesis. Theoretical prediction with different ρ_{tc} and ρ_{tt} couplings are shown with the grey bands representing the corresponding uncertainties due to the factorization and renormalization scales, and the PDFs. Right: Observed local significance extracted from the pDNN distribution. Expected significances are obtained with the injection of a $\sigma = 0.09$ (0.05) pb of g2HDM signal with $m_{H^\pm} = 600$ GeV (1 TeV). The injected cross sections are picked as the best fit value for $m_{H^\pm} = 600$ GeV, and the theoretical prediction for $m_{H^\pm} = 1$ TeV assuming $\rho_{tc} = \rho_{tt} = 0.6$. Local significance values in units of standard deviations (SD) are also shown with dashed horizontal lines on the vertical axis.

In order to provide cross section upper limits independent of the g2HDM, we separate the signal samples into two categories based on the number of b quarks at the parton level: one with two b quarks ($\sigma(pp \rightarrow H^\pm)$) and another with three or more b quarks ($\sigma(pp \rightarrow bH^\pm)$). The contribution of the processes in the two categories can vary depending on different signal hypothesis, while the ratio stays constant in the g2HDM for a fixed $m_{H^\pm}$. Using these two categories, we provide a two dimensional contour scan of two times the difference of negative log-likelihood ($2\Delta\text{NLL}$) for $\sigma(pp \rightarrow H^\pm) \mathcal{B}(H^\pm \rightarrow tb, t \rightarrow b\ell\nu)$ vs $\sigma(pp \rightarrow bH^\pm) \mathcal{B}(H^\pm \rightarrow tb, t \rightarrow b\ell\nu)$ processes in Fig. 8, for $m_{H^\pm} = 600$ and 1000 GeV. The best fit values for $m_{H^\pm} = 600$ and 1000 GeV are $\sigma(pp \rightarrow H^\pm) \mathcal{B}(H^\pm \rightarrow tb, t \rightarrow b\ell\nu) = 0.055^{+0.068}_{-0.055}$ and $0.000^{+0.009}_{-0.000}$ pb, and $\sigma(pp \rightarrow bH^\pm) \mathcal{B}(H^\pm \rightarrow tb, t \rightarrow b\ell\nu) = 0.032^{+0.035}_{-0.029}$ and $0.006^{+0.019}_{-0.006}$ pb, respectively, with the

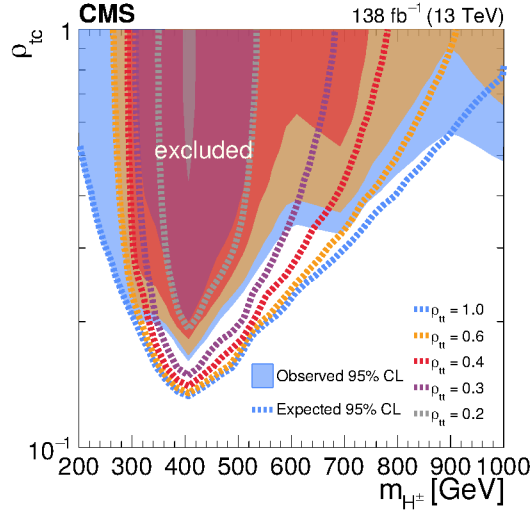


Figure 7: Observed and expected 95% CL excluded phase space regions, as functions of $m_{H^\pm}$ and ρ_{tc} for various assumed ρ_{tt} values represented with different colors. The limits are extracted from the pDNN distributions based on the g2HDM assuming all the extra Yukawa couplings except ρ_{tt} and ρ_{tc} are zero. The results are obtained from the 95% CL limits on the cross section times branching fraction in Fig. 6.

corresponding 68 and 95% CL contours also shown in Fig. 8.

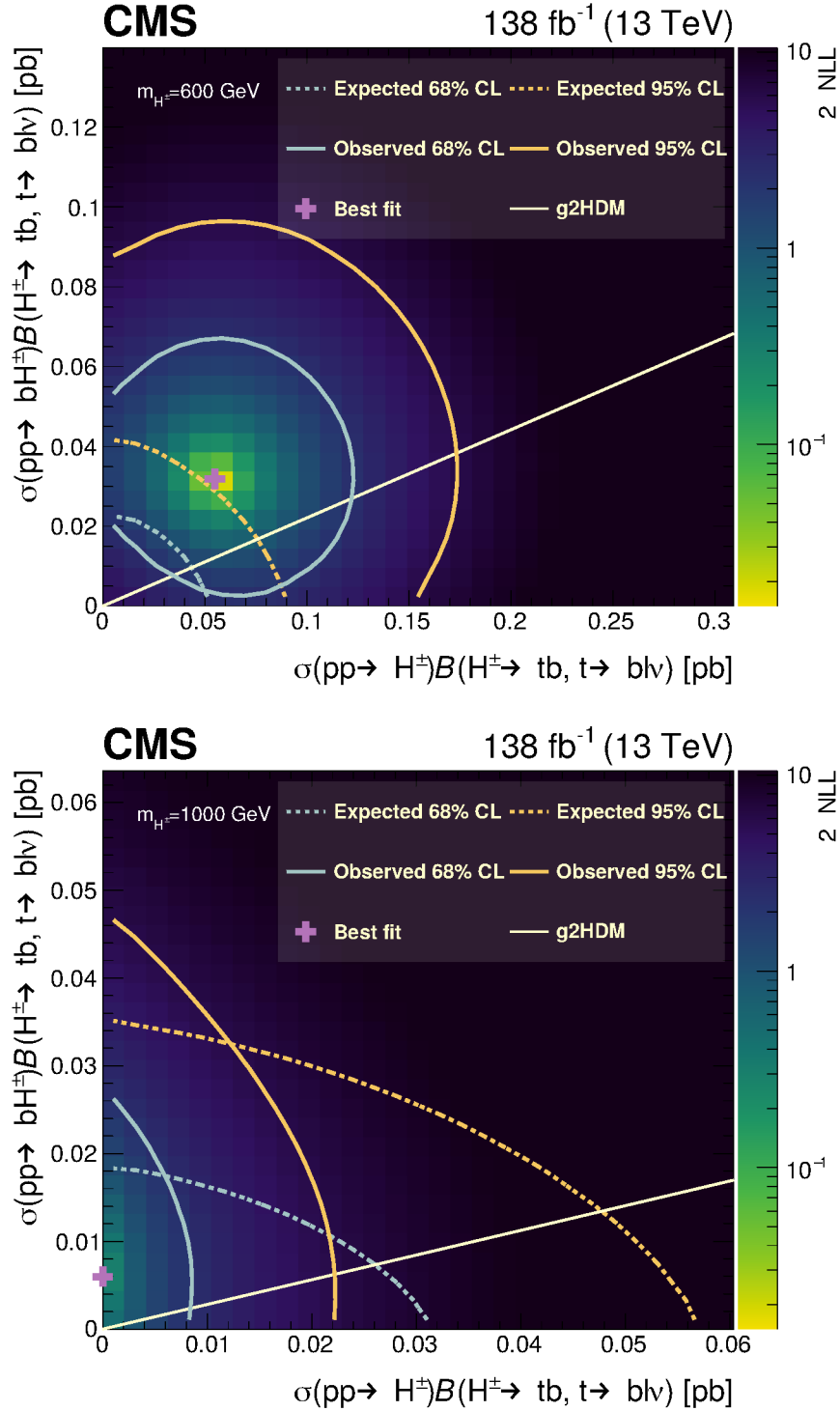


Figure 8: Two times the difference of the negative log-likelihood (NLL) as a function of $\sigma(pp \rightarrow H^\pm) B(H^\pm \rightarrow tb, t \rightarrow b\ell\nu)$ and $\sigma(pp \rightarrow bH^\pm) B(H^\pm \rightarrow tb, t \rightarrow b\ell\nu)$ with the best fit point extracted from the pDNN distribution for the $H^\pm$ boson mass $m_{H^\pm} = 600$ GeV (upper), and $m_{H^\pm} = 1000$ GeV (lower). The solid and dashed contours represent the observed and expected limits, respectively. The points along the contours represent 68 and 95% CL regions, extracted from the $2\Delta\text{NLL}$ values of 2.30 and 5.99, respectively. The g2HDM predictions are also shown. The points along the g2HDM prediction line represent different ρ_{tt}, ρ_{tc} coupling sets, with all other extra Yukawa couplings assumed to be zero.

Table 2: Summary of the systematic uncertainty decomposition with respect to the total uncertainty in the signal strength for the mass hypothesis $m_{H^\pm} = 200$ GeV.

Uncertainty source	Down variation [%]	Up variation [%]
Theoretical background cross sections	50.0	52.6
Statistical uncertainty	39.2	41.8
Top quark p_T reweighting	34.8	34.5
Heavy-flavor tagging	32.6	31.8
Nonprompt-lepton bkg. estimate	30.2	25.9
Parton shower ISR/FSR	26.7	23.1
μ_r/μ_f	25.8	23.5
Jet energy scale	23.9	22.0
Unclustered energy	18.2	20.7
Pileup	13.9	19.1
PDF	11.5	10.8
Jet energy resolution	10.7	10.0
Integrated luminosity	3.1	4.7
Electron reconstruction	4.2	3.0
Jet pileup identification	3.6	1.5
Lepton identification	3.4	1.6
Lepton trigger efficiencies	1.2	2.3
L1 trigger inefficiency	0.7	0.0
Lepton energy scale	0.7	0.0

Table 3: Summary of the systematic uncertainty decomposition with respect to the total uncertainty in the signal strength for the mass hypothesis $m_{H^\pm} = 600$ GeV.

Uncertainty source	Down variation [%]	Up variation [%]
Heavy-flavor tagging	56.4	56.7
Theoretical background cross sections	39.6	33.4
PDF	19.6	32.5
Statistical uncertainty	36.9	31.4
Top quark p_T reweighting	31.5	29.8
Jet energy scale	26.8	24.5
μ_r/μ_f	17.3	24.3
Unclustered energy	22.0	21.2
Nonprompt-lepton bkg. estimate	22.3	17.7
Parton shower ISR/FSR	11.0	17.1
Pileup	8.4	12.9
Jet pileup identification	12.3	12.1
Jet energy resolution	9.7	11.0
Integrated luminosity	4.4	5.5
L1 trigger inefficiency	5.2	3.5
Lepton energy scale	4.9	0.6
Lepton trigger efficiencies	4.0	3.8
Electron reconstruction	0.0	0.6
Lepton identification	0.0	0.0

Table 4: Summary of the systematic uncertainty decomposition with respect to the total uncertainty in the signal strength for the mass hypothesis $m_{H^\pm} = 1000$ GeV.

Uncertainty source	Down variation [%]	Up variation [%]
PDF	54.2	38.5
Top quark p_T reweighting	52.8	56.0
Jet energy scale	39.7	40.7
Theoretical background cross sections	34.1	31.0
Heavy-flavor tagging	26.3	32.1
Statistical uncertainty	6.0	30.7
Parton shower ISR/FSR	15.8	9.4
Nonprompt-lepton bkg. estimate	15.7	18.8
μ_r/μ_f	14.8	12.8
Lepton identification	7.9	3.6
Electron reconstruction	0.0	7.3
Jet pileup identification	1.1	5.8
L1 trigger inefficiency	3.8	5.7
Pileup	2.2	5.5
Lepton trigger efficiencies	3.9	3.8
Unclustered energy	3.3	0.0
Jet energy resolution	0.0	3.7
Integrated luminosity	2.4	1.4
Lepton energy scale	0.0	1.3

10 Summary

A search for charged Higgs bosons ($H^\pm$) in proton-proton (pp) collisions at a center-of-mass energy of 13 TeV has been presented. The processes considered are $pp \rightarrow (b)H^\pm$, with $H^\pm$ decaying into top (t) and bottom (b) quarks. We consider $t \rightarrow b\ell\nu$ decays, where $\ell = e, \mu$. The $H^\pm$ boson mass ($m_{H^\pm}$) is probed between 200 GeV and 1 TeV. The results of the search are interpreted in the generalized two-Higgs-doublet model (g2HDM), assuming the real parts of extra Yukawa couplings of $H^\pm$ to the top quark ρ_{tt} and to the top and charm quark ρ_{tc} are both less than one, and the imaginary parts and all other extra Yukawa couplings are zero. An excess is observed with respect to the standard model expectation with a local significance of 2.4 standard deviations for a signal with $m_{H^\pm} = 600$ GeV. The best fit cross section (σ) times branching fraction ($\mathcal{B}$) values corresponding to the excess at $m_{H^\pm} = 600$ GeV are $\sigma(pp \rightarrow H^\pm)\mathcal{B}(H^\pm \rightarrow tb, t \rightarrow b\ell\nu) = 0.055^{+0.068}_{-0.055}$ pb and $\sigma(pp \rightarrow bH^\pm)\mathcal{B}(H^\pm \rightarrow tb, t \rightarrow b\ell\nu) = 0.032^{+0.035}_{-0.029}$ pb, where $\ell = e, \mu$. Upper limits at 95% confidence level (CL) are set on $\sigma\mathcal{B}$ for $m_{H^\pm}$ up to 1 TeV. The values for $\rho_{tc} \gtrsim 0.15$ –0.5 are excluded, depending on the $m_{H^\pm}$ and ρ_{tt} assumptions. The strongest exclusion is achieved near $m_{H^\pm} = 400$ GeV, where values of $\rho_{tc} > 0.16$ for $\rho_{tt} = 1.0$ and $\rho_{tc} > 0.21$ for $\rho_{tt} = 0.3$ are excluded at 95% CL. For $\rho_{tt} = 1$, the analysis excludes $\rho_{tc} > 0.57$ at 95% CL across the mass range from 200 GeV to 1 TeV. This is the first search for $H^\pm$ bosons within the g2HDM framework.

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