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Abstract

This recommendation specifies two algorithms that can be used to generate a digital signature, both of which are stateful hash-based signature schemes: the Leighton-Micali Signature (LMS) system and the eXtended Merkle Signature Scheme (XMSS), along with their multi-tree variants, the Hierarchical Signature System (HSS) and multi-tree XMSS (XMSSMT).

Keywords

cryptography; digital signatures; hash-based signatures; public-key cryptography.
Document Conventions

The terms “shall” and “shall not” indicate requirements to be followed strictly in order to conform to the publication and from which no deviation is permitted.

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Conformance testing for implementations of the functions that are specified in this publication will be conducted within the framework of the Cryptographic Algorithm Validation Program (CAVP) and the Cryptographic Module Validation Program (CMVP). The requirements on these implementations are indicated by the word “shall.” Some of these requirements may be out-of-scope for CAVP or CMVP validation testing, and thus are the responsibility of entities using, implementing, installing, or configuring applications that incorporate this Recommendation.

Note to Reviewers

Sections 4 and 5 specify the parameter sets that are approved by this recommendation for LMS, HSS, XMSS, and XMSS\textsuperscript{MT}. Given the large number of parameter sets specified in these two sections, NIST would like feedback on whether there would be a benefit in reducing the number of parameter sets that are approved, and if so, which ones should be removed.

While this recommendation does not allow cryptographic modules to export private keying material, Section 7 describes a way in which a single key pair can be created with the one-time keys being spread across multiple cryptographic modules. The method described in Section 7 involves creating a 2-level HSS or XMSS\textsuperscript{MT} tree where the one-time keys associated with each of the bottom-level trees can be created on a different cryptographic module.

NIST believes that it would be possible to create a one-level XMSS or LMS tree in which the one-time keys are not all created and stored on the same cryptographic module. Key generation would be more complicated to implement, though, as would be the steps that end users would have to perform during the key generation process. However, a one-level tree would result in shorter signatures.

NIST would like feedback on whether there is a need to be able to create one-level XMSS or LMS keys in which the one-time keys are not all created and stored on the same cryptographic module even though such an option would be more complicated to implement and use than the two-level option that is already described in the draft.
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The assurance shall also indicate that it is intended to be binding on successors-in-interest regardless of whether such provisions are included in the relevant transfer documents.

Such statements should be addressed to: pqc-comments@nist.gov
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1 Introduction

This publication supplements FIPS 186-4 [4] by specifying two additional digital signature schemes, both of which are stateful hash-based signature (HBS) schemes: the Leighton-Micali Signature (LMS) system [2] and the eXtended Merkle Signature Scheme (XMSS) [1], along with their multi-tree variants, the Hierarchical Signature System (HSS) and multi-tree XMSS (XMSS\textsuperscript{MT}). All of the digital signature schemes specified in FIPS 186-4 will be broken if large-scale quantum computers are ever built. The security of the stateful HBS schemes in this publication, however, only depends on the security of the underlying hash functions—in particular, the infeasibility of finding a preimage or a second preimage—and it is believed that the security of hash functions will not be broken by the development of large-scale quantum computers [20].

This recommendation specifies profiles of LMS, HSS, XMSS, and XMSS\textsuperscript{MT} that are appropriate for use by the U.S. Federal Government. This profile approves the use of some but not all of the parameter sets defined in [1] and [2] and also defines some new parameter sets. The approved parameter sets use either SHA-256 or SHAKE256 with 192- or 256-bit outputs. It requires that key and signature generation be performed in hardware cryptographic modules that do not allow secret keying material to be exported.

1.1 Intended Applications for Stateful HBS Schemes

NIST is in the process of developing standards for post-quantum secure digital signature schemes [7] that can be used as replacements for the schemes that are specified in [4]. Stateful HBS schemes are not suitable for general use because they require careful state management that is often difficult to assure, as summarized in Section 1.2 and described in detail in [8].

Instead, stateful HBS schemes are primarily intended for applications with the following characteristics: 1) it is necessary to implement a digital signature scheme in the near future; 2) the implementation will have a long lifetime; and 3) it would not be practical to transition to a different digital signature scheme once the implementation has been deployed.

An application that may fit this profile is firmware updates for constrained devices. Some constrained devices that will be deployed in the near future will be in use for decades. These devices will need to have a secure mechanism for receiving firmware updates, and it may not be practical to change the code for verifying signatures on updates once the devices have been deployed.

1.2 The Importance of the Proper Maintenance of State

In a stateful HBS scheme, a key pair consists of a large set of one-time signature (OTS) key pairs. An HBS key pair may contain thousands, millions, or billions of OTS keys, and the signer needs to ensure that no individual OTS key is ever used to sign more than one message. If an attacker were able to obtain digital signatures for two different messages created using the same OTS key, then it would become computationally feasible for that attacker to forge signatures on arbitrary messages [13]. Therefore, as described in [8], when a stateful HBS scheme is implemented, extreme care needs to be taken in order to ensure that no OTS key is ever reused.
In order to obtain assurance that OTS keys are not reused, the signing process should be performed in a highly controlled environment. As described in [8], there are many ways in which seemingly routine operations could lead to the risk of one-time key reuse. The conformance requirements imposed in Section 8.1 on cryptographic modules that implement stateful HBS schemes are intended to help prevent one-time key reuse.

1.3 Outline of Text

The remainder of this document is divided into the following sections and appendices:

- Section 2, *Glossary of Terms, Acronyms, and Mathematical Symbols*, defines the terms, acronyms, and mathematical symbols used in this document. This section is *informative*.
- Section 3, *General Discussion*, gives a conceptual explanation of the elements used in stateful hash-based signature schemes (including hash chains, Merkle trees, and hash prefixes). This section may be used as either a high-level overview of stateful hash-based signature schemes or as an introduction to the detailed descriptions of LMS and XMSS provided in [1] and [2]. This section is *informative*.
- Section 4, *Leighton-Micali Signatures (LMS) Parameter Sets*, describes the parameter sets that are approved for use by this Special Publication with LMS and HSS.
- Section 5, *eXtended Merkle Signature Scheme (XMSS) Parameter Sets*, describes the parameter sets that are approved for use by this Special Publication with XMSS and XMSS\textsuperscript{MT}.
- Section 6, *Random Number Generation for Keys and Signatures*, states how the random data used in XMSS and LMS must be generated.
- Section 7, *Distributed Multi-Tree Hash-Based Signatures*, provides recommendations for distributing the implementation of a single HSS or XMSS\textsuperscript{MT} instance over multiple cryptographic modules.
- Section 8, *Conformance*, specifies requirements for cryptographic algorithm and module validation that are specific to modules that implement the algorithms in this document.
- Section 9, *Security Considerations*, enumerates security risks in various scenarios for stateful HBS schemes (with a focus on the problem of key reuse) and describes steps that should be taken to maximize the security of an implementation. This section is *informative*.
- Appendix A, *LMS XDR Syntax Additions*, describes additions that are required for the External Data Representation (XDR) syntax for LMS in order to support the new parameter sets specified in this document.
- Appendix B, *XMSS XDR Syntax Additions*, describes additions that are required for the XDR syntax for XMSS and XMSS\textsuperscript{MT} in order to support the new parameter sets specified in this document.
• Appendix C, *Provable Security Analysis*, provides information about the security proofs that are available for LMS and XMSS. This section is *informative*.
2 Glossary of Terms, Acronyms, and Mathematical Symbols

2.1 Terms and Definitions

approved

FIPS-approved or NIST-recommended. An algorithm or technique that is either 1) specified in a FIPS or NIST Recommendation, or 2) adopted in a FIPS or NIST Recommendation and specified either (a) in an appendix to the FIPS or NIST Recommendation, or (b) in a document referenced by the FIPS or NIST Recommendation.

2.2 Acronyms

Selected acronyms and abbreviations used in this publication are defined below.

EEPROM  Electronically erasable programmable read-only memory
EUF-CMA  Existential unforgeability under adaptive chosen message attacks
FIPS    Federal Information Processing Standard
HBS     Hash-based signature
HSS     Hierarchical Signature Scheme
IRTF    Internet Research Task Force
LM-OTS  Leighton-Micali One-Time Signature
LMS     Leighton-Micali signature
NIST    National Institute of Standards and Technology
OTS     One-time signature
QROM    Quantum random oracle model
RAM     Random access memory
RFC     Request for Comments
ROM     Random oracle model
SHA     Secure Hash Algorithm
SHAKE   Secure Hash Algorithm KECCAK
SP      Special publication
| **VM**  | Virtual machine |
| **WOTS** | Winternitz One-Time Signature Plus |
| **XDR**  | External Data Representation |
| **XMSS** | eXtended Merkle Signature Scheme |
| **XMSS**<sup>MT</sup> | Multi-tree XMSS |

### 2.3 Mathematical Symbols

<table>
<thead>
<tr>
<th>SHA-256(&lt;var&gt;M&lt;/var&gt;)</th>
<th>SHA-256 hash function as specified in [3]</th>
</tr>
</thead>
<tbody>
<tr>
<td>SHA-256/192(&lt;var&gt;M&lt;/var&gt;)</td>
<td>(T_{192}(\text{SHA-256}(&lt;var&gt;M&lt;/var&gt;))), the most significant (i.e., leftmost) 192 bits of the SHA-256 hash of (&lt;var&gt;M&lt;/var&gt;)</td>
</tr>
<tr>
<td>SHAKE256/256(&lt;var&gt;M&lt;/var&gt;)</td>
<td>SHAKE256(&lt;var&gt;M&lt;/var&gt;, 256), where SHAKE256 is specified in Section 6.2 of [5]</td>
</tr>
<tr>
<td>SHAKE256/192(&lt;var&gt;M&lt;/var&gt;)</td>
<td>SHAKE256(&lt;var&gt;M&lt;/var&gt;, 192), where SHAKE256 is specified in Section 6.2 of [5]</td>
</tr>
<tr>
<td>(T_{192}(X))</td>
<td>A truncation function that outputs the most significant (i.e., leftmost) 192 bits of the input bit string (&lt;var&gt;X&lt;/var&gt;)</td>
</tr>
</tbody>
</table>
3 General Discussion

At a high level, XMSS and LMS are very similar. They each consist of two components—a one-time signature (OTS) scheme and a method for creating a single, long-term public key from a large set of OTS public keys. A brief explanation of OTS schemes and the method for creating a long-term public key from a large set of OTS public keys can be found in Sections 3 and 4 of [14].

3.1 One-Time Signature Systems

Both LMS and XMSS make use of variants of the Winternitz signature scheme. In the Winternitz signature scheme, the message to be signed is hashed to create a digest; the digest is encoded as a base $b$ number; and then each digit of the digest is signed using a hash chain, as follows.

A hash chain is created by first randomly generating a secret value, $x$, which is the private key. The size of $x$ should generally correspond to the targeted strength of the scheme. So for the parameter sets approved by this recommendation, $x$ will be either 192 or 256 bits in length. The public key, $pub$, is then created by applying the hash function, $H$, to the secret $b - 1$ times, $H^{b-1}(x)$. Figure 1 shows an example of a hash chain for the $k$th digit of a digest where $b$ is 4.

The $k$th digit of the digest, $N_k$, is signed by applying the hash function, $H$, to the private key $N_k$ times, $H^{N_k}(x_k)$. In Figure 1, $N_k$ is 1, and so the signature is $s_k = H^1(x_k) = H(x_k)$. The signature can be verified by checking that $pub_k = H^{b-1-N_k}(s_k)$. So in Figure 1, the signature can be verified by checking that $pub_k = H^{4-1-1}(s_k) = H^2(s_k) = H(H(s_k))$.

As noted in [14], simply signing the individual digits of the digest is not sufficient as an attacker would be able to generate valid signatures for other message digests. For example, given $s_k = H(x_k)$, as in Figure 1, an attacker would be able to generate a signature for a message digest with a $k$th digit of 2 by applying $H$ to $s_k$ once or to a message digest with a $k$th digit of 3 by applying $H$ to $s_k$ twice. An attacker could not, however, generate a signature for a message digest with a $k$th digit of 0 as this would require finding some value $y$ such that $H(y) = s_k$, which would not be feasible as long as $H$ is preimage resistant.

In order to protect against the above attack, the Winternitz signature scheme computes a checksum of the message digest and signs the checksum along with the digest. For an $n$-digit message digest, the checksum is computed as $\sum_{k=0}^{n-1}(b - 1 - N_k)$. The checksum is designed so that the value is non-negative and any increase in a digit in the message digest will result in the checksum becoming smaller. This prevents an attacker from creating an effective forgery from a message signature since the attacker can only increase values within the message digest and cannot decrease values within the checksum.
Figure 2 shows an example of a signature for a 32-bit message digest using $b = 16$. The digest is written as eight hexadecimal digits, and a separate hash chain is used to sign each digit with each hash chain having its own private key.¹

<table>
<thead>
<tr>
<th>Digest</th>
<th>6</th>
<th>3</th>
<th>F</th>
<th>1</th>
<th>E</th>
<th>9</th>
<th>0</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>Private Key</td>
<td>$x_0$</td>
<td>$x_1$</td>
<td>$x_2$</td>
<td>$x_3$</td>
<td>$x_4$</td>
<td>$x_5$</td>
<td>$x_6$</td>
<td>$x_7$</td>
</tr>
<tr>
<td>Signature</td>
<td>$H^6(x_0)$</td>
<td>$H^7(x_1)$</td>
<td>$H^{15}(x_2)$</td>
<td>$H(x_3)$</td>
<td>$H^{14}(x_4)$</td>
<td>$H^6(x_5)$</td>
<td>$x_6$</td>
<td>$H^{11}(x_7)$</td>
</tr>
<tr>
<td>Public Key</td>
<td>$H^{15}(x_0)$</td>
<td>$H^{15}(x_1)$</td>
<td>$H^{15}(x_2)$</td>
<td>$H^{15}(x_3)$</td>
<td>$H^{15}(x_4)$</td>
<td>$H^{15}(x_5)$</td>
<td>$H^{15}(x_6)$</td>
<td>$H^{15}(x_7)$</td>
</tr>
</tbody>
</table>

Figure 2: A sample Winternitz signature

3.2 Merkle Trees

While a single, long-term public key could be created from a large set of OTS public keys by simply concatenating the keys together, the resulting public key would be unacceptably large. XMSS and LMS instead use Merkle hash trees [18], which allow for the long-term public key to be very short in exchange for requiring a small amount of additional information to be provided with each OTS key. To create a hash tree, the OTS public keys are hashed once to form the leaves of the tree, and these hashes are then hashed together in pairs to form the next level up. Those hash values are then hashed together in pairs, the resulting hash values are hashed together, and so on until all of the public keys have been used to generate a single hash value, which will be used as the long-term public key.

Figure 3 depicts a hash tree containing eight OTS public keys. The eight keys are each hashed to form the leaves of the tree, and the eight leaf values are hashed in pairs to create the next level up in the tree. These four hash values are again hashed in pairs to create $h_{0-3}$ and $h_{4-7}$, which are

![Figure 3: A Merkle Hash Tree](image)

¹ If SHA-256 were used as the hash function, then the message digest would be encoded as 64 hexadecimal digits, and the checksum would be encoded as three hexadecimal digits.
hashed together to create the long-term public key, $h_{0-7}$. In order for an entity that had already received $h_{0-7}$ in a secure manner to verify a message signed using $k_2$, the signer would need to provide $h_3$, $h_{01}$, and $h_{4-7}$ in addition to $k_2$. The verifier would compute $h'_2 = H(k_2)$, $h'_{23} = H(h'_2 || h_3)$, $h'_{0-3} = H(h_{01} || h'_{23})$, and $h'_{0-7} = H(h'_{0-3} || h_{4-7})$. If $h'_{0-7}$ is the same as $h_{0-7}$, then $k_2$ may be used to verify the message signature.

### 3.3 Two-Level Trees

Both [1] and [2] define single tree as well as multi-tree variants of their signature schemes. In an instance that involves two levels of trees, as shown in Figure 4, the OTS keys that form the leaves of the top-level tree sign the roots of the trees at the bottom level, and the OTS keys that form the leaves of the bottom-level trees are used to sign the messages. The root of the top-level tree is the public key for the signature scheme.²

As described in Section 7, the use of two levels of trees can make it easier to distribute OTS keys across multiple cryptographic modules in order to protect against private key loss. A set of OTS keys can be created in one cryptographic module, and the root of the Merkle tree formed from these keys can be published as the public key for the signature scheme. OTS keys can then be created on multiple other cryptographic modules with a separate Merkle tree being created for the OTS keys of each of the other cryptographic modules, and a different OTS key from the first cryptographic module can be used to sign each of the roots of the other cryptographic modules.

While there are benefits in the use of a two-level tree, it results in larger signatures and slower signature verification as each message signature will need to include two OTS signatures. For example, if a message were signed using OTS key $k_{1,6}$ in Figure 4, the signature would need to

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² While this section only describes two-level trees, HSS allows for up to eight levels of trees and XMSS⁷t allows for up to 12 levels of trees.
include the signature on $r_{1,1}$ using $k_{0,1}$ in addition to the signature on the message using $k_{1,6}$.

### 3.4 Prefixes and Bitmasks

In order to strengthen the security of the schemes in both XMSS and LMS whenever a value is hashed, a prefix is prepended to the value that is hashed. For example, when computing the public key for a Winternitz signature from the private key in LMS as described in Section 3.1, rather than just computing $pub_k = H^3(x_k) = H(H(H(x_k)))$ the public key is computed as $pub_k = H(p_3 || H(p_2 || H(p_1 || x_k)))$, where $p_1$, $p_2$, and $p_3$ are each different values. The prefix is formed by concatenating together various pieces of information, including a unique identifier for the long-term public key and an indicator of the purpose of the hash (e.g., Winternitz chain or Merkle tree). If the hash is part of a Winternitz chain, then the prefix also includes the number of the OTS key, which digit of the digest or checksum is being signed, and where in the chain the hash appears. The goal is to ensure that every single hash that is computed within the LMS scheme uses a different prefix.

XMSS generates its prefixes in a similar way. The information described above is used to form an address, which uniquely identifies where a particular hash invocation occurs within the scheme. This address is then hashed along with a unique identifier for the long-term public key (SEED) to create the prefix.

Unlike LMS, XMSS also uses bitmasks. In addition to creating the prefix, a slightly different address is also hashed along with the SEED to create a bitmask. The bitmask is then exclusive-ORed with the input before the input is hashed along with the prefix. Figure 5 illustrates an example of this computation. In [1], the hash function is referred to as $H$, $H_{msg}$, $F$, or $PRF$, depending on where it is being used. However, in each case it is the same function, just with a different prefix prepended in order to ensure separation between the uses.

\[ \text{Figure 5: XMSS hash computation with prefix and bitmask} \]
4 Leighton-Micali Signatures (LMS) Parameter Sets

The LMS and HSS algorithms are described in RFC 8554 [2]. This Special Publication approves the use of LMS and HSS with four different hash functions: SHA-256, SHA-256/192, SHAKE256/256, and SHAKE256/192 (see Section 2.3). The parameter sets that use SHA-256 are defined in RFC 8554 [2]. The parameter sets that use SHA-256/192, SHAKE256/256, and SHAKE256/192 are defined below.

When generating a key pair for an LMS instance, each LM-OTS key in the system shall use the same parameter set, and the hash function used for the LMS system shall be the same as the hash function used in the LM-OTS keys. The height of the tree (h) shall be 5, 10, 15, 20, or 25.

When generating a key pair for an HSS instance, the requirements specified in the previous paragraph apply to each LMS tree in the instance. If the HSS instance has more than one level, then the hash function used for the tree at level 0 shall be used for every LMS tree at every other level. For each level, the same LMS and LM-OTS parameter sets shall be used for every LMS tree at that level.

The LMS and LM-OTS parameter sets that are approved for use by this Special Publication are specified in Sections 4.1 through 4.4. The parameters n, w, p, ls, m, and h specified in the tables are defined in Sections 4.1 and 5.1 of [2].

Extensions to the XDR syntax in Section 3.3 of [2] needed to support the parameter sets defined in Sections 4.2 through 4.4 of this document are specified in Appendix A.

4.1 LMS with SHA-256

When generating LMS or HSS key pairs using SHA-256, the LMS and LM-OTS parameter sets shall be selected from the following two tables, which come from Sections 4 and 5 of [2].

<table>
<thead>
<tr>
<th>LM-OTS Parameter Sets</th>
<th>Numeric Identifier</th>
<th>n</th>
<th>w</th>
<th>p</th>
<th>ls</th>
<th>sig_len</th>
</tr>
</thead>
<tbody>
<tr>
<td>LMOTS_SHA256_N32_W1</td>
<td>0x00000001</td>
<td>32</td>
<td>1</td>
<td>265</td>
<td>7</td>
<td>8516</td>
</tr>
<tr>
<td>LMOTS_SHA256_N32_W2</td>
<td>0x00000002</td>
<td>32</td>
<td>2</td>
<td>133</td>
<td>6</td>
<td>4292</td>
</tr>
<tr>
<td>LMOTS_SHA256_N32_W4</td>
<td>0x00000003</td>
<td>32</td>
<td>4</td>
<td>67</td>
<td>4</td>
<td>2180</td>
</tr>
<tr>
<td>LMOTS_SHA256_N32_W8</td>
<td>0x00000004</td>
<td>32</td>
<td>8</td>
<td>34</td>
<td>0</td>
<td>1124</td>
</tr>
</tbody>
</table>
Table 2: LMS parameter sets for SHA-256

<table>
<thead>
<tr>
<th>LMS Parameter Sets</th>
<th>Numeric Identifier</th>
<th>m</th>
<th>h</th>
</tr>
</thead>
<tbody>
<tr>
<td>LMS_SHA256_M32_H5</td>
<td>0x00000005</td>
<td>32</td>
<td>5</td>
</tr>
<tr>
<td>LMS_SHA256_M32_H10</td>
<td>0x00000006</td>
<td>32</td>
<td>10</td>
</tr>
<tr>
<td>LMS_SHA256_M32_H15</td>
<td>0x00000007</td>
<td>32</td>
<td>15</td>
</tr>
<tr>
<td>LMS_SHA256_M32_H20</td>
<td>0x00000008</td>
<td>32</td>
<td>20</td>
</tr>
<tr>
<td>LMS_SHA256_M32_H25</td>
<td>0x00000009</td>
<td>32</td>
<td>25</td>
</tr>
</tbody>
</table>

4.2 LMS with SHA-256/192

When generating LMS or HSS key pairs using SHA-256/192, the LMS and LM-OTS parameter sets shall be selected from the following two tables.

Table 3: LM-OTS parameter sets for SHA-256/192

<table>
<thead>
<tr>
<th>LM-OTS Parameter Sets</th>
<th>Numeric Identifier</th>
<th>n</th>
<th>w</th>
<th>p</th>
<th>ls</th>
<th>sig_len</th>
</tr>
</thead>
<tbody>
<tr>
<td>LMOTS_SHA256_N24_W1</td>
<td>TBD</td>
<td>24</td>
<td>1</td>
<td>200</td>
<td>8</td>
<td>4828</td>
</tr>
<tr>
<td>LMOTS_SHA256_N24_W2</td>
<td>TBD</td>
<td>24</td>
<td>2</td>
<td>101</td>
<td>6</td>
<td>2452</td>
</tr>
<tr>
<td>LMOTS_SHA256_N24_W4</td>
<td>TBD</td>
<td>24</td>
<td>4</td>
<td>51</td>
<td>4</td>
<td>1252</td>
</tr>
<tr>
<td>LMOTS_SHA256_N24_W8</td>
<td>TBD</td>
<td>24</td>
<td>8</td>
<td>26</td>
<td>0</td>
<td>652</td>
</tr>
</tbody>
</table>

Table 4: LMS parameter sets for SHA-256/192

<table>
<thead>
<tr>
<th>LMS Parameter Sets</th>
<th>Numeric Identifier</th>
<th>m</th>
<th>h</th>
</tr>
</thead>
<tbody>
<tr>
<td>LMS_SHA256_M24_H5</td>
<td>TBD</td>
<td>24</td>
<td>5</td>
</tr>
<tr>
<td>LMS_SHA256_M24_H10</td>
<td>TBD</td>
<td>24</td>
<td>10</td>
</tr>
<tr>
<td>LMS_SHA256_M24_H15</td>
<td>TBD</td>
<td>24</td>
<td>15</td>
</tr>
<tr>
<td>LMS_SHA256_M24_H20</td>
<td>TBD</td>
<td>24</td>
<td>20</td>
</tr>
<tr>
<td>LMS_SHA256_M24_H25</td>
<td>TBD</td>
<td>24</td>
<td>25</td>
</tr>
</tbody>
</table>
4.3 LMS with SHAKE256/256

When generating LMS or HSS key pairs using SHAKE256/256, the LMS and LM-OTS parameter sets shall be selected from the following two tables.

Table 5: LM-OTS parameter sets for SHAKE256/256

<table>
<thead>
<tr>
<th>LM-OTS Parameter Sets</th>
<th>Numeric Identifier</th>
<th>n</th>
<th>w</th>
<th>p</th>
<th>ls</th>
<th>sig_len</th>
</tr>
</thead>
<tbody>
<tr>
<td>LMOTS_SHAKE_N32_W1</td>
<td>TBD</td>
<td>32</td>
<td>1</td>
<td>265</td>
<td>7</td>
<td>8516</td>
</tr>
<tr>
<td>LMOTS_SHAKE_N32_W2</td>
<td>TBD</td>
<td>32</td>
<td>2</td>
<td>133</td>
<td>6</td>
<td>4292</td>
</tr>
<tr>
<td>LMOTS_SHAKE_N32_W4</td>
<td>TBD</td>
<td>32</td>
<td>4</td>
<td>67</td>
<td>4</td>
<td>2180</td>
</tr>
<tr>
<td>LMOTS_SHAKE_N32_W8</td>
<td>TBD</td>
<td>32</td>
<td>8</td>
<td>34</td>
<td>0</td>
<td>1124</td>
</tr>
</tbody>
</table>

Table 6: LMS parameter sets for SHAKE256/256

<table>
<thead>
<tr>
<th>LMS Parameter Sets</th>
<th>Numeric Identifier</th>
<th>m</th>
<th>h</th>
</tr>
</thead>
<tbody>
<tr>
<td>LMS_SHAKE_M32_H5</td>
<td>TBD</td>
<td>32</td>
<td>5</td>
</tr>
<tr>
<td>LMS_SHAKE_M32_H10</td>
<td>TBD</td>
<td>32</td>
<td>10</td>
</tr>
<tr>
<td>LMS_SHAKE_M32_H15</td>
<td>TBD</td>
<td>32</td>
<td>15</td>
</tr>
<tr>
<td>LMS_SHAKE_M32_H20</td>
<td>TBD</td>
<td>32</td>
<td>20</td>
</tr>
<tr>
<td>LMS_SHAKE_M32_H25</td>
<td>TBD</td>
<td>32</td>
<td>25</td>
</tr>
</tbody>
</table>

4.4 LMS with SHAKE256/192

When generating LMS or HSS key pairs using SHAKE256/192, the LMS and LM-OTS parameter sets shall be selected from the following two tables.

Table 7: LM-OTS parameter sets for SHAKE256/192

<table>
<thead>
<tr>
<th>LM-OTS Parameter Sets</th>
<th>Numeric Identifier</th>
<th>n</th>
<th>w</th>
<th>p</th>
<th>ls</th>
<th>sig_len</th>
</tr>
</thead>
<tbody>
<tr>
<td>LMOTS_SHAKE_N24_W1</td>
<td>TBD</td>
<td>24</td>
<td>1</td>
<td>200</td>
<td>8</td>
<td>4828</td>
</tr>
<tr>
<td>LMOTS_SHAKE_N24_W2</td>
<td>TBD</td>
<td>24</td>
<td>2</td>
<td>101</td>
<td>6</td>
<td>2452</td>
</tr>
<tr>
<td>LMOTS_SHAKE_N24_W4</td>
<td>TBD</td>
<td>24</td>
<td>4</td>
<td>51</td>
<td>4</td>
<td>1252</td>
</tr>
<tr>
<td>LMOTS_SHAKE_N24_W8</td>
<td>TBD</td>
<td>24</td>
<td>8</td>
<td>26</td>
<td>0</td>
<td>652</td>
</tr>
</tbody>
</table>
Table 8: LMS parameter sets for SHAKE256/192

<table>
<thead>
<tr>
<th>LMS Parameter Sets</th>
<th>Numeric Identifier</th>
<th>m</th>
<th>h</th>
</tr>
</thead>
<tbody>
<tr>
<td>LMS_SHAKE_M24_H5</td>
<td>TBD</td>
<td>24</td>
<td>5</td>
</tr>
<tr>
<td>LMS_SHAKE_M24_H10</td>
<td>TBD</td>
<td>24</td>
<td>10</td>
</tr>
<tr>
<td>LMS_SHAKE_M24_H15</td>
<td>TBD</td>
<td>24</td>
<td>15</td>
</tr>
<tr>
<td>LMS_SHAKE_M24_H20</td>
<td>TBD</td>
<td>24</td>
<td>20</td>
</tr>
<tr>
<td>LMS_SHAKE_M24_H25</td>
<td>TBD</td>
<td>24</td>
<td>25</td>
</tr>
</tbody>
</table>
5 eXtended Merkle Signature Scheme (XMSS) Parameter Sets

The XMSS and XMSS\textsuperscript{MT} algorithms are described in RFC 8391 [1]. This Special Publication approves the use of XMSS and XMSS\textsuperscript{MT} with four different hash functions: SHA-256, SHA-256/192, SHAKE256/256, and SHAKE256/192 (see Section 2.3).\textsuperscript{3} The parameter sets that use SHA-256 are defined in RFC 8391 [1]. The parameter sets that use SHA-256/192, SHAKE256/256, and SHAKE256/192 are defined below.

The WOTS\textsuperscript{*} parameters corresponding to the use of each of these hash functions is specified in the following table.

Table 9: WOTS\textsuperscript{*} parameter sets

<table>
<thead>
<tr>
<th>Parameter Sets</th>
<th>Numeric Identifier</th>
<th>F / PRF</th>
<th>n</th>
<th>w</th>
<th>len</th>
</tr>
</thead>
<tbody>
<tr>
<td>WOTSP-SHA2_256</td>
<td>0x000000001</td>
<td>See Section 5.1</td>
<td>32</td>
<td>16</td>
<td>67</td>
</tr>
<tr>
<td>WOTSP-SHA2_192</td>
<td>TBD</td>
<td>See Section 5.2</td>
<td>24</td>
<td>16</td>
<td>51</td>
</tr>
<tr>
<td>WOTSP-SHAKE256_256</td>
<td>TBD</td>
<td>See Section 5.3</td>
<td>32</td>
<td>16</td>
<td>67</td>
</tr>
<tr>
<td>WOTSP-SHAKE256_192</td>
<td>TBD</td>
<td>See Section 5.4</td>
<td>24</td>
<td>16</td>
<td>51</td>
</tr>
</tbody>
</table>

The XMSS and XMSS\textsuperscript{MT} parameter sets that are approved for use by this Special Publication are specified in Sections 5.1 through 5.4. The parameters n, w, len, h, and d specified in the tables are defined in Sections 3.1.1, 4.1.1, and 4.2.1 of [1].

Extensions to the XDR syntax in Appendices A, B, and C of [1] needed to support the parameter sets defined in Sections 5.2 through 5.4 of this document are specified in Appendix B.

5.1 XMSS and XMSS\textsuperscript{MT} with SHA-256

When generating XMSS or XMSS\textsuperscript{MT} key pairs using SHA-256, the parameter sets shall be selected from the following two tables, which come from Section 5 of [1]. Each of these uses the WOTSP-SHA2_256 parameter set.

Table 10: XMSS parameter sets for SHA-256

<table>
<thead>
<tr>
<th>Parameter Sets</th>
<th>Numeric Identifier</th>
<th>n</th>
<th>w</th>
<th>len</th>
<th>h</th>
</tr>
</thead>
<tbody>
<tr>
<td>XMSS-SHA2_10_256</td>
<td>0x000000001</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>10</td>
</tr>
<tr>
<td>XMSS-SHA2_16_256</td>
<td>0x000000002</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>16</td>
</tr>
<tr>
<td>XMSS-SHA2_20_256</td>
<td>0x000000002</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>20</td>
</tr>
</tbody>
</table>

\textsuperscript{3} The parameter sets specified in RFC 8391 [1] that use SHAKE128, SHAKE256, and SHA-512 are not approved for use by this Special Publication.
Table 11: XMSS\textsuperscript{MT} parameter sets for SHA-256

<table>
<thead>
<tr>
<th>Parameter Sets</th>
<th>Numeric Identifier</th>
<th>n</th>
<th>w</th>
<th>len</th>
<th>h</th>
<th>d</th>
</tr>
</thead>
<tbody>
<tr>
<td>XMSSMT-SHA2_20/2_256</td>
<td>0x00000001</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>20</td>
<td>2</td>
</tr>
<tr>
<td>XMSSMT-SHA2_20/4_256</td>
<td>0x00000002</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>20</td>
<td>4</td>
</tr>
<tr>
<td>XMSSMT-SHA2_40/2_256</td>
<td>0x00000003</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>40</td>
<td>2</td>
</tr>
<tr>
<td>XMSSMT-SHA2_40/4_256</td>
<td>0x00000004</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>40</td>
<td>4</td>
</tr>
<tr>
<td>XMSSMT-SHA2_40/8_256</td>
<td>0x00000005</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>40</td>
<td>8</td>
</tr>
<tr>
<td>XMSSMT-SHA2_60/3_256</td>
<td>0x00000006</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>60</td>
<td>3</td>
</tr>
<tr>
<td>XMSSMT-SHA2_60/6_256</td>
<td>0x00000007</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>60</td>
<td>6</td>
</tr>
<tr>
<td>XMSSMT-SHA2_60/12_256</td>
<td>0x00000008</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>60</td>
<td>12</td>
</tr>
</tbody>
</table>

For the parameter sets in this section, the functions $F$, $H$, $H\_msg$, and $PRF$ are as defined in Section 5.1 of [1] for SHA2 with $n = 32$.

5.2 XMSS and XMSS\textsuperscript{MT} with SHA-256/192

When generating XMSS or XMSS\textsuperscript{MT} key pairs using SHA-256/192, the parameter sets shall be selected from the following two tables. Each of these uses the WOTSP-SHA2_192 parameter set.

Table 12: XMSS parameter sets for SHA-256/192

<table>
<thead>
<tr>
<th>Parameter Sets</th>
<th>Numeric Identifier</th>
<th>n</th>
<th>w</th>
<th>len</th>
<th>h</th>
</tr>
</thead>
<tbody>
<tr>
<td>XMSS-SHA2_10_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>10</td>
</tr>
<tr>
<td>XMSS-SHA2_16_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>16</td>
</tr>
<tr>
<td>XMSS-SHA2_20_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>20</td>
</tr>
</tbody>
</table>
Table 13: XMSS\textsuperscript{MT} parameter sets for SHA-256/192

<table>
<thead>
<tr>
<th>Parameter Sets</th>
<th>Numeric Identifier</th>
<th>n</th>
<th>w</th>
<th>len</th>
<th>h</th>
<th>d</th>
</tr>
</thead>
<tbody>
<tr>
<td>XMSSMT-SHA2_20/2_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>20</td>
<td>2</td>
</tr>
<tr>
<td>XMSSMT-SHA2_20/4_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>20</td>
<td>4</td>
</tr>
<tr>
<td>XMSSMT-SHA2_40/2_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>40</td>
<td>2</td>
</tr>
<tr>
<td>XMSSMT-SHA2_40/4_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>40</td>
<td>4</td>
</tr>
<tr>
<td>XMSSMT-SHA2_40/8_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>40</td>
<td>8</td>
</tr>
<tr>
<td>XMSSMT-SHA2_60/3_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>60</td>
<td>3</td>
</tr>
<tr>
<td>XMSSMT-SHA2_60/6_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>60</td>
<td>6</td>
</tr>
<tr>
<td>XMSSMT-SHA2_60/12_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>60</td>
<td>12</td>
</tr>
</tbody>
</table>

For the parameter sets in this section, the functions F, H, H\_msg, and PRF are defined as follows:

- \( F: T_{192}(SHA-256(toByte(0, 4) || KEY || M)) \)
- \( H: T_{192}(SHA-256(toByte(1, 4) || KEY || M)) \)
- \( H\_msg: T_{192}(SHA-256(toByte(2, 4) || KEY || M)) \)
- \( PRF: T_{192}(SHA-256(toByte(3, 4) || KEY || M)) \)

5.3 XMSS and XMSS\textsuperscript{MT} with SHAKE256/256

When generating XMSS or XMSS\textsuperscript{MT} key pairs using SHAKE256/256, the parameter sets shall be selected from the following two tables. Each of these uses the WOTSP-SHAKE256_256 parameter set.

Table 14: XMSS parameter sets for SHAKE256/256

<table>
<thead>
<tr>
<th>Parameter Sets</th>
<th>Numeric Identifier</th>
<th>n</th>
<th>w</th>
<th>len</th>
<th>h</th>
</tr>
</thead>
<tbody>
<tr>
<td>XMSS-SHAKE256_10_256</td>
<td>TBD</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>10</td>
</tr>
<tr>
<td>XMSS-SHAKE256_16_256</td>
<td>TBD</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>16</td>
</tr>
<tr>
<td>XMSS-SHAKE256_20_256</td>
<td>TBD</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>20</td>
</tr>
</tbody>
</table>
Table 15: XMSS\textsuperscript{MT} parameter sets for SHAKE256/256

<table>
<thead>
<tr>
<th>Parameter Sets</th>
<th>Numeric Identifier</th>
<th>n</th>
<th>w</th>
<th>len</th>
<th>h</th>
<th>d</th>
</tr>
</thead>
<tbody>
<tr>
<td>XMSSMT-SHAKE256_20/2_256</td>
<td>TBD</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>20</td>
<td>2</td>
</tr>
<tr>
<td>XMSSMT-SHAKE256_20/4_256</td>
<td>TBD</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>20</td>
<td>4</td>
</tr>
<tr>
<td>XMSSMT-SHAKE256_40/2_256</td>
<td>TBD</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>40</td>
<td>2</td>
</tr>
<tr>
<td>XMSSMT-SHAKE256_40/4_256</td>
<td>TBD</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>40</td>
<td>4</td>
</tr>
<tr>
<td>XMSSMT-SHAKE256_40/8_256</td>
<td>TBD</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>40</td>
<td>8</td>
</tr>
<tr>
<td>XMSSMT-SHAKE256_60/3_256</td>
<td>TBD</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>60</td>
<td>3</td>
</tr>
<tr>
<td>XMSSMT-SHAKE256_60/6_256</td>
<td>TBD</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>60</td>
<td>6</td>
</tr>
<tr>
<td>XMSSMT-SHAKE256_60/12_256</td>
<td>TBD</td>
<td>32</td>
<td>16</td>
<td>67</td>
<td>60</td>
<td>12</td>
</tr>
</tbody>
</table>

For the parameter sets in this section, the functions \(\text{F}, \text{H}, \text{H}_\text{msg},\) and \(\text{PRF}\) are defined as follows:

- \(\text{F}: \text{SHAKE256}(\text{toByte}(0, 32) || \text{KEY} || \text{M}, 256)\)
- \(\text{H}: \text{SHAKE256}(\text{toByte}(1, 32) || \text{KEY} || \text{M}, 256)\)
- \(\text{H}_\text{msg}: \text{SHAKE256}(\text{toByte}(2, 32) || \text{KEY} || \text{M}, 256)\)
- \(\text{PRF}: \text{SHAKE256}(\text{toByte}(3, 32) || \text{KEY} || \text{M}, 256)\)

5.4 XMSS and XMSS\textsuperscript{MT} with SHAKE256/192

When generating XMSS or XMSS\textsuperscript{MT} key pairs using SHAKE256/192, the parameter sets shall be selected from the following two tables. Each of these uses the WOTSP-SHAKE256_192 parameter set.

Table 16: XMSS parameter sets for SHAKE256/192

<table>
<thead>
<tr>
<th>Parameter Sets</th>
<th>Numeric Identifier</th>
<th>n</th>
<th>w</th>
<th>len</th>
<th>h</th>
</tr>
</thead>
<tbody>
<tr>
<td>XMSS-SHAKE256_10_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>10</td>
</tr>
<tr>
<td>XMSS-SHAKE256_16_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>16</td>
</tr>
<tr>
<td>XMSS-SHAKE256_20_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>20</td>
</tr>
</tbody>
</table>
Table 17: XMSS<sup>MT</sup> parameter sets for SHAKE256/192

<table>
<thead>
<tr>
<th>Parameter Sets</th>
<th>Numeric Identifier</th>
<th>n</th>
<th>w</th>
<th>len</th>
<th>h</th>
<th>d</th>
</tr>
</thead>
<tbody>
<tr>
<td>XMSSMT-SHAKE256_20/2_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>20</td>
<td>2</td>
</tr>
<tr>
<td>XMSSMT-SHAKE256_20/4_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>20</td>
<td>4</td>
</tr>
<tr>
<td>XMSSMT-SHAKE256_40/2_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>40</td>
<td>2</td>
</tr>
<tr>
<td>XMSSMT-SHAKE256_40/4_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>40</td>
<td>4</td>
</tr>
<tr>
<td>XMSSMT-SHAKE256_40/8_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>40</td>
<td>8</td>
</tr>
<tr>
<td>XMSSMT-SHAKE256_60/3_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>40</td>
<td>3</td>
</tr>
<tr>
<td>XMSSMT-SHAKE256_60/6_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>40</td>
<td>6</td>
</tr>
<tr>
<td>XMSSMT-SHAKE256_60/12_192</td>
<td>TBD</td>
<td>24</td>
<td>16</td>
<td>51</td>
<td>40</td>
<td>12</td>
</tr>
</tbody>
</table>

For the parameter sets in this section, the functions F, H, H<sub>msg</sub>, and PRF are defined as follows:

- F: SHAKE256(toByte(0, 4) || KEY || M, 192)
- H: SHAKE256(toByte(1, 4) || KEY || M, 192)
- H<sub>msg</sub>: SHAKE256(toByte(2, 4) || KEY || M, 192)
- PRF: SHAKE256(toByte(3, 4) || KEY || M, 192)
This section specifies requirements for the generation of random data that apply in addition to the requirements that are specified in [2] for LMS and HSS and in [1] for XMSS and XMSS\textsuperscript{MT}.

Note: Variables and notations used in this section are defined in the relevant documents mentioned above.

6.1 LMS and HSS Random Number Generation Requirements

The LMS key pair identifier, $I$, shall be generated using an approved random bit generator (see the SP 800-90 series of publications [6]) where the instantiation of the random bit generator supports at least 128 bits of security strength.

The $n$-byte private elements of the LM-OTS private keys ($x[i]$ in Section 4.2 of [2]) shall be generated using the pseudorandom key generation method specified in Appendix A of [2]. The same SEED value shall be used to generate every private element in a single LMS instance, and SEED shall be generated using an approved random bit generator [6] where the instantiation of the random bit generator supports at least $8n$ bits of security strength.

If more than one LMS instance is being created (e.g., for an HSS instance), then a separate key pair identifier, $I$, and SEED (if using the pseudorandom key generation method) shall be generated for each LMS instance.

When generating a signature, the $n$-byte randomizer $C$ (see Section 4.5 of [2]) shall be generated using an approved random bit generator [6] where the instantiation of the random bit generator supports at least $8n$ bits of security strength.

6.2 XMSS and XMSS\textsuperscript{MT} Random Number Generation Requirements

The $n$-byte values $SK\_PRF$ and SEED shall be generated using an approved random bit generator (see the SP 800-90 series of publications [6]) where the instantiation of the random bit generator supports at least $8n$ bits of security strength.

The private $n$-byte strings in the WOTS\textsuperscript{+} private keys ($sk[i]$ in Section 3.1.3 of [1]) shall be generated using the pseudorandom key generation method specified in Section 3.1.7 of [1]:

$$sk[i, j] = PRF(S\_ots[j], toByte(i, 32)),$$

where PRF is as defined in Section 5 for the parameter set being used. The private seed, $S\_ots[j]$, for each WOTS\textsuperscript{+} private key, $j$, shall be as specified in Section 4.1.11 of [1]:

$$S\_ots[j] = PRF(S\_XMSS, toByte(j, 32)),$$

where PRF is as defined in Section 5 for the parameter set being used. The private seed, $S\_XMSS$, shall be generated using an approved random bit generator [6] where the instantiation of the random bit generator supports at least $8n$ bits of security strength. If more than one XMSS key pair is being created within a cryptographic module (including XMSS keys that belong to a single XMSS\textsuperscript{MT} instance), then a separate random $S\_XMSS$ shall be generated for each XMSS key pair.
7 Distributed Multi-Tree Hash-Based Signatures

If a digital signature key will be used to generate signatures over a long period of time and replacing the public key would be difficult, then storing the private key in multiple places to protect against loss will be necessary. In the case of most digital signature schemes, this just involves making copies of the private key. However, in the case of stateful HBS schemes, simply copying the private key would create a risk of OTS key reuse. An alternative that avoids this risk is to have multiple cryptographic modules that each generate their own OTS keys and then create a single instance that includes all of the public keys from all of the modules.

While it would also be possible to have one cryptographic module generate all of the OTS keys and then distribute different OTS keys to each of the other cryptographic modules, doing so is not an option for cryptographic modules conforming to this recommendation. Due to the risks associated with copying OTS keys, this recommendation prohibits exporting private keying material (Section 8).

The easiest way to have OTS keys on multiple cryptographic modules without exporting private keys is to use HSS or XMSS\textsuperscript{MT} with two levels of trees where each tree is instantiated on a different cryptographic module. First, a top-level LMS or XMSS key pair would be created in a cryptographic module. The top level’s OTS keys would only be used to sign the roots of other trees. Then, bottom-level LMS or XMSS key pairs would be created in other cryptographic modules, and the public keys from those key pairs (i.e., the roots of their Merkle trees) would be signed by OTS keys of the top-level key pair. The OTS keys of the bottom-level key pairs would be used to sign ordinary messages. The number of bottom-level key pairs that could be created would only be limited by the number of OTS keys in the top-level key pair.

7.1 HSS

In the case of HSS, the scheme described above can be implemented using multiple cryptographic modules that each implement LMS without modifications. The top-level LMS public key can be converted to an HSS public key by an external, non-cryptographic device. This device can also submit the public keys of the bottom-level LMS keys to be signed by the top-level LMS key. In HSS, the operation for signing the root of a lower-level tree is the same as the operation for signing an ordinary message. Finally, this external device can submit ordinary messages to cryptographic modules holding the bottom-level LMS keys for signing and then combine the resulting LMS signatures with the top-level key’s signature on the bottom-level LMS public key in order to create the HSS signature for the ordinary messages (see Algorithm 8 and Algorithm 9 in [2]).

7.2 XMSS\textsuperscript{MT}

Distributing the implementation of an XMSS\textsuperscript{MT} instance across multiple cryptographic modules requires each cryptographic module to implement slightly modified versions of the XMSS key and signature generation algorithms provided in [1]. The modified versions of these algorithms are provided in Section 7.2.1. The modifications are primarily intended to ensure that each XMSS key uses the appropriate values for its layer and tree addresses when computing prefixes and bitmasks. The modifications also ensure that every XMSS key uses the same value for SEED and that the root of the top-level tree is used when computing the hashes of messages to be
signed.

Note that while Algorithm 15 in [1] indicates that an XMSS\textsuperscript{MT} secret key has a single SK\_PRF value that is shared by all of the XMSS secret keys, Algorithm 10' in Section 7.2.1 has each cryptographic module generate its own value for SK\_PRF. While generating a different SK\_PRF for each cryptographic module does not exactly align with the specification in [1], doing so does not affect either interoperability or security. SK\_PRF is only used to pseudorandomly generate the value $r$ in Algorithm 16, which is used for randomized hashing, and any secure method for generating random values could be used to generate $r$.

Section 7.2.2 describes the steps that an external, non-cryptographic device needs to perform in order to implement XMSS\textsuperscript{MT} key and signature generation using a set of cryptographic modules that implement the algorithms in Section 7.2.1. While Algorithms 10' and 12' in Section 7.2.1 have been designed to work with XMSS\textsuperscript{MT} instances that have more than two layers, the algorithms in Section 7.2.2 assume that an XMSS\textsuperscript{MT} instance with exactly two layers is being created.

### 7.2.1 Modified XMSS Key Generation and Signature Algorithms

Algorithm 10': XMSS'_keyGen

```plaintext
// L needs to be in the range [0 \ldots d-1]
// t needs to be in the range [0 \ldots 2^{((d-1-L)(h/d))} - 1]
Input: level L, tree t,
\quad public key of top-level tree PK_MT (if L \neq d - 1)
Output: XMSS public key PK

// Example initialization for SK-specific contents
idx = t * 2^{(h / d)};
for ( i = 0; i < 2^{(h / d)}; i++ ) {
    wots_sk[i] = WOTS_genSK();
}

Initialize SK\_PRF with an n-byte string using an approved random bit generator [6], where the instantiation of the random bit generator supports at least 8n bits of security strength.

setSK\_PRF(SK, SK\_PRF);

// SEED needs to be generated for the top-level XMSS key.
// For all other XMSS keys, the value needs to be copied from // the top-level XMSS key.
if ( L = d - 1 ) {
    Initialize SEED with an n-byte string using an approved random bit generator [6], where the instantiation of the random bit generator supports at least 8n bits of security strength.
} else {
```

21
\[
\text{SEED} = \text{getSEED} (\text{PK}_\text{MT});
\]

\[
\text{setSEED} (\text{SK}, \text{SEED});
\]

\[
\text{setWOTS}_\text{SK} (\text{SK}, \text{wots}_\text{sk});
\]

\[
\text{ADRS} = \text{toByte} (0, 32);
\]

\[
\text{ADRS}.\text{setLayerAddress} (\text{L});
\]

\[
\text{ADRS}.\text{setTreeAddress} (\text{t});
\]

\[
\text{root} = \text{treeHash} (\text{SK}, 0, h / d, \text{ADRS});
\]

// The "root" value in SK needs to be the root of the top-level
// XMSS tree, as this is the value used when hashing the message
// to be signed.

\[
\text{if} \ (L = d - 1) \{
\]

\[
\text{SK} = \text{L} || \text{t} || \text{idx} || \text{wots}_\text{sk} || \text{SK}_\text{PRF} || \text{root} || \text{SEED}
\]

\[
\text{else} \{
\]

\[
\text{SK} = \text{L} || \text{t} || \text{idx} || \text{wots}_\text{sk} || \text{SK}_\text{PRF} || \text{getRoot} (\text{PK}_\text{MT}) || \text{SEED}
\]

\[
\text{PK} = \text{OID} || \text{root} || \text{SEED}
\]

Algorithm 12': XMSS'\_sign

Input: Message \( M \)

Output: signature \( \text{Sig} \)

\[
\text{idx}_\text{sig} = \text{getIdx} (\text{SK});
\]

\[
\text{setIdx} (\text{SK}, \text{idx}_\text{sig} + 1);
\]

\[
\text{L} = \text{getLayerAddress} (\text{SK});
\]

\[
\text{t} = \text{getTreeAddress} (\text{SK});
\]

\[
\text{ADRS} = \text{toByte} (0, 32);
\]

\[
\text{ADRS}.\text{setLayerAddress} (\text{L});
\]

\[
\text{ADRS}.\text{setTreeAddress} (\text{t});
\]

\[
\text{if} \ (L > 0) \{
\]

// \( M \) must be the \( n \)-byte root from an XMSS public key

\[
\text{byte}[n] \ r = 0 \ // \ n \text{-byte string of zeros}
\]

\[
\text{byte}[n] \ M' = M
\]

\[
\text{else} \{
\]

\[
\text{byte}[n] \ r = \text{PRF} (\text{getSK}_\text{PRF} (\text{SK}), \text{toByte} (\text{idx}_\text{sig}, 32));
\]

\[
\text{byte}[n] \ M' = \text{H}_\text{msg} (r || \text{getRoot} (\text{SK}) || (\text{toByte} (\text{idx}_\text{sig}, n)), M);
\]

\[
\text{idx}_\text{leaf} = \text{idx}_\text{sig} - \text{t} * 2^{(h / d)};
\]

\[
\text{Sig} = \text{idx}_\text{sig} || r || \text{treeSig} (M', \text{SK}, \text{idx}_\text{leaf}, \text{ADRS});
\]

7.2.2 XMSS^MT External Device Operations

XMSS^MT external device keygen

Input: No input
// Generate top-level key pair on a cryptographic module
PK_MT = XMSS' keyGen(1, 0, NULL);

t = 0;
for each bottom-level key pair to be created {
    // Generate bottom-level key pair on a cryptographic module
    PK[t] = XMSS' keygen(0, t, PK_MT);

    // Submit root of bottom-level key pair's public key
    // to be signed by the top-level key pair.
    SigPK[t] = XMSS' sign(getRoot(PK[t]));

    // If the public key on the bottom-level tree was created using
    // a tree address of t, then its root needs to be signed by OTS
    // key t of the top-level tree. If it wasn't, then try again.
    if ( getIdx(SigPK[t]) ≠ t ) {
        t = getIdx(SigPK[t]) + 1;
        PK[t] = XMSS' keygen(0, t, PK_MT);
        SigPK[t] = XMSS' sign(getRoot(PK[t]));
    }
    t = t + 1;
}

XMSS^MT external device sign

Input: Message M
Output: signature Sig

// Send XMSS' sign() command to one of the bottom-level key pairs
Sig_tmp = XMSS' sign(M);
idx_sig = getIdx(Sig_tmp);
t = (h / d) most significant bits of idx_sig;

// Append the signature of the signing key pair's root
// (just the output of treeSig, not idxsig or r).
Sig = Sig_tmp || getSig(SigPK[t]);
8 Conformance

8.1 Key Generation and Signature Generation

Cryptographic modules implementing signature generation for a parameter set shall also implement key generation for that parameter set. Implementations of the key generation and signature algorithms in this document shall only be validated for use within hardware cryptographic modules. The cryptographic modules shall be validated to provide FIPS 140-2 or FIPS 140-3 [19] Level 3 or higher physical security, and the operational environment shall be limited.\(^4\) In addition, a cryptographic module implementing the key generation or signature algorithms shall only operate in an approved mode of operation and shall not implement a bypass mode. The cryptographic module shall not allow for the export of private keying material.

In order to prevent the possible reuse of an OTS key, when the cryptographic module accepts a request to sign a message, the cryptographic module shall update the state of the private key in non-volatile storage before exporting a signature value or accepting another request to sign a message.

Cryptographic modules implementing LMS key and signature generation shall support at least one of the LM-OTS parameter sets in Section 4. For each LM-OTS parameter set supported by a cryptographic module, the cryptographic module shall support at least one LMS parameter set from Section 4 that uses the same hash function as the LM-OTS parameter set. Cryptographic modules implementing LMS key and signature generation shall generate random data in accordance with Section 6.1.

Cryptographic modules implementing XMSS key and signature generation shall implement Algorithm 10 and Algorithm 12 from [1] for at least one of the XMSS parameter sets in Section 5. Cryptographic modules supporting implementation of XMSS\(^{MT}\) key and signature generation shall implement Algorithm 10' and Algorithm 12' from Section 7.2.1 of this document for at least one of the XMSS\(^{MT}\) parameter sets in Section 5. Cryptographic modules implementing XMSS or XMSS\(^{MT}\) key and signature generation shall generate random data in accordance with Section 6.2.

8.2 Signature Verification

Cryptographic modules implementing LMS signature verification shall support at least one of the LM-OTS parameter sets in Section 4. For each LM-OTS parameter set supported by a cryptographic module, the cryptographic module shall support at least one LMS parameter set from Section 4 that uses the same hash function as the LM-OTS parameter set.

Cryptographic modules implementing XMSS signature verification shall implement Algorithm 14 of [1] for at least one of the parameter sets in Section 5. Cryptographic modules implementing XMSS\(^{MT}\) signature verification shall implement Algorithm 17 of [1] for at least one of the parameter sets in Section 5.

\(^4\) See Section 4.6 of FIPS 140-2 [19].
9 Security Considerations

9.1 One-Time Signature Key Reuse

Both LMS and XMSS are stateful signature schemes. If an attacker were able to obtain signatures for two different messages created using the same one-time signature (OTS) key, then it would become computationally feasible for that attacker to create forgeries [13]. As noted in [8], extreme care needs to be taken in order to avoid the risk that an OTS key will be reused accidentally. While the conformance requirements in Section 8.1 prevent many of the actions that could result in accidental OTS key reuse, cryptographic modules still need to be carefully designed to ensure that unexpected behavior cannot result in an OTS key being reused.

In order to avoid reuse of an OTS key, the state of the private key must be updated each time a signature is generated. If the private key is stored in non-volatile memory, then the state of the key must be updated in the non-volatile memory to mark an OTS key as unavailable before the corresponding signature generated using the OTS key is exported. Depending on the environment, this can be nontrivial to implement. With many operating systems, simply writing the update to a file is not sufficient as the write operation will be cached with the actual write to non-volatile memory taking place later. If the cryptographic module loses power or crashes before the write to non-volatile memory, then the state update will be lost. If a signature were exported after the write operation was issued but before the update was written to non-volatile memory, there would be a risk that the OTS key would be used again after the cryptographic module starts up.

Some hardware cryptographic modules implement monotonic counters, which are guaranteed to increase each time the counter’s value is read. When available, using the current value of a monotonic counter to determine which OTS key to use for a signature may be very helpful in avoiding unintentional reuse of an OTS key.

9.2 Fault Injection Resistance

Fault injection attacks involve the intentional introduction of an error at some point during the execution of an algorithm, such as by varying the voltage supplied to a device executing the algorithm, causing it to produce the wrong output, and providing the attacker with additional information. These attacks are most relevant for users of embedded cryptographic devices where an adversary may have physical access to the signing device and thus can control its operations.

Fault injection attacks have been shown to be effective against hash-based signatures, though they are more severe when used against stateless schemes like SPHINCS and its variants [9][10]. With hash-based signatures, the attack works by forcing the cryptographic device to sign two different messages with the same OTS key. The attack takes advantage of the schemes where multiple levels of Merkle trees are used and the roots of lower-level trees are signed using a one-time signature (XMSS\textsuperscript{MT} and HSS) [10]. In some cases, the signatures on these roots are recomputed each time a message is signed. Under normal circumstances, this is acceptable since it just involves using an OTS key multiple times to sign the same message. However, by injecting a fault that introduces an error in the computation of the Merkle tree root at any of the non-top layers, an attacker can cause the device to sign a different message under the same key.

With both a valid and a faulty signature, the attacker can “graft” a new subtree into the hierarchy
and produce universal forgeries.

The faulted signature remains a valid signature, so checking that the signature verifies is insufficient to detect or prevent this attack. The only reliable way to prevent this attack is to compute each one-time signature once, cache the result, and output it whenever needed. When implementing multiple levels of trees as described in Section 7, this is the only option since no cryptographic module will use any OTS more than once. If multiple levels of trees are implemented within a single cryptographic module, it is recommended to cache a single, one-time signature per layer of subtrees, refreshing them when a new subtree is used for signing [10]. While this prevents an attacker from learning about the secret key when a corrupted signature is cached, it does result in the cached one-time signature being incorrect and thus prevents the hash-based signature scheme from working.

9.3 Hash Collisions

In LMS and XMSS, as in the other approved digital signature schemes [4], the signature generation algorithm is not applied directly to the message but to a message digest generated by the underlying hash function. The security of any signature scheme depends on the inability of an attacker to find distinct messages with the same message digest.

There are two ways that an attacker might find these distinct messages. The attacker could look for a message that has the same message digest as a message that has already been signed (a second preimage), or the attacker could look for any two messages that have the same message digest (a generic collision) and then try to get the private key holder (i.e., signer) to sign one of them [21]. Finding a second preimage is much more difficult than finding a generic collision, and it would be infeasible for an attacker to find a second preimage with any of the hash functions allowed for use in this recommendation.

LMS and XMSS both use randomized hashing. When a message is presented to be signed, a random value is created and prepended to the message, and the hash function is applied to this expanded message to produce the message digest. Prepending the random value makes it infeasible for anyone other than the signer to find a generic collision as finding a collision would require predicting the randomizing value. The randomized hashing process does not, however, impact the ability for a signer to create a generic collision since the signer, knowing the private key, could choose the random value to prepend to the message.

The 196-bit hash functions in this recommendation, SHA-256/196 and SHAKE256/196, offer significantly less resistance to generic collision searches than their 256-bit counterparts. In particular, a collision of the 196-bit functions may be found as the number of sampled inputs approaches $2^{96}$, as opposed to $2^{128}$ for the 256-bit functions, and it may be possible for a signer with access to an extremely large amount of computing resources to sample $2^{96}$ inputs.

Consequently, one tradeoff for the use of 196-bit hash functions in LMS and XMSS is the weakening of the verifier’s assurance that the signer will not be able to change the message once the signature is revealed. This possibility does not affect the formal security properties of the schemes because it remains the case that only the signer could produce a valid signature on a message.
References


[6] Special Publication 800-90 series:

Sönmez Turan M, Barker EB, Kelsey JM, McKay KA, Baish ML, Boyle M (2018) Recommendation for the Entropy Sources Used for Random Bit Generation. (National Institute of Standards and Technology, Gaithersburg, MD), NIST Special Publication (SP) 800-90B. https://doi.org/10.6028/NIST.SP.800-90B

Barker EB, Kelsey JM (2016) Recommendation for Random Bit Generator (RBG) Constructions. (National Institute of Standards and Technology, Gaithersburg, MD), (Second Draft) NIST Special Publication (SP) 800-90C. Available at https://csrc.nist.gov/publications/detail/sp/800-90c/draft


Appendix A—LMS XDR Syntax Additions

In order to support the LM-OTS and LMS parameter sets defined in Sections 4.2 through 4.4, the XDR syntax in Section 3.3 of [2] is extended as follows.

/* one-time signatures */

enum lmots_algorithm_type {
    lmots_sha256_n24_w1 = TBD,
    lmots_sha256_n24_w2 = TBD,
    lmots_sha256_n24_w4 = TBD,
    lmots_sha256_n24_w8 = TBD,
    lmots_shake_n32_w1  = TBD,
    lmots_shake_n32_w2  = TBD,
    lmots_shake_n32_w4  = TBD,
    lmots_shake_n32_w8  = TBD,
    lmots_shake_n24_w1  = TBD,
    lmots_shake_n24_w2  = TBD,
    lmots_shake_n24_w4  = TBD,
    lmots_shake_n24_w8  = TBD,
    lmots_shake_n24_w1  = TBD,
    lmots_shake_n24_w2  = TBD,
    lmots_shake_n24_w4  = TBD,
    lmots_shake_n24_w8  = TBD
};

typedef opaque bytestring24[24];

struct lmots_signature_n24_p200 {
    bytestring24 C;
    bytestring24 y[200];
};

struct lmots_signature_n24_p101 {
    bytestring24 C;
    bytestring24 y[101];
};

struct lmots_signature_n24_p51 {
    bytestring24 C;
    bytestring24 y[51];
};

struct lmots_signature_n24_p26 {
    bytestring24 C;
    bytestring24 y[26];
};

union lmots_signature switch (lmots_algorithm_type type) {
    case lmots_sha256_n24_w1:
        lmots_signature_n24_p200 sig_n24_p200;
case lmots_sha256_n24_w2:
    lmots_signature_n24_p101 sig_n24_p101;
case lmots_sha256_n24_w4:
    lmots_signature_n24_p51 sig_n24_p51;
case lmots_sha256_n24_w8:
    lmots_signature_n24_p26 sig_n24_p26;
case lmots_shake_n32_w1:
    lmots_signature_n32_p265 sig_n32_p265;
case lmots_shake_n32_w2:
    lmots_signature_n32_p133 sig_n32_p133;
case lmots_shake_n32_w4:
    lmots_signature_n32_p67 sig_n32_p67;
case lmots_shake_n32_w8:
    lmots_signature_n32_p34 sig_n32_p34;
case lmots_shake_n24_w1:
    lmots_signature_n24_p200 sig_n24_p200;
case lmots_shake_n24_w2:
    lmots_signature_n24_p101 sig_n24_p101;
case lmots_shake_n24_w4:
    lmots_signature_n24_p51 sig_n24_p51;
case lmots_shake_n24_w8:
    lmots_signature_n24_p26 sig_n24_p26;
};

/* hash-based signatures (hbs) */
enum lms_algorithm_type {
    lms_sha256_n24_h5  = TBD,
    lms_sha256_n24_h10 = TBD,
    lms_sha256_n24_h15 = TBD,
    lms_sha256_n24_h20 = TBD,
    lms_sha256_n24_h25 = TBD,
    lms_shake_n32_h5   = TBD,
    lms_shake_n32_h10  = TBD,
    lms_shake_n32_h15  = TBD,
    lms_shake_n32_h20  = TBD,
    lms_shake_n32_h25  = TBD,
    lms_shake_n24_h5   = TBD,
    lms_shake_n24_h10  = TBD,
    lms_shake_n24_h15  = TBD,
    lms_shake_n24_h20  = TBD,
    lms_shake_n24_h25  = TBD
};

/* leighton-micali signatures (lms) */
union lms_path switch (lms_algorithm_type type) {

case lms_sha256_n24_h5:
  case lms_shake_n24_h5:
    bytestring24 path_n24_h5[5];
  case lms_sha256_n24_h10:
  case lms_shake_n24_h10:
    bytestring24 path_n24_h10[10];
  case lms_sha256_n24_h15:
  case lms_shake_n24_h15:
    bytestring24 path_n24_h15[15];
  case lms_sha256_n24_h20:
  case lms_shake_n24_h20:
    bytestring24 path_n24_h20[20];
  case lms_sha256_n24_h25:
  case lms_shake_n24_h25:
    bytestring24 path_n24_h25[25];

case lms_sha256_n32_h5:
  bytestring32 path_n32_h5[5];
  case lms_sha256_n32_h10:
  case lms_sha256_n32_h15:
  case lms_sha256_n32_h20:
  case lms_sha256_n32_h25:
    bytestring32 path_n32_h25[25];

struct lms_key_n24 {
  lmots_algorithm_type ots_alg_type;
  opaque I[16];
  opaque K[24];
};

union lms_public_key switch (lms_algorithm_type type) {
  case lms_sha256_n24_h5:
  case lms_sha256_n24_h10:
  case lms_sha256_n24_h15:
  case lms_sha256_n24_h20:
  case lms_sha256_n24_h25:
  case lms_sha256_n24_h5:
  case lms_sha256_n24_h10:
  case lms_sha256_n24_h15:
  case lms_sha256_n24_h20:
  case lms_sha256_n24_h25:
  case lms_sha256_n24_h5:
  case lms_sha256_n24_h10:
  case lms_sha256_n24_h15:
  case lms_sha256_n24_h20:
  case lms_sha256_n24_h25:
    lms_key_n24 z_n24;
case lms_shake_n32_h5:
case lms_shake_n32_h10:
case lms_shake_n32_h15:
case lms_shake_n32_h20:
case lms_shake_n32_h25:
    lms_key_n32 z_n32;
};
Appendix B—XMSS XDR Syntax Additions

In order to support the XMSS parameter sets defined in Sections 5.2 through 5.4, the XDR syntax in Appendices A, B, and C of [1] is extended as follows.

B.1 WOTS+

/* ots_algorithm_type identifies a particular signature algorithm */
enum ots_algorithm_type {
  wotsp-sha2_192     = TBD,
  wotsp-shake256_256 = TBD,
  wotsp-shake256_192 = TBD,
};

/* Byte strings */
typedef opaque bytestring24[24];
union ots_signature switch (ots_algorithm_type type) {
  case wotsp-sha2_192:
  case wotsp-shake256_192:
    bytestring24 ots_sig_n24_len51[51];
  case wotsp-shake256_256:
    bytestring32 ots_sig_n32_len67[67];
};
union ots_pubkey switch (ots_algorithm_type type) {
  case wotsp-sha2_192:
  case wotsp-shake256_192:
    bytestring24 ots_pubk_n24_len51[51];
  case wotsp-shake256_256:
    bytestring32 ots_pubk_n32_len67[67];
};

B.2 XMSS

/* Definition of parameter sets */
enum xmss_algorithm_type {
  xmss-sha2_10_192     = TBD,
  xmss-sha2_16_192     = TBD,
  xmss-sha2_20_192     = TBD,
};
xmss-shake256_10_256 = TBD,
mxss-shake256_16_256 = TBD,
mxss-shake256_20_256 = TBD,

mxss-shake256_10_192 = TBD,
mxss-shake256_16_192 = TBD,
mxss-shake256_20_192 = TBD;

/* Authentication path types */

union xmss_path switch (xmss_algorithm_type type) {
  case xmss-sha2_10_192:
    case xmss-shake256_10_192:
      bytestring24 path_n24_t10[10];
    break;
  case xmss-shake256_10_256:
    bytestring32 path_n32_t10[10];
  case xmss-sha2_16_192:
    case xmss-shake256_16_192:
      bytestring24 path_n24_t16[16];
    break;
  case xmss-shake256_16_256:
    bytestring32 path_n32_t16[16];
  case xmss-sha2_20_192:
    case xmss-shake256_20_192:
      bytestring24 path_n24_t20[20];
    break;
  case xmss-shake256_20_256:
    bytestring32 path_n32_t20[20];
}

/* Types for XMSS random strings */

union random_string_xmss switch (xmss_algorithm_type type) {
  case xmss-sha2_10_192:
    case xmss-sha2_16_192:
    case xmss-sha2_20_192:
    case xmss-shake256_10_192:
    case xmss-shake256_16_192:
    case xmss-shake256_20_192:
      bytestring24 rand_n24;
    break;
  case xmss-shake256_10_256:
  case xmss-shake256_16_256:

case xmss-shake256_20_256:
    bytestring32 rand_n32;
};

/* Corresponding WOTS+ type for given XMSS type */

union xmss_ots_signature switch (xmss_algorithm_type type) {
    case xmss-sha2_10_192:
    case xmss-sha2_16_192:
    case xmss-sha2_20_192:
        wotsp-sha2_192;
    case xmss-shake256_10_256:
    case xmss-shake256_16_256:
    case xmss-shake256_20_256:
        wotsp-shake256_256;
    case xmss-shake256_10_192:
    case xmss-shake256_16_192:
    case xmss-shake256_20_192:
        wotsp-shake256_192;
};

/* Types for bitmask seed */

union seed switch (xmss_algorithm_type type) {
    case xmss-sha2_10_192:
    case xmss-sha2_16_192:
    case xmss-sha2_20_192:
    case xmss-shake256_10_192:
    case xmss-shake256_16_192:
    case xmss-shake256_20_192:
        bytestring24 seed_n24;
    case xmss-shake256_10_256:
    case xmss-shake256_16_256:
    case xmss-shake256_20_256:
        bytestring32 seed_n32;
};

/* Types for XMSS root node */

union xmss_root switch (xmss_algorithm_type type) {
    case xmss-sha2_10_192:
    case xmss-sha2_16_192:
    case xmss-sha2_20_192:
    case xmss-shake256_10_192:
    case xmss-shake256_16_192:
    case xmss-shake256_20_192:

case xmss-shake256_16_192:
    bytestring24 root_n24;

case xmss-shake256_10_256:
    case xmss-shake256_16_256:
    case xmss-shake256_20_256:
    bytestring32 root_n32;
}

B.3 XMSS\textsuperscript{MT}

/* Definition of parameter sets */
enum xmssmt_algorithm_type {
  xmssmt-sha2_20/2_192      = TBD,
  xmssmt-sha2_20/4_192      = TBD,
  xmssmt-sha2_40/2_192      = TBD,
  xmssmt-sha2_40/4_192      = TBD,
  xmssmt-sha2_40/8_192      = TBD,
  xmssmt-sha2_60/3_192      = TBD,
  xmssmt-sha2_60/6_192      = TBD,
  xmssmt-sha2_60/12_192     = TBD,
  xmssmt-sha256_20/2_256    = TBD,
  xmssmt-sha256_20/4_256    = TBD,
  xmssmt-sha256_40/2_256    = TBD,
  xmssmt-sha256_40/4_256    = TBD,
  xmssmt-sha256_40/8_256    = TBD,
  xmssmt-sha256_60/3_256    = TBD,
  xmssmt-sha256_60/6_256    = TBD,
  xmssmt-sha256_60/12_256   = TBD,
  xmssmt-sha256_20/2_192    = TBD,
  xmssmt-sha256_20/4_192    = TBD,
  xmssmt-sha256_40/2_192    = TBD,
  xmssmt-sha256_40/4_192    = TBD,
  xmssmt-sha256_40/8_192    = TBD,
  xmssmt-sha256_60/3_192    = TBD,
  xmssmt-sha256_60/6_192    = TBD,
  xmssmt-sha256_60/12_192   = TBD,
};

/* Type for XMSS\textsuperscript{MT} key pair index */
/* Depends solely on h */
union idx_sig_xmssmt switch (xmss_algorithm_type type) {
    case xmssmt-sha2_20/2_192:
    case xmssmt-sha2_20/4_192:
    case xmssmt-shake256_20/2_256:
    case xmssmt-shake256_20/4_256:
    case xmssmt-shake256_20/2_192:
    case xmssmt-shake256_20/4_192:
        bytestring3 idx3;
    case xmssmt-sha2_40/2_192:
    case xmssmt-sha2_40/4_192:
    case xmssmt-sha2_40/8_192:
    case xmssmt-shake256_40/2_256:
    case xmssmt-shake256_40/4_256:
    case xmssmt-shake256_40/8_256:
    case xmssmt-shake256_40/2_192:
    case xmssmt-shake256_40/4_192:
    case xmssmt-shake256_40/8_192:
        bytestring5 idx5;
    case xmssmt-sha2_60/3_192:
    case xmssmt-sha2_60/6_192:
    case xmssmt-sha2_60/12_192:
    case xmssmt-shake256_60/3_256:
    case xmssmt-shake256_60/6_256:
    case xmssmt-shake256_60/12_256:
    case xmssmt-shake256_60/3_192:
    case xmssmt-shake256_60/6_192:
    case xmssmt-shake256_60/12_192:
        bytestring8 idx8;
};

union random_string_xmssmt switch (xmssmt_algorithm_type type) {
    case xmssmt-sha2_20/2_192:
    case xmssmt-sha2_20/4_192:
    case xmssmt-sha2_40/2_192:
    case xmssmt-sha2_40/4_192:
    case xmssmt-sha2_40/8_192:
    case xmssmt-shake256_20/2_192:
    case xmssmt-shake256_20/4_192:
    case xmssmt-shake256_40/2_192:
    case xmssmt-shake256_40/4_192:
    case xmssmt-shake256_40/8_192:
    case xmssmt-shake256_60/3_192:

case xmssmt-shake256_60/6_192:
    bytestring24 rand_n24;

case xmssmt-shake256_60/12_192:

    bytestring24 rand_n24;

case xmssmt-shake256_20/2_256:
    case xmssmt-shake256_20/4_256:
    case xmssmt-shake256_40/2_256:
    case xmssmt-shake256_40/4_256:
    case xmssmt-shake256_40/8_256:
    case xmssmt-shake256_60/3_256:
    case xmssmt-shake256_60/6_256:
    case xmssmt-shake256_60/12_256:
    bytestring32 rand_n32;

    bytestring24 xmss_reduced_n24_t61[61];

    bytestring24 xmss_reduced_n24_t56[56];

    bytestring24 xmss_reduced_n24_t71[71];

    bytestring32 xmss_reduced_n32_t77[77];

    case xmssmt-shake256_20/4_256:
    case xmssmt-shake256_40/8_256:
    case xmssmt-shake256_60/12_256:
    case xmssmt-shake256_20/2_256:
    case xmssmt-shake256_40/4_256:
    case xmssmt-shake256_60/6_256:
    case xmssmt-shake256_20/4_256:
case xmssmt-shake256_60/12_256:
    bytestring32 xmss_reduced_n32_t72[72];
    case xmssmt-shake256_40/2_256:
    case xmssmt-shake256_60/3_256:
        bytestring32 xmss_reduced_n32_t87[87];
    }

} /* xmss_reduced_array depends on d */
union xmss_reduced_array (xmss_algorithm_type type) {
    case xmssmt-sha2_20/2_192:
    case xmssmt-sha2_40/2_192:
    case xmssmt-shake256_20/2_256:
    case xmssmt-shake256_40/2_256:
    case xmssmt-shake256_20/2_192:
    case xmssmt-shake256_40/2_192:
        xmss_reduced xmss_red_arr_d2[2];
    case xmssmt-sha2_60/3_192:
    case xmssmt-shake256_60/3_256:
    case xmssmt-shake256_60/3_192:
        xmss_reduced xmss_red_arr_d3[3];
    case xmssmt-sha2_20/4_192:
    case xmssmt-sha2_40/4_192:
    case xmssmt-shake256_20/4_256:
    case xmssmt-shake256_40/4_256:
    case xmssmt-shake256_20/4_192:
    case xmssmt-shake256_40/4_192:
        xmss_reduced xmss_red_arr_d4[4];
    case xmssmt-sha2_60/6_192:
    case xmssmt-shake256_60/6_256:
    case xmssmt-shake256_60/6_192:
        xmss_reduced xmss_red_arr_d6[6];
    case xmssmt-sha2_40/8_192:
    case xmssmt-shake256_40/8_256:
    case xmssmt-shake256_40/8_192:
        xmss_reduced xmss_red_arr_d8[8];
    case xmssmt-sha2_60/12_192:
    case xmssmt-shake256_60/12_256:
    case xmssmt-shake256_60/12_192:
        xmss_reduced xmss_red_arr_d12[12];
};
/* Types for bitmask seed */
union seed switch (xmssmt_algorithm_type type) {
    case xmssmt-sha2_20/2_192:
    case xmssmt-sha2_20/4_192:
    case xmssmt-sha2_40/2_192:
    case xmssmt-sha2_40/4_192:
    case xmssmt-sha2_40/8_192:
    case xmssmt-sha2_60/3_192:
    case xmssmt-sha2_60/6_192:
    case xmssmt-sha2_60/12_192:
    case xmssmt-shake256_20/2_192:
    case xmssmt-shake256_20/4_192:
    case xmssmt-shake256_40/2_192:
    case xmssmt-shake256_40/4_192:
    case xmssmt-shake256_40/8_192:
    case xmssmt-shake256_60/3_192:
    case xmssmt-shake256_60/6_192:
    case xmssmt-shake256_60/12_192:
        bytestring24 seed_n24;

    case xmssmt-shake256_20/2_256:
    case xmssmt-shake256_20/4_256:
    case xmssmt-shake256_40/2_256:
    case xmssmt-shake256_40/4_256:
    case xmssmt-shake256_40/8_256:
    case xmssmt-shake256_60/3_256:
    case xmssmt-shake256_60/6_256:
    case xmssmt-shake256_60/12_256:
        bytestring32 seed_n32;
};

/* Types for XMSS^MT root node */
union xmssmt_root switch (xmssmt_algorithm_type type) {
    case xmssmt-sha2_20/2_192:
    case xmssmt-sha2_20/4_192:
    case xmssmt-sha2_40/2_192:
    case xmssmt-sha2_40/4_192:
    case xmssmt-sha2_40/8_192:
    case xmssmt-sha2_60/3_192:
    case xmssmt-sha2_60/6_192:
    case xmssmt-sha2_60/12_192:
    case xmssmt-shake256_20/2_192:
    case xmssmt-shake256_20/4_192:
case xmssmt-shake256_40/2_192:
    bytestring24 root_n24;

case xmssmt-shake256_40/4_192:
    case xmssmt-shake256_40/8_192:
        case xmssmt-shake256_60/3_192:
            case xmssmt-shake256_60/6_192:
                case xmssmt-shake256_60/12_192:
                    bytestring24 root_n24;

            case xmssmt-shake256_20/2_256:
                case xmssmt-shake256_20/4_256:
                    case xmssmt-shake256_40/2_256:
                        case xmssmt-shake256_40/4_256:
                            case xmssmt-shake256_40/8_256:
                                case xmssmt-shake256_60/3_256:
                                    case xmssmt-shake256_60/6_256:
                                        case xmssmt-shake256_60/12_256:
                                            bytestring32 root_n32;
);
Appendix C—Provable Security Analysis

This appendix briefly summarizes the formal security model and proofs of security of the LMS and XMSS signature schemes and provides a short discussion comparing these models and proofs.

C.1 The Random Oracle Model

In the random oracle model (ROM), there is a publicly accessible random oracle that both the user and the adversary can send queries to and receive responses from at any time. A random oracle $H$ is a hypothetical, interactive black-box algorithm that obeys the following rules:

1. Every time the algorithm $H$ receives a new input string $s$, it generates an output $t$ uniformly at random from its output space and returns the response $t$. The algorithm $H$ then records the pair $(s, t)$ for future use.
2. If the algorithm $H$ is ever queried in the future with some prior input $s$, it will always return the same output $t$ according to its recorded memory.

Alternatively, the random oracle $H$ can be described as a non-interactive but exponentially large look-up table initialized with truly random outputs $t$ for each possible input string $s$.

To say that a cryptographic security proof is done in the random oracle model means that every use of a particular function (for example, in the case here, the compression function that is used to perform hashes) is replaced by a query to the random oracle $H$. This simplifies security claims as, for example, it becomes easy to prove upper bounds on the likelihood of producing a second preimage within a fixed number of queries to $H$. On the other hand, (compression) functions in the real world are neither interactive nor have exponentially large descriptions, so they cannot truly behave like a random oracle.

It is therefore desirable to have a cryptographic security proof that avoids using the random oracle model. However, this often leads to less efficient cryptographic systems, or it is not yet known how to perform a proof without appealing to the random oracle model, or both. So, as a matter of real-world pragmatism, the ROM is commonly used.

C.2 The Quantum Random Oracle Model

The quantum random oracle model (QROM) is similar to the ROM, except it is additionally assumed that all parties (in particular, the adversary) have quantum computers and can query the random oracle $H$ in superposition. (In the real world, the random oracle $H$ is still instantiated as a compression function or similar, as per the cryptosystem’s specification.) While this complicates security claims as compared to the ROM, it more accurately models the power of an adversary that has access to a large-scale quantum device for its cryptanalysis when attacking a real-world scheme.

C.3 LMS Security Proof

In [11], the author considers a particular experiment in the random oracle model in which the
adversary is given a series of strings with prefixes (in a randomly chosen but structured manner) and hash targets. The attacker’s goal is to find one more string that has the same prefix and hash target as any of its input strings. The author proves an upper bound on the adversary’s ability to compute first or second preimages from these strings (by querying the compression function modeled as a random oracle).

Then, the author reduces the problem of forging a signature in LMS to this stated experiment, concluding that the same upper bounds apply to the problem of producing forgeries against LMS. This random oracle model proof critically depends on the randomness of the prefixes used in LMS, which means that LMS in the real world critically depends on the pseudorandomness of the prefixes.

Further, in [15], the same proof is carried out in the QROM.

### C.4 XMSS Security Proof

In [12], a security analysis for the original (academic publication) version of XMSS is given under the following assumptions:

1. The function family \( \{f_k\} \) used to construct Winternitz signatures is pseudorandom. This means that if the bit string \( k \) is chosen uniformly at random, then an adversary given black-box access to the function \( f_k \) cannot distinguish this black box from a random function within a polynomial number of queries (except with negligible probability).

2. The hash function family \( \{h_k\} \) is second preimage-resistant. This means that if bit strings \( k \) and \( m \) are chosen uniformly at random, then an adversary given \( k \) and \( m \) cannot construct \( m' \neq m \) such that \( h_k(m') = h_k(m) \) in polynomial time (except with negligible probability).

The proof in [12] asserts that if both of these assumptions are true, then XMSS is existentially unforgeable under adaptive chosen message attacks (EUF-CMA) in the standard model.

However, in the current version of XMSS\(^{MT} \) [1], the security analysis differs somewhat. In the standard model, [17] shows that XMSS\(^{MT} \) is EUF-CMA. Further, [16] shows that XMSS\(^{MT} \) is post-quantum existentially unforgeable under adaptive chosen message attacks with respect to the QROM.

In a little more detail, the current version of XMSS uses two types of assumptions:

1. A standard model assumption – that the hash function \( h_k \), used for the one-time signatures and tree node computations, is post-quantum, multi-function, multi-target preimage-resistant.

2. A (quantum) random oracle model assumption – that the pseudorandom function \( f_k \), used to generate pseudorandom values for randomized hashing and computing bitmasks as blinding keys, may be validly modeled as a quantum random oracle \( H \).
C.5 Comparison of the Security Models and Proofs of LMS and XMSS

Generally speaking, both LMS and XMSS are supported by sound security proofs under commonly used cryptographic hardness assumptions. That is, if these cryptographic assumptions are true, then both schemes are provably shown to be existentially unforgeable under chosen message attack, even against an adversary that has access to a large-scale quantum computer for use in its forgery attack.

The main difference between these schemes’ security analyses comes down to the use (and the degree of use) of the random oracle or quantum random oracle models. Along these lines, the difference between the (standard model/real world) cryptographic assumption that some function family \( \{ f_k \} \) is pseudorandom and the use of the random oracle model is briefly pointed out. For a function \( f_k \) to be a pseudorandom function in the real world, it should be the case that the bit string \( k \) used as the key to the function remains private, meaning that it is not in the view of the adversary at any point of the security experiment. On the other hand, a random oracle \( H \) achieves the same pseudorandomness (or even randomness) properties of a pseudorandom function \( f_k \), but there is no key \( k \) necessarily associated with the random oracle. Indeed, all inputs to the random oracle \( H \) may be known to all parties and, in particular, to the adversary. Therefore, using the random oracle model clearly involves making a stronger assumption about the (limits of the) cryptanalytic power of the adversary.

That said, a security proof is either entirely a “real world proof,” which does not use the random oracle model, or it appeals to the random oracle methodology in some manner. The security analysis of the current version of XMSS only uses the random oracle \( H \) when performing randomized hashing and computing bitmasks, whereas LMS uses the random oracle \( H \) to a greater degree (modeling the compression function as a random oracle). However, it remains the case that both schemes in their modern form are ultimately proven secure using the ROM and QROM.

Therefore, the cryptographic hardness assumptions made by LMS and XMSS in order to achieve existential unforgeability under chosen message attack (EUF-CMA) may be viewed as substantially similar and worthy of essentially equal confidence. As such, the practitioner’s decision to deploy one scheme or the other should primarily depend on other factors, such as the efficiency demands for a given deployment environment or the other security considerations enumerated earlier in this document.