New Limit for Neutrinoless Double-Beta Decay of $^{100}$Mo from the CUPID-Mo Experiment

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The CUPID-Mo experiment at the Laboratoire Souterrain de Modane (France) is a demonstrator for CUPID, the next-generation ton-scale bolometric $0\nu\beta\beta$ experiment. It consists of a 4.2 kg array of 20 enriched Li$_2$MoO$_4$ scintillating bolometers to search for the lepton-number-violating process of $0\nu\beta\beta$ decay in $^{100}$Mo. With more than one year of operation ($^{100}$Mo exposure of 1.17 kg yr for physics data), no event in the region of interest and, hence, no evidence for $0\nu\beta\beta$ is observed. We report a new limit on the half-life of $0\nu\beta\beta$ decay in $^{100}$Mo of $T_{1/2} > 1.5 \times 10^{27}$ yr at 90% C.I. The limit corresponds to an effective Majorana neutrino mass $m_{\nu_0} < (0.31-0.54)$ eV, dependent on the nuclear matrix element in the light Majorana neutrino exchange interpretation.

DOI: 10.1103/PhysRevLett.126.181802

0031-9007/21/126(18)/181802(7) 181802-1 © 2021 American Physical Society
The discovery that neutrinos are massive particles through the evidence of neutrino flavor oscillations [1] opens the question of neutrino mass generation. Instead of having Dirac nature as charged leptons and quarks, the scale of neutrino masses could be well motivated by the Majorana theory [2,3]. In this scenario, neutrinos could coincide with their antimatter partner [4,5], which would have a tremendous impact on our vision of nature, implying the violation of the total lepton number \( L \) as well as for the matter-antimatter asymmetry in the Universe [6,7].

The distinction between Dirac and Majorana behavior is an extreme experimental challenge. Neutrinoless double-beta (\( \nu_{\beta\beta} \)) decay is the traditional and the most sensitive tool to probe the Majorana nature of neutrinos. This process is a nuclear transition consisting in the transformation of an even-even nucleus into a lighter isobar containing two more protons and accompanied by the emission of two electrons and no other particles, with a change of the lepton number.

A detector embedding a candidate with \( Q_{\beta\beta} > 2615 \text{ keV} \) is an optimal choice in terms of background control, as the bulk of the \( \gamma \) natural radioactivity ends at 2615 keV, corresponding to the energy of the \( ^{208}\text{Tl} \) line in the \( ^{232}\text{Th} \) decay chain. However, the energy region above \( \sim 2.6 \text{ MeV} \) is dominated by events due to surface radioactive contamination, especially energy-degraded \( \alpha \) particles [17,27], as shown by the results of CUORE, the largest \( \nu_{\beta\beta} \) bolometric experiment currently under way.

A dual readout of light—scintillation or Cherenkov— in addition to the thermal signal allows for the discrimination of \( \alpha \) events in various targets [25,26,28–33]. This technology has been developed for the scintillating \( \text{Li}_2^{100}\text{MoO}_4 \) crystals used in CUPID-Mo by the LUMINEU Collaboration [34,35], and its effectiveness is described together with the experimental setup in Ref. [36]. The isotope of interest \( ^{100}\text{Mo} \) features a \( Q_{\beta\beta} \) of \( (3034.40 \pm 0.17) \text{ keV} \) [37] and a natural abundance of 9.7%, making large-scale enrichment viable by gas centrifuge isotopic separation [38]. In CUPID-Mo, it is embedded into \( \text{Li}_2^{100}\text{MoO}_4 \) (LMO) crystals by a double low-thermal-gradient Czochralski crystallization process [39] from enriched Mo previously used in the NEMO-3 experiment [40]. A total of 20 cylindrical \( \sim 210 \text{ g} \) crystals are stacked into five towers, which results in a \( ^{100}\text{Mo} \) mass of \( (2.258 \pm 0.005) \text{ kg} \) with an average \( ^{100}\text{Mo} \) isotopic abundance of \( (96.6 \pm 0.2) \% \). Round Ge wafers, attached to the bottom of each LMO detector, are used as bolometric light detectors (LDs). Because of the stacking into the four-layer tower, most LMO detectors have a direct line of sight to a LD at both the top and bottom, except for the top crystal of each tower, which has a Cu lid on one side [36]. The LMO crystals as well as the LDs are instrumented with neutron-transmutation-doped-Ge sensors [41]. The towers are installed with a mechanical decoupling inside the EDELWEISS cryogenic infrastructure [42,43] at the Laboratoire Souterrain de Modane in France.

The data of the present analysis have been acquired over a 380 day period between March 2019 and April 2020 at operation temperatures of 20.7 and 22 mK. About 82% of the time was devoted to the \( \nu_{\beta\beta} \) search, split into 240 days of physics data and 73 days of calibration data. The physics data are grouped into a total of ten datasets with consistent operation conditions. In the following, we consider 213 out of the 240 days of physics data in seven (1–2-month-long) datasets and reject three (\( \sim 1 \)-week-long) datasets due to their small associated calibration statistics. From these seven datasets, we exclude periods of temperature instabilities, disturbances in the underground laboratory, and periods of excessive noise on the individual detectors, reducing the physics exposure by 6%. We reject one of the 20 LMO bolometers that shows an abnormal performance [36] and obtain a physics exposure of \( 2.16 \text{ kg} \times \text{yr} \ (\text{Li}_2^{100}\text{MoO}_4) \).
deviation. The extrapolation for the position of 609, 1461, and 2615 keV peaks and observe no systematic reconstructed-to-expected peak position of the 352, 583, 709, and 1120 keV peaks in calibration data. We perform a simultaneous unbinned fit for the energy and position with common parameters for the two LMOs and LD channels. We calibrate the response of the LMO signals. The data were triggered on a single crystal and in anticoincidence with a triple-module veto system [49] following event selections. For events (i) to be contained in the low-background regime. We consider detector- and dataset-based (19 × 7) energy resolutions, a preliminary estimate of our background index, and an exposure of 2.8 kg × yr, as we intend to replicate the present analysis for the full exposure of the now-completed CUPID-Mo experiment.

The most representative γ peak for the 100Mo region of interest (ROI) with sufficient statistics to extract detector- and dataset-based resolutions is the 2615 keV line from 208Tl. A ±50 keV region around $Q_{\beta\beta}$ has been blinded (gray).

All data are acquired as a continuous stream with 500 Hz sampling frequency and analyzed with a software package developed by the CUORE [44] and CUPID-0 [45] Collaborations, first used in CUPID-Mo in Refs. [36, 46]. We estimate pulse amplitudes with an optimum filter [47], designed to maximize the signal to noise ratio for a known signal and noise spectrum with 3-s-long pulse traces for neutron irradiation of the detectors [53]. For more details, we refer to a prior characterization of the backgrounds in the EDELWEISS facility [42].

We optimize the $0\nu\beta\beta$ search for a Poisson counting process in the low-background regime. We consider detector- and dataset-based (19 × 7) energy resolutions, a preliminary estimate of our background index, and an exposure of 2.8 kg × yr, as we intend to replicate the present analysis for the full exposure of the now-completed CUPID-Mo experiment.

The most representative γ peak for the 100Mo region of interest (ROI) with sufficient statistics to extract detector- and dataset-based resolutions is the 2615 keV line from 208Tl in calibration data. We perform a simultaneous unbinned extended maximum likelihood fit of this peak with individual parameters for the detector resolutions, peak amplitudes, and position and with common parameters for the peak-background ratio [46]. We then project these resolutions with a global scaling factor $s = \sigma_{\text{phys}}(3034 \text{ keV})/\sigma_{\text{cal}}(2615 \text{ keV})$ (common to all datasets and detectors) to $Q_{\beta\beta}$. In addition to the method described in Ref. [46], we extract $s$ from a polynomial fit of the global γ peaks in background and calibration data [17, 27]. We adopt the scaling factor from this latter method as a conservative choice, predicting a 0.2% worse resolution of $[7.6 \pm 0.7 \text{(stat)} \pm 0.2 \text{(syst)}] \text{ keV FWHM at } Q_{\beta\beta}$ for the overall data taking. The noted systematic uncertainty of 2% is due to pile-up-related non-Gaussian tails in calibration data that affect the calibration resolution estimates through the PC analysis cut.
The background index has been evaluated from the still-blinded data with a phenomenological fit model that contains an exponential to approximate both the high-energy part of the $2\nu\beta\beta$ spectrum as well as tails from U/Th contaminants in the setup and a constant as a conservative estimate for the coincident detection of two $2\nu\beta\beta$ events in the same crystal, remaining unvetted muon events and close contamination from the high-energy beta decays in the natural U/Th chains. The result of an unbinned extended maximum likelihood fit is strongly dependent on the low-energy and high-energy limit of the fit range. For a fit with the low-energy limit varied from 2.65 to 2.9 MeV and the high-energy limit from the upper end of the blinded region to 4 MeV, we obtain a background index of $2 \times 10^{-3}$ counts/(keV × kg × yr) to $6 \times 10^{-3}$ counts/(keV × kg × yr) in a 10 keV window around $Q_{\beta\beta}$. Considering the large remaining uncertainty, we round the background index for the ROI optimization to $5 \times 10^{-3}$ counts/(keV × kg × yr). We model the background as locally flat, consider detector- and dataset-based resolutions, and simulate the $0\nu\beta\beta$ peak containment in our GEANT4 Monte Carlo model. As this background index is both poorly constrained and indicative of a most probably background-free $0\nu\beta\beta$ search, we select the ROI maximizing the mean-limit-setting sensitivity for a Poisson process with zero background:

$$\overline{S}_{90} = \sum_{i=0}^{\infty} P(i, b, \Delta E_{ROI}) \cdot S_{90}(i)$$

with the sum running over the product of the Poisson probability $P(i, b, \Delta E_{ROI})$ of obtaining $i$ events for an ROI with width $\Delta E_{ROI}$ and a background index $b$ times the expected classical 90% confidence exclusion limit $S_{90}(i)$. We transfer this maximization from the optimization of the energy range for a peak search in 19 (detectors) times 7 (datasets) to the optimization of a single parameter by splitting the simulated smeared $0\nu\beta\beta$ peaks into 0.1 keV bins and ranking each bin associated with a triplet (detector, dataset, energy) in signal-background (B/S) likelihood space. The optimal cutoff parameter $(B/S)_{\text{cutoff}}$ results in an ROI that is on average (exposure weighted) 17.9 keV wide. It has a mean signal containment of 75.8% with a spread of ±1.0%. The ROI width corresponds to an average 2.7σ Gaussian coverage with the loss of $0\nu\beta\beta$ decay events in the full energy peak dominated by events with energy loss from bremsstrahlung and electron escape close to the surface of the crystals. The optimization exhibits only a mild dependence on the background index or the knowledge of the resolution, with the overall containment changing by ±0.7% for a 50% change in $b$ (2.2 keV wider, 1.5 keV narrower ROI). We truncate the computation of the mean-limit-setting sensitivity after the first three terms, as the probability of three or more background events is negligible for the considered ROI.

As the discussed Poisson sensitivity is by construction applicable only for limit setting, we implemented a binned likelihood analysis instead to extract either the final limit or a potential signal on the rate of $0\nu\beta\beta$ events. This analysis is built on the Bayesian analysis toolkit \[54\] and considers both the signal region as well as the sidebands of our 100-keV-wide blinded region. The likelihood function

$$L = \prod_{i=1}^{3} e^{\lambda_i} \frac{n_i}{n_i!}$$

is the product over three Poisson terms for the two sidebands and the signal ROI with observed events $n_i$ and expected events $\lambda_i$. The mean number of expected events $\lambda_i$ is computed considering the phenomenological background model described above and a Gaussian signal contribution, in which we leave the strength of the signal and flat background component free by using uninformative flat priors. After defining all analysis steps, we unblind and obtain the spectrum in Fig. 2. We observe no event in the signal region and a single event (cyan) in the right-hand side region. The corresponding marginalized posterior distribution for the number of signal events has a most probable value of zero with an upper limit of 2.4 events at 90% C.I., resulting in a half-life limit for $0\nu\beta\beta$ decay in $^{100}$Mo of $T_{1/2}^{\nu\beta\beta} > 1.4 \times 10^{24}$ yr (90% C.I.). The posterior for the flat background is nonzero with a 1σ interval of $3 \times 10^{-3}$ counts/(keV × kg × yr), and the posterior distributions for the parameters of the exponential are compatible with priors from a fit of the $2\nu\beta\beta$ spectrum in the 2650–2980 keV interval. We repeat the same fit for

FIG. 2. Physics spectrum for 2.16 kg × yr of data after unblinding. No event is observed in the detector- and dataset-based ROI. A single event, highlighted in cyan, has been observed in the analysis region. In a further refinement of the analysis, it was identified as a $\beta$ candidate out of the $^{212}$Bi → $^{208}$TI → $^{208}$Pb part of the natural decay chain (see the text). For visualization, the exposure-weighted mean ROI for $0\nu\beta\beta$ decay (17.9 keV wide) has been indicated with solid black lines.
the approximation of a Gaussian signal with a locally flat background over the 100 keV analysis region. The limit on 0νββ decay of 100Mo is unaffected.

The nuisance parameters considered in this limit are summarized in Table I. Uncertainties on the detector response, in particular, the energy scale and resolutions, are included in the simulation of 0νββ events. They are, hence, covered in the resulting containment in the optimized central ROI on a detector and dataset basis and not considered independently. The only remaining uncertainty for the detector response (index 1, Table I) is based on a potential non-Gaussianity of the 0νββ peak. In this analysis, we estimate this contribution based on the shape of the 2615 keV calibration peak. We observe evidence for non-Gaussian tails, which are dominated by unrejected pile-up events caused by the high trigger rate in calibration data.

We set a conservative systematic on the containment reduction of up to 5%. The second nuisance parameter on the containment (index 2) accounts for the GEANT4 modeling uncertainty of bremsstrahlung events. Reported accuracies for the GEANT4 bremsstrahlung production of a few MeV electrons in thick targets [55,56] of ~10% result in a systematic uncertainty in the overall containment of the 0νββ signal in the optimized ROI of (75.8 ± 1.1)% for our crystal geometry, which is applied as a single common multiplicative factor of 1.000 ± 0.015 in the limit setting. The inclusion of the analysis efficiency

\[ e = [90.6 ± 0.4(\text{stat})]^{+0.2}\%_{-0.2}\% (\text{syst})]\% \]

is split into two parts. For the evaluation of the mean value and its statistical uncertainty (index 3), we make use of the two independent signals in the LDs and LMOs to evaluate cut efficiencies on a clean sample of signal events in the 1.3–2 MeV 2νββ spectrum or from the 210Po peak [46]. Energy-independent cuts are evaluated directly from the ratio between passed and total events with binomial uncertainty. The pulse shape analysis efficiency is extracted from a linear fit extrapolated to \( Q_{\beta\beta} \) in order to account for the energy dependence in the reconstruction error. The systematic uncertainty associated with the excess broadening of the light yield cut has been evaluated with a set of pseudo-experiments considering the linear and modified photon statistics model introduced before. It is reflected in our limit setting as a multiplicative factor with uniform prior in 0.998–1.008 (index 4). Lastly, we include a subdominant uncertainty in the enrichment and number of 100Mo atoms of 0.2% (index 5).

We further refined our analysis after unblinding, implementing a cut designed to reject high-energy β events from the 212Bi [57] 208Tl [58] 208Pb branch in the thorium chain \( (\tau_{1/2}^{\text{208Pb}} = 183 \text{ s}, 5 \text{ MeV } Q \text{ value}) \). Similar to previous analyses with scintillating bolometers [28,31,45], we tag 212Bi α candidates with energies in the 6.0–6.3 MeV range and veto any decay in the same crystal in a 10-half-life period (1832 s). This cut has a negligible impact on the lifetime (0.02%) accidentally rejecting 2×10⁶ events, but it does reject the event close to the ROI in cyan in Fig. 2. The energy of the preceding α candidate is consistent with the \( Q \) value of 212Bi within 10 keV, and the time difference between the events is 113 s. We report a final 0νββ limit that is 1.3% stronger and rounds to

\[ T_{1/2}^{0\nu} > 1.5 \times 10^{24} \text{ yr (90\% C.I.}). \]

The posterior for the flat background of the Bayesian fit in this case is peaked at zero with a 90% C.I. of 1.1 \times 10^{-2} counts/(keV \times kg \times yr).

We interpret the obtained half-life limit in the framework of light Majorana neutrino exchange using \( g_\alpha = 1.27 \), phase space factors from Refs. [57,58], and nuclear matrix element calculations from Refs. [59–66]. The resulting limit on the effective Majorana neutrino mass of \( (m_{\nu\beta\beta}) < (0.31–0.54) \text{ eV} \) is the fourth most stringent limit worldwide, obtained with a modest 100Mo exposure of 1.17 kg \times yr. It is the leading constraint for 100Mo, exceeding the previous best limit from NEMO-3 [40] by 30% with almost 30 times lower 100Mo exposure. The technology of CUPID-Mo has proven that it can be operated reliably and reaches high efficiency for a 0νββ search of 68.6% (containment \times analysis efficiency) and a resolution of 0.11% (1σ) at \( Q_{\beta\beta} \). The present analysis strengthens the projection of the CUPID sensitivity [38], by demonstrating a detailed understanding of the 0νββ ROI and confirming key assumptions like the efficiency of Li$_{100}$MoO$_4$-based cryogenic scintillating bolometers. Extremely low U/Th contamination levels in the LMO crystals reported in Ref. [46] surpass the requirements for CUPID [38], and an efficient alpha separation has been demonstrated both in cylindrical [34,36] and recently also in cubic LMO detectors [67,68]. The preliminary estimate of the background in the ROI at the few 10^{-3} counts/(keV \times kg \times yr) level in CUPID-Mo, obtained in an experimental setup that was not designed for a 0νββ search, is encouraging and supports our belief that a 10^{-4} counts/(keV \times kg \times yr) background level for CUPID [38] seems feasible.

| Systematic | Index | Value | Prior |
|------------|-------|-------|-------|
| 0νββ detector response | 1 | 0.95–1.00 | Flat |
| 0νββ containment MC | 2 | 1.000 ± 0.015 | Gauss |
| Analysis efficiency | 3 | 0.906 ± 0.004 | Gauss |
| Light yield selection | 4 | 0.998–1.008 | Flat |
| Isotopic enrichment | 5 | 0.966 ± 0.002 | Gauss |

Dataset-dependent; exposure-weighted mean value presented.

We interpret the obtained half-life limit in the framework of light Majorana neutrino exchange using \( g_\alpha = 1.27 \).
Further analyses from CUPID-Mo will be focused on precisely reconstructing remaining backgrounds, comparing to the best reported background index for a bolometric $0\beta\beta$ search $[3.5 \times 10^{-3} \text{ counts/(keV} \times \text{ kg} \times \text{ yr})]$ in CUPID-0 $[31,32]$ and to optimally design and use the technology of the CUPID-Mo experiment in CUPID $[38]$.

The help of the technical staff of the Laboratoire Souterrain de Modane and of the other participant laboratories is gratefully acknowledged. This work has been partially performed in the framework of the LUMINEU program, funded by ANR (France). This work was also supported by CEA and IN2P3, by P2IO LabEx with the BSM-Nu project, by Istituto Nazionale di Fisica Nucleare, the Russian Science Foundation (Russia), the National Research Foundation (Ukraine), the U.S. Department of Energy (DOE) Office of Science, the DOE Office of Science, Office of Nuclear Physics, the National Science Foundation (USA), by the France-Berkeley fund, the Science, Office of Nuclear Physics, the National Science Foundation (U.S.A.) and of the other participant laboratories is gratefully acknowledged. This work has been supported by the National Academy of Sciences, Office of Science and Technology of the Embassy of France in the United States. Individuals have received support from the National Academy of Sciences of Ukraine and P2IO LabEx managed by the ANR (France). This work makes use of the DIANA data analysis software which has been developed by the Cuoricino, CUORE, LUCIFER, and CUPID-0 Collaborations.

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